SUPPORTING INFORMATION FOR CALCULATIONS

Metal-free α-Amination of Secondary Amines: Computational and Experimental Evidence for Azaquinone Methide and Azomethine Ylide Intermediates

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Contents

1 Computational Methods **6**

2 Cartesian Coordinates and Energies of Reactants **7**
2.1 Aminoaldehyde **1a** . . . 7
2.2 Aminoaldehyde **1b** . . . 7
2.3 Pyrrolidine . . . 8
2.4 Piperidine . . . 8
2.5 Morpholine . . . 9
2.6 Tetrahydroisoquinoline . . . 9
2.7 Tetrahydroquinoline . . . 10

3 Cartesian Coordinates and Energies of Products 2 **11**
3.1 Product 2a . . . 11
3.2 Product 2b . . . 11
3.3 Product 2c . . . 12
3.4 Product 2d . . . 13
3.5 Product 2e . . . 13
3.6 Product 2f . . . 14
3.7 Product 2g . . . 15
3.8 Product 2h . . . 16
3.9 Product 2i . . . 17

4 Cartesian Coordinates and Energies of Hemiaminals 3 **18**
4.1 Hemiaminal 3a . . . 18
4.2 Hemiaminal 3b . . . 18
4.3 Hemiaminal 3c . . . 19
4.4 Hemiaminal 3d . . . 20
4.5 Hemiaminal 3e . . . 21
4.6 Hemiaminal 3f . . . 22
4.7 Hemiaminal 3g . . . 22
4.8 Hemiaminal 3h . . . 23
4.9 Hemiaminal 3i . . . 24

5 Cartesian Coordinates and Energies of Azaquinone Methides 4 **26**
5.1 Azaquinone Methide *cis*-4a . . . 26
5.2 Azaquinone Methide *trans*-4a . . . 26
5.3 Azaquinone Methide *cis*-4b . . . 27
5.4 Azaquinone Methide *trans*-4b . . . 28

5.5 Azaquinone Methide *cis*-4c . . . 28
5.6 Azaquinone Methide *trans*-4c . . . 29
5.7 Azaquinone Methide *cis*-4d . . . 30
5.8 Azaquinone Methide *trans*-4d . . . 31
5.9 Azaquinone Methide *cis*-4e . . . 31
5.10 Azaquinone Methide *trans*-4e . . . 32
5.11 Azaquinone Methide *cis*-4f . . . 33
5.12 Azaquinone Methide *trans*-4f . . . 34
5.13 Azaquinone Methide *cis*-4g . . . 35
5.14 Azaquinone Methide *trans*-4g . . . 35
5.15 Azaquinone Methide *cis*-4h . . . 36
5.16 Azaquinone Methide *trans*-4h . . . 37
5.17 Azaquinone Methide *cis*-4i . . . 38
5.18 Azaquinone Methide *trans*-4i . . . 39

6 Cartesian Coordinates and Energies of Azomethine Ylides 5 40
6.1 Azomethine Ylide 5a . . . 40
6.2 Azomethine Ylide 5b . . . 40
6.3 Azomethine Ylide 5c . . . 41
6.4 Azomethine Ylide 5d . . . 42
6.5 Azomethine Ylide 5e . . . 42
6.6 Azomethine Ylide 5f . . . 43
6.7 Azomethine Ylide 5g . . . 44
6.8 Azomethine Ylide 5h . . . 45
6.9 Azomethine Ylide 5i . . . 46

7 Cartesian Coordinates and Energies of Zwitterions 7 47
7.1 Zwitterion 7a . . . 47
7.2 Zwitterion 7b . . . 47
7.3 Zwitterion 7c . . . 48
7.4 Zwitterion 7d . . . 49
7.5 Zwitterion 7e . . . 49
7.6 Zwitterion 7f . . . 50
7.7 Zwitterion 7g . . . 51
7.8 Zwitterion 7h . . . 52
7.9 Zwitterion 7i . . . 53

8 Cartesian Coordinates and Energies of Transition States TS-3 54
8.1 Transition State *cis*-3a . . . 54
8.2 Transition State *trans*-3a . . . 54
8.3 Transition State *cis*-3b . . . 55
8.4 Transition State *trans*-3b . . . 56
8.5 Transition State *cis*-3c . . . 57
8.6 Transition State *trans*-3c . . . 57

8.7 Transition State *cis*-3d . . . 58
8.8 Transition State *trans*-3d . . . 59
8.9 Transition State *cis*-3e . . . 60
8.10 Transition State *trans*-3e . . . 61
8.11 Transition State *cis*-3f . . . 62
8.12 Transition State *trans*-3f . . . 62
8.13 Transition State *cis*-3g . . . 63
8.14 Transition State *trans*-3g . . . 64
8.15 Transition State *cis*-3h . . . 65
8.16 Transition State *trans*-3h . . . 66
8.17 Transition State *cis*-3i . . . 67
8.18 Transition State *trans*-3i . . . 68

9 Cartesian Coordinates and Energies of Transition States TS-5 69
9.1 Transition State 5a . . . 69
9.2 Transition State 5b . . . 69
9.3 Transition State 5c . . . 70
9.4 Transition State 5d . . . 71
9.5 Transition State 5e . . . 71
9.6 Transition State 5f . . . 72
9.7 Transition State 5g . . . 73
9.8 Transition State 5h . . . 74
9.9 Transition State 5i . . . 75

10 Cartesian Coordinates and Energies of Transition States TS-6 76
10.1 Transition State 6a . . . 76
10.2 Transition State 6b . . . 77
10.3 Transition State 6c . . . 77
10.4 Transition State 6d . . . 78
10.5 Transition State 6e . . . 79
10.6 Transition State 6f . . . 80
10.7 Transition State 6g . . . 81
10.8 Transition State 6h . . . 82
10.9 Transition State 6i . . . 83

11 Cartesian Coordinates and Energies of Transition States TS-7 85
11.1 Transition State 7a . . . 85
11.2 Transition State 7b . . . 85
11.3 Transition State 7c . . . 86
11.4 Transition State 7d . . . 87
11.5 Transition State 7e . . . 87
11.6 Transition State 7f . . . 88
11.7 Transition State 7g . . . 89
11.8 Transition State 7h . . . 90

11.9 Transition State 7i 91

12 Cartesian Coordinates and Energies of the 1,3-dipolar Cycloaddition 92
12.1 Transition State TS-8 92
12.2 Transition State TS-9 93
12.3 Zwitterion 21 94
12.4 Cycloadduct 95

13 Reaction Enthalpies for the Formation of Iminium Ions in Model Systems 97

14 Gaussian 09 Reference 98

1 Computational Methods

Geometry optimizations were performed with the meta-hybrid density functional M06-2X and a 6-31+G(d,p) basis set. Solvation by ethanol was taken into account by the SMD solvent model, which was applied to both optimizations as well as frequency calculations. It was recently shown that the presence of a polarizable continuum model does not have a great impact on frequencies, while it might be mandatory to locate certain transition states that only exist in polar media. Thermal corrections were calculated from unscaled harmonic vibrational frequencies at the same level of theory for a standard state of 1 mol L−1 (17.12 mol L−1 for ethanol) and 298.15 K, as the experimental conditions of refluxing ethanol and high pressure in sealed tubes cannot be reproduced. The resulting free energies refer to Gibbs free energies. Free energies as well as enthalpies are corrected for zero-point vibrational energy. All stationary points were characterized and confirmed by vibrational analysis. An ultrafine grid corresponding to 99 radial shells and 590 angular points was used throughout this study for numerical integration of the density. Natural population analyses used the NBO program (version 3.1) as implemented in Gaussian 09. All calculations were performed with Gaussian 09.

2 Cartesian Coordinates and Energies of Reactants

2.1 Aminoaldehyde 1a

```
C 1.27886 0.88489 0.00000
C 0.92145 -0.48648 0.00000
Br 2.29477 -1.78335 0.00000
C -0.39176 -0.91020 -0.00000
H -0.61615 -1.97185 -0.00000
C -1.42460 0.03109 0.00000
Br -3.21814 -0.56481 0.00000
C -1.13233 1.37796 0.00000
H -1.92232 2.12418 0.00000
C 0.20025 1.81316 0.00000
C 0.41600 3.25773 0.00000
N 2.56578 1.28543 0.00000
H 3.31918 0.61451 0.00000
H 2.78113 2.27347 0.00000
O 1.51167 3.80907 -0.00000
H -0.50487 3.86585 0.00000
```

```
                           SCF energy:   -5543.213667 hartree
                zero-point correction:   +0.109165 hartree
                  enthalpy correction:   +0.120198 hartree
               free energy correction:   +0.071580 hartree
  quasiharmonic free energy correction:   +0.071580 hartree
```

2.2 Aminoaldehyde 1b

```
C -0.06130 0.85729 0.00000
C 1.29772 1.25574 0.00000
C 2.31083 0.31703 0.00000
H 3.34253 0.65827 0.00000
C 2.03457 -1.06356 0.00000
C 0.71493 -1.46851 0.00000
H 0.46382 -2.52722 0.00000
C -0.34442 -0.53766 0.00000
C -1.69803 -1.06272 0.00000
N -1.04120 1.79156 0.00000
H -0.79964 2.77185 0.00000
H -2.01269 1.51538 0.00000
O -2.72873 -0.38861 0.00000
H -1.77191 -2.16511 0.00000
H 2.84119 -1.78844 0.00000
```

```
H 1.52919 2.31759 -0.00000
```

```
                            SCF energy:   -400.803264 hartree
                 zero-point correction:   +0.127466 hartree
                   enthalpy correction:   +0.136177 hartree
                free energy correction:   +0.095339 hartree
  quasiharmonic free energy correction:   +0.095339 hartree
```

2.3 Pyrrolidine

```
C -0.77490 1.02160 -0.07164
C 0.77490 1.02160 -0.07164
C -1.15256 -0.45067 0.20083
H -1.16073 1.33811 -1.04549
H -1.19377 1.69281 0.68326
C 1.15256 -0.45067 0.20083
H 1.19378 1.69281 0.68325
H 1.16073 1.33810 -1.04550
N 0.00000 -1.26404 -0.21405
H -2.05687 -0.77179 -0.32163
H -1.30920 -0.60824 1.27457
H 1.30920 -0.60823 1.27458
H 2.05687 -0.77179 -0.32163
H 0.00000 -1.30468 -1.23334
```

```
                            SCF energy:   -212.501458 hartree
                 zero-point correction:   +0.130838 hartree
                   enthalpy correction:   +0.136672 hartree
                free energy correction:   +0.102787 hartree
  quasiharmonic free energy correction:   +0.103029 hartree
```

2.4 Piperidine

```
C -0.71501 1.25838 -0.22812
C 0.74729 1.20944 0.20484
C -1.45341 0.00000 0.23565
H -0.75898 1.32999 -1.32284
H -1.19013 2.15751 0.17969
C -0.71501 -1.25838 -0.22812
C 0.74729 -1.20944 0.20484
N 1.38443 0.00000 -0.32418
H 1.28964 -2.08288 -0.16987
H 0.79260 -1.23752 1.30931
H 0.79260 1.23752 1.30931
H 1.28964 2.08287 -0.16987
H -1.19013 -2.15751 0.17969
H -0.75898 -1.32999 -1.32284
H 2.36605 -0.00000 -0.05857
H -2.48511 0.00000 -0.13305
H -1.50512 0.00000 1.33370
```

```
                           SCF energy:   -251.806902 hartree
                 zero-point correction:   +0.160125 hartree
                   enthalpy correction:   +0.166560 hartree
                 free energy correction:   +0.131560 hartree
  quasiharmonic free energy correction:   +0.131560 hartree
```

2.5 Morpholine

```
C 1.17583 -0.75175 0.19829
C 1.19786 0.71365 -0.19891
O 0.00000 -1.39107 -0.29343
H 1.20904 -0.84568 1.29423
H 2.02620 -1.28682 -0.23103
C -1.17582 -0.75175 0.19829
C -1.19787 0.71364 -0.19891
N -0.00000 1.36606 0.33335
H -2.09038 1.19151 0.21548
H -1.24922 0.77972 -1.29908
H 1.24922 0.77972 -1.29908
H 2.09038 1.19151 0.21548
H -2.02619 -1.28683 -0.23103
H -1.20904 -0.84568 1.29423
H -0.00000 2.34594 0.06223
```

```
                           SCF energy:   -287.696860 hartree
                 zero-point correction:   +0.136732 hartree
                   enthalpy correction:   +0.142874 hartree
                 free energy correction:   +0.108381 hartree
  quasiharmonic free energy correction:   +0.108381 hartree
```

2.6 Tetrahydroisoquinoline

```
C 2.35550 0.62228 0.32137
N 2.29250 -0.63312 -0.42873
C 1.16927 1.49086 -0.07625
H 3.29367 1.13169 0.08723
H 2.33354 0.44125 1.41060
C -0.12866 0.71276 -0.03251
H 1.32655 1.86944 -1.09437
H 1.10013 2.36308 0.58293
C -0.11989 -0.68895 0.01222
C 1.18490 -1.45362 0.05723
H 1.10355 -2.35229 -0.56176
H 1.35496 -1.78903 1.09605
C -1.35783 1.38484 -0.04832
C -2.56169 0.68682 -0.01742
C -2.54975 -0.70947 0.03106
C -1.33355 -1.38612 0.04519
H -3.50434 1.22646 -0.02934
H -3.48262 -1.26539 0.05371
H -1.31842 -2.47381 0.07820
H -1.36312 2.47253 -0.08215
```

```
H 3.15873 -1.14843 -0.29542
```

```
                            SCF energy:   -404.188831 hartree
                 zero-point correction:   +0.183934 hartree
                   enthalpy correction:   +0.192531 hartree
                free energy correction:   +0.151735 hartree
  quasiharmonic free energy correction:   +0.151735 hartree
```

2.7 Tetrahydroquinoline

```
C 2.55080 0.70879 0.02161
C 2.54460 -0.68730 -0.03381
C 1.33321 1.38691 0.05259
C 0.10915 0.71341 0.03477
C 0.11301 -0.69606 -0.02965
C 1.34060 -1.38123 -0.06073
C -1.19729 1.47914 0.09608
C -2.38106 0.62431 -0.35760
H -1.11943 2.38518 -0.51437
H -1.36973 1.81324 1.12778
C -2.30965 -0.74524 0.30470
H -2.35860 0.49238 -1.44608
H -3.32457 1.11456 -0.10088
N -1.08110 -1.41126 -0.11416
H -3.15419 -1.37112 0.00577
H -2.34887 -0.62443 1.39941
H -1.00094 -2.37337 0.19399
H 3.48030 -1.23912 -0.05772
H 1.33385 -2.46787 -0.10983
H 3.48690 1.25828 0.03880
H 1.32281 2.47471 0.09444
```

```
                            SCF energy:   -404.196923 hartree
                 zero-point correction:   +0.183297 hartree
                   enthalpy correction:   +0.192058 hartree
                free energy correction:   +0.150968 hartree
  quasiharmonic free energy correction:   +0.150968 hartree
```

3 Cartesian Coordinates and Energies of Products 2

3.1 Product 2a

```
C 0.57206 0.26659 0.04559
C -0.52538 1.14037 0.00442
Br -0.21022 3.00614 -0.03315
C -1.83741 0.68835 -0.01484
H -2.66079 1.39347 -0.04413
C -2.06585 -0.68037 0.00077
Br -3.84816 -1.31984 -0.01706
C -1.00814 -1.58086 0.03346
H -1.19386 -2.65121 0.04004
C 0.30317 -1.11987 0.05573
C 1.44924 -2.10824 0.10634
N 2.67727 -1.46803 -0.33288
N 1.87985 0.72727 0.01552
C 3.89066 -2.24567 -0.08312
C 2.90078 -0.22989 0.39904
C 4.32080 0.16174 0.00903
C 5.02235 -1.20520 -0.19716
H 4.79776 0.77920 0.77321
H 4.28553 0.73110 -0.92443
H 3.97570 -3.06625 -0.80043
H 3.86498 -2.67970 0.93216
H 5.79653 -1.38796 0.55097
H 5.49489 -1.24891 -1.18091
H 2.02026 1.65951 0.38932
H 2.84655 -0.43008 1.49002
H 1.55335 -2.49337 1.13855
H 1.22899 -2.96288 -0.54090
```

```
                          SCF energy:   -5679.332791 hartree
                zero-point correction:   +0.217735 hartree
                  enthalpy correction:   +0.231407 hartree
               free energy correction:   +0.176519 hartree
  quasiharmonic free energy correction:   +0.177241 hartree
```

3.2 Product 2b

```
C 1.04964 -0.69916 -0.03646
C 2.26554 -1.39945 -0.06992
H 2.24614 -2.48605 -0.11085
C 3.47619 -0.71585 -0.05170
H 4.40678 -1.27586 -0.07598
C 3.49649 0.68037 -0.00408
H 4.43886 1.21898 0.00691
C 2.28861 1.37481 0.02608
H 2.28953 2.46261 0.06147
```

```
C 1.06211 0.70822 0.01435
C -0.23670 1.48411 0.08440
N -1.34872 0.64359 -0.33376
N -0.16822 -1.38959 -0.09945
C -2.66893 1.18249 -0.01328
C -1.31842 -0.63659 0.36325
C -2.67207 -1.25974 0.03453
C -3.60175 -0.03322 -0.15747
H -3.00910 -1.93239 0.82653
H -2.58364 -1.83593 -0.89136
H -2.92134 2.01158 -0.68006
H -2.68666 1.56216 1.02449
H -4.40539 -0.00108 0.58116
H -4.06148 -0.05230 -1.14835
H -0.11891 -2.32762 0.28650
H -1.24477 -0.45195 1.45731
H -0.39238 1.84747 1.11867
H -0.18346 2.36645 -0.56215
```

```
                          SCF energy:   -536.916765 hartree
               zero-point correction:   +0.236299 hartree
                 enthalpy correction:   +0.247304 hartree
              free energy correction:   +0.200639 hartree
quasiharmonic free energy correction:   +0.201069 hartree
```

3.3 Product 2c

```
C 0.32686 0.30807 0.14402
C -0.78738 1.15040 0.01376
Br -0.51263 3.02084 -0.06591
C -2.08465 0.66243 -0.05924
H -2.92279 1.34371 -0.15604
C -2.27862 -0.71099 -0.00494
Br -4.03918 -1.40123 -0.09647
C -1.20166 -1.58142 0.11493
H -1.36006 -2.65558 0.14881
C 0.09412 -1.08299 0.18891
C 1.26646 -2.03149 0.31027
N 2.49475 -1.36118 -0.08819
N 1.62262 0.79855 0.18204
C 3.67885 -2.20182 0.07773
C 2.63912 -0.12470 0.67740
C 4.71649 -0.04526 -0.75141
C 4.86365 -1.57501 -0.67661
H 3.44941 -3.19646 -0.31491
H 3.91333 -2.32746 1.15099
H 5.79391 -1.84026 -0.16252
H 4.92293 -1.99017 -1.68776
H 1.71086 1.73999 0.54983
H 1.33058 -2.40935 1.34856
H 1.10505 -2.89535 -0.34217
C 4.04516 0.46899 0.51977
H 4.10940 0.23370 -1.61902
```

```
H 5.69490 0.42728 -0.88042
H 3.97578 1.56200 0.52623
H 4.64850 0.18340 1.38857
H 2.44959 -0.34050 1.74877
```

```
                           SCF energy:   -5718.629577 hartree
                 zero-point correction:   +0.246959 hartree
                   enthalpy correction:   +0.261527 hartree
                 free energy correction:   +0.205050 hartree
  quasiharmonic free energy correction:   +0.205944 hartree
```

3.4 Product 2d

```
C 0.30603 0.32615 0.07791
C -0.82503 1.15256 0.00834
Br -0.58840 3.02853 -0.04328
C -2.11476 0.64037 -0.02704
H -2.96777 1.30799 -0.07940
C -2.28261 -0.73700 0.00470
Br -4.03297 -1.45681 -0.03999
C -1.18673 -1.59023 0.07039
H -1.32389 -2.66747 0.09389
C 0.09983 -1.06700 0.10959
C 1.29568 -1.98016 0.21564
N 2.50779 -1.32377 -0.26847
N 1.59079 0.83560 0.05519
C 3.67179 -2.17795 -0.02140
C 2.68999 -0.04432 0.40921
O 5.09510 -0.23930 0.20474
C 4.94132 -1.48410 -0.47281
H 3.54248 -3.11326 -0.57482
H 3.75413 -2.42356 1.05297
H 5.81737 -2.08780 -0.22678
H 4.91878 -1.30714 -1.55764
H 1.69305 1.78506 0.39636
H 1.41769 -2.29798 1.26783
H 1.12686 -2.88262 -0.37983
C 3.98919 0.60442 -0.05525
H 3.91598 0.81741 -1.13186
H 4.15728 1.53874 0.48733
H 2.73704 -0.20450 1.50576
```

```
                           SCF energy:   -5754.526331 hartree
                 zero-point correction:   +0.223442 hartree
                   enthalpy correction:   +0.237705 hartree
                 free energy correction:   +0.181704 hartree
  quasiharmonic free energy correction:   +0.182635 hartree
```

3.5 Product 2e

```
C 0.39502 0.14350 0.05860
C 1.39291 1.12168 -0.06600
```

```
Br 0.88356 2.93711 -0.21468
C 2.74328 0.80297 -0.08045
H 3.49030 1.58387 -0.17232
C 3.11042 -0.53182 0.02520
Br 4.94864 -0.98509 0.01674
C 2.15186 -1.53237 0.13389
H 2.44475 -2.57626 0.20194
C 0.80150 -1.20197 0.15102
C -0.24595 -2.28441 0.26089
N -1.54561 -1.80184 -0.19753
N -0.95290 0.45824 0.02797
H -1.17684 1.40113 0.32214
C -2.57828 -2.81582 0.00255
C -1.87371 -0.56886 0.50816
C -3.84911 -2.38600 -0.70954
H -2.77307 -2.97356 1.07964
H -2.20933 -3.76012 -0.40736
C -3.30888 -0.12811 0.28572
H -1.72331 -0.72208 1.59828
C -4.24619 -0.98931 -0.29799
H -4.66313 -3.08191 -0.48249
H -3.68491 -2.42059 -1.79357
C -5.56159 -0.54319 -0.47541
C -3.71064 1.14243 0.71733
C -5.02054 1.57528 0.53683
C -5.95057 0.72951 -0.07114
H -3.00324 1.80359 1.21378
H -5.31561 2.56424 0.87435
H -6.28644 -1.21458 -0.93035
H -6.97603 1.05704 -0.21524
H -0.30242 -2.63919 1.30685
H 0.04483 -3.13819 -0.35863
```

```
                           SCF energy:   -5871.016638 hartree
                zero-point correction:   +0.270460 hartree
                  enthalpy correction:   +0.287383 hartree
               free energy correction:   +0.225240 hartree
  quasiharmonic free energy correction:   +0.227264 hartree
```

3.6 Product 2f

```
C 0.37141 0.22643 0.54874
C 1.32184 1.14198 0.07215
Br 0.82053 2.95394 -0.14563
C 2.62158 0.76786 -0.24054
H 3.33208 1.50315 -0.60194
C 2.98383 -0.56278 -0.08243
Br 4.75127 -1.09803 -0.50653
C 2.07068 -1.50423 0.37825
H 2.35915 -2.54559 0.49262
C 0.77368 -1.11981 0.69635
C -0.22573 -2.13606 1.22592
N -1.61035 -1.68458 1.09919
```

```
N -0.93551 0.59017 0.82094
H -1.09208 1.57344 1.01036
C -1.72226 -0.33684 1.64182
C -2.05340 -1.75786 -0.29768
C -3.17460 0.10388 1.69075
H -1.31733 -0.37181 2.66179
C -3.38891 -1.09263 -0.52272
H -2.11932 -2.81661 -0.56881
H -1.31731 -1.30009 -0.98098
C -3.90815 -0.17975 0.40184
H -3.22715 1.17196 1.93107
H -3.65918 -0.42994 2.51599
C -5.12815 0.45112 0.12959
C -4.09776 -1.36161 -1.69956
C -5.31108 -0.73313 -1.96243
C -5.83024 0.18001 -1.04098
H -3.68699 -2.07153 -2.41469
H -5.85040 -0.95298 -2.87923
H -5.52608 1.16367 0.84908
H -6.77510 0.67882 -1.23654
H -0.01770 -2.33534 2.28321
H -0.11089 -3.08238 0.68826
```

```
                           SCF energy:   -5871.021824 hartree
                 zero-point correction:   +0.270729 hartree
                   enthalpy correction:   +0.287540 hartree
                 free energy correction:   +0.225195 hartree
  quasiharmonic free energy correction:   +0.227855 hartree
```

3.7 Product 2g

```
C -1.96413 -0.71840 -0.13998
C -2.90787 -1.73836 -0.33579
C -4.26841 -1.45509 -0.29201
H -4.98613 -2.25654 -0.44257
C -4.71063 -0.15036 -0.05681
C -3.77083 0.86111 0.13163
H -4.10045 1.88250 0.31145
C -2.40094 0.59577 0.09415
C -1.39044 1.69474 0.31810
N -0.06043 1.29746 -0.14295
N -0.59410 -0.99097 -0.21681
H -0.37167 -1.95177 0.01960
C 0.92907 2.30464 0.23021
C 0.27769 -0.00763 0.42103
C 2.24556 2.00805 -0.46544
H 1.06961 2.32954 1.32726
H 0.54736 3.28340 -0.07391
C 1.73652 -0.37392 0.20671
H 0.08352 0.01305 1.51606
C 2.66838 0.57966 -0.22353
H 3.02404 2.68865 -0.10544
```

```
H 2.13437 2.18410 -1.54248
C 4.00240 0.19525 -0.40804
C 2.16482 -1.67908 0.48192
C 3.49262 -2.05089 0.29544
C 4.41678 -1.10923 -0.16146
H 1.46221 -2.41838 0.85966
H 3.80495 -3.06834 0.51070
H 4.72070 0.93964 -0.74457
H 5.45580 -1.38831 -0.31054
H -1.36535 1.96168 1.39185
H -1.68904 2.59452 -0.22970
H -5.77202 0.07501 -0.02459
H -2.55969 -2.75176 -0.52126
```

```
                            SCF energy:   -728.594924 hartree
                  zero-point correction:   0.289581 hartree
                    enthalpy correction:   0.303664 hartree
                 free energy correction:   0.250027 hartree
   quasiharmonic free energy correction:   0.251016 hartree
```

3.8 Product 2h

```
C -1.94776 -0.68854 -0.20169
C -2.82746 -1.33466 -1.08475
C -4.07660 -0.78923 -1.36142
H -4.74532 -1.30572 -2.04437
C -4.46949 0.41356 -0.76860
C -3.59184 1.05747 0.10275
H -3.88282 1.99679 0.56966
C -2.33696 0.52460 0.40002
C -1.39979 1.21266 1.37821
N -0.01660 0.73942 1.27259
N -0.67487 -1.20686 0.04667
H -0.59894 -2.20844 -0.09868
C -0.00967 -0.72039 1.25895
C 0.63488 1.30208 0.08536
C 1.41299 -1.24934 1.33435
H -0.56345 -1.04153 2.15273
C 1.99024 0.69224 -0.17611
H 0.74382 2.37993 0.24511
H 0.01271 1.17486 -0.81732
C 2.35024 -0.53626 0.38910
H 1.41578 -2.32635 1.13021
H 1.76771 -1.12307 2.36364
C 3.60421 -1.08460 0.09220
C 2.88637 1.34849 -1.02835
C 4.13031 0.79700 -1.32030
C 4.49233 -0.42843 -0.75493
H 2.59932 2.30302 -1.46466
H 4.81513 1.31895 -1.98233
H 3.88042 -2.03984 0.53383
H 5.46055 -0.86869 -0.97508
```

```
H -1.74587 1.04154 2.40454
H -1.41144 2.29512 1.21326
H -5.44241 0.84357 -0.98523
H -2.51687 -2.26778 -1.54899
```

```
                           SCF energy:   -728.598803 hartree
                zero-point correction:   0.289710 hartree
                  enthalpy correction:   0.303672 hartree
               free energy correction:   0.250164 hartree
  quasiharmonic free energy correction:   0.251364 hartree
```

3.9 Product 2i

```
C 0.14660 0.60488 -0.55868
C 1.21482 1.24915 0.08430
Br 0.97149 3.01394 0.72032
C 2.44705 0.63846 0.27138
H 3.25066 1.16927 0.76952
C 2.62081 -0.66051 -0.18536
Br 4.29169 -1.51420 0.07033
C 1.58600 -1.34064 -0.81731
H 1.72434 -2.36113 -1.16394
C 0.35905 -0.71802 -1.00625
C -0.78044 -1.43229 -1.70721
N -2.07837 -0.85472 -1.37764
N -1.09406 1.19491 -0.69863
C -2.05479 0.59248 -1.62959
C -4.47702 0.25257 -0.93057
C -2.63273 -1.17397 -0.11390
C -3.89253 -0.60280 0.15664
C -4.51940 -0.86690 1.36953
C -2.02812 -2.00659 0.83255
C -2.68333 -2.27661 2.03763
C -3.92353 -1.70812 2.31474
H -1.05220 -2.44484 0.65071
H -2.20676 -2.92818 2.76454
H -5.48949 -0.41829 1.57143
H -4.42443 -1.91328 3.25599
C -3.43236 1.25244 -1.44626
H -5.36841 0.77782 -0.57780
H -4.78354 -0.39513 -1.76227
H -3.33392 2.07424 -0.72956
H -3.76445 1.68216 -2.39440
H -0.64949 -1.35469 -2.79208
H -0.77811 -2.49719 -1.46319
H -1.12342 2.20558 -0.63595
H -1.70534 0.71045 -2.66203
```

```
                           SCF energy:   -5871.022425 hartree
                zero-point correction:   +0.270676 hartree
                  enthalpy correction:   +0.287504 hartree
               free energy correction:   +0.225393 hartree
  quasiharmonic free energy correction:   +0.227765 hartree
```

4 Cartesian Coordinates and Energies of Hemiaminals 3

4.1 Hemiaminal 3a

```
C 1.04102 -1.29030 0.07044
C 1.99910 -0.26423 0.02493
Br 3.84059 -0.71073 0.06142
C 1.65928 1.08122 -0.03421
H 2.43312 1.84023 -0.06912
C 0.31699 1.42169 -0.04542
Br -0.18636 3.24499 -0.11210
C -0.66584 0.43972 -0.00079
H -1.70764 0.73244 0.00753
C -0.32298 -0.90536 0.04473
C -1.39175 -1.99250 0.18305
N -2.76803 -1.58653 0.18093
N 1.39586 -2.61745 0.20780
H 2.36195 -2.84336 0.00937
H 0.74016 -3.27635 -0.19688
C -3.27673 -0.87083 1.36638
C -3.36237 -1.05648 -1.05341
C -4.67895 -0.46252 -0.55415
H -3.51570 -1.85993 -1.77945
H -2.74345 -0.28712 -1.53988
C -4.28826 0.13800 0.80116
H -5.41566 -1.26194 -0.41657
H -5.09504 0.27274 -1.24707
H -2.47377 -0.37117 1.92328
H -3.75951 -1.57926 2.05155
H -5.13976 0.28848 1.46915
H -3.80821 1.11151 0.64798
O -1.17133 -2.91364 -0.87854
H -1.20782 -2.49342 1.14771
H -1.76815 -3.66528 -0.74302
```

```
                          SCF energy:   -5755.732602 hartree
                zero-point correction:   +0.243861 hartree
                  enthalpy correction:   +0.259923 hartree
               free energy correction:   +0.200301 hartree
  quasiharmonic free energy correction:   +0.201438 hartree
```

4.2 Hemiaminal 3b

```
C -2.22791 0.69707 -0.06033
C -3.41621 -0.05072 -0.01912
H -4.36457 0.47937 0.02916
C -3.38980 -1.44007 -0.04959
H -4.32404 -1.99387 -0.01634
C -2.17167 -2.11530 -0.12761
```

```
H -2.13992 -3.19969 -0.16348
C -0.98897 -1.37771 -0.16702
H -0.04021 -1.89611 -0.25809
C -0.98880 0.01783 -0.11732
C 0.29236 0.82678 -0.23177
N 1.48234 0.01727 -0.29927
N -2.29259 2.08728 -0.13344
H -3.19611 2.47208 0.11584
H -1.52760 2.56698 0.32649
C 2.65930 0.70790 -0.84185
C 1.96366 -0.55791 0.96328
C 3.29123 -1.19668 0.55037
H 1.24730 -1.26728 1.38469
H 2.13802 0.23211 1.71076
C 3.81381 -0.27455 -0.58141
H 3.11582 -2.20683 0.16871
H 3.98482 -1.27093 1.39139
H 2.84681 1.65602 -0.30855
H 2.51147 0.93729 -1.90081
H 4.04091 -0.85352 -1.48013
H 4.72267 0.25887 -0.29298
O 0.30336 1.76034 0.86289
H 0.24691 1.40343 -1.16770
H 0.96054 2.44768 0.68112
```

```
                            SCF energy:   -613.319781 hartree
                 zero-point correction:   +0.262555 hartree
                   enthalpy correction:   +0.276137 hartree
                 free energy correction:   +0.223679 hartree
  quasiharmonic free energy correction:   +0.224529 hartree
```

4.3 Hemiaminal 3c

```
C 1.10271 -1.33628 0.02954
C 2.21839 -0.48383 0.03368
Br 3.95615 -1.23374 0.12310
C 2.10690 0.89994 -0.01294
H 2.99562 1.52128 -0.00860
C 0.84057 1.45881 -0.06252
Br 0.65429 3.34151 -0.12569
C -0.29347 0.65385 -0.06183
H -1.27326 1.11295 -0.07030
C -0.17698 -0.72959 -0.02482
C -1.40769 -1.62671 0.08580
N -2.70334 -1.01186 0.12624
N 1.22539 -2.70599 0.14774
H 2.14585 -3.08627 -0.03062
H 0.48136 -3.23850 -0.28950
C -3.09916 -0.42879 1.40951
C -3.21096 -0.30053 -1.04584
C -4.73088 -0.51192 -1.12301
H -2.71479 -0.69197 -1.93706
H -2.99948 0.77857 -1.00571
```

```
C -4.47387 0.24107 1.27125
H -2.36549 0.30369 1.78519
H -3.14908 -1.24075 2.14726
O -1.33874 -2.54225 -1.00247
H -1.30553 -2.17918 1.03521
H -2.07327 -3.16705 -0.90286
C -5.34926 -0.54201 0.29189
H -4.35453 1.26940 0.90881
H -4.94047 0.30633 2.25877
H -6.36480 -0.13407 0.27383
H -5.43170 -1.57723 0.64390
H -4.94884 -1.45008 -1.64502
H -5.16941 0.29944 -1.71515
```

```
                           SCF energy:   -5795.028622 hartree
                zero-point correction:   +0.272896 hartree
                  enthalpy correction:   +0.290128 hartree
               free energy correction:   +0.227480 hartree
  quasiharmonic free energy correction:   +0.229461 hartree
```

4.4 Hemiaminal 3d

```
C 1.11648 -1.33246 0.04849
C 2.21764 -0.46099 0.03357
Br 3.96906 -1.18062 0.10223
C 2.08240 0.92030 -0.01921
H 2.96072 1.55620 -0.02838
C 0.80645 1.45791 -0.05674
Br 0.58758 3.33689 -0.12484
C -0.31352 0.63386 -0.04176
H -1.30017 1.07794 -0.04231
C -0.17363 -0.74741 0.00085
C -1.38954 -1.66316 0.11932
N -2.69391 -1.06257 0.13810
N 1.26542 -2.69806 0.17855
H 2.19170 -3.06307 -0.00132
H 0.52791 -3.25008 -0.24492
C -3.12149 -0.46165 1.40002
C -3.20880 -0.38812 -1.04612
C -4.73066 -0.56317 -1.04703
H -2.78902 -0.85334 -1.94072
H -2.95963 0.68175 -1.08445
C -4.46215 0.23954 1.16632
H -2.40521 0.27355 1.80156
H -3.23269 -1.25843 2.14563
O -1.30445 -2.59263 -0.95309
H -1.29050 -2.19750 1.07915
H -2.01690 -3.23983 -0.83694
O -5.26771 -0.52487 0.28128
H -4.31344 1.24875 0.75888
H -5.01224 0.33272 2.10479
H -5.00399 -1.54178 -1.45179
H -5.20113 0.22016 -1.65624
```

```
                           SCF energy:   -5830.917033 hartree
                 zero-point correction:   +0.249552 hartree
                   enthalpy correction:   +0.266502 hartree
                 free energy correction:   +0.204253 hartree
  quasiharmonic free energy correction:   +0.206225 hartree
```

4.5 Hemiaminal 3e

```
C -1.02752 1.11560 0.80970
C -2.13851 1.16442 -0.05531
Br -2.76767 2.85141 -0.64291
C -2.80781 0.03468 -0.50213
H -3.66052 0.12949 -1.16539
C -2.36023 -1.20745 -0.08095
Br -3.23965 -2.77102 -0.68109
C -1.26431 -1.30911 0.76464
H -0.92373 -2.28464 1.10046
C -0.58580 -0.17355 1.20175
C 0.65326 -0.44012 2.05363
N 1.90132 -0.58034 1.31182
N -0.38206 2.26835 1.19768
H -0.91043 3.12793 1.13133
H 0.18774 2.18907 2.03104
C 2.20649 0.55262 0.43873
C 1.99097 -1.83089 0.55542
C 4.12405 -0.88926 -0.38343
C 3.53906 0.37649 -0.25304
C 4.18079 1.49496 -0.79814
C 5.34860 -1.00846 -1.05279
C 5.98511 0.10634 -1.59061
C 5.39633 1.36719 -1.46370
H 5.80228 -1.99253 -1.15194
H 6.93390 -0.00542 -2.10752
H 3.71876 2.47455 -0.69355
H 5.88400 2.24431 -1.87907
O 0.78166 0.57926 3.02464
H 0.49764 -1.40437 2.55139
H 1.58753 0.40194 3.53275
H 2.22556 1.46816 1.03563
H 1.42294 0.67883 -0.33121
C 3.44835 -2.10565 0.20695
H 1.59343 -2.64699 1.16595
H 1.38478 -1.77713 -0.36666
H 3.50871 -2.94314 -0.49648
H 3.98281 -2.41042 1.11534
```

```
                           SCF energy:   -5947.423272 hartree
                 zero-point correction:   +0.295781 hartree
                   enthalpy correction:   +0.315279 hartree
                 free energy correction:   +0.247182 hartree
  quasiharmonic free energy correction:   +0.250574 hartree
```

4.6 Hemiaminal 3f

```
C 1.44195 -1.22360 0.56733
C 2.50646 -0.74056 -0.21973
Br 3.66662 -1.98311 -1.05580
C 2.75446 0.60917 -0.42115
H 3.59009 0.92516 -1.03555
C 1.91559 1.53323 0.18124
Br 2.21650 3.38291 -0.07804
C 0.84927 1.10637 0.96052
H 0.20227 1.83445 1.44162
C 0.58987 -0.24998 1.14810
C -0.66787 -0.56746 1.95408
N -1.89255 -0.70182 1.17314
N 1.23023 -2.57755 0.71249
H 2.02740 -3.17723 0.54669
H 0.67314 -2.84379 1.51546
C -1.83207 -1.67080 0.07621
C -2.38048 0.58310 0.67984
C -3.25020 -2.02761 -0.35195
H -1.31544 -2.56815 0.41885
H -1.26665 -1.25808 -0.77893
C -3.69774 0.43867 -0.04756
H -1.65379 1.04643 -0.01335
H -2.50036 1.26671 1.52748
C -4.10526 -0.79914 -0.56008
H -3.70824 -2.65799 0.42079
H -3.22070 -2.62122 -1.27191
C -5.32143 -0.88257 -1.24994
C -4.50188 1.56784 -0.23949
C -5.70819 1.47605 -0.92747
C -6.12099 0.24161 -1.43560
H -4.17550 2.52563 0.16063
H -6.32418 2.35977 -1.06608
H -5.63831 -1.84498 -1.64661
H -7.06048 0.15786 -1.97434
O -0.45288 -1.73822 2.71557
H -0.83942 0.28282 2.62541
H -1.26856 -1.92509 3.20409
```

```
                          SCF energy:  -5947.422568 hartree
                zero-point correction:  +0.296212 hartree
                  enthalpy correction:  +0.315704 hartree
               free energy correction:  +0.247228 hartree
quasiharmonic free energy correction:  +0.251004 hartree
```

4.7 Hemiaminal 3g

```
C -2.62460 1.02671 -0.01815
C -3.53160 1.19399 -1.08218
H -3.83795 2.20409 -1.34394
C -4.03173 0.10834 -1.78842
```

```
H -4.73124 0.27708 -2.60245
C -3.64619 -1.18888 -1.44607
H -4.03866 -2.04734 -1.98148
C -2.75383 -1.36172 -0.39172
H -2.45690 -2.36856 -0.10424
C -2.22164 -0.28451 0.32681
C -1.20688 -0.62953 1.41035
N 0.19292 -0.66607 0.98640
N -2.12529 2.16077 0.61315
H -2.70320 2.98548 0.50575
H -1.80197 2.02009 1.56219
C 0.65046 0.56665 0.34731
C 0.50035 -1.81287 0.13054
C 2.75526 -0.74869 -0.17817
C 2.11105 0.48693 -0.03617
C 2.81887 1.66839 -0.28789
C 4.10141 -0.77557 -0.56441
C 4.80183 0.40151 -0.81189
C 4.15554 1.63272 -0.67381
H 4.60006 -1.73657 -0.67392
H 5.84501 0.36145 -1.11200
H 2.31079 2.62412 -0.17602
H 4.69231 2.55783 -0.86308
O -1.35069 0.27095 2.49387
H -1.42958 -1.64832 1.75057
H -0.70021 0.02393 3.16791
H 0.49952 1.40273 1.03526
H 0.05832 0.78170 -0.56125
C 2.00741 -2.03279 0.09854
H 0.00202 -2.70024 0.53189
H 0.12073 -1.65330 -0.89479
H 2.25754 -2.78071 -0.66163
H 2.33125 -2.43813 1.06538
```

```
                          SCF energy:   -805.007307 hartree
                zero-point correction:   +0.315643 hartree
                  enthalpy correction:   +0.332288 hartree
               free energy correction:   +0.272859 hartree
  quasiharmonic free energy correction:   +0.274725 hartree
```

4.8 Hemiaminal 3h

```
C 2.97737 -0.48454 -0.45185
C 3.84819 0.26430 -1.26660
H 4.46612 -0.26790 -1.98615
C 3.93291 1.64634 -1.16435
H 4.61868 2.18843 -1.80957
C 3.15396 2.32896 -0.22900
H 3.22074 3.40721 -0.12645
C 2.29429 1.59441 0.58313
H 1.69555 2.11164 1.33042
C 2.17227 0.20283 0.48667
```

```
C 1.13774 -0.44965 1.39653
N -0.20829 -0.58962 0.84195
N 2.91755 -1.86228 -0.63819
H 3.73837 -2.25494 -1.08316
H 2.61235 -2.39252 0.16875
C -0.27571 -1.27964 -0.44757
C -0.90485 0.69093 0.75970
C -1.71013 -1.72481 -0.70595
H 0.38155 -2.14963 -0.41943
H 0.07260 -0.61981 -1.26276
C -2.32278 0.52597 0.26195
H -0.37928 1.38746 0.07994
H -0.91287 1.15518 1.75205
C -2.70319 -0.61238 -0.46000
H -1.94669 -2.56970 -0.04655
H -1.80544 -2.08827 -1.73488
C -4.01818 -0.71100 -0.93209
C -3.25597 1.54304 0.49420
C -4.56014 1.43748 0.01970
C -4.94404 0.30179 -0.69799
H -2.95196 2.42418 1.05565
H -5.27429 2.23338 0.20978
H -4.31190 -1.59601 -1.49289
H -5.95917 0.20898 -1.07323
O 1.61090 -1.71843 1.81033
H 1.02051 0.20166 2.27235
H 0.93253 -2.11286 2.37827
```

```
                          SCF energy:   -805.006897 hartree
               zero-point correction:   +0.315643 hartree
                 enthalpy correction:   +0.332323 hartree
              free energy correction:   +0.272818 hartree
quasiharmonic free energy correction:   +0.274601 hartree
```

4.9 Hemiaminal 3i

```
C -1.16847 -1.13111 -0.53337
C -2.49915 -0.86701 -0.14863
Br -3.69781 -2.31943 0.04963
C -2.98108 0.40834 0.10128
H -4.01500 0.55612 0.39370
C -2.11116 1.48090 -0.02848
Br -2.73094 3.23515 0.31622
C -0.79423 1.27444 -0.41075
H -0.11780 2.11747 -0.51902
C -0.31346 -0.00921 -0.65821
C 1.15004 -0.08994 -1.06794
N 2.04034 -0.17397 0.06695
N -0.71906 -2.42211 -0.69171
H -1.41994 -3.13287 -0.85252
H 0.12024 -2.52989 -1.24804
C 1.72228 -1.17133 1.09258
C 4.36449 -0.24327 0.83889
```

```
C 3.40974 0.09141 -0.15196
C 3.86589 0.71822 -1.32966
C 5.70712 0.07586 0.62795
C 6.15008 0.70446 -0.53307
C 5.21294 1.01865 -1.51373
H 6.42075 -0.18291 1.40774
H 7.20135 0.93736 -0.67008
H 3.18229 0.97989 -2.12941
H 5.52209 1.50131 -2.43653
O 1.31503 -1.16117 -1.99793
H 1.36574 0.84827 -1.58219
H 2.21408 -1.13101 -2.35757
C 3.97157 -0.95119 2.11781
C 2.47421 -0.85625 2.37500
H 4.25851 -2.00824 2.04075
H 4.54123 -0.53329 2.95418
H 2.20247 0.15305 2.70576
H 2.17209 -1.55743 3.15832
H 1.97703 -2.18569 0.74613
H 0.64723 -1.13860 1.27455
```

```
                           SCF energy:   -5947.424750 hartree
                zero-point correction:   +0.296110 hartree
                  enthalpy correction:   +0.315787 hartree
               free energy correction:   +0.247079 hartree
  quasiharmonic free energy correction:   +0.250602 hartree
```

5 Cartesian Coordinates and Energies of Azaquinone Methides 4

5.1 Azaquinone Methide *cis*-4a

```
C -0.38353 0.80980 -0.55338
C 0.94530 1.21328 -0.09233
C 1.96761 0.34156 0.12808
H 2.94757 0.70623 0.41930
C 1.75191 -1.05125 -0.03837
C 0.50927 -1.52412 -0.34348
H 0.32961 -2.59262 -0.42999
C -0.59110 -0.63525 -0.49587
C -1.84688 -1.27893 -0.64372
N -3.04128 -0.85530 -0.31287
H -1.82835 -2.30194 -1.02009
N -1.28962 1.60955 -1.04509
H -0.96106 2.57455 -1.00947
C -4.24947 -1.67618 -0.53951
C -3.34651 0.30177 0.54455
C -4.83931 0.15783 0.85636
H -3.08135 1.22653 0.02592
H -2.71297 0.22304 1.43662
C -5.12305 -1.33540 0.66000
H -5.42498 0.74512 0.14199
H -5.07457 0.51062 1.86235
H -3.96811 -2.72761 -0.62057
H -4.71974 -1.35658 -1.47590
H -6.17680 -1.55214 0.47444
H -4.79297 -1.90744 1.53357
Br 1.27169 3.06574 0.12621
Br 3.21444 -2.23049 0.19589
```

```
                          SCF energy:   -5679.288336 hartree
                zero-point correction:   +0.215101 hartree
                  enthalpy correction:   +0.229763 hartree
               free energy correction:   +0.171725 hartree
  quasiharmonic free energy correction:   +0.173892 hartree
```

5.2 Azaquinone Methide *trans*-4a

```
C 0.54734 -1.48323 0.00767
C 1.81840 -0.75821 0.01057
C 1.92044 0.59752 0.00443
H 2.89524 1.07451 0.02583
C 0.74566 1.39339 -0.02919
C -0.48782 0.81369 -0.07756
H -1.35938 1.44971 -0.13821
C -0.62899 -0.60239 -0.08349
C -1.85764 -1.27951 -0.25423
```

```
N -3.09586 -0.84940 -0.22564
H -1.76613 -2.34899 -0.43253
N 0.41904 -2.77753 0.09298
H 1.33408 -3.22414 0.10583
C -4.23797 -1.76301 -0.44150
C -3.57637 0.49944 0.13142
C -5.10196 0.35232 0.21382
H -3.28066 1.22140 -0.63294
H -3.12640 0.78349 1.08878
C -5.32598 -1.14823 0.42721
H -5.55446 0.66407 -0.73225
H -5.51937 0.96798 1.01241
H -3.95007 -2.77913 -0.16925
H -4.51706 -1.73532 -1.50108
H -6.32368 -1.47631 0.12960
H -5.16201 -1.41959 1.47535
Br 3.41444 -1.77785 0.05411
Br 0.93348 3.27729 -0.01862
```

```
                          SCF energy:  -5679.290708 hartree
                zero-point correction:  +0.215849 hartree
                  enthalpy correction:  +0.230523 hartree
               free energy correction:  +0.171923 hartree
  quasiharmonic free energy correction:  +0.174541 hartree
```

5.3 Azaquinone Methide *cis*-4b

```
C 1.43779 0.89345 -0.33507
C 2.77105 1.15566 0.19468
H 3.07967 2.19667 0.26721
C 3.63659 0.15211 0.51132
H 4.63818 0.39989 0.85545
C 3.26188 -1.22356 0.38167
H 3.97621 -2.01037 0.59895
C 1.97927 -1.51754 0.01236
H 1.65651 -2.55543 -0.04954
C 1.00063 -0.50041 -0.24130
C -0.31078 -0.97471 -0.44430
N -1.46747 -0.36739 -0.27406
H -0.41047 -2.02388 -0.72654
N 0.71242 1.80873 -0.93085
H 1.21822 2.69668 -0.90758
C -2.74685 -1.04515 -0.56455
C -1.68801 0.88265 0.46837
C -3.21128 0.98946 0.57742
H -1.20952 1.71626 -0.05297
H -1.20204 0.77621 1.44701
C -3.69229 -0.46202 0.47795
H -3.60401 1.57070 -0.26351
H -3.51556 1.48134 1.50347
H -2.61007 -2.12677 -0.50418
H -3.06707 -0.78305 -1.57939
H -4.73905 -0.55018 0.17982
```

```
H -3.55367 -0.97707 1.43480
```

```
                            SCF energy:   -536.870958 hartree
                 zero-point correction:   +0.234051 hartree
                   enthalpy correction:   +0.246059 hartree
                free energy correction:   +0.196665 hartree
  quasiharmonic free energy correction:   +0.197697 hartree
```

5.4 Azaquinone Methide *trans*-4b

```
C 2.10030 1.00535 0.12667
C 3.40294 0.36006 0.02653
H 4.28137 0.99945 0.08511
C 3.53660 -0.98885 -0.09998
H 4.53213 -1.42436 -0.14680
C 2.39513 -1.84929 -0.18354
H 2.52676 -2.91964 -0.30012
C 1.14450 -1.29812 -0.15365
H 0.28852 -1.95103 -0.27637
C 0.94139 0.11473 -0.03097
C -0.30393 0.75304 -0.15994
N -1.52858 0.26975 -0.11921
H -0.26247 1.82996 -0.32059
N 1.95033 2.28585 0.36427
H 2.86942 2.72906 0.39289
C -2.70266 1.14120 -0.36327
C -1.94437 -1.08203 0.28813
C -3.42205 -0.90665 0.63342
H -1.33112 -1.41697 1.12868
H -1.81856 -1.77862 -0.54847
C -3.87631 0.16703 -0.35911
H -3.52438 -0.53995 1.66022
H -3.97323 -1.84442 0.54071
H -2.57743 1.67700 -1.30587
H -2.77882 1.86652 0.45437
H -4.80870 0.65569 -0.07047
H -4.00495 -0.27072 -1.35455
```

```
                            SCF energy:   -536.873989 hartree
                 zero-point correction:   +0.234210 hartree
                   enthalpy correction:   +0.246323 hartree
                free energy correction:   +0.196467 hartree
  quasiharmonic free energy correction:   +0.197702 hartree
```

5.5 Azaquinone Methide *cis*-4c

```
C -0.20479 0.75003 -0.26406
C 1.16799 1.21571 -0.06352
C 2.24825 0.39354 0.05121
C 2.06973 -1.01080 -0.00366
C 0.81662 -1.53867 -0.12216
H 0.67482 -2.61566 -0.15340
```

```
C -0.33221 -0.70329 -0.16530
C -1.55819 -1.42602 -0.22602
N -2.77049 -1.11238 0.15644
N -1.22466 1.50546 -0.56608
H -0.93234 2.48059 -0.61935
C -3.89218 -2.02658 -0.12344
C -3.13374 -0.00438 1.05103
C -4.28908 0.80353 0.46949
C -5.04429 -1.25383 -0.75884
H -4.21156 -2.46059 0.83260
H -3.53360 -2.82520 -0.77391
H 3.24453 0.80844 0.16766
Br 1.46120 3.08737 -0.02426
Br 3.59526 -2.12959 0.08333
H -5.87070 -1.95006 -0.93297
H -4.72147 -0.87022 -1.73468
H -3.93535 1.31132 -0.43411
H -4.57101 1.57236 1.19617
H -1.48339 -2.43519 -0.63117
H -2.25872 0.60935 1.23705
H -3.44508 -0.48168 1.99019
C -5.48065 -0.09811 0.14268
H -6.27271 0.48125 -0.34188
H -5.89822 -0.50543 1.07330
```

```
                           SCF energy:   -5718.588530 hartree
                zero-point correction:   +0.244699 hartree
                  enthalpy correction:   +0.260225 hartree
                free energy correction:   +0.200716 hartree
quasiharmonic free energy correction:   +0.202779 hartree
```

5.6 Azaquinone Methide *trans*-4c

```
C 0.88620 -1.48656 0.14039
C 2.08164 -0.66325 0.00668
C 2.06362 0.69905 -0.03461
C 0.82801 1.38993 0.01263
C -0.35203 0.70148 0.07662
H -1.28702 1.24642 0.02088
C -0.35461 -0.71450 0.11864
C -1.53498 -1.49615 -0.00774
N -2.76786 -1.22896 0.34132
N 0.85564 -2.78462 0.29623
H 1.79561 -3.17000 0.21653
C -3.88103 -2.06949 -0.12938
C -3.22186 -0.07456 1.12806
C -4.10122 0.82627 0.26202
C -4.79230 -1.23195 -1.02671
H -4.42750 -2.41907 0.75401
H -3.46801 -2.92977 -0.65796
H 2.99181 1.25670 -0.11094
Br 3.75573 -1.54653 -0.08787
Br 0.84278 3.28212 -0.07858
```

```
H -5.63768 -1.85244 -1.33979
H -4.23438 -0.95125 -1.92874
H -3.50474 1.24073 -0.56043
H -4.45446 1.66347 0.87174
H -1.39788 -2.47853 -0.45809
H -2.36314 0.43597 1.55976
H -3.81891 -0.48653 1.95081
C -5.27928 0.02327 -0.29813
H -5.87237 0.64525 -0.97560
H -5.93674 -0.27275 0.52994
```

```
                          SCF energy:   -5718.592638 hartree
                zero-point correction:   +0.245400 hartree
                  enthalpy correction:   +0.260767 hartree
               free energy correction:   +0.201722 hartree
  quasiharmonic free energy correction:   +0.203485 hartree
```

5.7 Azaquinone Methide *cis*-4d

```
C -0.21469 0.74253 -0.25124
C 1.15790 1.21553 -0.05778
C 2.24073 0.39819 0.05134
C 2.06797 -1.00904 -0.00197
C 0.81877 -1.54322 -0.11035
H 0.68138 -2.62071 -0.13980
C -0.33676 -0.71233 -0.14684
C -1.55536 -1.43792 -0.19932
N -2.77417 -1.11306 0.16348
N -1.23657 1.49369 -0.55268
H -0.94757 2.46938 -0.61440
C -3.90409 -2.00801 -0.12370
C -3.15955 -0.00079 1.03622
C -4.33360 0.74356 0.41921
C -5.04135 -1.18546 -0.71295
H -4.22703 -2.47016 0.81631
H -3.58748 -2.78064 -0.82551
H 3.23619 0.81653 0.16220
Br 1.44195 3.08792 -0.02012
Br 3.60043 -2.11798 0.07315
O -5.42079 -0.14307 0.17404
H -5.91851 -1.81896 -0.85925
H -4.73631 -0.75992 -1.67974
H -4.02045 1.21982 -0.51884
H -4.69604 1.50608 1.11143
H -1.47931 -2.45693 -0.57892
H -2.31733 0.66272 1.19986
H -3.46928 -0.45286 1.98667
```

```
                          SCF energy:   -5754.475320 hartree
                zero-point correction:   +0.221157 hartree
                  enthalpy correction:   +0.236423 hartree
               free energy correction:   +0.176907 hartree
  quasiharmonic free energy correction:   +0.179447 hartree
```

5.8 Azaquinone Methide *trans*-4d

```
C 0.88425 -1.48819 0.12962
C 2.08055 -0.66173 0.00983
C 2.05948 0.69969 -0.02414
C 0.82056 1.38881 0.01075
C -0.35796 0.69954 0.06156
H -1.29275 1.24313 -0.00920
C -0.35876 -0.71836 0.10237
C -1.53500 -1.49826 -0.03091
N -2.77026 -1.22863 0.31896
N 0.85497 -2.78563 0.27932
H 1.79593 -3.16985 0.20466
C -3.89436 -2.03666 -0.17162
C -3.23519 -0.09070 1.11780
C -4.15987 0.76367 0.25900
C -4.80679 -1.12741 -0.98842
H -4.43424 -2.43532 0.69349
H -3.51446 -2.85621 -0.78341
H 2.98678 1.26036 -0.08810
Br 3.75578 -1.54184 -0.07577
Br 0.83387 3.28031 -0.07962
O -5.24796 -0.02151 -0.21187
H -5.69846 -1.67506 -1.29959
H -4.27191 -0.76803 -1.87935
H -3.60985 1.18850 -0.59321
H -4.58420 1.57379 0.85483
H -1.40167 -2.48083 -0.48225
H -2.39516 0.47129 1.51985
H -3.80853 -0.50894 1.95268
```

```
                          SCF energy:   -5754.477992 hartree
               zero-point correction:   +0.221867 hartree
                 enthalpy correction:   +0.236919 hartree
              free energy correction:   +0.178553 hartree
quasiharmonic free energy correction:   +0.180079 hartree
```

5.9 Azaquinone Methide *cis*-4e

```
C 0.72903 0.70951 -0.84838
C 1.95279 1.19502 -0.20990
Br 2.19226 3.06891 -0.08744
C 2.94629 0.37893 0.23638
H 3.85724 0.79871 0.65127
C 2.79526 -1.03028 0.14260
Br 4.22945 -2.13389 0.69910
C 1.63224 -1.57122 -0.31999
H 1.49455 -2.64882 -0.35282
C 0.54941 -0.73469 -0.70936
C -0.64935 -1.41863 -1.02948
N -1.89344 -1.01125 -0.91209
N -0.10232 1.43086 -1.54686
H 0.18845 2.40849 -1.53691
```

```
C -2.97025 -1.89637 -1.41654
C -2.25580 0.19623 -0.15751
C -4.26560 -1.11752 -1.60268
H -3.12121 -2.70454 -0.69201
H -2.63352 -2.32457 -2.36109
C -3.63234 0.10316 0.44736
H -2.17360 1.06043 -0.82940
H -1.50136 0.33752 0.62257
C -4.65884 -0.49702 -0.29072
H -5.03925 -1.79981 -1.96389
H -4.11897 -0.34378 -2.36755
C -5.95294 -0.53210 0.22835
C -3.90417 0.66485 1.69522
C -5.20320 0.64038 2.20411
C -6.22810 0.04236 1.47013
H -3.10040 1.12362 2.26594
H -5.41222 1.08064 3.17459
H -6.74528 -1.01133 -0.34156
H -7.23862 0.01547 1.86717
H -0.55221 -2.45071 -1.36929
```

```
                           SCF energy:   -5870.967822 hartree
                zero-point correction:   +0.267971 hartree
                  enthalpy correction:   +0.285885 hartree
               free energy correction:   +0.220008 hartree
  quasiharmonic free energy correction:   +0.223984 hartree
```

5.10 Azaquinone Methide *trans*-4e

```
C 1.68094 -1.47300 0.10355
C 2.92355 -0.70600 0.15910
Br 4.53719 -1.65781 0.44167
C 2.98063 0.64846 0.04931
H 3.93114 1.16661 0.13037
C 1.79039 1.38922 -0.17595
Br 1.91926 3.27134 -0.34083
C 0.58877 0.75828 -0.31499
H -0.28651 1.34462 -0.56212
C 0.50084 -0.65814 -0.21443
C -0.65393 -1.40658 -0.53794
N -1.92227 -1.06346 -0.58017
N 1.56493 -2.75246 0.32709
H 2.48328 -3.17335 0.46076
C -2.89867 -2.05869 -1.08456
C -2.42424 0.22848 -0.07988
C -4.16343 -1.37208 -1.58415
H -3.14630 -2.74368 -0.26638
H -2.41518 -2.62037 -1.88424
C -3.87590 0.17279 0.32160
H -2.30370 0.97931 -0.87166
H -1.80696 0.52530 0.77204
C -4.76468 -0.57254 -0.46114
H -4.86084 -2.13377 -1.94178
```

```
H -3.91545 -0.72266 -2.43406
C -6.12274 -0.57949 -0.14285
C -4.34480 0.90736 1.41061
C -5.70606 0.90853 1.71603
C -6.59507 0.16598 0.93811
H -3.64648 1.47886 2.01711
H -6.06960 1.48162 2.56370
H -6.81002 -1.17065 -0.74306
H -7.65417 0.15954 1.17846
H -0.46728 -2.44887 -0.79118
```

```
                          SCF energy:   -5870.969932 hartree
                zero-point correction:   +0.268716 hartree
                  enthalpy correction:   +0.286552 hartree
               free energy correction:   +0.221225 hartree
  quasiharmonic free energy correction:   +0.224473 hartree
```

5.11 Azaquinone Methide *cis*-4f

```
C 0.73671 0.76094 -0.50580
C 2.08899 1.20378 -0.16267
Br 2.40828 3.06840 -0.09518
C 3.13235 0.35412 0.04033
H 4.12698 0.74205 0.23641
C 2.91999 -1.04923 -0.02336
Br 4.41059 -2.20025 0.17481
C 1.66534 -1.55030 -0.20616
H 1.49096 -2.62299 -0.21044
C 0.54746 -0.67804 -0.33077
C -0.71133 -1.32647 -0.34549
N -1.88251 -0.88114 0.05360
N -0.20776 1.51232 -0.99685
H 0.10752 2.48108 -1.05095
C -2.04381 0.33842 0.85575
C -3.05629 -1.77541 -0.10996
C -3.31955 0.27339 1.69346
H -2.05715 1.20319 0.18519
H -1.15571 0.43138 1.48935
C -4.34038 -0.99427 -0.15292
H -3.06879 -2.46716 0.74318
H -2.92119 -2.35550 -1.02300
C -4.49876 0.02399 0.79506
H -3.42604 1.21733 2.23378
H -3.23432 -0.52860 2.43860
C -5.68555 0.75507 0.82823
C -5.36058 -1.28246 -1.05755
C -6.55259 -0.55755 -1.01048
C -6.71389 0.45947 -0.06883
H -5.22548 -2.07086 -1.79383
H -7.35019 -0.78166 -1.71243
H -5.80481 1.55467 1.55521
H -7.63875 1.02801 -0.03737
H -0.72005 -2.36701 -0.67085
```

```
                           SCF energy:   -5870.967500 hartree
                zero-point correction:   +0.268243 hartree
                  enthalpy correction:   +0.286074 hartree
               free energy correction:   +0.220667 hartree
 quasiharmonic free energy correction:   +0.224309 hartree
```

5.12 Azaquinone Methide *trans*-4f

```
C 1.66909 -1.46118 0.17509
C 2.94918 -0.78374 -0.02091
Br 4.50969 -1.85538 -0.10210
C 3.08423 0.56480 -0.13274
H 4.06645 1.00987 -0.25707
C 1.93202 1.39342 -0.09030
Br 2.16340 3.26630 -0.24653
C 0.68631 0.85404 0.04421
H -0.17372 1.50876 0.01179
C 0.51374 -0.55421 0.14891
C -0.73976 -1.20701 0.10195
N -1.95195 -0.76171 0.34788
N 1.51155 -2.73897 0.38263
H 2.40550 -3.22127 0.30582
C -2.23905 0.55726 0.93697
C -3.09032 -1.69426 0.14527
C -3.61013 0.56809 1.61059
H -2.22706 1.31352 0.14443
H -1.44727 0.78189 1.65680
C -4.36422 -0.95856 -0.16753
H -3.21472 -2.26912 1.07228
H -2.82856 -2.38487 -0.65606
C -4.65918 0.16708 0.61142
H -3.79601 1.57111 2.00229
H -3.60480 -0.12662 2.46046
C -5.85038 0.85950 0.39857
C -5.25420 -1.39039 -1.14938
C -6.45213 -0.70208 -1.34913
C -6.74919 0.42038 -0.57545
H -5.01368 -2.26194 -1.75319
H -7.14833 -1.03802 -2.11178
H -6.07519 1.74063 0.99433
H -7.67851 0.95944 -0.73504
H -0.69563 -2.25980 -0.17177
```

```
                           SCF energy:   -5870.970183 hartree
                zero-point correction:   +0.268473 hartree
                  enthalpy correction:   +0.286372 hartree
               free energy correction:   +0.220402 hartree
 quasiharmonic free energy correction:   +0.224224 hartree
```

5.13 Azaquinone Methide *cis*-4g

```
C 2.51066 -0.67144 0.75548
C 3.67249 -1.49529 0.44483
C 4.68827 -1.04419 -0.34289
H 5.55924 -1.67481 -0.50570
C 4.64278 0.25409 -0.94593
C 3.51368 1.00738 -0.79205
H 3.43607 1.97729 -1.27984
C 2.37343 0.53770 -0.05801
C 1.23283 1.35849 -0.14378
N -0.04877 1.05627 -0.01032
N 1.69248 -0.93047 1.74686
H 1.97896 -1.80298 2.19574
C -1.04466 2.13908 -0.11779
C -0.51531 -0.33165 -0.00264
C -2.26240 1.82177 0.73782
H -1.34505 2.24313 -1.16767
H -0.56786 3.06396 0.20669
C -2.00624 -0.48059 -0.15921
H -0.17723 -0.79424 0.93749
H 0.01217 -0.86643 -0.80342
C -2.87611 0.53220 0.26119
H -2.98045 2.64289 0.66049
H -1.95705 1.74416 1.78918
C -4.25624 0.33303 0.17941
C -2.52530 -1.67953 -0.65548
C -3.90313 -1.87753 -0.72267
C -4.77215 -0.86921 -0.30223
H -1.84543 -2.46081 -0.98767
H -4.29705 -2.81294 -1.10896
H -4.92751 1.12889 0.49339
H -5.84683 -1.01526 -0.35911
H 1.40416 2.39608 -0.43210
H 5.47869 0.61384 -1.53615
H 3.73369 -2.46929 0.92578
```

```
                          SCF energy:   -728.550196 hartree
                zero-point correction:   +0.286805 hartree
                  enthalpy correction:   +0.302044 hartree
               free energy correction:   +0.244430 hartree
  quasiharmonic free energy correction:   +0.247112 hartree
```

5.14 Azaquinone Methide *trans*-4g

```
C -3.51545 0.66419 0.54150
C -4.71842 -0.11909 0.29153
C -4.67415 -1.34268 -0.30121
H -5.59575 -1.90279 -0.44192
C -3.43860 -1.90739 -0.75603
C -2.28313 -1.19293 -0.61162
H -1.37149 -1.60912 -1.02188
C -2.26564 0.10822 -0.00528
```

```
C -1.17311 0.99011 0.01051
N 0.12228 0.79953 -0.18170
N -3.51974 1.78015 1.22707
H -4.48282 2.01900 1.46737
C 1.00956 1.98233 -0.19319
C 0.72513 -0.53804 -0.28730
C 2.27223 1.70331 -0.99855
H 1.27882 2.23229 0.83982
H 0.44997 2.81422 -0.62217
C 2.20173 -0.54823 0.02123
H 0.57584 -0.91097 -1.30921
H 0.19466 -1.20530 0.39787
C 2.99169 0.53186 -0.38859
H 2.90380 2.59550 -0.99378
H 2.00095 1.49243 -2.04136
C 4.36982 0.49816 -0.17269
C 2.79090 -1.65181 0.63949
C 4.17068 -1.68609 0.84154
C 4.96083 -0.61082 0.43347
H 2.17000 -2.48440 0.96132
H 4.62589 -2.54633 1.32324
H 4.97946 1.34490 -0.47875
H 6.03443 -0.63100 0.59659
H -1.43183 2.02545 0.22755
H -3.43032 -2.87736 -1.24148
H -5.66385 0.29917 0.63050
```

```
                            SCF energy:   -728.551657 hartree
                 zero-point correction:   +0.287514 hartree
                   enthalpy correction:   +0.302789 hartree
                 free energy correction:   +0.245060 hartree
  quasiharmonic free energy correction:   +0.247538 hartree
```

5.15 Azaquinone Methide *cis*-4h

```
C -2.63864 -0.80368 -0.62567
C -3.99342 -1.29706 -0.39871
C -5.00204 -0.47596 0.00489
H -6.00749 -0.87690 0.11045
C -4.77198 0.91278 0.27524
C -3.49317 1.38792 0.21097
H -3.28491 2.42732 0.45871
C -2.37811 0.54280 -0.10949
C -1.11399 1.13797 0.04254
N 0.06758 0.58264 0.26174
N -1.74058 -1.45981 -1.31548
H -2.13558 -2.35795 -1.60278
C 0.22111 -0.81168 0.69122
C 1.24722 1.47588 0.34085
C 1.52571 -1.00618 1.46347
H 0.18224 -1.46351 -0.18703
H -0.64506 -1.06017 1.31418
C 2.51745 0.73221 0.03066
```

```
H 1.29704 1.88628 1.35915
H 1.10142 2.30216 -0.35552
C 2.68167 -0.52122 0.63342
H 1.63033 -2.06638 1.70764
H 1.48186 -0.45015 2.40945
C 3.85246 -1.24501 0.41003
C 3.51791 1.25957 -0.78403
C 4.69440 0.53748 -0.99279
C 4.86041 -0.71301 -0.39666
H 3.37910 2.23026 -1.25386
H 5.47553 0.94695 -1.62645
H 3.97604 -2.22352 0.86749
H 5.77248 -1.27819 -0.56542
H -1.08966 2.22855 0.04369
H -5.59648 1.56032 0.55351
H -4.18797 -2.34181 -0.63261
```

```
                            SCF energy:   -728.550048 hartree
                 zero-point correction:   +0.287459 hartree
                   enthalpy correction:   +0.302540 hartree
                free energy correction:   +0.245966 hartree
  quasiharmonic free energy correction:   +0.247954 hartree
```

5.16 Azaquinone Methide *trans*-4h

```
C -3.48829 0.96138 0.08999
C -4.73438 0.37651 -0.38910
C -4.82841 -0.93137 -0.75056
H -5.78683 -1.32840 -1.07722
C -3.68803 -1.79790 -0.71912
C -2.47539 -1.29357 -0.34342
H -1.61587 -1.95043 -0.38044
C -2.30712 0.08119 0.03439
C -1.08142 0.72837 0.25639
N 0.14183 0.26610 0.45952
N -3.40882 2.17993 0.56324
H -4.31785 2.63447 0.46827
C 0.45518 -1.15566 0.67035
C 1.24508 1.24452 0.60642
C 1.83870 -1.32959 1.29747
H 0.43472 -1.67497 -0.29417
H -0.31728 -1.58214 1.31690
C 2.53927 0.68882 0.07830
H 1.35209 1.47982 1.67406
H 0.96854 2.15855 0.08048
C 2.86510 -0.61869 0.46025
H 2.05576 -2.39785 1.37204
H 1.83048 -0.91972 2.31590
C 4.06338 -1.18528 0.02776
C 3.40735 1.42644 -0.72444
C 4.61312 0.86035 -1.14268
C 4.93953 -0.44325 -0.76724
H 3.14282 2.43846 -1.02080
```

```
H 5.29224 1.43356 -1.76681
H 4.31145 -2.20479 0.31283
H 5.87420 -0.88571 -1.09942
H -1.14505 1.81492 0.27038
H -3.78420 -2.83527 -1.02115
H -5.60836 1.02380 -0.41874
```

```
                            SCF energy:   -728.552369 hartree
                 zero-point correction:   +0.287512 hartree
                   enthalpy correction:   +0.302738 hartree
                free energy correction:   +0.245113 hartree
  quasiharmonic free energy correction:   +0.247720 hartree
```

5.17 Azaquinone Methide *cis*-4i

```
C 0.75888 0.97755 -0.43051
C 2.21064 1.06230 -0.22523
Br 3.01554 2.76864 -0.37424
C 3.00355 -0.01221 0.01438
H 4.07702 0.10742 0.12167
C 2.42532 -1.31258 0.10948
Br 3.58176 -2.78850 0.36683
C 1.08039 -1.47969 0.02340
H 0.63502 -2.46613 0.12041
C 0.21046 -0.35748 -0.15379
C -1.15700 -0.66800 -0.14995
N -2.19933 0.12332 0.10260
N 0.00607 1.93835 -0.87157
C -2.08937 1.31652 0.95520
C -4.48122 1.07675 1.64859
C -3.51195 -0.30691 -0.25527
H 0.56343 2.77667 -1.03582
C -4.62471 0.12324 0.48657
C -5.88711 -0.33609 0.10159
C -3.67811 -1.13341 -1.37442
C -4.94483 -1.58289 -1.72978
C -6.05717 -1.18803 -0.98625
H -2.82057 -1.39522 -1.98645
H -5.06144 -2.22268 -2.59894
H -6.75103 -0.01472 0.67876
H -7.05066 -1.52881 -1.26099
C -3.04087 1.15647 2.13516
H -5.15310 0.77155 2.45657
H -4.81031 2.07186 1.32183
H -2.76942 0.25040 2.68967
H -2.90830 2.00959 2.80624
H -2.32214 2.20812 0.36517
H -1.06129 1.38770 1.29998
H -1.42131 -1.70555 -0.35108
```

```
                           SCF energy:   -5870.970442 hartree
                 zero-point correction:   +0.268340 hartree
                   enthalpy correction:   +0.286069 hartree
                free energy correction:   +0.221432 hartree
  quasiharmonic free energy correction:   +0.224252 hartree
```

5.18 Azaquinone Methide *trans*-4i

```
C 1.16441 -1.37862 0.34537
C 2.56106 -1.00129 0.11837
Br 3.86687 -2.36712 0.20406
C 2.96316 0.27399 -0.11450
H 4.01609 0.50386 -0.24331
C 1.99883 1.32102 -0.20366
Br 2.61808 3.07162 -0.56696
C 0.67024 1.06222 -0.07118
H -0.05158 1.85651 -0.22535
C 0.21811 -0.27075 0.16959
C -1.12906 -0.64126 0.07624
N -2.21205 0.11819 0.23515
N 0.73942 -2.55603 0.69707
C -2.20484 1.35808 1.03258
C -4.66817 1.16930 1.41821
C -3.47470 -0.33059 -0.26220
H 1.50795 -3.22634 0.69992
C -4.66693 0.14933 0.30451
C -5.87725 -0.32630 -0.20857
C -3.51132 -1.21992 -1.34543
C -4.72889 -1.68268 -1.83022
C -5.92115 -1.24051 -1.25655
H -2.59132 -1.52591 -1.83236
H -4.74227 -2.37297 -2.66796
H -6.80204 0.03455 0.23542
H -6.87638 -1.59383 -1.63237
C -3.30424 1.27941 2.08318
H -5.43848 0.90769 2.14983
H -4.95041 2.14270 0.99652
H -3.11488 0.40961 2.72244
H -3.25064 2.17293 2.71096
H -2.34989 2.21871 0.36945
H -1.23313 1.43712 1.51588
H -1.32367 -1.68598 -0.15732
```

```
                           SCF energy:   -5870.971898 hartree
                 zero-point correction:   +0.268389 hartree
                   enthalpy correction:   +0.286184 hartree
                free energy correction:   +0.221273 hartree
  quasiharmonic free energy correction:   +0.224083 hartree
```

6 Cartesian Coordinates and Energies of Azomethine Ylides 5

6.1 Azomethine Ylide 5a

```
C -0.38471 0.69919 -0.41323
C 0.87764 1.20246 -0.08130
Br 1.10407 3.08110 0.05657
C 1.99564 0.39765 0.10759
H 2.96020 0.83130 0.34309
C 1.82518 -0.97551 -0.02414
Br 3.32961 -2.11115 0.19728
C 0.58657 -1.53244 -0.29123
H 0.47200 -2.61025 -0.34981
C -0.55178 -0.72060 -0.46871
C -1.81674 -1.33248 -0.78746
N -2.98865 -0.98819 -0.16653
H -1.83320 -2.31840 -1.23615
N -1.46251 1.52535 -0.68555
H -1.22601 2.46781 -0.97139
H -2.14598 1.10124 -1.30738
C -4.25967 -1.55943 -0.69797
C -3.23930 -0.15232 0.81717
C -4.70564 -0.00997 1.07773
H -2.43505 0.34753 1.33740
C -5.26619 -1.27938 0.41241
H -5.10719 0.89806 0.60499
H -4.93112 0.05057 2.14574
H -4.10323 -2.61609 -0.92082
H -4.49313 -1.02597 -1.62429
H -6.27744 -1.15320 0.02244
H -5.26675 -2.10383 1.13108
```

```
                          SCF energy:   -5679.277754 hartree
                zero-point correction:   +0.213918 hartree
                  enthalpy correction:   +0.228825 hartree
               free energy correction:   +0.170950 hartree
  quasiharmonic free energy correction:   +0.172773 hartree
```

6.2 Azomethine Ylide 5b

```
C 2.10723 0.88689 0.05370
C 3.35979 0.28235 0.10522
H 4.23509 0.91794 0.22300
C 3.50962 -1.10619 0.01248
H 4.49899 -1.55057 0.06433
C 2.37837 -1.89453 -0.16200
H 2.46686 -2.97247 -0.26458
C 1.11225 -1.30503 -0.21121
H 0.26600 -1.95099 -0.39966
```

```
C 0.92183 0.09047 -0.08199
C -0.34593 0.76092 -0.11629
N -1.57613 0.19332 -0.00666
H -0.39548 1.83293 -0.22724
N 2.00544 2.28016 0.21619
H 2.90151 2.74448 0.11263
H 1.32363 2.72967 -0.38516
C -2.74192 1.13135 -0.07775
C -2.01523 -1.03086 0.24488
C -3.50702 -1.08790 0.36905
H -1.34489 -1.84453 0.46542
C -3.93393 0.21686 -0.31811
H -3.81563 -1.10022 1.42514
H -3.93334 -1.97762 -0.10351
H -2.56084 1.86064 -0.86724
H -2.79649 1.64365 0.88738
H -4.85615 0.63813 0.08583
H -4.06466 0.04870 -1.39091
```

```
                          SCF energy:  -536.857724 hartree
                zero-point correction:  +0.233275 hartree
                  enthalpy correction:  +0.245716 hartree
               free energy correction:  +0.195553 hartree
  quasiharmonic free energy correction:  +0.196827 hartree
```

6.3 Azomethine Ylide 5c

```
C -0.12035 0.69895 -0.41086
C 1.14755 1.19759 -0.10077
C 2.26203 0.38800 0.09728
C 2.07784 -0.98528 -0.00247
C 0.83266 -1.53807 -0.24956
H 0.71051 -2.61603 -0.28538
C -0.30060 -0.72194 -0.44352
C -1.56190 -1.32898 -0.78089
N -2.76030 -0.98732 -0.18032
H -1.56226 -2.32834 -1.20140
N -1.19703 1.52702 -0.68313
H -0.95785 2.46409 -0.98439
H -1.88584 1.09719 -1.29590
C -3.94807 -1.68799 -0.74999
C -2.91126 -0.16898 0.83646
C -4.22982 0.34775 1.32362
H -2.00185 0.19669 1.29675
C -5.22079 -0.87748 -0.59469
H -4.02795 -2.64369 -0.22133
H -3.72151 -1.88289 -1.79805
H 3.23180 0.81896 0.31535
Br 1.39218 3.07698 -0.00806
Br 3.57454 -2.12954 0.23062
H -6.05430 -1.48009 -0.96758
H -5.16111 0.02561 -1.21558
H -4.35114 1.38017 0.95947
```

```
H -4.18759 0.41770 2.41554
C -5.41663 -0.49644 0.86795
H -6.34859 0.05846 1.00856
H -5.47994 -1.40912 1.47310
```

```
                           SCF energy:   -5718.573809 hartree
                 zero-point correction:   +0.243403 hartree
                   enthalpy correction:   +0.259314 hartree
                 free energy correction:   +0.199273 hartree
  quasiharmonic free energy correction:   +0.201292 hartree
```

6.4 Azomethine Ylide 5d

```
C -0.12358 0.70902 -0.42769
C 1.14598 1.19968 -0.10225
C 2.25038 0.38000 0.09903
C 2.06185 -0.99257 -0.01139
C 0.81542 -1.53557 -0.27221
H 0.68431 -2.61216 -0.31645
C -0.30814 -0.70845 -0.46694
C -1.57689 -1.30817 -0.80246
N -2.75849 -0.97259 -0.18859
H -1.59117 -2.28579 -1.26957
N -1.19104 1.54536 -0.70281
H -0.94732 2.48415 -0.99455
H -1.88728 1.12505 -1.31308
C -3.95597 -1.68439 -0.71027
C -2.92599 -0.15215 0.82682
C -4.27419 0.30824 1.29249
H -2.04480 0.27164 1.28923
C -5.20350 -0.85988 -0.48733
H -4.02288 -2.63809 -0.17980
H -3.79773 -1.86537 -1.77372
H 3.22129 0.80292 0.32865
Br 1.40075 3.07657 0.00442
Br 3.54959 -2.14427 0.23196
O -5.33099 -0.54516 0.89042
H -6.08343 -1.43735 -0.77665
H -5.17244 0.06486 -1.08201
H -4.47088 1.32856 0.91931
H -4.28704 0.34866 2.38487
```

```
                           SCF energy:   -5754.459697 hartree
                 zero-point correction:   +0.219697 hartree
                   enthalpy correction:   +0.235327 hartree
                 free energy correction:   +0.175927 hartree
  quasiharmonic free energy correction:   +0.177722 hartree
```

6.5 Azomethine Ylide 5e

```
C 0.65473 0.57403 -0.67566
C 1.82868 1.20803 -0.24300
```

```
Br 1.90228 3.10083 -0.26311
C 2.96116 0.51470 0.16080
H 3.85403 1.04651 0.46846
C 2.91191 -0.87519 0.14921
Br 4.44626 -1.85484 0.67845
C 1.76136 -1.55171 -0.21565
H 1.72866 -2.63624 -0.18613
C 0.60673 -0.85079 -0.60740
C -0.55810 -1.60697 -1.01850
N -1.81711 -1.34830 -0.60253
N -0.42916 1.28257 -1.14506
H -0.24582 2.22107 -1.47668
H -1.04493 0.76257 -1.76168
C -2.88953 -2.21783 -1.16399
C -2.18932 -0.45847 0.32440
C -4.12334 -1.39669 -1.49280
H -3.11416 -2.97227 -0.40325
H -2.48745 -2.70562 -2.05030
C -3.57645 -0.17784 0.59929
H -1.40688 0.03311 0.88705
C -4.58538 -0.63717 -0.27701
H -4.90502 -2.06810 -1.85932
H -3.88499 -0.69570 -2.30452
C -5.91953 -0.34833 -0.01342
C -3.94794 0.57893 1.72704
C -5.28683 0.86463 1.97596
C -6.28122 0.40148 1.11025
H -3.17659 0.93785 2.40422
H -5.55690 1.44858 2.85140
H -6.68519 -0.71032 -0.69624
H -7.32622 0.62087 1.30686
H -0.42479 -2.55647 -1.52102
```

```
                           SCF energy:   -5870.970947 hartree
                zero-point correction:   +0.267258 hartree
                  enthalpy correction:   +0.285290 hartree
               free energy correction:   +0.220115 hartree
  quasiharmonic free energy correction:   +0.223288 hartree
```

6.6 Azomethine Ylide 5f

```
C 0.60132 0.58100 -0.26832
C 1.83785 1.21685 -0.12064
Br 1.89524 3.11302 -0.10853
C 3.04405 0.53140 -0.02649
H 3.98106 1.06681 0.06853
C 2.99596 -0.85692 -0.06621
Br 4.62144 -1.83184 0.03705
C 1.79610 -1.54150 -0.15676
H 1.78280 -2.62689 -0.14791
C 0.57016 -0.85061 -0.23829
C -0.65487 -1.59131 -0.40031
N -1.79317 -1.32411 0.33189
```

```
N -0.57816 1.28506 -0.43341
H -0.47738 2.23290 -0.77577
H -1.28793 0.76912 -0.94725
C -1.91572 -0.48354 1.33397
C -3.01802 -2.06018 -0.07725
C -3.26460 -0.13365 1.88550
H -1.01566 -0.03454 1.73148
C -4.17439 -1.10519 -0.20336
H -3.21748 -2.80667 0.70034
H -2.81020 -2.56729 -1.01856
C -4.31257 -0.14095 0.79990
H -3.21169 0.84412 2.37141
H -3.55387 -0.85470 2.66808
C -5.37787 0.75714 0.75174
C -5.09222 -1.17204 -1.25057
C -6.16268 -0.27728 -1.29017
C -6.30445 0.68549 -0.28997
H -4.97143 -1.92023 -2.02994
H -6.88013 -0.32711 -2.10379
H -5.48053 1.51343 1.52601
H -7.13267 1.38725 -0.32469
H -0.61777 -2.59651 -0.80227
```

```
                           SCF energy:   -5870.956613 hartree
                zero-point correction:   +0.266646 hartree
                  enthalpy correction:   +0.284766 hartree
               free energy correction:   +0.219109 hartree
quasiharmonic free energy correction:   +0.222604 hartree
```

6.7 Azomethine Ylide 5g

```
C 2.45308 -0.58603 0.75147
C 3.58174 -1.41982 0.66962
C 4.63859 -1.11732 -0.17861
H 5.50403 -1.77288 -0.21161
C 4.59385 0.03643 -0.97096
C 3.46827 0.84752 -0.92272
H 3.41482 1.73529 -1.54862
C 2.36280 0.55005 -0.09810
C 1.23959 1.47355 -0.07367
N -0.05096 1.10714 -0.15256
N 1.44029 -0.88489 1.65025
H 1.72408 -1.46570 2.43020
H 0.87435 -0.09640 1.94511
C -1.05501 2.20671 -0.12452
C -0.52944 -0.13306 -0.36079
C -2.25597 1.81262 0.71722
H -1.35030 2.38943 -1.16295
H -0.56394 3.09335 0.27301
C -1.93654 -0.42480 -0.30760
H 0.18960 -0.90846 -0.58629
C -2.84938 0.52454 0.21069
H -2.98873 2.62428 0.68849
```

```
H -1.93721 1.69283 1.76211
C -4.20642 0.22960 0.26973
C -2.43563 -1.67043 -0.74206
C -3.79558 -1.95441 -0.66925
C -4.69286 -1.00723 -0.16738
H -1.74429 -2.41001 -1.13918
H -4.15947 -2.91980 -1.01066
H -4.89223 0.97414 0.66902
H -5.75478 -1.22726 -0.11603
H 1.42307 2.53553 -0.18015
H 5.42161 0.28894 -1.62642
H 3.62764 -2.29654 1.31172
```

```
                          SCF energy:   -728.554132 hartree
                zero-point correction:   +0.286242 hartree
                  enthalpy correction:   +0.301597 hartree
               free energy correction:   +0.244756 hartree
  quasiharmonic free energy correction:   +0.246703 hartree
```

6.8 Azomethine Ylide 5h

```
C -2.45467 -0.80722 -0.51049
C -3.71173 -1.42878 -0.49044
C -4.86529 -0.71073 -0.19174
H -5.82866 -1.21243 -0.19731
C -4.77677 0.65561 0.09604
C -3.52946 1.26933 0.11986
H -3.45439 2.32571 0.36894
C -2.33537 0.56649 -0.15234
C -1.06811 1.27137 -0.18176
N 0.04911 0.82266 0.47963
N -1.32222 -1.53205 -0.87157
H -1.51657 -2.34954 -1.43839
H -0.58231 -0.96301 -1.27453
C 0.16459 -0.24072 1.25091
C 1.27726 1.63935 0.29541
C 1.50775 -0.69264 1.74543
H -0.73443 -0.79145 1.48829
C 2.44942 0.75348 -0.02694
H 1.44654 2.17663 1.23618
H 1.09087 2.35925 -0.50024
C 2.58108 -0.42173 0.71954
H 1.46296 -1.75775 1.98812
H 1.77173 -0.17277 2.68200
C 3.65824 -1.27389 0.47841
C 3.38451 1.07662 -1.00894
C 4.46646 0.22583 -1.24089
C 4.60227 -0.94727 -0.49731
H 3.26655 1.98829 -1.58924
H 5.19649 0.47427 -2.00542
H 3.75754 -2.19303 1.05066
H 5.43975 -1.61359 -0.68278
H -1.06009 2.33661 -0.37880
```

```
H -5.67060 1.23118 0.31839
H -3.77462 -2.48333 -0.75066
```

```
                            SCF energy:   -728.537936 hartree
                 zero-point correction:   +0.285951 hartree
                   enthalpy correction:   +0.301316 hartree
                free energy correction:   +0.244385 hartree
  quasiharmonic free energy correction:   +0.246266 hartree
```

6.9 Azomethine Ylide 5i

```
C 0.66636 0.79732 -0.31508
C 2.02311 1.10841 -0.20113
Br 2.55796 2.92312 -0.33917
C 3.01818 0.15024 -0.03776
H 4.06108 0.43562 0.02603
C 2.61674 -1.17855 0.03070
Br 3.94262 -2.52242 0.23072
C 1.28270 -1.54297 -0.01623
H 0.99557 -2.58525 0.08059
C 0.26933 -0.57193 -0.16654
C -1.09941 -0.99430 -0.28741
N -2.13860 -0.35584 0.38246
N -0.30247 1.75901 -0.54688
C -1.96402 0.55786 1.31851
C -4.06898 1.66726 0.66221
C -3.50329 -0.67367 -0.01294
C -4.47181 0.33166 0.09858
C -5.78080 0.04004 -0.28846
C -3.83565 -1.94632 -0.47391
C -5.15049 -2.21735 -0.84643
C -6.12364 -1.22285 -0.76573
H -3.09670 -2.73626 -0.53294
H -5.40877 -3.21139 -1.19760
H -6.53523 0.81808 -0.20605
H -7.14721 -1.43379 -1.05989
C -3.07835 1.42640 1.79932
H -4.95086 2.21054 1.01023
H -3.58733 2.27309 -0.11678
H -3.59413 0.95408 2.64924
H -2.65534 2.36608 2.16496
H -1.28977 -2.01982 -0.56369
H -0.96096 0.66180 1.71067
H -1.10107 1.40270 -1.06720
H 0.03811 2.63004 -0.93702
```

```
                            SCF energy:   -5870.950816 hartree
                 zero-point correction:   +0.266781 hartree
                   enthalpy correction:   +0.284820 hartree
                free energy correction:   +0.219929 hartree
  quasiharmonic free energy correction:   +0.222634 hartree
```

7 Cartesian Coordinates and Energies of Zwitterions 7

7.1 Zwitterion 7a

```
C -0.43726 0.82207 -0.56227
C 0.87546 1.22871 -0.13563
Br 1.19235 3.08632 0.10924
C 1.92463 0.35936 0.09336
H 2.89080 0.74313 0.40555
C 1.72910 -1.01053 -0.07338
Br 3.16247 -2.21221 0.24360
C 0.48464 -1.48891 -0.46792
H 0.32377 -2.55567 -0.60160
C -0.56368 -0.61051 -0.70722
C -1.86962 -1.14552 -1.19921
N -2.99015 -0.93983 -0.26215
N -1.48636 1.60397 -0.79440
H -1.21734 2.57705 -0.65807
C -4.37926 -1.17145 -0.71621
C -2.93061 -0.40607 0.89878
C -4.27732 -0.21592 1.50108
H -1.97772 -0.12647 1.33629
C -5.18252 -1.05914 0.58298
H -4.50505 0.85745 1.45477
H -4.29560 -0.51071 2.55232
H -4.43879 -2.14415 -1.20752
H -4.61536 -0.38601 -1.44171
H -6.15847 -0.60269 0.41900
H -5.32803 -2.05095 1.01721
H -2.18191 -0.63629 -2.11901
H -1.82092 -2.22012 -1.39688
```

```
                          SCF energy:   -5679.284778 hartree
                zero-point correction:   +0.214663 hartree
                  enthalpy correction:   +0.229530 hartree
               free energy correction:   +0.170341 hartree
  quasiharmonic free energy correction:   +0.173365 hartree
```

7.2 Zwitterion 7b

```
C 1.36570 0.84890 -0.49989
C 2.67391 1.18804 -0.00963
H 2.99307 2.22617 -0.09043
C 3.52395 0.24873 0.54783
H 4.50377 0.56765 0.89881
C 3.14868 -1.10029 0.66844
H 3.81868 -1.83350 1.10514
C 1.88528 -1.46654 0.20313
H 1.56513 -2.50552 0.27442
```

```
C 1.00949 -0.54195 -0.36523
C -0.30482 -0.99453 -0.91178
N -1.47515 -0.44787 -0.19255
N 0.49216 1.71623 -1.02903
H 0.92964 2.63849 -1.05530
C -2.83464 -0.63620 -0.74394
C -1.45116 0.35115 0.80621
C -2.80970 0.83099 1.17807
H -0.51250 0.62748 1.27417
C -3.73371 -0.10725 0.37828
H -2.88466 1.87824 0.85687
H -2.96592 0.80724 2.25855
H -2.98039 -1.69094 -0.98378
H -2.89594 -0.04631 -1.66424
H -4.61457 0.40184 -0.01259
H -4.06084 -0.93387 1.01311
H -0.40821 -2.08341 -0.88546
H -0.44408 -0.65843 -1.94721
```

```
                          SCF energy:  -536.861143 hartree
                zero-point correction:  +0.233447 hartree
                  enthalpy correction:  +0.245584 hartree
               free energy correction:  +0.195698 hartree
  quasiharmonic free energy correction:  +0.197011 hartree
```

7.3 Zwitterion 7c

```
C -0.07387 0.94890 -0.60647
C 1.26224 1.20409 -0.13539
C 2.19970 0.22163 0.11661
C 1.86073 -1.11719 -0.07530
C 0.58634 -1.45076 -0.51833
H 0.31540 -2.49162 -0.67691
C -0.35143 -0.45948 -0.77846
C -1.68303 -0.84099 -1.33458
N -2.84007 -0.65053 -0.41503
N -1.02419 1.84199 -0.85684
H -0.65768 2.77909 -0.69780
C -4.14296 -1.04428 -0.99722
C -2.71704 -0.16214 0.76264
C -3.84999 0.05081 1.69997
C -5.30735 -0.40497 -0.26144
H -4.18574 -2.13794 -0.95512
H -4.11469 -0.74438 -2.04684
H 3.19145 0.49346 0.46398
Br 1.77614 3.01314 0.13944
Br 3.14392 -2.47193 0.26855
H -6.23232 -0.85618 -0.62955
H -5.34154 0.66582 -0.49483
H -3.95788 1.14146 1.79072
H -3.52429 -0.29787 2.68576
H -1.92173 -0.23081 -2.21215
H -1.70932 -1.89568 -1.62378
```

```
H -1.71177 0.10364 1.07818
C -5.14851 -0.60544 1.24221
H -5.99189 -0.17541 1.78737
H -5.11951 -1.67753 1.46886
```

```
                           SCF energy:   -5718.586421 hartree
                 zero-point correction:   +0.244372 hartree
                   enthalpy correction:   +0.260114 hartree
                 free energy correction:   +0.199741 hartree
  quasiharmonic free energy correction:   +0.202231 hartree
```

7.4 Zwitterion 7d

```
C -0.11664 0.91428 -0.60615
C 1.21226 1.21524 -0.14103
C 2.18180 0.26500 0.11092
C 1.88717 -1.08538 -0.07626
C 0.62361 -1.46253 -0.51328
H 0.38621 -2.51211 -0.66754
C -0.34711 -0.50291 -0.77332
C -1.66703 -0.92961 -1.32187
N -2.82074 -0.74092 -0.39848
N -1.09799 1.77405 -0.85365
H -0.76244 2.72360 -0.69967
C -4.13715 -1.12343 -0.94630
C -2.70744 -0.24088 0.77176
C -3.87172 -0.04464 1.67921
C -5.23358 -0.41670 -0.17751
H -4.22290 -2.21101 -0.86878
H -4.14905 -0.83689 -1.99995
H 3.16474 0.57060 0.45511
Br 1.66810 3.04051 0.12527
Br 3.21421 -2.39600 0.26996
O -5.05597 -0.64668 1.21518
H -6.20705 -0.82233 -0.45392
H -5.21695 0.66180 -0.38427
H -3.99338 1.04182 1.81880
H -3.62474 -0.47967 2.65225
H -1.92790 -0.34337 -2.20959
H -1.67362 -1.99110 -1.58582
H -1.71968 0.05181 1.11668
```

```
                           SCF energy:   -5754.468026 hartree
                 zero-point correction:   +0.220852 hartree
                   enthalpy correction:   +0.236195 hartree
                 free energy correction:   +0.176888 hartree
  quasiharmonic free energy correction:   +0.178985 hartree
```

7.5 Zwitterion 7e

```
C -0.53311 0.81944 0.88017
```

```
C -1.63064 1.33076 0.10250
Br -1.59567 3.16726 -0.38351
C -2.71595 0.57781 -0.30140
H -3.51442 1.03868 -0.87426
C -2.77469 -0.77457 0.03290
Br -4.26468 -1.81443 -0.51368
C -1.73883 -1.35549 0.75573
H -1.76873 -2.41294 1.00737
C -0.65458 -0.59170 1.16552
C 0.46902 -1.23920 1.91565
N 1.68381 -1.23379 1.06908
N 0.52048 1.49876 1.32588
H 0.44297 2.47051 1.02918
C 1.63218 -1.98399 -0.20295
C 2.63114 -0.38427 1.28585
C 3.03040 -2.38894 -0.63951
H 1.15710 -1.33323 -0.94646
H 0.99488 -2.85541 -0.04250
C 3.74802 -0.22759 0.37234
H 2.57669 0.20971 2.19155
C 3.95839 -1.20255 -0.61900
H 2.97888 -2.82496 -1.63997
H 3.41941 -3.16038 0.03783
C 5.03829 -1.05189 -1.48379
C 4.60550 0.87142 0.50583
C 5.67286 1.01483 -0.37298
C 5.88437 0.05290 -1.36423
H 4.42059 1.60515 1.28582
H 6.33855 1.86743 -0.28831
H 5.21856 -1.79686 -2.25387
H 6.71865 0.16326 -2.05073
H 0.24213 -2.28052 2.15583
H 0.72264 -0.69630 2.82980
```

```
                          SCF energy:  -5870.962695 hartree
               zero-point correction:  0.268819 hartree
                 enthalpy correction:  0.286491 hartree
              free energy correction:  0.221309 hartree
quasiharmonic free energy correction:  0.225022 hartree
```

7.6 Zwitterion 7f

```
C 0.94947 -1.17468 0.74539
C 2.13127 -1.12194 -0.07465
Br 2.77321 -2.75174 -0.81180
C 2.83826 0.03262 -0.34964
H 3.72915 -0.00961 -0.96822
C 2.39832 1.24759 0.17374
Br 3.36120 2.83895 -0.19988
C 1.24973 1.28871 0.95597
H 0.89236 2.23338 1.35820
C 0.54756 0.12426 1.23376
```

```
C -0.69560 0.18754 2.06507
N -1.87548 -0.13726 1.22368
N 0.23963 -2.25295 1.06659
H 0.66892 -3.07416 0.64288
C -2.48107 -1.26078 1.33778
C -2.16345 0.78474 0.10863
C -3.56735 -1.66881 0.40957
H -2.16947 -1.91425 2.14552
C -3.61169 0.72473 -0.29420
H -1.51161 0.49468 -0.72472
H -1.87922 1.78928 0.42890
C -4.30004 -0.48241 -0.16368
H -4.24093 -2.35644 0.92567
H -3.08000 -2.25006 -0.39020
C -5.63863 -0.56215 -0.55054
C -4.25739 1.84838 -0.81217
C -5.58920 1.76188 -1.21223
C -6.28010 0.55556 -1.08103
H -3.71638 2.78699 -0.90072
H -6.08984 2.63588 -1.61762
H -6.17500 -1.50049 -0.43557
H -7.32054 0.48819 -1.38445
H -0.85785 1.18888 2.47090
H -0.68354 -0.54477 2.87582
```

```
                           SCF energy:   -5870.957117 hartree
                zero-point correction:   0.267689 hartree
                  enthalpy correction:   0.285684 hartree
                free energy correction:   0.218293 hartree
quasiharmonic free energy correction:   0.223745 hartree
```

7.7 Zwitterion 7g

```
C -2.75502 0.87120 -0.21109
C -3.77701 0.47280 -1.14084
C -4.29849 -0.80867 -1.16352
H -5.07585 -1.04879 -1.88665
C -3.84693 -1.80144 -0.27599
C -2.84581 -1.45479 0.63175
H -2.46701 -2.20105 1.32981
C -2.31106 -0.16828 0.68366
C -1.21399 0.16099 1.64537
N 0.04880 0.38463 0.89111
N -2.21516 2.09712 -0.13699
H -2.66438 2.68740 -0.83922
C 0.49222 1.56964 0.68329
C 0.61199 -0.78076 0.18347
C 1.65291 1.82873 -0.21020
H -0.01238 2.38460 1.18957
C 2.09189 -0.62125 -0.03847
H 0.07941 -0.86781 -0.77160
H 0.38828 -1.66795 0.77924
C 2.60481 0.65965 -0.25127
```

```
H 2.14977 2.74941 0.10293
H 1.23269 2.02278 -1.21026
C 3.97130 0.83032 -0.47799
C 2.94102 -1.72881 -0.05732
C 4.30240 -1.55721 -0.30028
C 4.81756 -0.27664 -0.51034
H 2.53479 -2.72168 0.11809
H 4.96190 -2.41956 -0.31646
H 4.36912 1.83052 -0.62907
H 5.87940 -0.13981 -0.69151
H -1.02548 -0.65521 2.34709
H -1.40495 1.08588 2.19638
H -4.26280 -2.80344 -0.29527
H -4.14478 1.21955 -1.84324
```

```
                            SCF energy:   -728.542788 hartree
                 zero-point correction:   +0.286424 hartree
                   enthalpy correction:   +0.301644 hartree
                free energy correction:   +0.244199 hartree
  quasiharmonic free energy correction:   +0.246846 hartree
```

7.8 Zwitterion 7h

```
C -2.22757 1.15020 0.10883
C -3.17216 1.50801 -0.91455
C -4.13347 0.62657 -1.37555
H -4.82678 0.95793 -2.14639
C -4.23131 -0.68233 -0.87054
C -3.31902 -1.07062 0.11055
H -3.35894 -2.08128 0.51628
C -2.34910 -0.19826 0.60351
C -1.35341 -0.66644 1.61822
N -0.01497 -0.73222 0.98215
N -1.28187 1.96468 0.60166
H -1.35588 2.86595 0.12644
C 0.16551 -1.68799 -0.12944
C 0.84885 0.20721 1.17836
C 1.63046 -2.06653 -0.27265
H -0.20895 -1.20638 -1.04024
H -0.45499 -2.55970 0.08516
C 2.09058 0.28031 0.42795
H 0.62696 0.94003 1.94548
C 2.49506 -0.83406 -0.32800
H 1.75678 -2.67071 -1.17421
H 1.93784 -2.68121 0.58370
C 3.69395 -0.76431 -1.03216
C 2.87513 1.43866 0.48983
C 4.06430 1.49821 -0.22761
C 4.46876 0.39652 -0.98626
H 2.53988 2.28230 1.08739
H 4.67525 2.39444 -0.19723
H 4.02319 -1.61792 -1.61837
H 5.39854 0.44109 -1.54576
```

```
H -1.58904 -1.66933 1.98323
H -1.25758 0.02045 2.46405
H -4.99054 -1.36815 -1.23193
H -3.11715 2.51445 -1.32718
```

```
                            SCF energy:   -728.548640 hartree
                 zero-point correction:   +0.287054 hartree
                   enthalpy correction:   +0.302129 hartree
                free energy correction:   +0.245240 hartree
  quasiharmonic free energy correction:   +0.247531 hartree
```

7.9 Zwitterion 7i

```
C 0.60707 0.86521 -0.51111
C 2.00071 1.14177 -0.28497
Br 2.56480 2.95509 -0.33911
C 2.95794 0.17538 -0.04702
H 3.99331 0.46214 0.10677
C 2.58106 -1.16630 -0.00141
Br 3.88902 -2.49997 0.33263
C 1.25148 -1.51912 -0.19694
H 0.95037 -2.56293 -0.16337
C 0.29399 -0.54436 -0.44867
C -1.10822 -0.96161 -0.74911
N -2.12297 -0.46423 0.23664
N -0.36365 1.74572 -0.72928
C -1.76548 0.12970 1.32182
C -3.93026 1.30222 1.47713
C -3.51503 -0.58212 -0.11880
C -4.43343 0.28517 0.48824
C -5.77665 0.17566 0.13416
C -3.92049 -1.54187 -1.04490
C -5.26931 -1.63382 -1.38067
C -6.19710 -0.77432 -0.79581
H -3.20820 -2.21856 -1.50197
H -5.58931 -2.38125 -2.09928
H -6.49643 0.84530 0.59708
H -7.24792 -0.84538 -1.05906
C -2.75857 0.71448 2.25768
H -4.73083 1.60086 2.15685
H -3.59632 2.19908 0.93998
H -3.09566 -0.09759 2.92028
H -2.25981 1.45889 2.87998
H 0.03223 2.68420 -0.75461
H -1.43898 -0.55078 -1.70848
H -1.19428 -2.04995 -0.77385
H -0.70165 0.15971 1.53716
```

```
                            SCF energy:   -5870.962350 hartree
                 zero-point correction:   +0.267906 hartree
                   enthalpy correction:   +0.285752 hartree
                free energy correction:   +0.220189 hartree
  quasiharmonic free energy correction:   +0.223820 hartree
```

8 Cartesian Coordinates and Energies of Transition States TS-3

8.1 Transition State *cis*-3a

```
C -0.20209 0.90073 0.41829
C 1.11350 1.20497 0.00612
C 2.09105 0.23881 -0.16429
H 3.09053 0.52397 -0.47473
C 1.77571 -1.09410 0.07968
C 0.49401 -1.45551 0.46522
H 0.23875 -2.49642 0.64120
C -0.49124 -0.47711 0.59533
C -1.85555 -0.96400 0.88093
N -2.83161 -0.84031 0.04033
N -1.17389 1.82381 0.65197
H -0.86718 2.78708 0.70255
H -1.84310 1.47854 1.41759
C -4.15613 -1.46177 0.28222
C -2.83158 -0.04221 -1.20103
C -4.06101 -0.56411 -1.93825
H -1.88668 -0.18418 -1.73019
H -2.93701 1.01408 -0.93407
C -5.04365 -0.84371 -0.79611
H -3.81801 -1.49136 -2.46804
H -4.43649 0.16329 -2.66007
H -4.47220 -1.24243 1.30344
H -4.05256 -2.54363 0.15536
H -5.85792 -1.51241 -1.08065
H -5.47304 0.09548 -0.43329
O -2.52726 0.53581 2.46348
H -1.98506 -1.70105 1.66715
H -1.98425 0.52484 3.26345
Br 1.56514 3.01348 -0.31027
Br 3.10751 -2.42031 -0.13809
```

```
                          SCF energy:   -5755.695827 hartree
                zero-point correction:   +0.238687 hartree
                  enthalpy correction:   +0.255163 hartree
               free energy correction:   +0.194201 hartree
  quasiharmonic free energy correction:   +0.195793 hartree
```

8.2 Transition State *trans*-3a

```
C -0.57964 -1.30718 -0.15574
C -1.85954 -0.71977 -0.03415
C -2.05449 0.64711 0.02196
H -3.05642 1.05133 0.12098
C -0.94905 1.49224 -0.05568
C 0.32615 0.97601 -0.20019
```

```
H 1.16706 1.64814 -0.32304
C 0.52159 -0.40882 -0.25029
C 1.83430 -0.96427 -0.60167
N 2.97049 -0.35017 -0.42911
N -0.35397 -2.64305 -0.20642
H -1.14341 -3.24047 0.00265
H 0.59938 -2.89082 0.22292
C 4.21633 -0.92996 -0.98883
C 3.27793 0.62144 0.64247
C 4.70780 0.25378 1.03026
H 2.55005 0.52200 1.45059
H 3.23972 1.63884 0.24042
C 5.32876 -0.12932 -0.31620
H 4.70019 -0.60903 1.70490
H 5.21856 1.08287 1.52356
H 4.20441 -0.84668 -2.07717
H 4.24795 -1.98632 -0.70406
H 6.24338 -0.71674 -0.21772
H 5.55371 0.77118 -0.89678
O 2.01421 -2.68660 0.79904
H 1.84119 -1.77075 -1.33102
H 1.93536 -2.28606 1.67588
Br -3.36969 -1.85400 0.05619
Br -1.21178 3.36515 0.00417
```

```
                           SCF energy:   -5755.697042 hartree
                zero-point correction:   +0.238830 hartree
                  enthalpy correction:   +0.255244 hartree
                free energy correction:   +0.194251 hartree
quasiharmonic free energy correction:   +0.195934 hartree
```

8.3 Transition State *cis*-3b

```
C -1.51944 0.55924 0.64602
C -2.80149 0.19336 1.10230
H -3.18103 0.65372 2.01102
C -3.57914 -0.71270 0.39556
H -4.56569 -0.97058 0.77094
C -3.12036 -1.27414 -0.80242
H -3.73947 -1.96563 -1.36395
C -1.85451 -0.93060 -1.26058
H -1.47234 -1.36001 -2.18372
C -1.03402 -0.05962 -0.53029
C 0.33407 0.13809 -1.03553
N 1.39616 -0.19805 -0.37187
N -0.74624 1.49457 1.29408
H -1.25016 2.06077 1.96657
H -0.16124 2.03016 0.61408
C 2.74850 -0.12209 -0.97420
C 1.46122 -0.63530 1.03439
C 2.84138 -1.27925 1.12268
H 0.62666 -1.30662 1.24861
H 1.38260 0.24481 1.68016
```

```
C 3.68362 -0.38718 0.20417
H 2.80628 -2.30275 0.73415
H 3.20836 -1.30727 2.15020
H 2.87972 0.85752 -1.43738
H 2.82597 -0.90016 -1.73999
H 4.61578 -0.85496 -0.11745
H 3.92158 0.55289 0.71202
O 0.53248 2.42360 -0.92007
H 0.47061 0.28649 -2.10244
H -0.13587 2.87841 -1.45030
```

```
                            SCF energy:   -613.281014 hartree
                 zero-point correction:   +0.257883 hartree
                   enthalpy correction:   +0.272023 hartree
                free energy correction:   +0.218355 hartree
  quasiharmonic free energy correction:   +0.219320 hartree
```

8.4 Transition State *trans*-3b

```
C 2.09808 0.78000 -0.11158
C 3.38127 0.21332 0.03574
H 4.23721 0.87819 0.11703
C 3.54930 -1.16008 0.08609
H 4.54903 -1.56964 0.20189
C 2.44782 -2.02265 -0.01048
H 2.58441 -3.09844 0.01489
C 1.17993 -1.48281 -0.16280
H 0.33531 -2.15133 -0.28928
C 0.98009 -0.09157 -0.21451
C -0.31890 0.48748 -0.55806
N -1.46930 -0.12091 -0.44268
N 1.90657 2.13566 -0.17182
H 2.71563 2.69194 0.07737
H 0.99875 2.41408 0.27115
C -2.69402 0.50433 -0.99775
C -1.81307 -1.13030 0.58061
C -3.24575 -0.75891 0.95523
H -1.10131 -1.07333 1.40707
H -1.77920 -2.13186 0.14014
C -3.83261 -0.30847 -0.38574
H -3.24027 0.07419 1.66647
H -3.77890 -1.60058 1.40168
H -2.66341 0.47312 -2.08869
H -2.71845 1.54665 -0.66416
H -4.74135 0.28711 -0.28101
H -4.05733 -1.17965 -1.00995
O -0.51366 2.14162 0.93729
H -0.31013 1.33255 -1.24215
H -0.37432 1.68861 1.78025
```

```
                            SCF energy:   -613.283151 hartree
                 zero-point correction:   +0.258231 hartree
                   enthalpy correction:   +0.272226 hartree
                 free energy correction:   +0.218920 hartree
  quasiharmonic free energy correction:   +0.219888 hartree
```

8.5 Transition State *cis*-3c

```
C 0.03647 0.80998 0.40011
C -1.26663 1.22364 0.05175
Br -1.59553 3.07212 -0.16812
C -2.31675 0.33773 -0.12829
H -3.30303 0.70660 -0.38906
C -2.08770 -1.02309 0.03987
Br -3.51656 -2.24315 -0.18699
C -0.82162 -1.49032 0.36143
H -0.63638 -2.55390 0.48162
C 0.23263 -0.59021 0.50280
C 1.56304 -1.19463 0.73997
N 2.52829 -1.17793 -0.12182
N 1.08400 1.65280 0.61268
H 0.84663 2.63137 0.71746
H 1.75919 1.24218 1.33572
C 3.74780 -1.98489 0.13450
C 2.56785 -0.36666 -1.34773
C 3.68649 0.68343 -1.26160
H 1.59098 0.08453 -1.51380
H 2.76173 -1.07151 -2.16216
C 4.96684 -1.35538 -0.54021
H 3.55916 -2.99963 -0.22924
H 3.88395 -2.01547 1.21851
O 2.30524 0.25726 2.43070
H 1.64933 -1.92033 1.54278
H 3.23919 0.02201 2.35322
C 4.87791 0.16586 -0.43670
H 5.02442 -1.65825 -1.59171
H 5.86134 -1.74077 -0.04350
H 5.80553 0.63565 -0.77407
H 4.74494 0.43868 0.61798
H 3.29093 1.60333 -0.82540
H 3.99946 0.90666 -2.28656
```

```
                            SCF energy:   -5794.989438 hartree
                 zero-point correction:   +0.267958 hartree
                   enthalpy correction:   +0.285641 hartree
                 free energy correction:   +0.221620 hartree
  quasiharmonic free energy correction:   +0.224240 hartree
```

8.6 Transition State *trans*-3c

```
C 0.97946 -1.31001 -0.09388
C 2.15040 -0.51830 -0.05627
```

```
Br 3.82968 -1.38801 -0.09140
C 2.12326 0.86240 -0.00692
H 3.04917 1.42689 0.02267
C 0.89175 1.51375 -0.00689
Br 0.84199 3.40454 0.02309
C -0.28709 0.79296 -0.06516
H -1.23401 1.31612 -0.13576
C -0.25692 -0.60538 -0.09941
C -1.48812 -1.36380 -0.35935
N -2.69297 -0.96532 -0.06667
N 0.97947 -2.66457 -0.15897
H 1.87102 -3.11919 -0.00909
H 0.11374 -3.07858 0.32285
C -3.84725 -1.69560 -0.63377
C -3.04952 -0.09617 1.06400
C -3.92813 1.06580 0.58149
H -2.14884 0.23081 1.58096
H -3.60885 -0.73577 1.75657
C -5.12435 -0.85633 -0.50758
H -3.93946 -2.65024 -0.10218
H -3.61719 -1.89518 -1.68272
O -1.21411 -3.06396 1.09597
H -1.42192 -2.13298 -1.12652
H -1.89186 -3.65226 0.73790
C -4.78551 0.63057 -0.62053
H -5.61545 -1.05048 0.45258
H -5.81791 -1.16874 -1.29256
H -5.69590 1.23342 -0.67461
H -4.23299 0.79915 -1.55330
H -3.31181 1.93047 0.31476
H -4.56672 1.36953 1.41695
```

```
                          SCF energy:   -5794.990802 hartree
               zero-point correction:   +0.268655 hartree
                 enthalpy correction:   +0.285954 hartree
              free energy correction:   +0.223067 hartree
quasiharmonic free energy correction:   +0.225094 hartree
```

8.7 Transition State *cis*-3d

```
C -0.16656 1.06131 0.45487
C -1.49002 1.09974 -0.03810
Br -2.23494 2.77865 -0.48243
C -2.26455 -0.03579 -0.20101
H -3.27894 0.04617 -0.57691
C -1.73052 -1.27677 0.13576
Br -2.79218 -2.82968 -0.06631
C -0.43011 -1.37977 0.60289
H -0.00062 -2.34638 0.84969
C 0.35519 -0.23186 0.71915
C 1.76232 -0.44950 1.09920
N 2.75673 -0.18963 0.30760
N 0.60588 2.15442 0.68776
```

```
H 0.13166 3.04847 0.66112
H 1.29069 1.97317 1.50360
C 4.13203 -0.51778 0.69190
C 2.63468 0.52804 -0.97306
C 3.87022 0.22588 -1.81846
H 2.53687 1.60127 -0.78104
H 1.72922 0.17109 -1.47007
C 4.74757 -1.42478 -0.38116
H 4.12813 -1.01019 1.66436
H 4.67842 0.42540 0.78468
O 2.09155 1.25678 2.60973
H 1.97234 -1.09833 1.94252
H 1.53911 1.21828 3.40228
O 4.21517 -1.14299 -1.67502
H 4.51396 -2.47227 -0.17825
H 5.83645 -1.29194 -0.38238
H 4.71776 0.86504 -1.53991
H 3.64062 0.40007 -2.87069
```

```
                          SCF energy:  -5830.876548 hartree
                zero-point correction:  +0.244144 hartree
                  enthalpy correction:  +0.261544 hartree
               free energy correction:  +0.197967 hartree
  quasiharmonic free energy correction:  +0.200430 hartree
```

8.8 Transition State *trans*-3d

```
C -0.62506 -1.29366 0.18306
C -1.96514 -0.87146 0.00858
Br -3.31498 -2.18768 -0.13204
C -2.32899 0.45864 -0.05619
H -3.36919 0.73344 -0.19558
C -1.34412 1.43806 0.06712
Br -1.84189 3.26246 -0.00477
C -0.02153 1.08765 0.26434
H 0.71660 1.86335 0.42676
C 0.34994 -0.26189 0.32110
C 1.70079 -0.64851 0.74338
N 2.76594 0.10118 0.62596
N -0.23711 -2.58734 0.24561
H -0.93844 -3.27939 0.01499
H 0.77409 -2.71453 -0.13095
C 4.01023 -0.28084 1.29964
C 2.95237 1.11967 -0.42370
C 4.38548 1.02274 -0.95672
H 2.77660 2.12217 -0.02071
H 2.23563 0.91729 -1.22238
C 4.99137 -0.87794 0.27717
H 3.79044 -0.99882 2.09006
H 4.42080 0.62270 1.75851
O 2.15780 -2.38427 -0.58802
H 1.76267 -1.43912 1.48539
H 2.14459 -2.01812 -1.48301
```

```
O 4.77551 -0.33690 -1.02396
H 4.84941 -1.95595 0.18671
H 6.01889 -0.67245 0.60462
H 5.08616 1.58949 -0.32988
H 4.42171 1.43043 -1.96827
```

```
                            SCF energy:   -5830.877372 hartree
                 zero-point correction:   +0.244744 hartree
                   enthalpy correction:   +0.261706 hartree
                free energy correction:   +0.199811 hartree
  quasiharmonic free energy correction:   +0.201248 hartree
```

8.9 Transition State *cis*-3e

```
C 0.96583 -1.12814 0.52788
C 2.13103 -1.04683 -0.26536
Br 2.75452 -2.61696 -1.11096
C 2.84221 0.12856 -0.43946
H 3.74025 0.13678 -1.04809
C 2.39515 1.28938 0.18431
Br 3.36635 2.89847 -0.03383
C 1.23818 1.27879 0.94734
H 0.87333 2.18726 1.41745
C 0.51148 0.09626 1.08239
C -0.77475 0.20383 1.79663
N -1.92865 0.01497 1.23519
N 0.27178 -2.27147 0.77257
H 0.73818 -3.13177 0.51255
H -0.18020 -2.23504 1.75033
C -2.09108 -0.53760 -0.12420
C -3.15090 0.28016 2.03799
C -4.47930 0.13834 -0.04878
C -3.29811 0.05924 -0.79609
C -3.26956 0.48897 -2.12148
C -5.63251 0.65513 -0.63762
C -5.60978 1.07371 -1.96954
C -4.43084 0.99096 -2.71113
H -6.54791 0.72860 -0.05567
H -6.51134 1.47193 -2.42581
H -2.34430 0.43072 -2.68935
H -4.41280 1.32422 -3.74439
O -0.53466 -1.69640 3.15891
H -0.78612 0.71739 2.75293
H -1.45908 -1.83697 3.40223
H -2.19424 -1.62568 -0.02771
H -1.18464 -0.33250 -0.69454
C -4.38817 -0.32227 1.38039
H -2.98851 -0.14030 3.03285
H -3.25855 1.36539 2.12305
H -5.26745 -0.01966 1.95415
H -4.32514 -1.41734 1.42227
```

```
                           SCF energy:   -5947.374446 hartree
                 zero-point correction:   +0.291255 hartree
                   enthalpy correction:   +0.311027 hartree
                 free energy correction:   +0.242055 hartree
  quasiharmonic free energy correction:   +0.245643 hartree
```

8.10 Transition State *trans*-3e

```
C 1.54452 -1.31398 -0.24398
C 2.80133 -0.75752 0.08986
Br 4.24335 -1.92959 0.43993
C 3.01882 0.60411 0.17404
H 3.99925 0.98506 0.43985
C 1.96563 1.47786 -0.09242
Br 2.26584 3.34338 -0.00506
C 0.72005 0.99336 -0.44644
H -0.07032 1.68457 -0.71568
C 0.49767 -0.38735 -0.51409
C -0.74523 -0.90824 -1.08877
N -1.89501 -0.29224 -1.09595
N 1.29978 -2.64256 -0.34266
H 2.03137 -3.25752 -0.01026
H 0.28093 -2.87452 -0.08046
C -2.29661 0.66351 -0.04109
C -2.94548 -0.82283 -1.99916
C -4.66941 0.04049 -0.45407
C -3.67192 0.33679 0.48193
C -3.96824 0.36805 1.84338
C -5.96674 -0.22445 -0.01770
C -6.26956 -0.17752 1.34439
C -5.27179 0.11705 2.27420
H -6.73905 -0.46659 -0.74350
H -7.28251 -0.37984 1.67999
H -3.18320 0.58819 2.56237
H -5.50558 0.14311 3.33434
O -1.14840 -2.59574 0.38025
H -0.63520 -1.70279 -1.82448
H -1.84496 -3.04122 -0.11947
H -2.29082 1.67518 -0.46492
H -1.56236 0.61778 0.76405
C -4.23107 -0.01065 -1.89139
H -2.55196 -0.80132 -3.01710
H -3.13690 -1.86293 -1.71209
H -4.99188 -0.47592 -2.52274
H -4.05680 1.00341 -2.27416
```

```
                           SCF energy:   -5947.374883 hartree
                 zero-point correction:   +0.291875 hartree
                   enthalpy correction:   +0.311433 hartree
                 free energy correction:   +0.243159 hartree
  quasiharmonic free energy correction:   +0.246239 hartree
```

8.11 Transition State *cis*-3f

```
C -0.77402 0.84072 0.48663
C -2.06366 1.25275 0.08330
Br -2.38476 3.10090 -0.14650
C -3.10411 0.36758 -0.14164
H -4.07891 0.73676 -0.44215
C -2.88165 -0.99457 0.03285
Br -4.29853 -2.21455 -0.25835
C -1.63082 -1.46119 0.40523
H -1.44942 -2.52502 0.52834
C -0.58206 -0.56078 0.59277
C 0.73545 -1.16940 0.87691
N 1.70562 -1.16735 0.01634
N 0.25365 1.68919 0.75853
H 0.00467 2.66515 0.86182
H 0.91811 1.26624 1.49506
C 1.67258 -0.36012 -1.22641
C 2.95841 -1.88824 0.33506
C 2.96321 -0.53434 -2.02677
H 1.55343 0.68812 -0.93766
H 0.79932 -0.67155 -1.80581
C 4.13549 -0.98338 0.09230
H 3.00827 -2.76635 -0.31977
H 2.90739 -2.22481 1.37090
C 4.15315 -0.30587 -1.13372
H 2.94761 0.17299 -2.85926
H 3.00079 -1.54524 -2.45203
C 5.22013 0.53890 -1.43565
C 5.17008 -0.81902 1.01045
C 6.24224 0.01861 0.69701
C 6.26639 0.69429 -0.52354
H 5.13885 -1.34270 1.96274
H 7.05283 0.14879 1.40759
H 5.23307 1.07474 -2.38136
H 7.09799 1.35042 -0.76336
O 1.49244 0.27996 2.52985
H 0.80369 -1.88163 1.69168
H 2.43819 0.12349 2.40124
```

```
                            SCF energy:   -5947.374273 hartree
                 zero-point correction:   +0.291342 hartree
                   enthalpy correction:   +0.311058 hartree
                free energy correction:   +0.240551 hartree
  quasiharmonic free energy correction:   +0.245916 hartree
```

8.12 Transition State *trans*-3f

```
C 1.76141 -1.28494 -0.10503
C 2.99606 -0.59555 -0.08737
Br 4.59605 -1.60303 -0.09019
C 3.08454 0.78261 -0.06704
H 4.05440 1.26817 -0.04779
```

```
C 1.91232 1.53625 -0.07865
Br 2.02958 3.42414 -0.06908
C 0.67553 0.91984 -0.12108
H -0.21969 1.52503 -0.19637
C 0.58775 -0.47767 -0.13167
C -0.69046 -1.14679 -0.38972
N -1.87221 -0.65636 -0.13290
N 1.64207 -2.63467 -0.12393
H 2.49200 -3.16193 0.03071
H 0.74863 -2.95151 0.38643
C -2.12060 0.29922 0.96650
C -3.03324 -1.39115 -0.69546
C -3.41461 -0.05919 1.69541
H -2.21032 1.30965 0.55624
H -1.26543 0.25993 1.64386
C -4.32592 -0.64462 -0.51842
H -3.08847 -2.35350 -0.16817
H -2.83323 -1.58774 -1.74988
C -4.55286 -0.01947 0.71389
H -3.56672 0.65557 2.50808
H -3.31505 -1.05830 2.13960
C -5.76144 0.63804 0.94034
C -5.30111 -0.61399 -1.51403
C -6.51539 0.03173 -1.27673
C -6.74503 0.65602 -0.05027
H -5.11346 -1.09615 -2.47020
H -7.27676 0.05369 -2.05075
H -5.93159 1.13661 1.89142
H -7.68669 1.16569 0.13208
O -0.56035 -2.79028 1.16813
H -0.66514 -1.95960 -1.11272
H -1.26765 -3.36696 0.85083
```

```
                          SCF energy:   -5947.375476 hartree
                zero-point correction:   +0.291793 hartree
                  enthalpy correction:   +0.311410 hartree
               free energy correction:   +0.242769 hartree
  quasiharmonic free energy correction:   +0.246095 hartree
```

8.13 Transition State *cis*-3g

```
C -2.59921 -0.14953 -0.80200
C -3.57233 -1.15227 -0.98337
C -4.08406 -1.85352 0.09883
H -4.83863 -2.61628 -0.07252
C -3.66328 -1.57124 1.40444
C -2.69783 -0.59210 1.59946
H -2.35018 -0.35778 2.60291
C -2.12791 0.08371 0.51117
C -1.04161 1.02439 0.81976
N 0.17958 0.91966 0.38861
N -2.10522 0.59771 -1.84686
H -2.64993 0.52857 -2.69869
```

```
H -1.90278 1.57488 -1.53886
C 0.60338 -0.05658 -0.63288
C 1.18489 1.88834 0.89646
C 2.96223 0.42654 -0.02333
C 2.00220 -0.53830 -0.35190
C 2.35655 -1.88303 -0.44423
C 4.27872 0.03534 0.21617
C 4.63794 -1.30997 0.11213
C 3.67911 -2.26824 -0.21807
H 5.02200 0.78291 0.48185
H 5.66552 -1.61032 0.29524
H 1.60203 -2.62504 -0.69308
H 3.95785 -3.31521 -0.29148
O -1.88403 2.86965 -0.40190
H -1.18446 1.69984 1.65784
H -1.11518 3.45428 -0.39472
H 0.54917 0.43852 -1.61043
H -0.10610 -0.88438 -0.63494
C 2.46711 1.84335 0.07172
H 0.73287 2.88206 0.86314
H 1.39649 1.62883 1.93803
H 3.20752 2.49393 0.54333
H 2.26700 2.24056 -0.93190
H -4.08327 -2.10509 2.25019
H -3.93363 -1.35047 -1.98925
```

```
                            SCF energy:   -804.959589 hartree
                 zero-point correction:   +0.311282 hartree
                   enthalpy correction:   +0.328384 hartree
                 free energy correction:   +0.267841 hartree
  quasiharmonic free energy correction:   +0.269742 hartree
```

8.14 Transition State *trans*-3g

```
C 3.22953 -0.53341 0.55615
C 4.42610 0.21476 0.57893
C 4.54894 1.37989 -0.15753
H 5.48201 1.93554 -0.12148
C 3.48844 1.84685 -0.94874
C 2.30646 1.12486 -0.98408
H 1.50485 1.45680 -1.63615
C 2.15148 -0.05912 -0.23860
C 0.99493 -0.93099 -0.42212
N -0.18435 -0.56467 -0.85181
N 3.09531 -1.70302 1.25430
H 3.83642 -1.89200 1.91833
H 2.11600 -1.85028 1.59560
C -0.73264 0.78654 -0.61164
C -1.11939 -1.63567 -1.27217
C -3.01726 -0.19732 -0.61188
C -2.12074 0.70584 -0.02848
C -2.52830 1.52319 1.02440
C -4.32457 -0.27709 -0.13336
```

```
C -4.73852 0.55137 0.91147
C -3.84187 1.45002 1.49061
H -5.01809 -0.98665 -0.57796
H -5.75879 0.48929 1.27867
H -1.82149 2.21351 1.47808
H -4.16131 2.08729 2.30976
O 0.52650 -1.40925 1.76256
H 1.20430 -1.99580 -0.50462
H -0.18699 -2.04293 1.61346
H -0.76106 1.32987 -1.56414
H -0.06309 1.31285 0.06906
C -2.46148 -1.05990 -1.71119
H -0.64833 -2.19270 -2.08433
H -1.26540 -2.30805 -0.41896
H -3.13597 -1.88617 -1.94867
H -2.32379 -0.47015 -2.62704
H 3.59505 2.75062 -1.53901
H 5.25029 -0.14217 1.19093
```

```
                          SCF energy:   -804.960978 hartree
                zero-point correction:   +0.311445 hartree
                  enthalpy correction:   +0.328502 hartree
               free energy correction:   +0.267747 hartree
  quasiharmonic free energy correction:   +0.270047 hartree
```

8.15 Transition State *cis*-3h

```
C 2.52042 -0.21726 0.98423
C 3.79125 -0.78916 1.19742
C 4.78981 -0.69517 0.23956
H 5.75936 -1.14371 0.43820
C 4.56996 -0.01098 -0.96211
C 3.32163 0.55365 -1.19100
H 3.12590 1.08804 -2.11782
C 2.28500 0.42164 -0.25576
C 0.97893 0.97611 -0.65607
N -0.06779 0.24380 -0.89663
N 1.52959 -0.26494 1.93793
H 1.85745 -0.50797 2.86553
H 0.91969 0.58569 1.89059
C -0.12772 -1.20006 -0.57569
C -1.30228 0.89192 -1.39277
C -1.47810 -1.79385 -0.97640
H 0.02346 -1.31007 0.50203
H 0.69468 -1.69554 -1.09878
C -2.48457 0.42026 -0.59048
H -1.42156 0.61608 -2.44754
H -1.17275 1.97270 -1.32687
C -2.59136 -0.96326 -0.39715
H -1.52109 -2.82462 -0.61704
H -1.56007 -1.82150 -2.07054
C -3.66768 -1.47435 0.32643
C -3.44226 1.28632 -0.06762
```

```
C -4.52562 0.76744 0.64421
C -4.63692 -0.60960 0.83972
H -3.34217 2.35878 -0.21577
H -5.27599 1.43791 1.05224
H -3.74769 -2.54629 0.48923
H -5.47598 -1.01149 1.40013
O 0.39527 2.08355 1.30439
H 0.95797 1.98589 -1.05007
H -0.55719 2.12635 1.14280
H 5.35790 0.07955 -1.70222
H 3.98032 -1.29214 2.14245
```

```
                          SCF energy:   -804.959567 hartree
                zero-point correction:   +0.311228 hartree
                  enthalpy correction:   +0.328373 hartree
               free energy correction:   +0.267547 hartree
  quasiharmonic free energy correction:   +0.269759 hartree
```

8.16 Transition State *trans*-3h

```
C -3.47297 0.58662 -0.18436
C -4.67537 -0.14938 -0.24191
C -4.65902 -1.52945 -0.34273
H -5.60004 -2.07105 -0.38561
C -3.44586 -2.23199 -0.39225
C -2.25505 -1.52543 -0.33808
H -1.31928 -2.06584 -0.42968
C -2.24192 -0.12236 -0.22945
C -1.01017 0.64969 -0.37292
N 0.20360 0.21058 -0.15419
N -3.46626 1.95393 -0.10703
H -4.36803 2.37345 0.08514
H -2.66057 2.30457 0.46429
C 0.50340 -0.83959 0.83995
C 1.31445 1.08406 -0.60531
C 1.74884 -0.46883 1.64373
H 0.67816 -1.79013 0.32657
H -0.36634 -0.93920 1.49177
C 2.66057 0.42951 -0.46329
H 1.28365 1.99323 0.01131
H 1.12655 1.36666 -1.64248
C 2.90923 -0.30643 0.70170
H 1.94053 -1.25737 2.37587
H 1.55961 0.46235 2.19378
C 4.16432 -0.88183 0.89788
C 3.66177 0.59284 -1.41979
C 4.92109 0.02866 -1.21124
C 5.17155 -0.70780 -0.05292
H 3.45779 1.16141 -2.32382
H 5.70159 0.15675 -1.95533
H 4.35269 -1.46574 1.79547
H 6.14870 -1.15435 0.10664
O -1.27164 2.09701 1.35725
```

```
H -1.07418 1.54122 -0.99316
H -0.56522 2.72751 1.16551
H -3.43588 -3.31237 -0.48917
H -5.61714 0.39159 -0.20062
```

```
                            SCF energy:   -804.961489 hartree
                 zero-point correction:   +0.311689 hartree
                   enthalpy correction:   +0.328681 hartree
                free energy correction:   +0.268287 hartree
  quasiharmonic free energy correction:   +0.270286 hartree
```

8.17 Transition State *cis*-3i

```
C -0.99896 -1.07479 -0.42806
C -2.35793 -0.95107 -0.05087
Br -3.35822 -2.53095 0.22573
C -2.98877 0.26939 0.10785
H -4.03669 0.30821 0.38685
C -2.26648 1.44062 -0.11050
Br -3.12474 3.11581 0.07975
C -0.92729 1.38614 -0.45667
H -0.35614 2.29677 -0.61312
C -0.28783 0.14837 -0.56456
C 1.16381 0.22484 -0.79011
C 1.63485 -0.87857 1.32308
N -0.36548 -2.24712 -0.66935
H -0.96445 -3.06159 -0.72864
H 0.41359 -2.10715 -1.44798
N 2.05218 -0.16508 0.08140
C 2.78716 -1.08403 2.29308
C 4.25980 0.34651 0.96930
C 3.44453 0.11735 -0.14747
C 3.94805 0.19789 -1.44664
C 5.59682 0.67838 0.75104
C 6.10921 0.78562 -0.54102
C 5.28456 0.54013 -1.63797
H 6.23870 0.85215 1.61061
H 7.15243 1.04659 -0.69046
H 3.31220 -0.01587 -2.29918
H 5.67884 0.60241 -2.64721
O 1.27480 -1.51447 -2.45751
H 1.51299 0.88589 -1.57666
H 2.16917 -1.86065 -2.33942
C 3.67242 0.15957 2.34034
H 2.35427 -1.30444 3.27232
H 3.38999 -1.94772 1.99328
H 4.47175 0.05492 3.07814
H 3.06872 1.03229 2.62339
H 1.19223 -1.82978 1.01809
H 0.85677 -0.25928 1.77919
```

```
                            SCF energy:   -5947.372340 hartree
                  zero-point correction:   +0.290375 hartree
                    enthalpy correction:   +0.310045 hartree
                 free energy correction:   +0.241667 hartree
   quasiharmonic free energy correction:   +0.244663 hartree
```

8.18 Transition State *trans*-3i

```
C 1.55824 -1.29124 -0.11095
C 2.62264 -0.35699 -0.03563
Br 4.38018 -1.01185 0.20403
C 2.43128 1.00530 -0.13156
H 3.27752 1.68075 -0.06182
C 1.13820 1.49986 -0.32180
Br 0.87345 3.36610 -0.48394
C 0.06378 0.64103 -0.42325
H -0.92693 1.03449 -0.62200
C 0.26068 -0.74338 -0.31778
C -0.82466 -1.67060 -0.62659
C -3.04798 -2.32561 -1.24453
N 1.70771 -2.63024 -0.01347
H 2.62870 -2.95827 0.24876
H 0.82748 -3.10891 0.43058
N -2.10490 -1.42495 -0.51824
C -4.44226 -1.71081 -1.37327
C -3.77781 0.25075 -0.08336
C -2.66231 -0.45607 0.37726
C -2.12226 -0.24354 1.64471
C -4.32668 1.22889 0.74635
C -3.76857 1.49129 1.99722
C -2.67542 0.74837 2.44949
H -5.19742 1.78371 0.40707
H -4.19902 2.26212 2.62930
H -1.28030 -0.83859 1.98452
H -2.25930 0.93279 3.43493
O -0.50492 -3.27064 1.04279
H -0.56793 -2.51713 -1.25874
H -1.02051 -3.98035 0.63765
C -4.36146 -0.17865 -1.40069
H -4.90171 -2.09974 -2.28551
H -5.06996 -2.01395 -0.53009
H -5.34907 0.26597 -1.54356
H -3.72282 0.14470 -2.23363
H -3.07685 -3.27663 -0.70393
H -2.61155 -2.48988 -2.23083
```

```
                            SCF energy:   -5947.374382 hartree
                  zero-point correction:   +0.290332 hartree
                    enthalpy correction:   +0.310222 hartree
                 free energy correction:   +0.240745 hartree
   quasiharmonic free energy correction:   +0.244540 hartree
```

9 Cartesian Coordinates and Energies of Transition States TS-5

9.1 Transition State 5a

```
C -0.44628 0.64349 -0.40793
C 0.82635 1.20529 -0.08669
C 1.96320 0.45093 0.07858
H 2.91900 0.92730 0.26696
C 1.86606 -0.94820 -0.01635
C 0.65715 -1.56013 -0.23191
H 0.58078 -2.64258 -0.27748
C -0.52013 -0.78860 -0.37147
C -1.75327 -1.50181 -0.55336
N -2.94053 -1.09515 -0.15229
N -1.52989 1.35896 -0.78751
H -1.38176 2.36171 -0.68766
C -4.18060 -1.78379 -0.59762
C -3.23325 0.02956 0.63107
C -4.74283 0.07426 0.80454
H -2.52023 0.98300 -0.15561
H -2.59938 0.08558 1.51954
C -5.19775 -1.35381 0.45032
H -5.19794 0.79305 0.11166
H -5.03041 0.36614 1.81761
H -3.99027 -2.85710 -0.64964
H -4.43490 -1.41185 -1.59541
H -6.21998 -1.40250 0.06922
H -5.11774 -2.00248 1.32835
H -1.72527 -2.49343 -0.99733
Br 0.97615 3.08935 0.04124
Br 3.44039 -1.98526 0.17686
```

```
                          SCF energy:   -5679.263909 hartree
                zero-point correction:   +0.210104 hartree
                  enthalpy correction:   +0.224033 hartree
               free energy correction:   +0.168525 hartree
  quasiharmonic free energy correction:   +0.169511 hartree
```

9.2 Transition State 5b

```
C 1.33563 0.81102 -0.32587
C 2.64998 1.23137 0.03453
C 3.63198 0.32232 0.35763
H 4.63488 0.67371 0.58521
C 3.35168 -1.06476 0.37957
C 2.06914 -1.49242 0.11921
H 1.82780 -2.55264 0.16113
C 1.02082 -0.57920 -0.17377
C -0.29555 -1.11279 -0.36984
```

```
N -1.42790 -0.48725 -0.11581
N 0.41601 1.66082 -0.85580
H 0.74347 2.62636 -0.81647
C -2.73252 -1.03702 -0.56596
C -1.58662 0.75998 0.51967
C -3.08169 1.03916 0.56605
H -0.66725 1.50812 -0.28170
H -1.02986 0.79832 1.46065
C -3.72502 -0.34377 0.35692
H -3.38358 1.71378 -0.24549
H -3.38399 1.50384 1.50788
H -2.70715 -2.12549 -0.48899
H -2.88265 -0.75402 -1.61317
H -4.72560 -0.29926 -0.07898
H -3.77926 -0.88143 1.30933
H -0.40002 -2.14574 -0.69444
H 4.13422 -1.77873 0.61574
H 2.87530 2.29496 -0.00812
```

```
                          SCF energy:  -536.847217 hartree
               zero-point correction:  +0.229007 hartree
                 enthalpy correction:  +0.240260 hartree
              free energy correction:  +0.193155 hartree
quasiharmonic free energy correction:  +0.193403 hartree
```

9.3 Transition State 5c

```
C -0.14589 0.68954 -0.40509
C 1.15092 1.20025 -0.10144
C 2.25366 0.39909 0.07430
C 2.08973 -0.99560 0.00596
C 0.85420 -1.55643 -0.19358
H 0.73146 -2.63521 -0.22081
C -0.29005 -0.73601 -0.34261
C -1.54620 -1.40868 -0.51912
N -2.74917 -0.98526 -0.15835
H -1.51819 -2.42128 -0.91376
N -1.20459 1.43868 -0.78413
H -1.03056 2.43706 -0.67914
H -2.18439 1.06128 -0.13656
C -3.88425 -1.86964 -0.55549
C -2.94097 0.15141 0.64037
C -4.35353 0.63122 0.92365
H -2.25462 0.13639 1.49072
C -5.22807 -1.16692 -0.52315
H -3.88587 -2.69921 0.16064
H -3.66250 -2.26185 -1.54858
H 3.23202 0.83332 0.24868
Br 1.38368 3.07769 -0.01759
Br 3.61559 -2.10129 0.20802
H -5.99775 -1.92550 -0.69551
H -5.29347 -0.43793 -1.34076
H -4.62527 1.42860 0.21647
```

```
H -4.35958 1.08738 1.91806
C -5.41451 -0.46106 0.81497
H -6.41633 -0.02646 0.88974
H -5.30348 -1.18758 1.63083
```

```
                           SCF energy:   -5718.556823 hartree
                 zero-point correction:   +0.239356 hartree
                   enthalpy correction:   +0.254466 hartree
                 free energy correction:   +0.195954 hartree
  quasiharmonic free energy correction:   +0.197778 hartree
```

9.4 Transition State 5d

```
C -0.14672 0.71199 -0.36441
C 1.16405 1.20251 -0.09082
C 2.25762 0.38461 0.06636
C 2.07490 -1.00662 0.00274
C 0.82825 -1.54764 -0.18315
H 0.68945 -2.62421 -0.21417
C -0.30541 -0.71123 -0.31623
C -1.56397 -1.38390 -0.49528
N -2.76695 -0.96313 -0.15378
H -1.52857 -2.40028 -0.88060
N -1.20071 1.48526 -0.70649
H -1.01524 2.48026 -0.59569
H -2.16660 1.11294 -0.09732
C -3.89781 -1.87440 -0.47862
C -2.98976 0.16756 0.65398
C -4.41948 0.61832 0.79509
H -2.39876 0.11328 1.57054
C -5.23136 -1.15637 -0.43306
H -3.88168 -2.66673 0.27656
H -3.73065 -2.30643 -1.46651
H 3.24472 0.80561 0.22361
Br 1.42914 3.07491 -0.01473
Br 3.58545 -2.13470 0.18654
O -5.37106 -0.45066 0.78725
H -6.03315 -1.89562 -0.49077
H -5.33099 -0.45916 -1.27787
H -4.70193 1.30485 -0.01884
H -4.53709 1.14931 1.74166
```

```
                           SCF energy:   -5754.445761 hartree
                 zero-point correction:   +0.216041 hartree
                   enthalpy correction:   +0.230786 hartree
                 free energy correction:   +0.173081 hartree
  quasiharmonic free energy correction:   +0.174680 hartree
```

9.5 Transition State 5e

```
C 0.57692 0.50511 -0.57849
C 1.77684 1.20925 -0.23680
```

```
Br 1.75536 3.10047 -0.30123
C 2.95343 0.58105 0.08423
H 3.84812 1.15894 0.28919
C 2.98700 -0.82571 0.12828
Br 4.62288 -1.68446 0.54650
C 1.85683 -1.56352 -0.10960
H 1.87722 -2.64826 -0.05505
C 0.62984 -0.91963 -0.39899
C -0.50686 -1.77658 -0.58459
N -1.76500 -1.49680 -0.31991
N -0.53103 1.07014 -1.08542
H -0.48101 2.08771 -1.07662
C -2.81128 -2.46607 -0.71635
C -2.16518 -0.31275 0.35471
C -3.99220 -1.72493 -1.32498
H -3.12355 -3.00082 0.18721
H -2.36973 -3.16947 -1.42133
C -3.61480 -0.10410 0.52492
H -1.55593 0.59757 -0.43115
H -1.56596 -0.15944 1.25715
C -4.53827 -0.73785 -0.32549
H -4.75767 -2.45241 -1.60947
H -3.66475 -1.21318 -2.23938
C -5.89999 -0.46436 -0.20009
C -4.08608 0.79790 1.49059
C -5.44676 1.07203 1.60186
C -6.36140 0.44370 0.75359
H -3.37606 1.28563 2.15483
H -5.79477 1.77328 2.35504
H -6.60442 -0.97159 -0.85589
H -7.42364 0.65160 0.84041
H -0.32218 -2.79454 -0.91893
```

```
                          SCF energy:   -5870.954334 hartree
                zero-point correction:   +0.263326 hartree
                  enthalpy correction:   +0.280461 hartree
               free energy correction:   +0.217294 hartree
  quasiharmonic free energy correction:   +0.219903 hartree
```

9.6 Transition State 5f

```
C 0.59466 0.60505 -0.23292
C 1.88419 1.20700 -0.12768
Br 2.00232 3.09670 -0.14362
C 3.05076 0.48290 -0.07287
H 4.01158 0.98486 -0.04927
C 2.97462 -0.92080 -0.06470
Br 4.58626 -1.91727 -0.02416
C 1.76318 -1.56477 -0.07293
H 1.70840 -2.64912 -0.04022
C 0.55938 -0.82178 -0.09552
C -0.66885 -1.56614 -0.06547
N -1.80822 -1.17407 0.48224
```

```
N -0.54976 1.27332 -0.50190
H -0.42111 2.28362 -0.47893
C -1.95810 -0.00679 1.24223
C -3.01634 -2.00546 0.25195
C -3.35436 0.23777 1.78225
H -1.42511 0.90739 0.28236
H -1.14563 0.09946 1.96618
C -4.18835 -1.12744 -0.09270
H -3.20951 -2.54828 1.18578
H -2.80416 -2.72137 -0.54139
C -4.37903 0.00869 0.70318
H -3.41461 1.26024 2.16464
H -3.57410 -0.43287 2.62981
C -5.45981 0.85144 0.44628
C -5.06724 -1.42215 -1.13294
C -6.15460 -0.58129 -1.37726
C -6.34905 0.55328 -0.58859
H -4.90275 -2.30333 -1.74802
H -6.84264 -0.80721 -2.18645
H -5.60524 1.74164 1.05339
H -7.19048 1.21179 -0.78413
H -0.66526 -2.57875 -0.45770
```

```
                           SCF energy:   -5870.944405 hartree
                zero-point correction:   +0.263196 hartree
                  enthalpy correction:   +0.280289 hartree
               free energy correction:   +0.217403 hartree
  quasiharmonic free energy correction:   +0.219822 hartree
```

9.7 Transition State 5g

```
C 2.33483 -0.73116 0.61828
C 3.49116 -1.56787 0.51240
C 4.65167 -1.11940 -0.06991
H 5.52306 -1.76851 -0.09527
C 4.73311 0.18485 -0.62115
C 3.61433 0.98284 -0.60937
H 3.64669 1.97689 -1.05048
C 2.37823 0.53253 -0.06557
C 1.26813 1.42794 -0.16609
N -0.01372 1.12265 -0.21539
N 1.26047 -1.05566 1.36557
H 1.33131 -2.01289 1.71265
C -1.01327 2.21063 -0.17970
C -0.48107 -0.21658 -0.35565
C -2.15034 1.83229 0.75813
H -1.39341 2.34728 -1.19828
H -0.51233 3.12231 0.14458
C -1.94203 -0.41139 -0.30580
H 0.18715 -0.80603 0.64900
H 0.01782 -0.70997 -1.19608
C -2.78272 0.54516 0.29235
H -2.88579 2.64209 0.76920
```

```
H -1.75715 1.72741 1.77779
C -4.15086 0.29596 0.40429
C -2.50600 -1.60414 -0.78567
C -3.87113 -1.84745 -0.66184
C -4.70192 -0.89811 -0.06156
H -1.86205 -2.34413 -1.25594
H -4.28865 -2.77677 -1.03921
H -4.79023 1.05042 0.85783
H -5.76798 -1.08172 0.03287
H 1.48713 2.48756 -0.27921
H 5.66089 0.53920 -1.05821
H 3.44351 -2.55875 0.95879
```

```
                          SCF energy:  -728.537791 hartree
               zero-point correction:  +0.282295 hartree
                 enthalpy correction:  +0.296719 hartree
              free energy correction:  +0.242007 hartree
 quasiharmonic free energy correction:  +0.243369 hartree
```

9.8 Transition State 5h

```
C -2.40557 -0.80447 -0.47019
C -3.69695 -1.40799 -0.50636
C -4.84192 -0.66103 -0.34573
H -5.81253 -1.14372 -0.42310
C -4.76652 0.73074 -0.09868
C -3.52996 1.32303 0.02714
H -3.45317 2.38590 0.24746
C -2.32748 0.57368 -0.08528
C -1.08841 1.26825 0.10820
N 0.03640 0.75489 0.58333
N -1.27623 -1.46296 -0.84089
H -1.46078 -2.45520 -0.99113
C 0.14802 -0.54425 1.11360
C 1.26231 1.58895 0.53841
C 1.53088 -0.90578 1.62649
H -0.39905 -1.26390 0.00831
H -0.67136 -0.74628 1.81031
C 2.42836 0.76861 0.05656
H 1.44635 1.94419 1.56037
H 1.08144 2.44648 -0.10962
C 2.58161 -0.50087 0.62784
H 1.57197 -1.98180 1.81682
H 1.74563 -0.40538 2.58587
C 3.65315 -1.30298 0.23709
C 3.33628 1.23402 -0.89260
C 4.41475 0.43144 -1.26961
C 4.57155 -0.83491 -0.70524
H 3.20164 2.21799 -1.33509
H 5.12564 0.79137 -2.00742
H 3.76955 -2.29377 0.66950
H 5.40646 -1.46242 -1.00366
H -1.06359 2.33816 -0.07953
```

```
H -5.67265 1.31801 0.00816
H -3.75719 -2.47185 -0.72424
```

```
                            SCF energy:   -728.527389 hartree
                 zero-point correction:   +0.282154 hartree
                   enthalpy correction:   +0.296538 hartree
                free energy correction:   +0.241874 hartree
  quasiharmonic free energy correction:   +0.243260 hartree
```

9.9 Transition State 5i

```
C 0.73205 0.87659 0.38828
C 2.13495 1.06592 0.21150
Br 2.83507 2.82000 0.35048
C 3.01289 0.03102 0.00166
H 4.07885 0.21575 -0.07287
C 2.50213 -1.27658 -0.09832
Br 3.71787 -2.70595 -0.36094
C 1.15636 -1.52107 -0.02543
H 0.76665 -2.52922 -0.13035
C 0.24115 -0.45383 0.16483
C -1.14507 -0.79671 0.20947
N -2.16463 -0.01690 -0.16458
N -0.12716 1.84074 0.78939
C -1.97701 1.17248 -0.88482
C -4.27883 0.85537 -1.80562
C -3.49874 -0.42689 0.19800
H 0.30528 2.76253 0.81742
C -4.55858 -0.06184 -0.64509
C -5.83875 -0.51092 -0.32121
C -3.71647 -1.16732 1.35971
C -5.00216 -1.61259 1.65766
C -6.06298 -1.29361 0.81125
H -2.89570 -1.37503 2.03875
H -5.17300 -2.19103 2.56008
H -6.66942 -0.23166 -0.96418
H -7.06810 -1.63083 1.04564
C -3.23481 1.87452 -1.34157
H -5.20715 1.33742 -2.12628
H -3.88456 0.28615 -2.65793
H -3.66917 2.48179 -0.53681
H -2.96380 2.55734 -2.15075
H -1.21847 1.02418 -1.65757
H -1.09847 1.82214 0.07438
H -1.41036 -1.81547 0.47094
```

```
                            SCF energy:   -5870.943383 hartree
                 zero-point correction:   +0.263133 hartree
                   enthalpy correction:   +0.280199 hartree
                free energy correction:   +0.217450 hartree
  quasiharmonic free energy correction:   +0.219715 hartree
```

10 Cartesian Coordinates and Energies of Transition States TS-6

10.1 Transition State 6a

```
C 0.07759 0.79427 -0.10641
C -1.25595 1.16971 -0.32486
Br -1.64496 2.96929 -0.76565
C -2.31695 0.27781 -0.21811
H -3.33478 0.61328 -0.38454
C -2.03960 -1.04034 0.10861
Br -3.46658 -2.27660 0.26230
C -0.73077 -1.46707 0.30323
H -0.52064 -2.50662 0.53654
C 0.33200 -0.57083 0.19556
C 1.72904 -1.03338 0.44310
N 2.54816 -1.07844 -0.74916
H 1.75234 -2.03242 0.88568
N 1.13082 1.68092 -0.22766
H 1.93076 1.48184 0.38068
H 0.87702 2.66098 -0.21822
C 3.94574 -1.56239 -0.61137
C 2.32176 -0.59978 -1.92179
C 3.50938 -0.69548 -2.81892
H 1.35924 -0.17000 -2.17628
H 2.41059 -0.18558 1.23713
C 4.41688 -1.68193 -2.06102
H 3.95843 0.30202 -2.91117
H 3.23102 -1.02570 -3.82211
H 3.94003 -2.50065 -0.05413
H 4.49184 -0.80717 -0.03769
H 5.47662 -1.44877 -2.16524
H 4.24423 -2.69766 -2.42508
H 1.10407 0.77111 2.70224
C 2.55073 0.39990 4.24861
C 2.14507 1.06894 2.93986
O 3.00337 0.73561 1.87865
H 2.12241 2.16214 3.08410
H 1.86993 0.67215 5.06370
H 3.56573 0.69881 4.53362
H 2.53595 -0.69048 4.13776
```

```
                          SCF energy:   -5834.261287 hartree
                zero-point correction:   +0.291699 hartree
                  enthalpy correction:   +0.311455 hartree
               free energy correction:   +0.241644 hartree
  quasiharmonic free energy correction:   +0.245541 hartree
```

10.2 Transition State 6b

```
C 1.27486 -0.73165 0.80547
C 2.41220 -1.48917 1.12570
H 2.74652 -1.51819 2.16029
C 3.11800 -2.17325 0.14035
H 4.00146 -2.74362 0.41349
C 2.69897 -2.11684 -1.19007
H 3.24744 -2.64214 -1.96594
C 1.55619 -1.38484 -1.50890
H 1.21260 -1.34338 -2.54037
C 0.82042 -0.69431 -0.53691
C -0.36603 0.12587 -0.91740
N -1.62528 -0.37842 -0.42169
H -0.46578 0.23350 -2.00094
N 0.55938 -0.07329 1.80719
H 0.15102 0.81481 1.50817
H 1.08130 0.03522 2.66978
C -2.85611 0.38511 -0.74702
C -1.85603 -1.31126 0.43531
C -3.29207 -1.37854 0.83588
H -1.05324 -1.93604 0.80946
H -0.28191 1.35787 -0.35248
C -3.97623 -0.53011 -0.25182
H -3.39808 -0.93905 1.83639
H -3.65077 -2.40873 0.88846
H -2.87149 0.58895 -1.81904
H -2.79931 1.33333 -0.20311
H -4.82885 0.03576 0.12421
H -4.31595 -1.17589 -1.06553
H 1.61878 2.27465 -0.80217
C 1.31795 4.31909 -0.20373
C 1.19524 2.82372 0.06142
O -0.13558 2.43382 0.27915
H 1.83184 2.56369 0.92816
H 2.36349 4.60881 -0.36030
H 0.92683 4.89047 0.64532
H 0.74596 4.59865 -1.09533
```

```
                            SCF energy:   -691.844827 hartree
                 zero-point correction:   +0.310745 hartree
                   enthalpy correction:   +0.327859 hartree
                free energy correction:   +0.266061 hartree
  quasiharmonic free energy correction:   +0.268741 hartree
```

10.3 Transition State 6c

```
C -0.11975 0.74585 -0.24099
C -1.44289 0.98838 -0.63800
C -2.47867 0.09207 -0.40193
C -2.18391 -1.09804 0.24502
C -0.88216 -1.39840 0.62737
H -0.65841 -2.34262 1.11440
```

```
C 0.15743 -0.49746 0.39179
C 1.53163 -0.80389 0.87727
N 2.52189 -1.06737 -0.16181
N 0.91071 1.63264 -0.50249
H 0.61840 2.57310 -0.73915
H 1.64640 1.63696 0.20909
C 3.83080 -1.50613 0.38853
C 2.34401 -0.89005 -1.42468
C 3.39913 -1.05701 -2.46469
C 4.98090 -1.22192 -0.55986
H 3.73337 -2.57762 0.59335
H 3.95286 -0.98461 1.33913
H -3.48941 0.32765 -0.71573
Br -1.85619 2.61107 -1.52164
Br -3.57550 -2.33778 0.58755
H 5.88097 -1.69018 -0.15239
H 5.15884 -0.14046 -0.60417
H 3.63235 -0.04792 -2.83425
H 2.94515 -1.58709 -3.30831
H 2.03271 0.28444 1.54012
H 1.53794 -1.67289 1.54116
H 1.35017 -0.59163 -1.74339
C 4.65367 -1.75446 -1.95031
H 5.48260 -1.58656 -2.64224
H 4.48059 -2.83567 -1.89673
O 2.40566 1.35634 2.04619
C 1.32496 1.79152 2.83278
C 1.79060 2.50768 4.09304
H 0.69270 0.93120 3.12493
H 0.66731 2.47232 2.25934
H 2.40520 1.84135 4.70830
H 0.93792 2.84357 4.69406
H 2.39338 3.38511 3.83403
```

```
                          SCF energy:   -5873.560923 hartree
                zero-point correction:   +0.321310 hartree
                  enthalpy correction:   +0.342051 hartree
               free energy correction:   +0.270002 hartree
  quasiharmonic free energy correction:   +0.274408 hartree
```

10.4 Transition State 6d

```
C -0.11394 0.75200 -0.22874
C -1.43804 1.00587 -0.61844
C -2.47829 0.11629 -0.37954
C -2.19091 -1.07830 0.26338
C -0.89006 -1.38911 0.63903
H -0.66992 -2.33555 1.12336
C 0.15385 -0.49482 0.39913
C 1.53071 -0.81875 0.86819
N 2.49229 -1.10515 -0.18751
N 0.92228 1.62998 -0.49306
H 0.63733 2.57015 -0.73924
```

```
H 1.66141 1.63245 0.21656
C 3.80196 -1.58280 0.31401
C 2.31960 -0.90995 -1.44591
C 3.39004 -1.12879 -2.46435
C 4.89202 -1.27769 -0.68941
H 3.70818 -2.65797 0.49047
H 3.98983 -1.07695 1.26280
H -3.48874 0.35997 -0.68824
Br -1.84385 2.63455 -1.49358
Br -3.59013 -2.30865 0.60589
O 4.52297 -1.79740 -1.96019
H 5.81994 -1.76769 -0.39242
H 5.06220 -0.19462 -0.76099
H 3.66159 -0.14554 -2.88165
H 2.97625 -1.73281 -3.27690
H 2.06360 0.24860 1.50177
H 1.53843 -1.68313 1.53766
H 1.35168 -0.56196 -1.79208
O 2.47445 1.33387 1.99422
C 1.43164 1.77649 2.82558
C 1.95317 2.46924 4.07723
H 0.79565 0.92298 3.13090
H 0.76404 2.47481 2.28554
H 2.57711 1.78538 4.66308
H 1.12754 2.81203 4.71136
H 2.56138 3.33973 3.80773
```

```
                            SCF energy:   -5909.443866 hartree
                 zero-point correction:   +0.297654 hartree
                   enthalpy correction:   +0.318077 hartree
                free energy correction:   +0.246533 hartree
  quasiharmonic free energy correction:   +0.250916 hartree
```

10.5 Transition State 6e

```
C 0.74782 0.47604 0.62224
C 1.90587 -0.04451 1.22021
Br 2.14546 0.15381 3.08706
C 2.90374 -0.68732 0.49789
H 3.78828 -1.06326 0.99976
C 2.74124 -0.82809 -0.87188
Br 4.09020 -1.69216 -1.88209
C 1.59867 -0.35597 -1.50589
H 1.46958 -0.48816 -2.57586
C 0.59732 0.28816 -0.77908
C -0.59210 0.84138 -1.48509
N -1.84885 0.17307 -1.20352
N -0.25585 1.08798 1.34915
H -0.00206 1.37160 2.28756
H -0.75429 1.82922 0.84598
C -3.00258 0.65426 -2.00413
C -2.04127 -0.73561 -0.30333
C -4.24923 0.77431 -1.14658
```

```
C -3.36778 -1.23782 0.01967
C -4.49533 -0.50770 -0.39555
H -5.09915 1.02086 -1.78781
H -4.12445 1.59786 -0.43100
C -5.76185 -0.97273 -0.05552
C -3.50895 -2.41186 0.76954
C -4.78141 -2.87241 1.09246
C -5.90449 -2.15158 0.68041
H -2.62374 -2.95597 1.08815
H -4.89969 -3.78622 1.66589
H -6.63987 -0.41307 -0.36694
H -6.89832 -2.50772 0.93510
H -0.46219 0.84345 -2.57090
H -0.83761 2.08210 -1.07026
O -1.07051 3.21358 -0.51690
C 0.16063 3.88741 -0.48947
C 0.00939 5.36895 -0.80894
H 0.86292 3.43697 -1.21853
H 0.64640 3.78666 0.49985
H -0.41319 5.50478 -1.81052
H 0.97674 5.88312 -0.76949
H -0.66235 5.84678 -0.08724
H -3.14318 -0.06985 -2.81441
H -2.71819 1.61491 -2.43229
H -1.17481 -1.13744 0.21301
```

```
                            SCF energy:   -6025.947670 hartree
                 zero-point correction:   +0.345108 hartree
                   enthalpy correction:   +0.368017 hartree
                free energy correction:   +0.290416 hartree
  quasiharmonic free energy correction:   +0.296318 hartree
```

10.6 Transition State 6f

```
C -1.10160 0.83040 0.29701
C -2.39855 1.17495 -0.11723
Br -2.78199 2.98062 -0.54027
C -3.42745 0.24822 -0.22215
H -4.41794 0.56070 -0.53428
C -3.15615 -1.07672 0.08409
Br -4.53966 -2.36307 -0.05128
C -1.87934 -1.47253 0.46270
H -1.67025 -2.51605 0.67846
C -0.84421 -0.54201 0.56193
C 0.51109 -0.99715 1.00256
N 1.50289 -1.05817 -0.06351
N -0.08219 1.75751 0.39080
H -0.38006 2.72520 0.37713
H 0.58970 1.57047 1.14509
C 1.44563 -0.44757 -1.19466
C 2.69683 -1.88127 0.24914
C 2.58044 -0.48599 -2.16549
H 0.53868 0.09445 -1.43869
```

```
C 3.95851 -1.22553 -0.23889
H 2.53457 -2.84781 -0.24415
H 2.71784 -2.04226 1.32687
C 3.90798 -0.53920 -1.45276
H 2.51286 0.37857 -2.82925
H 2.44975 -1.38026 -2.79546
C 5.05124 0.09326 -1.94018
C 5.14745 -1.28677 0.48730
C 6.29422 -0.66803 -0.00958
C 6.24478 0.02291 -1.22161
H 5.17380 -1.81293 1.43823
H 7.22142 -0.71524 0.55343
H 5.00535 0.64175 -2.87740
H 7.13446 0.51447 -1.60387
H 0.45947 -1.99994 1.43235
H 1.02443 -0.13086 1.90856
O 1.44470 0.80755 2.65176
C 2.84357 0.89835 2.55815
C 3.30244 1.80454 1.41887
H 3.29327 -0.10268 2.42071
H 3.25680 1.28310 3.50452
H 2.91961 1.44474 0.45554
H 4.39711 1.83947 1.35540
H 2.93305 2.82570 1.57084
```

```
                            SCF energy:   -6025.941958 hartree
                 zero-point correction:   +0.344886 hartree
                   enthalpy correction:   +0.367485 hartree
                 free energy correction:   +0.291857 hartree
  quasiharmonic free energy correction:   +0.296458 hartree
```

10.7 Transition State 6g

```
C -1.90248 -1.13015 -0.76607
C -2.64645 -2.25400 -1.16009
C -3.27554 -3.06165 -0.21804
H -3.85430 -3.91902 -0.55023
C -3.17334 -2.76604 1.14282
C -2.41648 -1.66551 1.54017
H -2.31939 -1.43110 2.59801
C -1.76363 -0.84026 0.61498
C -1.01256 0.36480 1.06940
N 0.42525 0.30723 0.89749
N -1.25004 -0.34578 -1.71618
H -1.58654 -0.49041 -2.66154
H -1.20777 0.64914 -1.48251
C 1.17486 1.43620 1.50067
C 1.07340 -0.59536 0.23392
C 2.28899 1.90677 0.58331
C 2.50323 -0.49489 -0.01881
C 3.14575 0.74310 0.15890
H 2.88301 2.66213 1.10385
H 1.85380 2.38222 -0.30605
```

```
C 4.50740 0.84157 -0.11049
C 3.21575 -1.61353 -0.46751
C 4.57913 -1.50458 -0.72324
C 5.22204 -0.27778 -0.54438
H 2.69802 -2.55882 -0.60775
H 5.13911 -2.36981 -1.06359
H 5.01221 1.79535 0.01913
H 6.28563 -0.19077 -0.74608
H -1.19998 0.60234 2.12113
H -1.34679 1.42875 0.32666
O -1.65923 2.35866 -0.48478
C -3.06016 2.33636 -0.56660
C -3.65410 3.73926 -0.58292
H -3.48729 1.78105 0.29167
H -3.39642 1.79860 -1.47327
H -3.37983 4.28151 0.32880
H -4.74790 3.70609 -0.64859
H -3.27570 4.30351 -1.44247
H 1.57094 1.07155 2.45526
H 0.45662 2.23171 1.69637
H 0.52103 -1.45668 -0.12773
H -3.66751 -3.38768 1.88295
H -2.73840 -2.47494 -2.22104
```

```
                          SCF energy:   -883.530872 hartree
                zero-point correction:   +0.364397 hartree
                  enthalpy correction:   +0.384524 hartree
               free energy correction:   +0.315499 hartree
  quasiharmonic free energy correction:   +0.319576 hartree
```

10.8 Transition State 6h

```
C 2.35238 -0.57483 0.88802
C 3.53641 -1.14619 1.38031
C 4.52728 -1.59799 0.51396
H 5.43908 -2.02568 0.92153
C 4.35488 -1.49213 -0.86740
C 3.17070 -0.94708 -1.36075
H 3.01892 -0.87008 -2.43530
C 2.15219 -0.49081 -0.51346
C 0.92816 0.15103 -1.07130
N -0.30163 -0.61059 -0.89851
N 1.35206 -0.15544 1.76459
H 1.67132 -0.04213 2.72017
H 0.83052 0.66386 1.44520
C -0.44885 -1.66686 -0.17835
C -1.48476 -0.01855 -1.56529
C -1.79191 -2.27976 0.04937
H 0.44001 -2.11250 0.25511
C -2.70155 -0.08886 -0.68339
H -1.63556 -0.58621 -2.49191
H -1.23737 1.01118 -1.82353
C -2.86981 -1.22661 0.10761
```

```
H -1.76419 -2.87792 0.96254
H -1.98800 -2.97662 -0.78101
C -3.99240 -1.34171 0.92717
C -3.64865 0.93448 -0.65571
C -4.77821 0.81026 0.15241
C -4.95013 -0.32788 0.94216
H -3.50028 1.82424 -1.26196
H -5.51790 1.60492 0.17369
H -4.11457 -2.22245 1.55237
H -5.82508 -0.42123 1.57858
H 1.02196 0.35562 -2.14171
H 0.64058 1.31002 -0.41164
O 0.40725 2.30617 0.30089
C 1.61959 3.01016 0.37978
C 1.44128 4.49678 0.09708
H 2.34861 2.59722 -0.34487
H 2.08190 2.88995 1.37691
H 1.03833 4.64899 -0.91026
H 2.39585 5.03080 0.17139
H 0.74282 4.94138 0.81459
H 5.12588 -1.83674 -1.54960
H 3.67659 -1.21442 2.45676
```

```
                          SCF energy:   -883.523914 hartree
                zero-point correction:   +0.363820 hartree
                  enthalpy correction:   +0.384085 hartree
               free energy correction:   +0.314386 hartree
  quasiharmonic free energy correction:   +0.319062 hartree
```

10.9 Transition State 6i

```
C -1.01417 0.83631 0.19555
C -2.38458 1.11098 0.08723
Br -2.96748 2.91295 0.08567
C -3.34814 0.11367 -0.00548
H -4.39907 0.37144 -0.07539
C -2.92979 -1.20789 -0.00079
Br -4.21876 -2.58988 -0.12790
C -1.57981 -1.53031 0.07037
H -1.26184 -2.56810 0.05033
C -0.61338 -0.52758 0.16328
C 0.82063 -0.89190 0.33192
N 1.69043 -0.46975 -0.77922
N -0.05864 1.83542 0.25557
C 1.27123 0.19846 -1.80450
C 3.45448 1.30897 -2.06089
C 3.11212 -0.70176 -0.61544
C 4.00739 0.17932 -1.23610
C 5.37432 -0.03352 -1.06339
C 3.56399 -1.78449 0.13628
C 4.93442 -1.98131 0.29038
C 5.84070 -1.10265 -0.30011
H 2.87204 -2.47551 0.60108
```

```
H 5.28797 -2.82377 0.87629
H 6.07451 0.64925 -1.53708
H 6.90848 -1.25377 -0.17428
C 2.20338 0.81978 -2.78398
H 4.20230 1.66289 -2.77345
H 3.19098 2.15010 -1.40562
H 2.46091 0.06322 -3.54009
H 1.68076 1.62943 -3.29681
H 0.92819 -1.96866 0.45972
H 0.19764 0.28954 -1.92906
H 0.76684 1.60780 0.81123
H -0.41245 2.75712 0.48214
H 4.35187 0.61491 1.62442
H 1.31380 -0.19674 1.38178
H 2.83563 -1.06691 2.74256
O 1.72949 0.61022 2.25725
C 4.12296 0.65983 2.69590
C 2.77234 0.01204 2.98072
H 4.93044 0.15690 3.24185
H 4.11033 1.71392 2.99614
H 2.57195 0.07052 4.06431
```

```
                           SCF energy:   -6025.937376 hartree
                zero-point correction:   +0.344845 hartree
                  enthalpy correction:   +0.367522 hartree
               free energy correction:   +0.292354 hartree
 quasiharmonic free energy correction:   +0.296092 hartree
```

11 Cartesian Coordinates and Energies of Transition States TS-7

11.1 Transition State 7a

```
C 0.58012 0.47073 -0.42370
C -0.62158 1.19214 -0.14233
C -1.85889 0.59773 0.02826
C -1.95786 -0.78982 -0.02968
C -0.82659 -1.56375 -0.25771
H -0.89880 -2.64767 -0.29200
C 0.40817 -0.95827 -0.45854
C 1.59237 -1.81263 -0.80217
N 2.80772 -1.47409 -0.04491
N 1.80856 0.98518 -0.59257
C 4.12697 -1.67437 -0.67292
C 2.84203 -0.52229 0.84303
C 4.24507 -0.10956 1.14949
C 5.08483 -1.16408 0.40350
H 4.42635 -0.07387 2.22602
H 4.39328 0.89994 0.75085
H 4.16228 -1.06811 -1.58689
H 4.25671 -2.72653 -0.93359
H 5.35008 -1.97851 1.08268
H 5.99984 -0.75266 -0.02379
H 1.78301 1.99507 -0.45687
H 1.97012 -0.28425 1.43797
H 1.37365 -2.87625 -0.67566
H 1.86891 -1.64771 -1.85237
H -2.73629 1.20803 0.21560
Br -0.52409 3.08507 -0.03131
Br -3.64594 -1.61708 0.22409
```

```
                           SCF energy:   -5679.280166 hartree
                zero-point correction:   +0.214837 hartree
                  enthalpy correction:   +0.228631 hartree
               free energy correction:   +0.173402 hartree
  quasiharmonic free energy correction:   +0.174399 hartree
```

11.2 Transition State 7b

```
C -1.13841 0.73552 -0.47378
C -2.41283 1.33253 -0.22285
H -2.52454 2.39760 -0.41963
C -3.49251 0.59796 0.24090
H -4.44454 1.09978 0.40094
C -3.37359 -0.77347 0.51352
H -4.21890 -1.34617 0.88102
C -2.13522 -1.38037 0.30605
H -2.01206 -2.44156 0.51786
```

```
C -1.03827 -0.66763 -0.17919
C 0.24958 -1.37841 -0.46763
N 1.43669 -0.68815 0.06702
N -0.04340 1.40179 -0.90360
C 2.73455 -0.83661 -0.61648
C 1.37086 0.42431 0.73502
C 2.70361 1.09447 0.81856
C 3.65804 0.03480 0.23539
H 2.93941 1.39216 1.84271
H 2.66343 2.00231 0.20663
H 2.62408 -0.45551 -1.63940
H 3.01276 -1.89168 -0.65408
H 4.09118 -0.56126 1.04284
H 4.46786 0.46954 -0.35127
H -0.27457 2.39321 -0.98893
H 0.49988 0.66688 1.32851
H 0.24222 -2.40741 -0.09666
H 0.42595 -1.41202 -1.55157
```

```
                           SCF energy:   -536.857885 hartree
                zero-point correction:   +0.233427 hartree
                  enthalpy correction:   +0.244573 hartree
               free energy correction:   +0.197706 hartree
  quasiharmonic free energy correction:   +0.197968 hartree
```

11.3 Transition State 7c

```
C -0.44901 0.56713 -0.81220
C 0.62593 1.27484 -0.17923
Br 0.36815 3.11207 0.22773
C 1.84693 0.71029 0.13938
H 2.62511 1.31479 0.59334
C 2.06261 -0.63979 -0.12607
Br 3.73466 -1.42443 0.30735
C 1.04985 -1.40924 -0.68661
H 1.19821 -2.47190 -0.86110
C -0.16713 -0.83179 -1.02319
C -1.27958 -1.69901 -1.53876
N -2.42899 -1.53958 -0.62022
N -1.62719 1.07600 -1.18829
C -2.24201 -2.03668 0.75747
C -3.30561 -0.63206 -0.92624
C -3.51188 -1.88571 1.57788
H -1.42348 -1.47078 1.21533
H -1.92891 -3.08125 0.67288
H -4.27672 -2.58342 1.21552
H -3.28280 -2.15130 2.61337
H -1.62272 -1.39903 -2.53356
H -0.98770 -2.75154 -1.55786
C -4.35420 -0.15153 0.01358
H -4.50696 0.91417 -0.17874
H -5.28431 -0.65534 -0.28804
H -3.38667 -0.37158 -1.97364
```

```
H -1.69288 2.05185 -0.90359
C -4.02252 -0.45126 1.47108
H -4.90818 -0.29903 2.09292
H -3.24715 0.24084 1.82225
```

```
                           SCF energy:   -5718.586289 hartree
                zero-point correction:   +0.244294 hartree
                  enthalpy correction:   +0.259030 hartree
                free energy correction:   +0.201639 hartree
  quasiharmonic free energy correction:   +0.203169 hartree
```

11.4 Transition State 7d

```
C 0.43270 0.62319 0.81072
C -0.66608 1.28784 0.17029
Br -0.47104 3.12830 -0.25400
C -1.86496 0.67732 -0.14494
H -2.66270 1.24931 -0.60730
C -2.03462 -0.67762 0.13392
Br -3.67483 -1.52590 -0.29868
C -0.99994 -1.40480 0.70881
H -1.11323 -2.46913 0.89860
C 0.19481 -0.78012 1.04268
C 1.33350 -1.59668 1.57721
N 2.45902 -1.44840 0.62634
N 1.59572 1.17069 1.17695
C 2.28245 -1.99896 -0.72823
C 3.33893 -0.53135 0.86249
C 3.58027 -1.86283 -1.49679
H 1.48094 -1.45039 -1.23159
H 1.98939 -3.04728 -0.62439
H 4.36311 -2.50310 -1.06766
H 3.42721 -2.13332 -2.54192
H 1.69288 -1.24209 2.54792
H 1.07398 -2.65530 1.64550
C 4.34208 -0.11194 -0.15846
H 4.43277 0.97648 -0.13691
H 5.31205 -0.54024 0.14430
H 3.47197 -0.19565 1.88260
H 1.62654 2.14655 0.88632
O 3.99908 -0.50256 -1.46757
```

```
                           SCF energy:   -5754.468305 hartree
                zero-point correction:   +0.220598 hartree
                  enthalpy correction:   +0.235071 hartree
                free energy correction:   +0.177989 hartree
  quasiharmonic free energy correction:   +0.179682 hartree
```

11.5 Transition State 7e

```
C -0.35828 0.55738 0.95949
C -1.30786 1.29842 0.18157
```

```
Br -0.89861 3.10192 -0.24374
C -2.51069 0.78466 -0.26289
H -3.19616 1.40896 -0.82705
C -2.83047 -0.54281 0.01909
Br -4.48365 -1.25139 -0.58193
C -1.93825 -1.34280 0.72151
H -2.16628 -2.38889 0.91057
C -0.73904 -0.81442 1.18319
C 0.26853 -1.71104 1.83951
N 1.49031 -1.67357 1.00618
N 0.79615 1.01210 1.45647
H 0.96562 1.96473 1.13704
C 1.37157 -2.13035 -0.39136
C 2.39945 -0.78839 1.31175
C 2.74971 -2.42326 -0.96043
H 0.87428 -1.34417 -0.97317
H 0.73826 -3.01981 -0.39217
C 3.47106 -0.44865 0.38370
H 2.45326 -0.45433 2.33886
C 3.65992 -1.23969 -0.76172
H 2.65809 -2.66591 -2.02211
H 3.18004 -3.29879 -0.45669
C 4.70662 -0.92585 -1.62725
C 4.32338 0.62544 0.66817
C 5.35708 0.93275 -0.20805
C 5.54477 0.15565 -1.35533
H 4.15807 1.21619 1.56561
H 6.01564 1.77042 -0.00208
H 4.86616 -1.53026 -2.51627
H 6.35295 0.39312 -2.04093
H -0.08766 -2.74189 1.89394
H 0.55654 -1.36996 2.83841
```

```
                          SCF energy:   -5870.971488 hartree
                zero-point correction:   +0.268264 hartree
                  enthalpy correction:   +0.285138 hartree
               free energy correction:   +0.222685 hartree
  quasiharmonic free energy correction:   +0.225291 hartree
```

11.6 Transition State 7f

```
C -0.71349 1.00477 0.89509
C -1.78743 1.22123 -0.02937
Br -1.99023 2.95699 -0.77158
C -2.69720 0.24910 -0.39943
H -3.50372 0.48936 -1.08447
C -2.56388 -1.03985 0.11385
Br -3.80830 -2.38007 -0.38742
C -1.51476 -1.34426 0.97183
H -1.38345 -2.35731 1.34354
C -0.61706 -0.35680 1.35763
C 0.57616 -0.71767 2.19125
N 1.77298 -0.36960 1.39188
```

```
N 0.16799 1.91362 1.32590
H 0.02166 2.80046 0.84615
C 2.27908 0.81708 1.54350
C 1.97560 -1.10518 0.13171
C 3.25346 1.36159 0.54849
H 2.14177 1.30200 2.49965
C 3.40098 -0.96720 -0.32887
H 1.28814 -0.69882 -0.62230
H 1.70837 -2.14897 0.31034
C 4.03700 0.25945 -0.12341
H 3.90880 2.08470 1.03778
H 2.66941 1.91268 -0.20202
C 5.35459 0.43604 -0.54667
C 4.07772 -2.01262 -0.95698
C 5.38972 -1.82910 -1.39178
C 6.02807 -0.60515 -1.18475
H 3.57776 -2.96656 -1.10423
H 5.91580 -2.64246 -1.88236
H 5.85157 1.38792 -0.37735
H 7.05281 -0.46313 -1.51494
H 0.60276 -1.78555 2.41790
H 0.63850 -0.14320 3.12010
```

```
                           SCF energy:   -5870.964786 hartree
                 zero-point correction:   +0.267527 hartree
                   enthalpy correction:   +0.284567 hartree
                 free energy correction:   +0.221395 hartree
  quasiharmonic free energy correction:   +0.224392 hartree
```

11.7 Transition State 7g

```
C 1.97338 -1.09880 0.21497
C 2.76650 -1.65612 -0.84178
C 3.83818 -0.97661 -1.39308
H 4.42068 -1.45429 -2.17833
C 4.18108 0.31730 -0.96306
C 3.39869 0.90751 0.02792
H 3.61649 1.92340 0.35630
C 2.33233 0.23292 0.62425
C 1.43271 0.93634 1.59373
N 0.08433 0.98696 0.97962
N 0.94177 -1.72594 0.81266
H 0.77905 -2.61852 0.34339
C -0.05316 1.71286 -0.29661
C -0.74964 0.02567 1.26029
C -1.51358 2.04578 -0.55304
H 0.34430 1.07987 -1.09936
H 0.55839 2.61463 -0.22802
C -1.96684 -0.17766 0.48370
H -0.60609 -0.51218 2.18743
C -2.36284 0.80725 -0.43677
H -1.61372 2.49115 -1.54601
H -1.85726 2.78906 0.17834
```

```
C -3.54252 0.61902 -1.15500
C -2.74601 -1.32227 0.69378
C -3.91520 -1.50164 -0.03564
C -4.30962 -0.52985 -0.96047
H -2.41970 -2.06618 1.41608
H -4.51881 -2.39130 0.11269
H -3.86098 1.37458 -1.86831
H -5.22329 -0.66793 -1.53124
H 1.76319 1.96019 1.78481
H 1.31937 0.40665 2.54475
H 5.02304 0.84571 -1.39787
H 2.51183 -2.65209 -1.19963
```

```
                            SCF energy:   -728.547932 hartree
                 zero-point correction:   +0.286831 hartree
                   enthalpy correction:   +0.301029 hartree
                 free energy correction:   +0.246777 hartree
  quasiharmonic free energy correction:   +0.248216 hartree
```

11.8 Transition State 7h

```
C -2.50638 0.87864 -0.20822
C -3.40315 0.59044 -1.28886
C -4.07427 -0.61595 -1.38617
H -4.75931 -0.77490 -2.21653
C -3.88178 -1.63658 -0.43925
C -2.98057 -1.40561 0.59897
H -2.78309 -2.18974 1.32926
C -2.31552 -0.18698 0.73961
C -1.26200 -0.00996 1.78948
N 0.01754 0.23116 1.07627
N -1.84828 2.04319 -0.04574
H -2.04294 2.64911 -0.84462
C 0.36087 1.45703 0.83030
C 0.54641 -0.86834 0.25141
C 1.44503 1.76516 -0.15206
H -0.02826 2.22531 1.48261
C 2.01080 -0.65931 -0.02409
H -0.02031 -0.89977 -0.68844
H 0.36708 -1.80225 0.78855
C 2.45770 0.64803 -0.23139
H 1.91233 2.71734 0.10661
H 0.96149 1.89984 -1.13016
C 3.80553 0.88462 -0.50367
C 2.90671 -1.72630 -0.09409
C 4.25024 -1.48859 -0.38124
C 4.69929 -0.18271 -0.58517
H 2.55222 -2.73956 0.07723
H 4.94728 -2.31940 -0.43594
H 4.15306 1.90376 -0.65267
H 5.74691 0.00550 -0.80042
H -1.14884 -0.90168 2.41051
H -1.42626 0.86361 2.42798
```

```
H -4.41036 -2.58094 -0.51980
H -3.55920 1.36180 -2.04145
```

```
                            SCF energy:   -728.541429 hartree
                 zero-point correction:   +0.286250 hartree
                   enthalpy correction:   +0.300565 hartree
                free energy correction:   +0.245859 hartree
  quasiharmonic free energy correction:   +0.247544 hartree
```

11.9 Transition State 7i

```
C 0.51782 0.72972 -0.37517
C 1.88681 1.13440 -0.26455
Br 2.28030 2.98686 -0.39714
C 2.94363 0.25933 -0.09521
H 3.96037 0.63475 -0.04081
C 2.68348 -1.10452 0.01574
Br 4.12272 -2.31519 0.26395
C 1.37746 -1.57428 -0.04437
H 1.17113 -2.63700 0.05049
C 0.32193 -0.69209 -0.24216
C -1.05821 -1.25236 -0.41698
N -2.10447 -0.57724 0.40199
N -0.54865 1.52473 -0.52179
C -1.75932 0.34257 1.25389
C -3.89864 1.54815 0.94194
C -3.47413 -0.73758 0.00135
C -4.38688 0.29214 0.26841
C -5.71461 0.11467 -0.11757
C -3.87517 -1.91444 -0.63076
C -5.20680 -2.06763 -1.01059
C -6.12822 -1.05348 -0.75656
H -3.16604 -2.71130 -0.82498
H -5.51901 -2.98364 -1.50195
H -6.42826 0.90881 0.08571
H -7.16642 -1.17165 -1.05116
C -2.77250 1.20638 1.91186
H -4.72015 2.03865 1.46871
H -3.52569 2.24797 0.18419
H -3.15752 0.64475 2.77698
H -2.27465 2.09715 2.29865
H -0.24959 2.49894 -0.54079
H -1.39018 -1.10375 -1.45134
H -1.07219 -2.32161 -0.19532
H -0.73576 0.33104 1.60608
```

```
                            SCF energy:   -5870.961087 hartree
                 zero-point correction:   +0.267717 hartree
                   enthalpy correction:   +0.284702 hartree
                free energy correction:   +0.222192 hartree
  quasiharmonic free energy correction:   +0.224309 hartree
```

12 Cartesian Coordinates and Energies of the 1,3-dipolar Cycloaddition

12.1 Transition State TS-8

C 2.52329 1.19552 0.26174
C 3.88578 1.28739 −0.01850
C 4.71946 0.17586 −0.14209
H 5.77158 0.29595 −0.37104
C 4.14978 −1.07010 0.03068
C 2.79632 −1.22374 0.31091
H 2.41976 −2.22189 0.48094
C 1.95769 −0.10863 0.44381
C 0.54230 −0.16729 0.74755
N −0.12456 −1.33485 1.10552
N 1.73599 2.32486 0.44577
C −0.00992 −2.55437 0.66276
C −1.24514 −1.21548 2.08571
C −2.00787 −2.53443 1.94785
H −1.83273 −0.32926 1.83253
H −0.79292 −1.07322 3.07124
C −1.00983 −3.48470 1.26030
H −2.88442 −2.39775 1.31087
H −2.34205 −2.90513 2.91754
H −1.47424 −4.10482 0.48774
H −0.51115 −4.15849 1.96832
Br 4.67640 2.99777 −0.23201
Br 5.24235 −2.61278 −0.12125
C −0.32920 −0.10432 −1.35720
H 0.12992 0.68207 1.28067
O 0.03811 −1.19383 −1.85114
H 0.72974 −2.82555 −0.07455
C −1.74274 0.15441 −0.95672
H 0.26484 0.80670 −1.53357
C −2.73478 −0.86012 −0.96527
C −2.06019 1.45189 −0.55217
C −3.33073 1.76721 −0.10629
C −4.00594 −0.49470 −0.47006
C −4.31813 0.78796 −0.05171
H −1.28734 2.21493 −0.59379
H −5.31637 1.01906 0.30386
N −2.47409 −2.13906 −1.37653
H −3.25088 −2.70967 −1.67896
H −1.58668 −2.27811 −1.84671
Br −5.37481 −1.80392 −0.43911
Br −3.74034 3.53780 0.42059
H 2.12510 3.18269 0.07383
H 0.76449 2.22183 0.18119

```
                          SCF energy:   -11222.509770 hartree
               zero-point correction:   +0.324507 hartree
                 enthalpy correction:   +0.350234 hartree
              free energy correction:   +0.266874 hartree
quasiharmonic free energy correction:   +0.272462 hartree
```

12.2 Transition State TS-9

```
C 2.46817 1.15836 -0.18525
C 3.85806 1.32953 -0.29139
C 4.76159 0.28940 -0.12424
H 5.82712 0.46603 -0.21990
C 4.26359 -0.96643 0.17417
C 2.89647 -1.18206 0.29445
H 2.55257 -2.16615 0.58268
C 1.98772 -0.14470 0.10471
C 0.49636 -0.32992 0.31774
N 0.10600 -1.61022 0.86442
N 1.60702 2.24413 -0.24942
C 0.18960 -2.69004 0.12379
C -0.92098 -1.72012 1.92855
C -1.66424 -3.02168 1.59001
H -1.56145 -0.83590 1.91294
H -0.40217 -1.76226 2.89038
C -0.73879 -3.75462 0.60039
H -2.61414 -2.79194 1.10297
H -1.86319 -3.61307 2.48438
H -1.26847 -4.20115 -0.24602
H -0.14388 -4.54809 1.06930
Br 4.56210 3.04790 -0.66625
Br 5.46115 -2.40879 0.42845
C -0.38238 -0.30038 -1.05066
H 0.16006 0.44782 1.01074
O -0.22931 -1.48118 -1.69098
H 1.01675 -2.87601 -0.54250
C -1.83614 0.06586 -0.67314
H 0.02598 0.53791 -1.64173
C -2.93390 -0.81142 -0.87531
C -2.06125 1.32135 -0.10947
C -3.32844 1.73089 0.27820
C -4.19904 -0.36045 -0.44146
C -4.41727 0.88653 0.12247
H -1.22649 2.00093 0.03465
H -5.41348 1.18533 0.42913
N -2.78593 -2.06724 -1.41833
H -3.58697 -2.45536 -1.89704
H -1.86965 -2.20251 -1.84608
Br -5.69627 -1.50355 -0.66214
Br -3.57479 3.45054 1.03223
H 2.02742 3.09994 -0.59106
H 0.72342 2.08309 -0.71299
```

```
                          SCF energy:   -11222.518087 hartree
               zero-point correction:   +0.327102 hartree
                 enthalpy correction:   +0.351786 hartree
              free energy correction:   +0.270662 hartree
quasiharmonic free energy correction:   +0.275919 hartree
```

12.3 Zwitterion 21

```
C 2.55353 1.26623 0.02304
C 3.95381 1.30510 -0.07400
C 4.74097 0.16121 -0.08295
H 5.81976 0.23856 -0.16154
C 4.11336 -1.06843 0.01121
C 2.73000 -1.15729 0.11255
H 2.28177 -2.13783 0.20575
C 1.94403 -0.01119 0.12193
C 0.43680 -0.04688 0.22172
N -0.11320 -1.22917 0.89600
N 1.80599 2.42852 0.10482
C -0.12559 -2.43988 0.45904
C -0.86049 -1.08418 2.17474
C -1.65706 -2.38888 2.25081
H -1.47777 -0.18531 2.11917
H -0.12562 -0.97037 2.97803
C -0.84788 -3.36146 1.37671
H -2.64765 -2.24041 1.81065
H -1.77619 -2.73702 3.27671
H -1.44919 -4.08474 0.82350
H -0.09394 -3.91807 1.95000
Br 4.83250 2.97835 -0.18724
Br 5.15015 -2.65019 0.00457
C -0.28208 0.07080 -1.19368
H 0.12139 0.79417 0.84653
O 0.02770 -0.95275 -2.02369
H 0.36737 -2.70011 -0.47031
C -1.78085 0.24965 -0.86316
H 0.05693 1.05491 -1.57895
C -2.69714 -0.82872 -0.90558
C -2.20589 1.50716 -0.44603
C -3.51811 1.72178 -0.04334
C -4.00737 -0.57083 -0.46362
C -4.43484 0.68088 -0.04180
H -1.49043 2.32730 -0.43591
H -5.46092 0.83500 0.27365
N -2.29026 -2.08825 -1.30016
H -3.01191 -2.69626 -1.66657
H -1.42082 -2.03324 -1.84478
Br -5.26622 -1.98713 -0.48022
Br -4.06532 3.44744 0.51370
H 2.28249 3.27565 -0.17777
H 0.86582 2.39539 -0.26729
```

```
                           SCF energy:   -11222.527464 hartree
                zero-point correction:   +0.326989 hartree
                  enthalpy correction:   +0.352544 hartree
               free energy correction:   +0.269045 hartree
 quasiharmonic free energy correction:   +0.274987 hartree
```

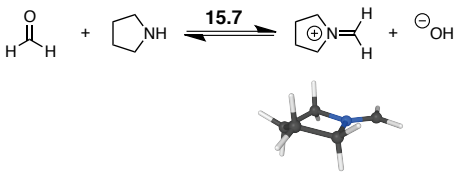
12.4 Cycloadduct

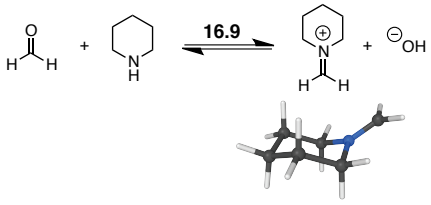
```
C -2.56285 1.01682 0.04207
C -3.31210 -0.16457 0.18467
C -2.81465 -1.31076 0.79253
H -3.42406 -2.20575 0.85445
C -1.53055 -1.27658 1.31425
C -0.77638 -0.11298 1.25085
H 0.23014 -0.09128 1.66116
C -1.26554 1.01950 0.60557
C -0.26098 2.11379 0.32913
N -0.71993 3.50760 0.27640
N -3.02469 2.10081 -0.67231
C -0.02710 4.12471 -0.88550
C -0.36382 4.30088 1.47803
C 0.91248 5.05483 1.10227
H -0.25613 3.63894 2.34148
H -1.17357 5.00691 1.69369
C 0.64628 5.38688 -0.36941
H 1.78472 4.39681 1.19419
H 1.08017 5.93986 1.72039
H 1.53885 5.61866 -0.95558
H -0.05087 6.22730 -0.45229
Br -5.06928 -0.21742 -0.51743
Br -0.81664 -2.80692 2.16985
C 0.36327 1.91146 -1.07434
H 0.55006 2.01893 1.06616
O 0.95379 3.17719 -1.32684
H -0.72931 4.29331 -1.71106
C 1.30006 0.73646 -1.07650
H -0.43873 1.73504 -1.80592
C 2.56509 0.77833 -0.44516
C 0.75784 -0.47414 -1.49874
C 1.42533 -1.66759 -1.26173
C 3.22886 -0.45089 -0.28121
C 2.67713 -1.66624 -0.66589
H -0.22405 -0.47917 -1.96420
H 3.21969 -2.59009 -0.49774
N 3.07507 1.95403 0.05817
H 4.06783 1.98020 0.24902
H 2.70197 2.80524 -0.34612
Br 4.93307 -0.46433 0.54237
Br 0.63845 -3.30311 -1.79707
H -4.02612 2.16592 -0.80035
H -2.56431 2.97719 -0.43393
```

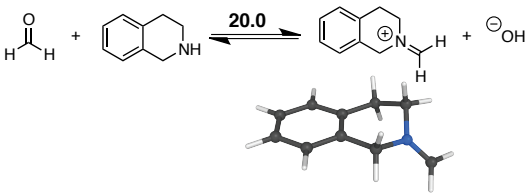
```
                          SCF energy:  -11222.573349 hartree
               zero-point correction:  +0.328735 hartree
                 enthalpy correction:  +0.353529 hartree
              free energy correction:  +0.271108 hartree
quasiharmonic free energy correction:  +0.277736 hartree
```

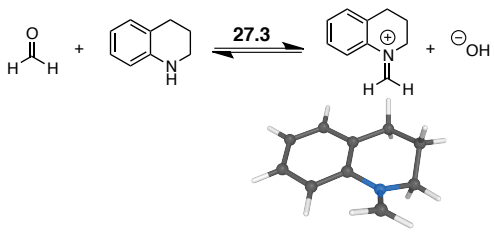
13 Reaction Enthalpies for the Formation of Iminium Ions in Model Systems

Exocyclic Iminium Ions:

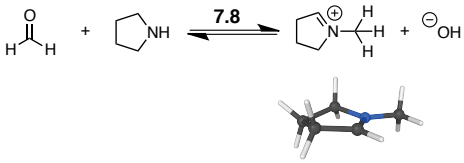


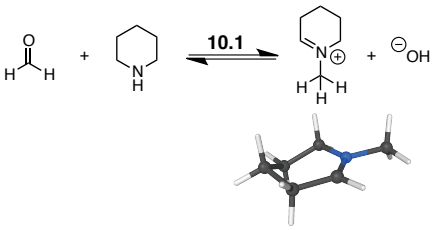


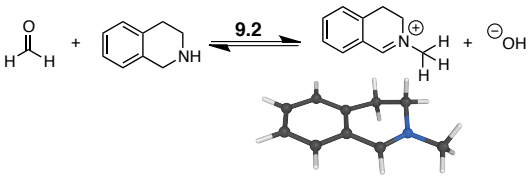


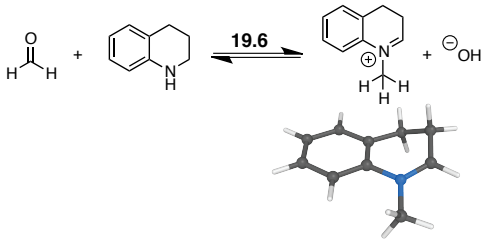


Endocyclic Iminium Ions:









14 Gaussian 09 Reference

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