

Supporting Information for

**Quantum Tunneling in Testosterone 6 $\beta$ -Hydroxylation by  
Cytochrome P450: Reaction Dynamics Calculations  
Employing Multi-Configuration Molecular-Mechanical  
Potential Energy Surfaces**

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**Preparation Date:** Feb. 4, 2009

**Running Head:** Quantum Tunneling in Testosterone 6 $\beta$ -Hydroxylation

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I. Added MM3 parameters in the MM3 parameter file (MM3-1996) in the TINKER format for the MCMM calculation

```

#####
##                               ##
## Atom Type Definitions      ##
##                               ##
#####

# The parameters are from the Charmm27 parameter file
#STARTATM
atom      159    S      "Thiolate Sulfur"          16      32.060      2
atom      160    Fe      "Heme Group Iron"            26      55.847      6
atom      161    O      "Heme CO/O2 Oxygen"          8       15.999      1
# For Hydroxo Compound I.
atom      162    Fe      "Heme Group Iron"            26      55.847      6
atom      163    O      "Heme CO/O2 Oxygen"          8       15.999      2
#ENDATM

#####
##                               ##
## Atomic Partial Charge Parameters ##
##                               ##
#####
# For compound I
charge    159          -1.000
charge    160          +3.000
charge    161          -2.000

#For Hydroxo Compound I.
charge    162          +3.000
charge    163          -2.000

#####
##                               ##
## Bond Stretching Parameters      ##
##                               ##
#####

# For compound I.
# Fe-S k l from QM calculation. S-H k l from MM3.
# O-Fe and Fe-N k l from CHARMM27. O-Fe from the supporting
# information of JACS 2005 127 12900-12908 by Harvey etc.
# k is divided by the factor 71.94
bond      159  160      0.723      2.5816
bond      159   44      3.8700     1.3420
bond      161  160      4.8650     1.6300
bond      160   40      3.753      1.9580

# For Hydroxo Cpd I.
# Kb from QM calculation. b0 from the QM optimization for
# hydroxo compound I.
bond      159  162      1.0336     2.2992
# Kb and b0 (162 40) from Fe-N (160 40) for compound I.
bond      162   40      3.753      1.9580
# Kb(162 163) from Fe-O(161 160) for compound I. b0 from QM calculation
bond      162  163      4.8650     1.8053
# Kb and b0 (163 21) from MM3 O-H(6-21)
bond      163   21      7.6300     0.9470

```

```

# For testosterone radical
# For 2 Beta H abstraction.
# Kb of C-C* (3 29) from MM3 C-C* (1 29). b0 from QM optimization.
bond      3      29      5.2000      1.4289
# For 6 Beta H abstraction.
# C-C* (2 29) from MM3 C-C (2 3).
bond      2      29      8.5000      1.3540
# For 15 Beta H abstraction.
# C-C* (1 29) from MM3 C-C (1 2).
bond5     1      29      6.3000      1.4990

#####
##                               ##
## Angle Bending Parameters     ##
##                               ##
#####

# For Compound I.
# from the supporting information of JACS 2005 127 12900-12908 by Harvey etc.
# k is divided by the factor 71.94.
angle     159    160    40    0.0695    90.000    0.000    0.000
angle     40     160    161   0.6950    90.000    0.000    0.000
#from charmm27.prm. k is divided by the factor 71.94
angle     40     160    40    0.200    90.000    0.000    0.000
angle     160    40     2    1.337   128.0500    0.000    0.000
# k from 1C 15S 44H of MM3 parameters. Theta(0) from QM calculation for the Cpd I
(4A)
angle     160    159    44    0.650    98.417    0.000    0.000
# Kb from 9N 1C 15S of MM3 parameters. Theta0 from QM calculation (angle O-Fe-S)
# for the Cpd I (4A)
angle     159    160    161    0.580    173.500    0.000    0.000

# For Hydroxo Cpd I.
# Kb and A0 from Fe-S-H (160 159 44) for Compound I.
angle     162    159    44    0.650    98.417    0.000    0.000
# Kb and A0 from S-Fe-N (159 160 40) for Compound I.
angle     159    162    40    0.0695    90.000    0.000    0.000
# Kb and A0 from S-Fe-O (159 160 161) for Compound I.
angle     159    162    163    0.580    173.500    0.000    0.000
# Kb and A0 from N-Fe-N(40 160 40) for Compound I.
angle     40     162    40    0.200    90.000    0.000    0.000
# Kb and A0 from N-Fe-O(40 160 161) for Compound I.
angle     40     162    163    0.6950    90.000    0.000    0.000
#Kb and A0 from Fe-N-c(160 40 2) for Compound I.
angle     162    40     2    1.337   128.0500    0.000    0.000
# Kb from MM3 O-O-H (6-6-21). A0 from QM calculation for hydroxox compound I..
angle     162    163    21    0.852   110.5376    0.000    0.000

# For testosterone radical
# For 1 Beta H abstraction.
# C-C-C* (2 1 29) from MM3 C-C-C* (1 1 29).
angle     2      1      29    0.450   110.000    0.000    0.000
# C-C-C* (3 1 29) from MM3 C-C-C* (1 1 29).
angle     3      1      29    0.450   110.000    0.000    0.000
# For 2 Beta H abstraction.
# C-C-C* (2 3 29) from MM3 C-C-C (2 3 2).
angle     2      3      29    0.850   114.700    0.000    0.000
# C*-C-O (29 3 7) from C-C-O (2 3 7).
angle     29     3      7    1.300   122.000   123.500    0.000
# C-C*-C (3 29 1) from MM3 C-C*-C (1 29 1).

```

```

angle      3  29  1  0.500  119.000  0.000  0.000
# C-C*-H (3 29 5) from MM3 C-C*-H (1 29 5).
angle      3  29  5  0.420  118.000  0.000  0.000
# For 6 Beta H abstraction.
# Kb of C-C*-C (1 29 2) from MM3 C-C-C (1 3 2). A0 from QM optimization.
angle      1  29  2  0.500  125.150  0.000  0.000
# C-C*-H (2 29 5) from MM3 C-C-H (2 2 5).
angle      2  29  5  0.490  120.000  120.500  0.000
# C-C-C* (2 2 29) from MM3 C-C-C (2 2 2)
angle      2  2  29  0.760  122.000  121.700  0.000
# C-C-C* (1 2 29) from MM3 C-C-C (1 2 2).
angle      1  2  29  0.470  122.300  0.000  0.000
# For 15 Beta H abstraction.
# C-C-C* (1 1 29) from MM3 C-C-C* (1 1 2).
angle5     1  1  29  0.540  110.200  110.200  110.600
# C-C*-C (1 29 1) from MM3 5-Ring -C-C (1 3 1).
angle5     1  29  1  1.250  112.700  0.000  0.000

#####
##                               ##
##  Torsional Parameters        ##
##                               ##
#####
# For compound I
#N-Fe-N-C parameters from CHARMM27.
#
torsion    40 160  40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    160 40  2  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    44 159 160 40 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    44 159 160 161 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    159 160 40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    161 160 40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3

# For Hydroxo Cpd I
# Set torsion to be 0.
torsion    44 159 162 40 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    44 159 162 163 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    159 162 40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    40 162 40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    163 162 40  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    159 162 163 21 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    40 162 163 21 0.000 0.0 1  0.000 180.0 2  0.000 0.0 3
torsion    162 40  2  2  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3

# For testosterone radical
# For 1 Beta H abstraction.
# C-C-C-C* (2 3 1 29) from MM3 C-C-C-C*(1 1 1 29).
torsion    2  3  1  29  0.500 0.0 1  -0.200 180.0 2  0.100 0.0 3
# C-C-C-C* (2 2 1 29) from MM3 C-C-C-C*(1 1 1 29).
torsion    2  2  1  29  0.500 0.0 1  -0.200 180.0 2  0.100 0.0 3
# C-C-C-C* (1 2 1 29) from MM3 C-C-C-C*(1 1 1 29).
torsion    1  2  1  29  0.500 0.0 1  -0.200 180.0 2  0.100 0.0 3
# C-C-C*-C (3 1 29 1) from MM3 C-C-C*-C (1 1 29 1).
torsion    3  1  29  1  0.400 0.0 1  0.150 180.0 2  0.500 0.0 3
# C-C-C*-C (2 1 29 1) from MM3 C-C-C*-C (1 1 29 1).
torsion    2  1  29  1  0.400 0.0 1  0.150 180.0 2  0.500 0.0 3
# C-C-C*-H (3 1 29 5) from MM3 C-C-C*-H (1 1 29 5).
torsion    3  1  29  5  0.000 0.0 1  0.200 180.0 2  0.300 0.0 3
# C-C-C*-H (2 1 29 5) from MM3 C-C-C*-H (1 1 29 5).
torsion    2  1  29  5  0.000 0.0 1  0.200 180.0 2  0.300 0.0 3
# Set O-C-C-C* (7 3 1 29) to be 0.
torsion    7  3  1  29  0.000 0.0 1  0.000 180.0 2  0.000 0.0 3

```

```

# For 2 Beta H abstraction.
# C-C-C-C* (2 2 3 29) from MM3 C-C-C-C(2 2 3 2).
torsion      2  2  3  29      0.000 0.0 1      9.820 180.0 2      0.000 0.0 3
# C-C-C*-C (2 3 29 1) from MM3 C-C-C-C (2 3 2 1).
torsion      2  3  29  1      0.000 0.0 1      9.820 180.0 2      0.000 0.0 3
# C-C-C*-H (2 3 29 5) from MM3 C-C-C-H (2 3 3 5).
torsion      2  3  29  5      0.000 0.0 1      5.000 180.0 2      0.000 0.0 3
# C-C-C*-C (1 1 29 3) from MM3 C-C-C-C (1 1 2 3).
torsion      1  1  29  3      0.000 0.0 1      0.000 180.0 2      0.457 0.0 3
# C-C-C-C* (2 1 1 29) from MM3 C-C-C-C(2 1 1 2).
torsion      2  1  1  29      1.100 0.0 1      0.000 180.0 2      1.500 0.0 3
# H-C-C-C* (5 2 3 29) from MM3 H-C-C-C(5 2 3 2).
torsion      5  2  3  29      0.400 0.0 1      9.820 180.0 2      0.000 0.0 3
# C-C*-C-H (3 29 1 5) from MM3 C-C*-C-H (3 2 1 5).
torsion      5  1  29  3      0.000 0.0 1      0.000 180.0 2      0.274 0.0 3
# O-C-C*-C (7 3 29 1) from MM3 O-C-C-C (7 3 1 1).
torsion      1  29  3  7      -0.457 0.0 1      1.106 180.0 2      -0.160 0.0 3
# O-C-C*-H (7 3 29 5) from MM3 O-C-C-H (7 3 1 5).
torsion      5  29  3  7      -0.154 0.0 1      0.044 180.0 2      -0.086 0.0 3
# For 6 Beta H abstraction.
# C-C-C-C* (3 2 2 29) from MM3 C-C-C-C ( 2 2 2 3).
torsion      3  2  2  29      0.000 0.0 1      10.000 180.0 2      0.000 0.0 3
# H-C-C-C* (5 2 2 29) from MM3 H-C-C-C (5 2 2 2).
torsion      5  2  2  29      0.250 0.0 1      9.000 180.0 2      -0.550 0.0 3
# C-C-C-C* (1 1 2 29) from MM3 C-C-C-C (1 1 2 2).
torsion      1  1  2  29      -0.700 0.0 1      -0.200 180.0 2      -0.550 0.0 3
# C-C-C-C* (1 1 29 2) from MM3 C-C-C-C (1 1 2 2).
torsion      1  1  29  2      -0.700 0.0 1      -0.200 180.0 2      -0.550 0.0 3
# H-C-C*-C (5 1 29 2) from MM3 H-C-C-C (5 1 2 2).
torsion      5  1  29  2      0.000 0.0 1      0.000 180.0 2      -0.090 0.0 3
# C-C*-C-C (1 29 2 2) from MM3 C-C-C-C (1 2 2 2).
torsion      1  29  2  2      -0.610 0.0 1      7.000 180.0 2      0.000 0.0 3
# C-C*-C-C (1 29 2 1) from MM3 C-C-C-C (1 2 2 1).
torsion      1  29  2  1      -0.300 0.0 1      9.500 180.0 2      0.000 0.0 3
# H-C*-C-C (5 29 2 2) from MM3 H-C-C-C (5 2 2 2).
torsion      5  29  2  2      0.250 0.0 1      9.000 180.0 2      -0.550 0.0 3
# H-C*-C-C (5 29 2 1) from MM3 H-C-C-C (5 2 2 1).
torsion      5  29  2  1      0.000 0.0 1      10.000 180.0 2      0.000 0.0 3
# For 15 Beta H abstraction.
# O-C-C-C* (6 1 1 29) from MM3 O-C-C-C (6 1 1 2).
torsion      6  1  1  29      0.000 0.0 1      0.000 180.0 2      0.180 0.0 3

#####
##                               ##
## Out-of-Plane Bend Parameters ##
##                               ##
#####

#set Out-of-Plane Bend Parameters zero
opbend      40    160    0.000

# For Hydroxo Cpd I
# Set to be 0.
opbend      40    162    0.000

# For testosterone radical
# For 2 Beta H abstraction.
# C*-C (29 3) from MM3 C*-C (29 1).
opbend      29    3      0.130
#set C-C* (3 29) to be 0.
opbend      3     29     0.000
# For 6 Beta H abstraction.

```



```
# C*-C (29 2) from MM3 C-C (2 2)
opbend      29    2          0.200
# C-C* (2 29) from MM3 C-C (2 2)
opbend      2    29          0.200

#####
##                               ##
##  Van der Waals Parameters    ##
##                               ##
#####
#
# Only O vdw paramters from mm3
#
vdw          161          1.820    0.059
vdw          163          1.820    0.059
```

II. Input geometries (in Å), absolute energy (in a.u.), and frequencies ( $\text{cm}^{-1}$ ) in the MCMM calculations for 6 $\beta$ -H abstraction of testosterone (and 6 $\beta$ -D abstraction of 6 $\beta$ - $d_1$ -testosterone) by Compound I. The QM level of theory was B3LYP/6-31G.

## II.A. QM optimized geometry, energy, and frequencies for testosterone and its isotope

### II.A.1. QM optimized geometry and energy for testosterone

Absolute energy: -891.0915883

C	-1.034755	-2.025362	-0.598636
C	-2.372164	-1.457301	-0.792935
C	-2.601401	-0.069466	-0.224993
C	3.782622	2.405884	0.272807
O	-3.286550	-2.105636	-1.346724
C	-1.321719	0.779822	-0.278639
C	-0.087863	0.111160	0.398769
C	1.217639	0.865538	-0.084105
C	2.542591	0.134128	0.304858
C	2.529968	-1.305837	-0.240593
C	1.298355	-2.084471	0.260494
C	0.000431	-1.363768	-0.027483
C	1.234875	2.366837	0.317253
C	2.494986	3.120298	-0.174698
C	3.730932	0.941753	-0.244585
C	3.959410	2.512440	1.806414
C	-0.247101	0.161885	1.947776
C	5.087372	2.881544	-0.427184
C	6.068994	1.677777	-0.279311
C	5.176111	0.415330	-0.051434
H	-1.074854	0.970986	-1.332628
H	1.179388	0.832563	-1.187388
H	2.624217	0.082841	1.401822
H	2.521482	-1.274995	-1.340351
H	3.443631	-1.835306	0.056669
H	1.394929	-2.221016	1.349856
H	1.269632	-3.089076	-0.176256
H	-0.922012	-3.061914	-0.906339
H	-3.419791	0.404272	-0.776508
H	-2.947829	-0.182734	0.813539
H	1.164733	2.460714	1.407805
H	0.348941	2.866761	-0.090538
H	2.481883	3.171368	-1.273990
H	3.109313	2.095292	2.352457
H	0.625097	-0.252548	2.462963
H	-1.121517	-0.417018	2.263496
H	4.869415	3.065904	-1.484401
H	6.710024	1.583692	-1.161235
H	6.736717	1.851181	0.574967
H	5.313791	0.012433	0.960011
H	5.417771	-0.390688	-0.751427
H	3.570740	1.017861	-1.335661
H	4.044216	3.567741	2.092341
H	4.856597	1.990737	2.159148
H	-0.386027	1.191418	2.292933
O	5.624172	4.150753	0.027281
H	-1.511827	1.754364	0.183638
H	2.478336	4.156004	0.188415
H	5.992026	4.053438	0.928862

### II.A.2. QM frequencies for testosterone

Frequencies:		
35.4143	50.0938	83.1024
124.9656	130.6700	158.2164
178.7427	197.0196	215.3313

216.7845	233.3197	246.1413
266.5749	271.1457	275.8694
299.1299	312.6540	324.0623
333.2638	381.1394	385.4580
399.6776	413.1879	444.0331
468.9830	470.5078	507.0547
518.0235	549.1978	557.7823
572.5397	577.8510	620.6098
646.7890	667.1028	698.2941
729.1597	765.6886	798.7200
822.1680	850.8153	852.6867
857.5016	886.8428	914.6920
927.6507	933.4147	953.4112
964.0680	973.7169	989.9033
991.4248	1002.5077	1028.0530
1036.8373	1047.2269	1052.8542
1057.6735	1062.6750	1075.7007
1087.8284	1100.1720	1125.9045
1131.9583	1143.6515	1166.6766
1168.2133	1177.3015	1185.8038
1206.8568	1227.9194	1237.1034
1243.8857	1250.8842	1266.6742
1280.0779	1286.3195	1296.3423
1304.4876	1320.5962	1325.6594
1331.7867	1345.4954	1352.3212
1357.8357	1362.9921	1378.0557
1379.8889	1388.1426	1392.9992
1396.2463	1400.9340	1408.2449
1412.4523	1419.4415	1423.1051
1437.4822	1454.0890	1455.4244
1511.6850	1526.6313	1532.0274
1535.7969	1537.5078	1539.7374
1542.5310	1547.6526	1549.9593
1552.5926	1562.6042	1565.4820
1672.4980	1695.3883	2963.0664
2974.4031	3007.7063	3016.6190
3021.9580	3029.6579	3030.6537
3038.6517	3045.2137	3050.1107
3053.9847	3058.5506	3059.9625
3077.3169	3080.7524	3082.2330
3089.1213	3094.5722	3098.9083
3103.8794	3111.6784	3115.7538
3121.0480	3129.3333	3135.0143
3140.8618	3190.2810	3631.4187

II.A.3. QM frequencies for  $6\beta$ - $d_1$ -testosterone

Frequencies:

35.3465	50.0219	82.6174
124.7940	130.4152	157.5182
178.3944	195.9322	215.2323
216.5644	232.3883	246.0341
259.1261	271.0201	273.6754
296.9440	311.6589	323.8669
332.9497	378.3429	384.7957
399.4722	403.8954	436.9059
467.8117	468.6947	505.8100
517.1493	531.3929	555.6617
568.6181	572.7206	620.4794
644.7255	664.8670	689.2774
727.2368	759.3240	793.7190
810.9742	847.0021	850.8765
854.0500	874.8850	890.9822
914.5783	933.0810	949.2185
952.8176	965.6956	977.9707
990.8578	992.1504	1001.9500
1022.3535	1036.0357	1048.2476
1051.4368	1057.7149	1062.1740
1080.6466	1086.7298	1099.9884
1124.8098	1136.7051	1142.3018
1167.0684	1171.4658	1183.6909
1201.9285	1210.0322	1228.4136
1238.7940	1250.7099	1264.3705
1276.3207	1281.8507	1291.5175
1299.6354	1307.4266	1321.4489
1325.7271	1331.6201	1346.9852
1354.9781	1358.0022	1363.3333
1369.3331	1380.6254	1387.7833
1394.4328	1400.8234	1403.1039
1407.1114	1412.6661	1418.2274
1422.9675	1437.2444	1454.3311
1455.9964	1511.8054	1532.0100
1535.2774	1537.4839	1539.5650
1542.2974	1546.6251	1549.8773
1552.4734	1562.5964	1565.4792
1672.0284	1695.1827	2210.0509
2963.0672	2974.4004	3016.5100
3021.9418	3029.5292	3030.4678
3038.6486	3045.2043	3050.1056
3053.9586	3058.4904	3059.9592
3077.3156	3080.5398	3081.0750
3084.8986	3094.5231	3098.9086
3103.8793	3111.6803	3115.7514
3121.0473	3129.2854	3134.9009
3140.8602	3190.2797	3631.4138

II.B. Input geometries and frequencies of the MM reactant-complex, MM product-complex, Cpd I, products, and transition structure for the  $6\beta$ -H(D) abstraction by Cpd I of the  $^2A$  state.

II.B.1. Atom types, MM optimized coordinates, and connectivities for the MM reactant-complex in the TINKER xyz file format.

89	reactant complex	at MM optimized geometry									
1	C	-3.795558	3.928697	.980697	2	2	12	56			
2	C	-4.736765	4.618896	.288156	3	1	3	5			
3	C	-5.152545	4.074867	-1.070821	1	2	6	57	58		
4	C	-3.301486	-2.465637	-.456938	1	14	15	16	18		
5	O	-5.138256	5.687583	.689557	7	2					
6	C	-5.116279	2.546521	-1.089042	1	3	7	49	74		
7	C	-3.749271	1.970359	-.640772	1	6	8	12	17		
8	C	-3.965222	.464586	-.266747	1	7	9	13	50		
9	C	-2.728692	-.143625	.446757	1	8	10	15	51		
10	C	-2.414262	.669215	1.712870	1	9	11	52	53		
11	C	-2.127645	2.128819	1.357124	1	10	12	54	55		
12	C	-3.286860	2.750339	.592759	2	1	7	11			
13	C	-4.393740	-.410357	-1.474937	1	8	14	59	60		
14	C	-4.566599	-1.902114	-1.123508	1	4	13	61	75		
15	C	-3.022081	-1.609379	.797174	1	4	9	20	70		
16	C	-2.123032	-2.478641	-1.462973	1	4	62	71	72		
17	C	-2.710397	2.157068	-1.769885	1	7	63	64	73		
18	C	-3.472460	-3.857006	.203144	1	4	19	21	65		
19	C	-2.334078	-3.910370	1.266328	1	18	20	66	67		
20	C	-1.952354	-2.424991	1.545529	1	15	19	68	69		
21	O	-3.393957	-4.928481	-.723288	6	18	76				
22	S	4.789244	-.977830	.263786	159	23	77				
23	Fe	2.183985	-.179016	.082322	160	22	28	33	38	43	48
24	C	1.989870	-2.129440	2.705206	2	29	47	78			
25	C	3.095196	2.282402	2.036476	2	32	34	79			
26	C	3.126671	1.585817	-2.507380	2	37	39	80			
27	C	2.016599	-2.824853	-1.838569	2	42	44	81			
28	N	2.636385	-.000774	2.015334	40	23	29	32			
29	C	2.304790	-.855405	2.912187	2	24	28	30			
30	C	2.292088	-.287169	4.125353	2	29	31	82			
31	C	2.612426	.987849	3.932410	2	30	32	83			
32	C	2.801308	1.121905	2.612912	2	25	28	31			
33	N	3.120194	1.561232	-.178411	40	23	34	37			
34	C	3.226774	2.463411	.726757	2	25	33	35			
35	C	3.463521	3.660854	.174537	2	34	36	84			
36	C	3.472481	3.459738	-1.138936	2	35	37	85			
37	C	3.240913	2.151384	-1.310533	2	26	33	36			
38	N	2.666961	-.588030	-1.808162	40	23	39	42			
39	C	2.839106	.304918	-2.712841	2	26	38	40			
40	C	2.664402	-.217681	-3.933985	2	39	41	86			
41	C	2.342595	-1.492115	-3.740435	2	40	42	87			
42	C	2.340401	-1.671238	-2.412764	2	27	38	41			
43	N	2.187959	-2.150691	.384151	40	23	44	47			
44	C	1.942979	-3.019940	-.526494	2	27	43	45			
45	C	1.560378	-4.182049	.019571	2	44	46	88			
46	C	1.554779	-3.981295	1.333089	2	45	47	89			
47	C	1.932806	-2.708189	1.510645	2	24	43	46			
48	O	.563328	.182954	.026271	161	23					
49	H	-5.919107	2.176291	-.409696	5	6					
50	H	-4.805108	.426245	.470168	5	8					
51	H	-1.850081	-.100283	-.230354	5	9					
52	H	-3.269341	.615789	2.424975	5	10					
53	H	-1.530733	.237582	2.236441	5	10					
54	H	-1.204853	2.195573	.738649	5	11					
55	H	-1.917813	2.701122	2.289103	5	11					
56	H	-3.422858	4.404446	1.903507	5	1					
57	H	-6.181138	4.425454	-1.317993	5	3					
58	H	-4.480638	4.488398	-1.856413	5	3					
59	H	-3.650504	-.316813	-2.295557	5	13					
60	H	-5.357397	-.036382	-1.888713	5	13					
61	H	-5.438543	-2.016294	-.439768	5	14					

62	H	-1.854138	-1.468718	-1.834905	5	16
63	H	-1.736705	1.675067	-1.538631	5	17
64	H	-2.493977	3.232526	-1.953087	5	17
65	H	-4.457733	-3.900779	.723905	5	18
66	H	-2.689719	-4.414543	2.193155	5	19
67	H	-1.445013	-4.470642	.900401	5	19
68	H	-.938333	-2.197780	1.149599	5	20
69	H	-1.950468	-2.202638	2.635828	5	20
70	H	-3.939538	-1.620961	1.436068	5	15
71	H	-2.366031	-3.082392	-2.365010	5	16
72	H	-1.194941	-2.909300	-1.030601	5	16
73	H	-3.059028	1.737106	-2.737806	5	17
74	H	-5.376441	2.184638	-2.109227	5	6
75	H	-4.806256	-2.486729	-2.040651	5	14
76	H	-2.494803	-5.039550	-.997955	21	21
77	H	5.277381	.081829	.927548	44	22
78	H	1.715302	-2.738904	3.583576	5	24
79	H	3.194206	3.167485	2.688535	5	25
80	H	3.234205	2.235336	-3.393319	5	26
81	H	1.750276	-3.669012	-2.498014	5	27
82	H	2.043174	-.757317	5.087181	5	30
83	H	2.676738	1.766610	4.705418	5	31
84	H	3.591784	4.625465	.685609	5	35
85	H	3.609600	4.227485	-1.913464	5	36
86	H	2.737776	.294625	-4.903680	5	40
87	H	2.101467	-2.228073	-4.520427	5	41
88	H	1.276482	-5.109225	-.498028	5	45
89	H	1.263909	-4.710978	2.101968	5	46

II.B.2. Atom types, MM optimized coordinates, and connectivities for the MM product-complex in the TINKER xyz file format.

89 intermediate complex at MM optimized geometry for 6b2a										
1	C	.695913	2.803749	-1.235509	2	2	12	56		
2	C	.488329	3.865358	-.414941	3	1	3	5		
3	C	1.384800	4.028378	.807118	1	2	6	57	58	
4	C	5.793273	-1.138440	.358746	1	14	15	16	18	
5	O	-.347541	4.697446	-.685659	7	2				
6	C	2.698379	3.250064	.667331	1	3	7	49	74	
7	C	2.458671	1.787514	.235320	1	6	8	12	17	
8	C	3.821803	1.095144	-.083159	1	7	9	13	50	
9	C	3.591259	-.323096	-.671644	1	8	10	15	51	
10	C	2.793649	-.224458	-1.985455	1	9	11	52	53	
11	C*	1.763975	.870270	-1.983250	29	10	12	55		
12	C	1.589441	1.823585	-1.024711	2	1	7	11		
13	C	4.784778	1.056114	1.133950	1	8	14	59	60	
14	C	6.089801	.279670	.869494	1	4	13	61	75	
15	C	4.950081	-.994220	-.925135	1	4	9	20	70	
16	C	5.094377	-1.973088	1.459836	1	4	62	71	72	
17	C	1.679446	1.047300	1.350094	1	7	63	64	73	
18	C	7.017960	-1.898807	-.208943	1	4	19	21	65	
19	C	6.390885	-2.958317	-1.165464	1	18	20	66	67	
20	C	4.974211	-2.413070	-1.523004	1	15	19	68	69	
21	O	7.821078	-2.483817	.804397	6	18	76			
22	S	-4.936299	-.544265	.893781	159	23	77			
23	Fe	-2.728031	-.323403	.047092	162	22	28	33	38	43 48
24	C	-2.443865	-3.498898	.696049	2	29	47	78		
25	C	-3.689732	-1.033156	-2.980899	2	32	34	79		
26	C	-3.012879	2.843570	-.604300	2	37	39	80		
27	C	-1.766060	.381430	3.068579	2	42	44	81		
28	N	-3.251020	-1.976386	-.885765	40	23	29	32		
29	C	-2.998362	-3.162079	-.469973	2	24	28	30		
30	C	-3.300444	-4.050643	-1.427405	2	29	31	82		
31	C	-3.661459	-3.336578	-2.492038	2	30	32	83		
32	C	-3.560986	-2.050410	-2.127224	2	25	28	31		
33	N	-3.065266	.726835	-1.582496	40	23	34	37		
34	C	-3.468815	.251502	-2.700125	2	25	33	35		
35	C	-3.707287	1.257402	-3.554012	2	34	36	84		
36	C	-3.510244	2.381333	-2.865221	2	35	37	85		
37	C	-3.164690	2.001764	-1.626983	2	26	33	36		
38	N	-2.706428	1.312754	1.138375	40	23	39	42		
39	C	-2.771366	2.501037	.662472	2	26	38	40		
40	C	-2.466009	3.390593	1.617466	2	39	41	86		
41	C	-2.104150	2.677495	2.681628	2	40	42	87		
42	C	-2.208473	1.391715	2.317181	2	27	38	41		
43	N	-1.994718	-1.370485	1.543146	40	23	44	47		
44	C	-1.698056	-.897290	2.695339	2	27	43	45		
45	C	-1.358107	-1.899675	3.518208	2	44	46	88		
46	C	-1.554846	-3.024175	2.830512	2	45	47	89		
47	C	-2.002495	-2.648313	1.623742	2	24	43	46		
48	O	-.971840	-.271223	-.498763	163	23	54			
49	H	3.342768	3.760879	-.085562	5	6				
50	H	4.328410	1.699787	-.875393	5	8				
51	H	3.010016	-.942443	.045480	5	9				
52	H	3.495051	-.034196	-2.829866	5	10				
53	H	2.304721	-1.202873	-2.196908	5	10				
54	H	-.665120	.624684	-.522282	21	48				
55	H	1.147142	.916380	-2.898841	5	11				
56	H	.068871	2.766967	-2.142614	5	1				
57	H	1.613322	5.108525	.959330	5	3				
58	H	.831970	3.699819	1.715526	5	3				
59	H	4.272951	.610905	2.013492	5	13				
60	H	5.056182	2.094609	1.430246	5	13				
61	H	6.698909	.834484	.119839	5	14				
62	H	4.118537	-1.548893	1.774001	5	16				
63	H	1.492497	-.019779	1.107265	5	17				
64	H	.678970	1.497020	1.524887	5	17				
65	H	7.645117	-1.196282	-.806500	5	18				

66	H	7.017287	-3.077615	-2.078309	5	19
67	H	6.302906	-3.958934	-.685903	5	19
68	H	4.181688	-3.047601	-1.067128	5	20
69	H	4.807859	-2.398604	-2.623247	5	20
70	H	5.516610	-.338021	-1.631533	5	15
71	H	5.716297	-2.031219	2.380326	5	16
72	H	4.893566	-3.018669	1.142731	5	16
73	H	2.207697	1.074070	2.326944	5	17
74	H	3.245418	3.289928	1.635697	5	6
75	H	6.701623	.229917	1.798795	5	14
76	H	7.409734	-3.278953	1.112352	21	21
77	H	-5.596946	-.078943	-.177715	44	22
78	H	-2.329060	-4.576412	.907412	5	24
79	H	-3.989671	-1.276957	-4.014994	5	25
80	H	-3.065311	3.922309	-.832165	5	26
81	H	-1.406027	.627427	4.082840	5	27
82	H	-3.180142	-5.142748	-1.391556	5	30
83	H	-3.891285	-3.735448	-3.490330	5	31
84	H	-4.066118	1.187295	-4.590670	5	35
85	H	-3.675860	3.404816	-3.230370	5	36
86	H	-2.406390	4.483854	1.519806	5	40
87	H	-1.695281	3.079357	3.619563	5	41
88	H	-1.056999	-1.829218	4.573100	5	45
89	H	-1.445456	-4.047597	3.216627	5	46



II.B.3. QM optimized geometry, absolute energy, and frequencies for the Cpd I of the  $^2A$  state.

Absolute energy: -1585.5202197

Geometry:

S	19.968009	8.667022	71.051951
Fe	18.737987	8.629950	68.759641
C	21.557985	9.509913	67.021936
C	19.584188	5.312248	68.453442
C	16.079898	7.754489	70.764146
C	18.012302	11.947356	69.268347
N	20.268503	7.617334	67.925915
C	21.326227	8.155874	67.212837
C	22.157663	7.096941	66.683286
C	21.595048	5.915414	67.074446
C	20.418946	6.244830	67.850016
N	18.023488	6.895925	69.516376
C	18.477326	5.611997	69.228686
C	17.614953	4.633089	69.852651
C	16.630667	5.320771	70.502193
C	16.878828	6.729125	70.284915
N	17.357570	9.643056	69.833177
C	16.308057	9.106267	70.563147
C	15.476403	10.167949	71.089128
C	16.020298	11.347392	70.671566
C	17.189175	11.020359	69.883203
N	19.610761	10.372172	68.256804
C	19.139704	11.644955	68.514463
C	20.007351	12.630066	67.905302
C	21.009869	11.944722	67.280838
C	20.758906	10.536688	67.501497
O	17.797888	8.558714	67.406820
H	20.361599	7.342657	71.103142
H	22.431941	9.788483	66.442493
H	19.821799	4.263721	68.307797
H	15.210441	7.476725	71.350318
H	17.760677	12.995724	69.389015
H	23.049064	7.252756	66.093533
H	21.934391	4.910619	66.869690
H	17.756277	3.563999	69.790462
H	15.806531	4.926302	71.078221
H	14.598135	10.012883	71.698366
H	15.676319	12.351850	70.869953
H	19.858323	13.698336	67.961816
H	21.845902	12.339494	66.722461

Frequencies:

18.1028	42.9826	51.1754
86.7437	97.3790	126.4735
147.6495	148.6505	160.9240
174.9216	182.9342	220.0937
232.3331	272.1937	279.8282
281.3026	287.3450	295.4300
307.7383	310.8543	357.8617
371.8882	372.1697	376.8279
413.5557	415.3143	433.8026
436.9755	439.7370	440.6105
485.9070	488.7532	679.0649
679.3358	686.1495	690.3410
691.9377	725.3942	725.4781
734.5643	741.3097	760.6464
766.8364	767.7564	801.5779
811.4547	811.6799	819.8656
820.4031	835.1436	835.4549
852.3875	869.3386	903.5277
916.7293	916.8126	934.5689
940.3336	951.8644	952.1800
956.3478	1018.8457	1020.2580

1023.0083	1025.6749	1033.6423
1057.9410	1059.1830	1078.7312
1117.8754	1117.9772	1119.9693
1123.5585	1157.2486	1191.0707
1191.6082	1216.6719	1245.7773
1298.6126	1299.5073	1314.5915
1352.2082	1353.5611	1388.4488
1391.0191	1412.3367	1422.3038
1427.7617	1438.7020	1502.9418
1503.4865	1504.6292	1538.5664
1560.3112	1594.6614	1595.0475
1612.2559	1618.9645	1648.2095
1650.3738	1719.2484	2493.9128
3212.6642	3212.7881	3213.6679
3214.1425	3263.9187	3264.0558
3264.4328	3264.5526	3286.9738
3287.1433	3287.5376	3287.7614

II.B.4. QM optimized geometry, absolute energy, and frequencies for the products ( $\text{Fe}^{\text{IV}}$ ) of the  $^2A$  state.

Absolute energy:-2476.6274751

Geometry:

C	.712924	3.417137	-1.225569
C	.700785	4.545582	-.334785
C	1.792045	4.637114	.720915
C	5.377419	-1.189930	.232479
O	-.201633	5.432876	-.413579
C	2.955935	3.655818	.483200
C	2.481558	2.207864	.155538
C	3.712473	1.292313	-.192199
C	3.250929	-.093408	-.748773
C	2.418779	.089221	-2.037036
C	1.518245	1.283659	-2.021627
C	1.555839	2.292688	-1.073587
C	4.728537	1.157363	.977283
C	5.896887	.185761	.685257
C	4.478277	-.977453	-1.015474
C	4.655450	-1.914045	1.394019
C	1.659690	1.645027	1.352227
C	6.448708	-2.137957	-.378112
C	5.631458	-3.126649	-1.266818
C	4.285854	-2.402250	-1.596026
O	7.340290	-2.781994	.568746
S	-4.748409	-.443332	.537104
Fe	-2.427344	-.557062	.156767
C	-2.344163	-3.915806	.868243
C	-2.969539	-1.271820	-3.170504
C	-2.589266	2.816176	-.560210
C	-1.970815	.167724	3.476516
N	-2.683153	-2.241499	-.914497
C	-2.586409	-3.543061	-.444112
C	-2.750165	-4.468969	-1.541568
C	-2.925490	-3.726373	-2.675201
C	-2.871558	-2.335065	-2.288228
N	-2.664433	.546910	-1.530780
C	-2.882483	.064716	-2.813782
C	-3.039784	1.172942	-3.728057
C	-2.937827	2.321610	-2.993166
C	-2.718450	1.932006	-1.618882
N	-2.357449	1.137972	1.240822
C	-2.419287	2.439603	.762106
C	-2.246039	3.368592	1.856331
C	-2.080883	2.625393	2.991907
C	-2.141918	1.233079	2.606438
N	-2.168950	-1.649315	1.819944
C	-1.983713	-1.165263	3.105355
C	-1.825348	-2.273035	4.022960
C	-1.928055	-3.420639	3.290774
C	-2.151340	-3.030447	1.914932
O	-.626050	-.557071	-.107257
H	3.571895	4.016918	-.353064
H	4.243752	1.794830	-1.020662
H	2.612094	-.584511	-.003474
H	3.102587	.188491	-2.900912
H	1.833047	-.819476	-2.238425
H	-.320729	.134787	-.735328
H	.834755	1.397066	-2.863354
H	.004237	3.443199	-2.048028
H	2.152195	5.672766	.743065
H	1.327340	4.460776	1.700827
H	4.207817	.824908	1.882966
H	5.146088	2.143996	1.210912
H	6.531106	.603167	-.111690
H	3.814407	-1.335955	1.784382

H	1.285438	.637135	1.153791
H	.781013	2.266786	1.546674
H	7.128912	-1.544039	-.997672
H	6.191806	-3.400603	-2.166137
H	5.454829	-4.057905	-.712494
H	3.438487	-2.907210	-1.115699
H	4.079044	-2.384853	-2.671076
H	5.102860	-.424680	-1.741899
H	5.357357	-2.071378	2.221928
H	4.259147	-2.890078	1.091222
H	2.261868	1.627566	2.267204
H	3.598961	3.642148	1.369432
H	6.533178	.088252	1.574428
H	6.846386	-3.444957	1.092390
H	-5.115626	-1.560707	-.187978
H	-2.301065	-4.976206	1.090054
H	-3.131579	-1.502438	-4.217594
H	-2.590756	3.877519	-.780109
H	-1.814645	.396489	4.524771
H	-2.722427	-5.544277	-1.442255
H	-3.070270	-4.073171	-3.687979
H	-3.218879	1.069533	-4.788383
H	-3.017106	3.344526	-3.331136
H	-2.234217	4.442336	1.741169
H	-1.923144	2.972262	4.002667
H	-1.664816	-2.167110	5.085908
H	-1.868377	-4.443248	3.633674

## Frequencies:

8.7864	11.0828	16.2061
26.3549	29.2662	35.8123
46.6769	54.4201	56.3430
73.3394	98.4235	99.4669
100.2045	109.0684	119.1290
125.3841	137.6391	145.8989
152.2838	157.1679	171.6926
177.8582	186.4042	206.0827
215.7347	216.9491	223.8354
232.3769	238.7090	249.3525
259.7163	263.7231	269.1316
277.1616	279.3167	285.3772
286.8829	289.6902	290.6879
293.7443	297.6672	299.1877
317.0996	329.2213	338.1288
356.4092	366.7308	368.0759
372.4427	376.3872	377.9477
385.1695	396.9988	411.5888
418.7258	429.1936	438.2936
439.4309	440.8949	441.4806
449.1437	469.7284	482.8175
484.8211	509.7522	518.7986
548.3673	561.2473	575.7211
605.7405	620.1613	620.9297
632.4698	648.1059	662.0285
671.5238	679.0973	680.1301
691.6660	702.4966	711.8568
718.9633	722.9920	727.6816
731.5497	743.8599	758.5430
761.6728	763.8205	764.2651
792.4901	794.5999	805.0191
807.1493	810.1909	819.5073
824.7404	830.8056	831.3516
837.2840	843.1712	849.4426
850.9817	852.4733	865.2213
882.0730	888.2461	900.7657
905.4730	912.5365	918.6458
935.8138	940.3456	946.4778
947.6106	948.5933	953.6673
960.5042	974.1831	978.3079
994.3952	1001.8390	1014.6843
1019.3277	1020.6200	1022.9548

1034.3574	1038.1460	1039.6046
1044.7398	1048.1434	1060.9298
1062.5173	1063.4153	1063.7506
1077.2849	1080.8983	1085.4221
1103.8064	1115.3386	1116.6588
1119.0604	1122.9269	1125.4054
1144.7991	1153.1210	1175.2068
1181.2804	1184.2307	1185.8604
1190.1637	1193.0729	1202.2064
1215.2648	1215.5321	1229.4702
1245.1389	1251.2061	1254.5772
1263.8056	1270.2165	1280.6158
1291.0857	1292.5285	1296.4993
1308.3279	1319.5892	1330.5780
1331.8213	1344.6151	1357.1528
1359.2210	1359.5655	1359.6901
1362.0628	1377.9213	1379.7208
1386.7122	1388.3525	1389.0173
1390.4670	1395.5469	1399.4253
1404.6759	1414.1284	1417.1021
1418.3137	1420.5223	1427.6451
1430.7381	1436.8085	1438.4379
1451.0078	1458.9105	1466.5283
1491.0745	1505.0232	1505.9811
1508.3257	1515.0592	1522.9589
1530.9549	1535.1653	1537.1643
1541.5491	1547.6937	1548.5406
1551.3226	1557.4304	1558.2690
1561.0533	1565.2631	1573.1222
1593.5000	1595.9637	1623.3934
1640.1356	1641.9231	1667.7433
1715.4734	2511.9805	2953.9824
2961.5524	2971.0950	3019.0101
3033.7195	3037.9227	3046.0226
3048.7674	3050.2954	3053.6031
3059.1694	3061.7745	3065.6874
3074.9687	3079.5931	3092.1753
3096.9681	3097.4008	3105.2238
3115.1032	3120.3470	3136.4860
3146.9860	3151.7629	3154.8967
3206.3557	3217.1655	3218.7800
3219.0261	3228.6503	3263.1691
3263.3532	3263.9692	3267.6458
3286.2583	3286.6388	3286.9033
3291.2127	3585.0728	3632.2018

II.B.5. Frequencies of the products ( $\text{Fe}^{\text{IV}}$ ) with  $6\beta\text{-d}_1\text{-testosterone}$  of the  ${}^2A$  state

Frequencies:

8.7927	11.0907	16.1996
26.3340	29.2546	35.7890
46.6698	54.3661	56.3326
73.2930	98.2606	99.3920
100.1527	109.0544	119.0802
125.2820	136.7506	145.8779
151.0885	156.9757	166.8409
173.9034	186.2719	205.2653
213.2551	215.7413	223.8002
230.3568	233.5622	239.7458
255.9546	260.2435	269.0788
274.7138	277.9923	284.6355
285.3840	288.0511	290.6645
291.9505	295.8162	297.9817
312.5974	317.2845	329.2284
338.1517	360.7493	367.4181
371.8807	373.4182	377.9439
384.9530	396.9845	410.9320
416.0376	429.1734	438.2072
439.3465	440.7296	441.3079
449.1320	469.7187	482.8167
484.8184	509.7158	518.7757
548.3499	561.2382	575.7172
592.2707	609.4893	620.8086
621.4912	632.4724	648.1395
662.0469	671.9189	679.2647
680.1282	691.6666	702.6219
711.9460	721.4793	723.0685
729.9631	731.5651	744.4888
758.6740	761.6812	763.9187
764.6413	793.8324	795.0221
805.0175	807.5569	810.3889
820.0412	830.7798	831.3212
837.2832	843.1654	849.4109
850.9697	852.4331	865.2109
882.0564	888.2422	900.7619
905.4719	912.5341	918.6344
935.8119	940.3458	946.4762
947.6097	948.5925	953.6586
960.4935	974.1512	978.3067
994.3234	1001.8043	1014.6620
1019.3084	1020.6146	1022.9425
1034.3550	1038.1445	1039.6022
1044.7369	1048.1402	1060.9295
1062.5016	1063.4154	1063.7367
1077.2523	1080.8848	1085.4202
1103.7896	1115.3365	1116.6575
1119.0602	1122.9246	1125.4050
1144.7946	1153.1205	1175.2060
1181.2644	1184.2209	1185.8595
1190.1410	1193.0579	1202.2011
1215.1846	1215.5276	1229.4714
1245.1377	1251.2040	1254.5743
1263.8035	1270.2144	1280.6131
1291.0714	1292.5080	1296.4989
1308.3262	1319.5870	1330.5647
1331.8185	1344.6137	1357.1491
1359.2212	1359.5395	1359.6864
1362.0625	1377.9201	1379.7205
1386.7117	1388.3081	1388.9748
1390.4449	1395.5444	1399.4248
1404.6694	1414.1278	1417.0995
1418.3105	1420.5185	1427.5965
1430.7215	1436.7374	1438.4351
1451.0014	1458.9104	1466.4933
1491.0383	1505.0220	1505.9805
1508.3160	1515.0477	1522.9337

1530.9549	1535.1555	1537.1588
1541.5339	1547.6614	1548.5378
1551.3204	1557.4211	1558.2433
1561.0458	1565.2628	1573.1074
1593.4988	1595.9617	1623.3879
1640.1312	1641.9167	1667.7434
1715.4708	2511.9799	2609.2297
2953.9825	2961.5543	2971.0949
3019.0101	3033.7196	3037.9242
3046.0225	3048.7682	3050.2952
3053.6031	3059.1673	3061.7730
3065.6896	3074.9689	3079.5930
3092.1757	3096.9681	3097.4011
3105.2241	3115.1032	3120.3470
3136.4857	3146.9861	3151.7640
3154.9008	3206.3556	3217.1658
3218.7801	3219.0263	3228.6510
3263.1691	3263.3533	3263.9690
3267.6458	3286.2584	3286.6387
3286.9042	3291.2129	3632.2019

## II.B.6. QM optimized geometry, absolute energy, and frequencies for the transition structure of the $^2A$ state

Absolute energy: -2476.5973756

Geometry:

C	.360032	3.326033	-1.229569
C	.391893	4.599435	-.527795
C	1.449032	4.775308	.547637
C	5.343349	-.865866	.191082
O	-.456420	5.497266	-.764368
C	2.619731	3.789623	.395694
C	2.173407	2.306732	.226200
C	3.420420	1.428326	-.183013
C	3.018988	-.027467	-.583261
C	2.037433	.005355	-1.769847
C	.866874	.953527	-1.551528
C	1.122257	2.236303	-.895732
C	4.564456	1.462156	.870079
C	5.778922	.577611	.495981
C	4.285152	-.819814	-.944494
C	4.841294	-1.568767	1.474808
C	1.515158	1.796677	1.542933
C	6.418551	-1.757658	-.492945
C	5.597275	-2.873952	-1.209338
C	4.161536	-2.292199	-1.414505
O	7.475053	-2.254160	.370567
S	-4.632545	-.902678	.693157
Fe	-2.231030	-.647158	.106653
C	-2.664961	-1.405340	-3.201289
C	-2.819402	2.680600	-.574445
C	-1.957129	.092671	3.447383
C	-1.852813	-3.988097	.831166
N	-2.646966	.420554	-1.544038
C	-2.769529	-.070810	-2.837647
C	-3.040006	1.013563	-3.756683
C	-3.087709	2.162156	-3.017899
C	-2.848710	1.788523	-1.640649
N	-2.422738	1.032068	1.211347
C	-2.625671	2.327706	.751612
C	-2.580964	3.259383	1.857343
C	-2.341802	2.528281	2.986224
C	-2.233318	1.141445	2.585322
N	-1.966401	-1.734657	1.801741
C	-1.843184	-1.243094	3.087130
C	-1.592048	-2.331353	4.012754
C	-1.569168	-3.481506	3.279476
C	-1.800421	-3.106648	1.898134
N	-2.267103	-2.351632	-.964953
C	-2.066181	-3.636342	-.497388
C	-2.107917	-4.576531	-1.597154
C	-2.333713	-3.851479	-2.732923
C	-2.432038	-2.464001	-2.333341
O	-.480512	-.529248	.011349
H	3.213067	4.074276	-.485197
H	3.824074	1.891744	-1.101839
H	2.514377	-.515136	.261481
H	2.586530	.326747	-2.673003
H	1.656621	-1.001635	-1.976615
H	.102917	.276136	-.732206
H	.207479	1.037909	-2.420000
H	-.371083	3.247912	-2.027594
H	1.798244	5.813863	.520422
H	.955939	4.646815	1.522116
H	4.179977	1.145043	1.846823
H	4.913036	2.493463	.998676
H	6.272264	.994211	-.395374
H	4.007548	-1.037234	1.940257
H	1.141316	.774868	1.439335



H	.656180	2.420366	1.809928
H	6.960232	-1.152906	-1.227874
H	6.071127	-3.166021	-2.151696
H	5.574680	-3.772959	-.579021
H	3.424427	-2.833182	-.808288
H	3.832180	-2.364680	-2.455880
H	4.765568	-.267429	-1.773512
H	5.653557	-1.611862	2.210723
H	4.500416	-2.592332	1.281180
H	2.228160	1.836201	2.373317
H	3.278993	3.878208	1.265589
H	6.520653	.598507	1.304999
H	7.111225	-2.917223	.991602
H	-5.077189	.324657	.236717
H	-2.782671	-1.643187	-4.253579
H	-2.931691	3.735919	-.798756
H	-1.830762	.336111	4.497262
H	-1.712914	-5.042147	1.047815
H	-3.181021	.895429	-4.821175
H	-3.272927	3.171300	-3.355542
H	-2.707916	4.327466	1.759763
H	-2.243236	2.880406	4.002712
H	-1.462431	-2.212777	5.078581
H	-1.415373	-4.493693	3.623920
H	-1.981897	-5.644712	-1.497445
H	-2.429136	-4.207616	-3.748256

## Frequencies:

-1615.9577	10.2263	15.6391
19.5244	35.6573	38.2096
43.6026	53.5743	58.1191
59.8103	73.3541	81.6646
92.8837	101.0878	115.5070
130.7474	140.7765	141.4833
154.8845	157.2605	164.5795
174.3448	188.9846	203.0381
207.8241	211.1875	219.3853
224.7562	231.8357	235.1482
246.1151	265.7776	269.9949
273.2244	279.9737	281.7609
282.9996	287.7526	297.4157
298.5472	304.4840	315.2652
321.7635	329.5500	341.3152
360.9550	368.8380	370.0944
373.2495	380.0054	384.2387
399.0437	411.1928	416.2075
423.8174	433.5046	436.0221
438.1593	439.6179	443.6550
463.1123	475.0755	486.0915
505.9135	519.5416	532.3874
557.7207	560.2010	562.2027
578.0389	618.1032	628.2212
656.0147	662.7722	678.2045
678.9464	687.9328	689.7285
690.0741	694.9610	704.5062
725.3095	726.0677	730.4089
735.4372	740.1768	760.8630
765.9118	766.5602	766.8944
801.1349	802.3409	810.9423
812.6994	818.1822	821.0283
827.5738	834.3059	835.1897
849.7273	852.2484	853.1868
862.9533	887.8811	905.2948
905.8074	917.5292	919.9993
934.0617	936.2786	937.0528
940.8302	952.2933	952.4130
953.2088	958.2924	968.6357
975.2526	985.5738	992.8026
1003.8635	1016.4213	1019.6181
1021.4826	1023.3702	1027.9298
1032.3003	1038.9928	1049.6180

1050.7554	1056.6865	1057.5364
1062.3390	1063.7796	1076.3883
1077.1392	1087.0709	1101.5182
1116.6539	1117.2052	1119.2241
1122.8250	1128.1821	1134.5592
1151.2622	1155.3128	1161.5156
1172.5984	1175.8845	1189.3482
1190.8982	1200.2691	1211.7121
1215.5442	1215.7846	1238.6186
1242.4422	1244.4099	1255.9396
1264.0965	1275.5860	1279.8702
1294.8557	1296.1990	1299.3298
1307.0048	1311.1098	1316.5479
1321.6549	1330.5207	1332.9026
1337.9014	1345.4286	1347.7155
1349.3490	1357.6348	1363.2278
1377.9784	1379.1106	1385.4950
1387.8402	1389.7322	1394.8836
1398.7469	1400.6952	1409.5075
1411.1269	1416.1438	1420.3038
1422.7748	1427.0866	1430.5650
1436.0575	1437.8919	1453.7383
1463.6242	1497.9104	1499.2504
1501.4656	1510.0733	1522.8535
1529.8283	1533.2399	1534.2781
1536.7282	1540.7635	1545.6768
1550.6697	1557.1969	1557.9508
1562.2126	1565.0629	1589.9042
1591.5036	1602.9273	1606.7813
1614.3553	1642.8848	1643.4482
1645.7903	1714.4029	2501.4838
2953.7934	2964.5477	2977.5574
3020.0872	3032.9288	3041.8584
3044.2612	3048.1985	3053.1359
3056.5490	3061.2798	3062.1780
3075.0336	3079.1773	3083.0214
3094.5040	3097.8600	3098.8225
3103.8811	3112.9675	3113.5074
3119.8652	3130.2738	3143.7617
3151.6332	3210.1372	3210.3844
3210.9001	3211.8279	3222.3067
3263.6496	3263.7706	3265.0634
3266.1832	3286.7705	3287.0519
3287.9734	3289.1791	3630.5459

II.B.7. QM frequencies for the transition structure with 6 $\beta$ -d<sub>1</sub>-testosterone of the <sup>2</sup>A state

Frequencies:		
-1226.2736	10.2264	15.6330
19.5169	35.6547	38.2076
43.5689	53.5650	58.1091
59.8072	73.3293	81.6672
92.8293	100.9735	115.4748
130.5210	140.7108	141.2832
154.8491	157.2560	164.3232
174.2571	188.8034	203.0131
207.6821	211.0980	219.3348
224.3097	231.7411	233.5412
245.8891	265.7028	269.8520
273.0155	279.8054	281.7403
282.9549	287.3054	297.3314
298.3725	304.3862	315.1629
320.0565	329.4428	341.2820
360.9174	368.7757	370.0529
372.9000	379.6795	383.9582
398.9317	411.1903	415.7065
421.9896	433.5014	436.0186
438.0633	439.5942	442.7730
461.2932	472.6815	486.0912
505.8384	518.9176	529.4966
554.2668	557.5539	561.6830
576.7336	601.8611	621.8529
643.6881	654.6392	677.8415
678.8360	683.2289	687.9134
689.7283	690.0738	700.4646
725.2081	725.5341	729.0574
735.3596	740.0838	760.8062
762.3537	766.4242	766.8296
791.7771	802.2671	810.8456
812.3672	813.6156	818.1823
821.0363	834.3027	835.1677
846.8755	849.7386	852.2541
853.2096	854.7905	876.9456
905.7919	909.4054	917.5254
919.9941	922.9788	934.5382
936.3294	940.8308	951.9304
952.3262	952.6678	958.2873
962.1655	974.4208	982.8583
989.4885	998.4656	1015.6037
1016.5025	1019.6379	1021.4998
1023.4085	1032.2975	1038.1570
1047.7199	1049.9342	1056.6932
1057.5392	1060.2849	1062.5569
1076.5251	1077.4269	1086.0320
1101.2516	1116.6456	1117.1902
1119.2244	1122.8237	1123.8750
1135.8790	1148.9898	1154.0301
1155.3196	1172.0858	1176.1861
1189.3446	1190.8890	1199.0002
1203.8157	1215.3349	1215.5602
1237.6856	1242.2811	1244.4139
1255.8369	1262.7872	1273.0027
1279.8122	1294.7765	1296.1238
1299.4230	1306.9339	1311.1033
1315.2253	1322.0767	1331.7139
1336.5092	1345.3845	1347.6978
1349.3442	1357.6305	1362.7270
1376.1462	1378.6379	1385.4950
1387.5673	1389.2446	1394.7859
1398.7398	1400.6058	1409.3151
1411.1273	1415.9909	1420.2322
1422.7244	1427.0067	1429.4192
1436.0289	1437.7970	1453.7378
1463.3668	1497.9006	1499.2318
1501.4677	1510.0359	1522.7023

1529.8276	1533.2370	1534.1829
1536.7125	1540.7121	1545.6388
1550.6637	1557.1196	1557.9357
1562.2035	1565.0625	1589.9005
1591.4840	1598.7743	1606.7794
1614.3543	1642.8709	1643.4269
1645.7832	1714.4029	2501.5174
2953.7920	2964.5458	2977.5210
3020.0840	3032.9294	3041.8562
3044.2600	3048.1988	3053.1382
3056.5403	3061.2800	3062.1792
3075.0335	3079.1771	3083.0097
3094.5021	3097.8592	3098.8217
3103.8772	3112.9648	3113.3338
3119.8636	3130.2741	3143.7616
3151.6321	3210.1280	3210.3860
3210.8992	3211.8270	3222.3123
3263.6451	3263.7701	3265.0543
3266.1840	3286.7725	3287.0504
3287.9715	3289.1847	3630.5471

II.C. Input geometries and frequencies of the MM reactant-complex, MM product-complex, Cpd I, products, and transition structure for the  $6\beta$ -H(D) abstraction by Cpd I of the  $^4A$  state.

II.C.1. Atom types, MM optimized coordinates, and connectivities for the MM reactant-complex in the TINKER xyz file format

89	reactant complex	at MM optimized geometry									
1	C	-3.051065	4.216395	.916744	2	2	12	56			
2	C	-3.974146	5.040367	.359100	3	1	3	5			
3	C	-4.662417	4.570891	-.914281	1	2	6	57	58		
4	C	-3.677784	-2.171187	-.509413	1	14	15	16	18		
5	O	-4.152461	6.153419	.799277	7	2					
6	C	-4.847721	3.053216	-.914997	1	3	7	49	74		
7	C	-3.525494	2.284421	-.666210	1	6	8	12	17		
8	C	-3.895101	.820584	-.247536	1	7	9	13	50		
9	C	-2.663770	.038773	.281998	1	8	10	15	51		
10	C	-2.064788	.785468	1.483797	1	9	11	52	53		
11	C	-1.624284	2.191111	1.074231	1	10	12	54	55		
12	C	-2.779600	2.979547	.476044	2	1	7	11			
13	C	-4.618932	.026699	-1.367594	1	8	14	59	60		
14	C	-4.940205	-1.431365	-.979809	1	4	13	61	75		
15	C	-3.098287	-1.378340	.681831	1	4	9	20	70		
16	C	-2.677752	-2.326444	-1.682655	1	4	62	71	72		
17	C	-2.647907	2.333322	-1.937612	1	7	63	64	73		
18	C	-3.932352	-3.535735	.179376	1	4	19	21	65		
19	C	-2.659467	-3.759021	1.050084	1	18	20	66	67		
20	C	-2.047972	-2.341594	1.264633	1	15	19	68	69		
21	O	-4.148667	-4.597995	-.735086	6	18	76				
22	S	4.617219	-.895170	1.044799	159	23	77				
23	Fe	2.135359	-.494672	-.025968	160	22	28	33	38	43	48
24	C	1.339353	-2.006827	2.768086	2	29	47	78			
25	C	2.267025	2.342245	1.603205	2	32	34	79			
26	C	3.661724	.932724	-2.544164	2	37	39	80			
27	C	2.708860	-3.413520	-1.388074	2	42	44	81			
28	N	1.999861	.046478	1.888762	40	23	29	32			
29	C	1.501969	-.689181	2.813520	2	24	28	30			
30	C	1.118893	.058909	3.856959	2	29	31	82			
31	C	1.385515	1.316330	3.519947	2	30	32	83			
32	C	1.915746	1.261239	2.290856	2	25	28	31			
33	N	2.978688	1.283008	-.345488	40	23	34	37			
34	C	2.746444	2.325706	.364256	2	25	33	35			
35	C	3.034330	3.439265	-.322556	2	34	36	84			
36	C	3.438956	3.032119	-1.520902	2	35	37	85			
37	C	3.373703	1.694260	-1.494149	2	26	33	36			
38	N	3.174215	-1.140596	-1.599834	40	23	39	42			
39	C	3.545839	-.390754	-2.571961	2	26	38	40			
40	C	3.780689	-1.121427	-3.670114	2	39	41	86			
41	C	3.504469	-2.377496	-3.336252	2	40	42	87			
42	C	3.118051	-2.338879	-2.054032	2	27	38	41			
43	N	2.191924	-2.376580	.631605	40	23	44	47			
44	C	2.263513	-3.401453	-.136283	2	27	43	45			
45	C	1.798703	-4.493472	.485305	2	44	46	88			
46	C	1.405225	-4.086518	1.687242	2	45	47	89			
47	C	1.652341	-2.770293	1.726760	2	24	43	46			
48	O	.576673	-.340032	-.583325	161	23					
49	H	-5.584713	2.797106	-.118501	5	6					
50	H	-4.613012	.894173	.606366	5	8					
51	H	-1.892481	-.027384	-.514075	5	9					
52	H	-2.810371	.848368	2.309043	5	10					
53	H	-1.189451	.225901	1.882920	5	10					
54	H	-.799494	2.127668	.329349	5	11					
55	H	-1.203039	2.718886	1.959709	5	11					
56	H	-2.483322	4.627860	1.768393	5	1					
57	H	-5.655775	5.066907	-1.010174	5	3					
58	H	-4.063927	4.889201	-1.797501	5	3					
59	H	-4.004172	.027090	-2.293040	5	13					
60	H	-5.573598	.534585	-1.632925	5	13					
61	H	-5.704958	-1.433005	-.169895	5	14					

62	H	-2.335587	-1.355446	-2.095635	5	16
63	H	-1.728143	1.717226	-1.845874	5	17
64	H	-2.311628	3.369216	-2.163085	5	17
65	H	-4.819496	-3.450872	.850022	5	18
66	H	-2.928507	-4.231962	2.021487	5	19
67	H	-1.918449	-4.421034	.548079	5	19
68	H	-1.082711	-2.246119	.720547	5	20
69	H	-1.855912	-2.139350	2.341881	5	20
70	H	-3.901614	-1.274354	1.452438	5	15
71	H	-3.134242	-2.877104	-2.534544	5	16
72	H	-1.760570	-2.883695	-1.394996	5	16
73	H	-3.190479	1.975688	-2.838997	5	17
74	H	-5.305890	2.739053	-1.879789	5	6
75	H	-5.394992	-1.966480	-1.844195	5	14
76	H	-3.338407	-4.792661	-1.184122	21	21
77	H	4.801609	.319415	1.585623	44	22
78	H	.868245	-2.495323	3.638621	5	24
79	H	2.112650	3.325545	2.080282	5	25
80	H	3.975175	1.439168	-3.473462	5	26
81	H	2.698184	-4.377097	-1.926374	5	27
82	H	.649531	-.278621	4.791742	5	30
83	H	1.178241	2.209882	4.125514	5	31
84	H	2.934224	4.481808	.010911	5	35
85	H	3.734299	3.676339	-2.361059	5	36
86	H	4.101058	-.767193	-4.660083	5	40
87	H	3.554866	-3.252968	-3.998929	5	41
88	H	1.724127	-5.515511	.087789	5	45
89	H	.943467	-4.709196	2.466499	5	46

## II.C.2. Atom types, MM optimized coordinates, and connectivities for the MM product-complex in the TINKER xyz file format

89 intermediate complex at MM optimized geometry											
1	C	.687175	2.787831	-1.269744	2	2	12	56			
2	C	.477236	3.859847	-.463368	3	1	3	5			
3	C	1.379515	4.046898	.751087	1	2	6	57	58		
4	C	5.791363	-1.121989	.381903	1	14	15	16	18		
5	O	-.365305	4.682785	-.741374	7	2					
6	C	2.694742	3.269861	.619446	1	3	7	49	74		
7	C	2.457401	1.800297	.211054	1	6	8	12	17		
8	C	3.821212	1.104883	-.097471	1	7	9	13	50		
9	C	3.591179	-.322315	-.664042	1	8	10	15	51		
10	C	2.795494	-.242978	-1.980221	1	9	11	52	53		
11	C*	1.762525	.848623	-1.992898	29	10	12	55			
12	C	1.586105	1.815025	-1.047875	2	1	7	11			
13	C	4.784706	1.085971	1.119737	1	8	14	59	60		
14	C	6.089172	.304263	.868499	1	4	13	61	75		
15	C	4.949685	-.998506	-.905113	1	4	9	20	70		
16	C	5.090209	-1.936789	1.496351	1	4	62	71	72		
17	C	1.680005	1.076311	1.337677	1	7	63	64	73		
18	C	7.015696	-1.893436	-.171294	1	4	19	21	65		
19	C	6.388312	-2.968360	-1.110187	1	18	20	66	67		
20	C	4.972878	-2.427298	-1.478893	1	15	19	68	69		
21	O	7.816823	-2.462021	.852918	6	18	76				
22	S	-4.917880	-.565525	.927090	159	23	77				
23	Fe	-2.725588	-.331934	.043182	162	22	28	33	38	43	48
24	C	-2.423074	-3.514151	.649659	2	29	47	78			
25	C	-3.740735	-1.008640	-2.974960	2	32	34	79			
26	C	-3.026507	2.841774	-.566654	2	37	39	80			
27	C	-1.711012	.339917	3.054959	2	42	44	81			
28	N	-3.262248	-1.975160	-.899228	40	23	29	32			
29	C	-2.999421	-3.165054	-.502071	2	24	28	30			
30	C	-3.316644	-4.043109	-1.464291	2	29	31	82			
31	C	-3.698549	-3.317492	-2.513711	2	30	32	83			
32	C	-3.594364	-2.035450	-2.135690	2	25	28	31			
33	N	-3.093030	.736255	-1.568062	40	23	34	37			
34	C	-3.516925	.273103	-2.683333	2	25	33	35			
35	C	-3.773301	1.288323	-3.520846	2	34	36	84			
36	C	-3.565355	2.404591	-2.822904	2	35	37	85			
37	C	-3.195863	2.011405	-1.595891	2	26	33	36			
38	N	-2.687506	1.291664	1.152785	40	23	39	42			
39	C	-2.761599	2.485187	.691489	2	26	38	40			
40	C	-2.439437	3.364354	1.650551	2	39	41	86			
41	C	-2.058252	2.639752	2.700087	2	40	42	87			
42	C	-2.168389	1.357985	2.323248	2	27	38	41			
43	N	-1.964329	-1.394781	1.513915	40	23	44	47			
44	C	-1.647455	-.934308	2.665855	2	27	43	45			
45	C	-1.289700	-1.945429	3.470309	2	44	46	88			
46	C	-1.496159	-3.062298	2.773037	2	45	47	89			
47	C	-1.967125	-2.673466	1.579311	2	24	43	46			
48	O	-.979253	-.269920	-.532198	163	23	54				
49	H	3.335630	3.770339	-.143308	5	6					
50	H	4.326750	1.697767	-.899191	5	8					
51	H	3.008418	-.930233	.061572	5	9					
52	H	3.497514	-.061348	-2.826012	5	10					
53	H	2.309742	-1.225465	-2.179699	5	10					
54	H	-.669218	.625101	-.533929	21	48					
55	H	1.144051	.879166	-2.908024	5	11					
56	H	.056473	2.734341	-2.173474	5	1					
57	H	1.605811	5.130193	.882755	5	3					
58	H	.832041	3.733387	1.668021	5	3					
59	H	4.273034	.656059	2.006899	5	13					
60	H	5.056602	2.129268	1.398256	5	13					
61	H	6.698797	.845672	.109538	5	14					
62	H	4.114226	-1.506453	1.801610	5	16					
63	H	1.492631	.005791	1.110767	5	17					
64	H	.679698	1.528288	1.506758	5	17					
65	H	7.644416	-1.201989	-.780013	5	18					
66	H	7.015728	-3.104231	-2.019983	5	19					

67	H	6.298322	-3.960480	-.613605	5	19
68	H	4.178923	-3.052980	-1.013380	5	20
69	H	4.807933	-2.431165	-2.579437	5	20
70	H	5.517402	-.354709	-1.621859	5	15
71	H	5.710657	-1.979228	2.418689	5	16
72	H	4.889131	-2.987604	1.197200	5	16
73	H	2.209205	1.117848	2.313486	5	17
74	H	3.244573	3.326273	1.585399	5	6
75	H	6.700916	.269720	1.798538	5	14
76	H	7.404511	-3.251778	1.173205	21	21
77	H	-5.595482	-.048393	-.109527	44	22
78	H	-2.301466	-4.593764	.845892	5	24
79	H	-4.059329	-1.241028	-4.006114	5	25
80	H	-3.084592	3.922951	-.781226	5	26
81	H	-1.332407	.575068	4.065023	5	27
82	H	-3.193103	-5.135259	-1.443584	5	30
83	H	-3.945478	-3.705091	-3.512329	5	31
84	H	-4.151476	1.229528	-4.551315	5	35
85	H	-3.739690	3.431935	-3.172829	5	36
86	H	-2.382064	4.458658	1.563747	5	40
87	H	-1.632481	3.031585	3.634766	5	41
88	H	-.968757	-1.886487	4.520050	5	45
89	H	-1.376488	-4.089923	3.144702	5	46



II.C.3. QM optimized geometry, absolute energy, and frequencies for Cpd I of the  $^4A$  state.

Absolute energy: -1585.5207546

## Geometry:

S	20.395528	8.721945	70.734517
Fe	18.715095	8.626496	68.776996
C	21.533828	9.506575	67.014111
C	19.574818	5.310154	68.474741
C	16.061482	7.752846	70.769501
C	18.008337	11.945367	69.291142
N	20.271623	7.621084	67.974426
C	21.324467	8.157957	67.240804
C	22.162721	7.094763	66.732095
C	21.612796	5.915004	67.142124
C	20.428942	6.238705	67.907244
N	17.985299	6.887768	69.497668
C	18.439853	5.611364	69.217616
C	17.573649	4.628939	69.832520
C	16.592216	5.316872	70.487084
C	16.847624	6.724747	70.272983
N	17.325190	9.642125	69.825859
C	16.280968	9.106101	70.558016
C	15.447176	10.166608	71.082925
C	15.993129	11.345780	70.664029
C	17.164872	11.013192	69.881739
N	19.606939	10.367660	68.282946
C	19.139304	11.646715	68.550840
C	20.007136	12.628773	67.936764
C	20.994415	11.942212	67.291814
C	20.742931	10.533302	67.508466
O	17.788500	8.567629	67.411429
H	20.533984	7.362663	70.948938
H	22.392987	9.784019	66.412694
H	19.813790	4.261277	68.333742
H	15.199478	7.475868	71.367466
H	17.760089	12.993580	69.420894
H	23.051368	7.248384	66.137645
H	21.960950	4.910733	66.949698
H	17.713176	3.559898	69.765605
H	15.766936	4.923823	71.062586
H	14.567506	10.012490	71.690483
H	15.650789	12.351394	70.859557
H	19.865453	13.697636	68.001211
H	21.824057	12.335721	66.723079

## Frequencies:

40.5214	51.6792	69.9259
87.7475	98.1806	146.7491
150.4533	159.5457	167.7040
186.3466	189.9396	220.8751
232.8255	271.3130	279.6962
280.7083	286.9852	297.2013
325.7595	326.7798	358.3828
372.0284	372.5578	377.2764
418.5211	420.1555	434.1261
436.8656	440.0905	440.7830
485.6243	504.2515	678.6052
679.1935	685.7631	689.8434
691.5601	724.8210	725.5779
733.8455	740.9540	759.7370
766.7159	767.2372	801.6783
811.8775	812.0307	820.5530
821.6531	834.5040	834.7142
852.2569	857.6088	903.9427
917.0969	917.1734	934.7047
940.8052	952.0912	952.5587
956.6749	1017.0431	1019.6779
1022.8422	1024.8822	1033.1415

1056.7278	1059.3323	1078.4371
1117.0621	1117.1248	1119.4914
1123.0809	1159.1796	1188.8437
1189.9108	1215.1143	1245.3380
1296.9982	1299.0941	1318.8834
1350.0994	1352.5775	1387.5705
1389.4687	1411.5514	1417.9263
1426.7258	1438.0115	1503.0245
1503.9334	1504.7551	1538.7841
1560.6818	1594.6863	1594.9200
1615.5403	1619.4809	1646.0421
1648.7439	1718.5279	2504.5213
3212.5160	3213.1119	3213.2365
3214.3251	3263.8097	3264.2368
3264.2940	3264.5598	3286.9291
3287.3185	3287.4661	3287.7910

II.C.4. QM optimized geometry, energy, and frequencies for the products ( $\text{Fe}^{\text{IV}}$ ) of the  $^4A$  state.

Absolute energy: -2476.627407

Geometry:

C	.705723	3.416294	-1.226566
C	.691370	4.543927	-.334933
C	1.784203	4.638612	.718882
C	5.378148	-1.183217	.230215
O	-.213191	5.429200	-.412722
C	2.949837	3.659461	.480446
C	2.477988	2.210625	.152895
C	3.710291	1.297038	-.194665
C	3.250826	-.089083	-.752022
C	2.419386	.092999	-2.040787
C	1.517912	1.286572	-2.025698
C	1.552119	2.293994	-1.076177
C	4.725950	1.163059	.975291
C	5.895663	.192991	.683641
C	4.479473	-.971504	-1.018190
C	4.656409	-1.908568	1.391125
C	1.657111	1.646369	1.349650
C	6.450987	-2.129716	-.380017
C	5.635549	-3.119127	-1.269590
C	4.289201	-2.396355	-1.599312
O	7.342780	-2.772958	.567192
S	-4.745606	-.450628	.542214
Fe	-2.427759	-.560476	.159297
C	-2.330486	-3.918844	.868058
C	-2.974516	-1.274809	-3.167664
C	-2.599105	2.813108	-.556737
C	-1.963099	.164687	3.477248
N	-2.680077	-2.244735	-.912510
C	-2.577771	-3.546221	-.443415
C	-2.741269	-4.471982	-1.541041
C	-2.921829	-3.729255	-2.673745
C	-2.871412	-2.337998	-2.286072
N	-2.671243	.544207	-1.528252
C	-2.890338	.062036	-2.810783
C	-3.051774	1.170157	-3.724514
C	-2.950818	2.318842	-2.989463
C	-2.728158	1.929154	-1.615743
N	-2.359311	1.134720	1.243418
C	-2.425488	2.436458	.765048
C	-2.252049	3.365543	1.859100
C	-2.082218	2.622395	2.994062
C	-2.140311	1.230087	2.608228
N	-2.159649	-1.651948	1.819812
C	-1.972038	-1.167899	3.105142
C	-1.806864	-2.275649	4.021606
C	-1.907918	-3.423194	3.289207
C	-2.137036	-3.033205	1.914249
O	-.627593	-.551796	-.112346
H	3.564650	4.021721	-.356156
H	4.241261	1.800617	-1.022683
H	2.611934	-.581186	-.007402
H	3.103683	.192625	-2.904248
H	1.834196	-.815989	-2.242413
H	-.329274	.141992	-.741242
H	.834094	1.399042	-2.867313
H	-.004369	3.440743	-2.047893
H	2.142304	5.675012	.739556
H	1.321309	4.462321	1.699655
H	4.205170	.829711	1.880610
H	5.142088	2.150184	1.209403
H	6.529781	.611393	-.112863
H	3.814421	-1.331631	1.781149
H	1.284924	.637739	1.151251
H	.777218	2.266402	1.543880
H	7.130850	-1.534749	-.998943

H	6.196782	-3.391973	-2.168694
H	5.459823	-4.050842	-.715755
H	3.442230	-2.902563	-1.119598
H	4.082946	-2.378875	-2.674466
H	5.103805	-.417725	-1.744064
H	5.358034	-2.065276	2.219388
H	4.261496	-2.885006	1.087811
H	2.259225	1.630300	2.264707
H	3.593437	3.647002	1.366285
H	6.531613	.096025	1.573115
H	6.849423	-3.436860	1.090164
H	-5.112517	-1.567207	-.184231
H	-2.283261	-4.979177	1.089330
H	-3.138000	-1.505593	-4.214497
H	-2.603166	3.874530	-.776167
H	-1.804656	.393295	4.525195
H	-2.709678	-5.547256	-1.442487
H	-3.067886	-4.075890	-3.686396
H	-3.232565	1.066670	-4.784548
H	-3.032815	3.341697	-3.326955
H	-2.243246	4.439343	1.744292
H	-1.922740	2.969351	4.004521
H	-1.643328	-2.169698	5.084095
H	-1.843665	-4.445757	3.631417

## Frequencies:

8.7642	10.9593	15.9946
26.2710	29.3829	35.8630
46.8327	54.3234	56.3378
73.3651	98.5439	99.4029
100.4232	109.2350	119.2178
125.2904	138.3844	145.8664
152.5623	157.6103	172.9115
178.0142	186.2913	205.8920
215.6835	216.8479	223.7749
232.6682	238.4949	251.3403
259.6654	263.4062	269.0352
277.4238	279.3383	285.3801
287.4765	290.2850	291.5791
294.5275	297.7739	299.6278
316.9635	329.3806	338.2750
355.4089	366.3802	368.4862
372.4318	375.8939	377.9194
385.0768	396.9540	411.7519
418.7854	429.1177	438.3047
439.4496	440.9351	441.4535
449.0773	469.7353	482.8242
484.8546	509.6866	518.7277
548.1233	561.2013	575.6869
605.7874	620.7538	621.4104
632.4876	647.9656	661.8307
671.5571	679.0942	680.1090
691.6377	702.4386	711.8929
718.8873	723.0051	727.7849
731.5278	743.8668	758.5838
761.6100	763.8123	764.2731
792.3481	794.5588	804.9982
807.1033	810.1428	819.4654
824.9332	830.8472	831.4234
837.2854	842.9628	849.4178
850.9915	852.4222	865.0132
881.8402	888.2186	900.7286
905.4045	912.5205	918.5865
935.7668	940.3098	946.3866
947.5546	948.5727	953.5159
960.5294	974.1542	978.2302
994.4879	1001.8317	1014.6989
1019.0825	1020.9738	1023.0160
1034.3813	1038.1283	1039.6007
1044.7286	1048.0422	1060.9059
1062.5429	1063.4113	1063.7451

1077.2611	1080.8846	1085.3659
1103.8155	1115.3499	1116.6674
1119.0338	1122.8973	1125.3582
1144.7739	1153.0322	1175.2212
1181.2553	1184.2314	1185.8307
1190.2331	1193.0943	1202.1724
1215.3122	1215.4966	1229.4655
1245.1423	1251.1928	1254.5778
1263.7699	1270.1632	1280.5788
1291.0913	1292.6089	1296.4958
1308.2959	1319.5541	1330.6151
1331.8209	1344.6005	1357.1040
1359.2418	1359.6421	1359.6789
1362.0192	1377.8230	1379.6967
1386.7557	1388.3128	1389.0322
1390.4598	1395.4729	1399.3913
1404.6077	1414.1312	1417.0474
1418.2244	1420.4809	1427.7355
1430.6733	1436.8883	1438.4457
1450.9092	1458.8390	1466.4579
1491.2775	1505.0449	1505.9816
1508.3706	1515.0399	1523.0457
1530.9392	1535.1094	1537.1356
1541.5091	1547.6419	1548.5532
1551.3037	1557.4371	1558.2178
1560.9921	1565.2422	1573.1295
1593.5049	1596.0055	1623.4283
1640.2972	1642.0578	1667.7549
1715.4798	2512.0523	2953.9873
2961.4729	2971.0627	3018.9921
3033.7269	3037.9894	3046.0243
3048.7726	3050.3142	3053.5968
3059.0829	3061.7921	3065.5953
3074.9709	3079.6108	3092.1144
3096.9682	3097.3966	3105.1780
3115.1310	3120.3707	3136.6867
3146.9777	3152.1346	3154.6549
3206.1378	3217.1230	3218.7661
3219.0850	3228.8291	3263.1807
3263.3635	3263.9889	3267.6624
3286.2251	3286.6425	3286.9238
3291.2666	3590.5019	3632.1999

II.C.5. QM frequencies for the products ( $\text{Fe}^{\text{IV}}$ ) with  $6\beta$ - $d_1$ -tetsosterone of the  $^4A$  state

Frequencies:

8.7633	10.9542	15.9814
26.2564	29.3702	35.8410
46.8277	54.2675	56.3273
73.3223	98.4311	99.2710
100.3830	109.2269	119.1759
125.1966	137.3778	145.8596
151.5351	157.4535	167.7436
173.9974	186.2130	204.9210
212.7150	215.7037	223.7406
229.9076	234.0054	239.8997
256.5346	260.0565	269.0215
275.8164	277.7515	285.3733
286.1552	288.1576	290.6757
292.8074	296.2351	298.0279
312.9535	317.1356	329.3879
338.3007	361.1386	367.7661
371.9121	373.4595	377.9147
384.8938	396.9443	411.1009
416.2360	429.0996	438.2242
439.3711	440.7613	441.2850
449.0661	469.7241	482.8232
484.8516	509.6527	518.7054
548.1026	561.1923	575.6832
592.3824	609.5364	620.8101
622.4978	632.4876	647.9964
661.8456	671.9646	679.2580
680.1090	691.6374	702.5681
711.9956	721.4589	723.0890
729.9925	731.5457	744.4824
758.7119	761.6193	763.9278
764.6496	793.7350	794.9890
804.9959	807.5196	810.3344
819.9723	830.8203	831.3884
837.2847	842.9572	849.3827
850.9799	852.3802	865.0003
881.8270	888.2147	900.7253
905.4036	912.5181	918.5752
935.7648	940.3097	946.3851
947.5532	948.5721	953.5069
960.5183	974.1224	978.2290
994.4181	1001.7970	1014.6774
1019.0658	1020.9695	1023.0033
1034.3789	1038.1275	1039.5987
1044.7255	1048.0392	1060.9056
1062.5272	1063.4111	1063.7313
1077.2285	1080.8714	1085.3639
1103.7989	1115.3475	1116.6663
1119.0337	1122.8955	1125.3578
1144.7693	1153.0317	1175.2204
1181.2388	1184.2222	1185.8298
1190.2114	1193.0785	1202.1669
1215.2340	1215.4922	1229.4648
1245.1413	1251.1909	1254.5750
1263.7680	1270.1618	1280.5756
1291.0771	1292.5892	1296.4954
1308.2941	1319.5516	1330.6000
1331.8177	1344.5989	1357.1006
1359.2416	1359.6289	1359.6622
1362.0188	1377.8216	1379.6967
1386.7555	1388.2733	1388.9879
1390.4383	1395.4704	1399.3909
1404.6012	1414.1306	1417.0448
1418.2212	1420.4778	1427.6884
1430.6558	1436.8159	1438.4427
1450.9047	1458.8388	1466.4229
1491.2458	1505.0438	1505.9809
1508.3610	1515.0285	1523.0212

1530.9391	1535.0994	1537.1301
1541.4939	1547.6097	1548.5487
1551.3016	1557.4263	1558.1934
1560.9848	1565.2418	1573.1138
1593.5036	1596.0045	1623.4227
1640.2933	1642.0509	1667.7548
1715.4770	2512.0517	2613.2467
2953.9876	2961.4746	2971.0627
3018.9922	3033.7269	3037.9909
3046.0242	3048.7727	3050.3141
3053.5970	3059.0815	3061.7915
3065.5972	3074.9708	3079.6107
3092.1146	3096.9690	3097.3970
3105.1783	3115.1307	3120.3699
3136.6856	3146.9777	3152.1355
3154.6593	3206.1375	3217.1231
3218.7661	3219.0852	3228.8286
3263.1808	3263.3637	3263.9891
3267.6624	3286.2251	3286.6426
3286.9240	3291.2667	3632.1998

## II.C.6. QM optimized geometry, absolute energy, and frequencies for the transition structure of the ${}^4A$ state

Absolute energy: -2476.5984352

Geometry:

C	.377903	3.373609	-1.224970
C	.417473	4.639061	-.510924
C	1.467032	4.793970	.575097
C	5.311502	-.880311	.212409
O	-.416571	5.549650	-.749972
C	2.631271	3.801144	.419771
C	2.174092	2.323765	.231694
C	3.417517	1.436712	-.167884
C	3.006664	-.011145	-.586757
C	2.043319	.042644	-1.787335
C	.882110	1.006333	-1.581572
C	1.135395	2.272937	-.903489
C	4.547420	1.449673	.900885
C	5.757674	.555937	.535300
C	4.269411	-.814076	-.936908
C	4.784885	-1.588466	1.483357
C	1.493479	1.810819	1.536313
C	6.386843	-1.777722	-.464149
C	5.564168	-2.878950	-1.202054
C	4.136936	-2.281227	-1.420480
O	7.425226	-2.293404	.410122
S	-4.650585	-.738002	.303658
Fe	-2.231665	-.675948	.164076
C	-1.850948	-3.994487	.905109
C	-2.523128	-1.449130	-3.184201
C	-2.818146	2.645352	-.588395
C	-2.059009	.109708	3.489856
N	-2.236818	-2.375542	-.911090
C	-2.037913	-3.657742	-.428559
C	-2.023358	-4.600889	-1.524711
C	-2.199683	-3.883078	-2.673766
C	-2.329099	-2.493966	-2.292441
N	-2.611974	.384764	-1.544984
C	-2.666869	-.113419	-2.837626
C	-2.913588	.966142	-3.770341
C	-3.007693	2.115565	-3.037338
C	-2.818950	1.751155	-1.648916
N	-2.444720	1.020200	1.235641
C	-2.649827	2.302040	.744463
C	-2.644783	3.252139	1.835879
C	-2.438962	2.541584	2.984686
C	-2.307575	1.150714	2.606514
N	-1.975016	-1.721252	1.843008
C	-1.906490	-1.220296	3.133284
C	-1.681909	-2.301999	4.070805
C	-1.628238	-3.456148	3.345885
C	-1.817140	-3.094203	1.955943
O	-.515566	-.465880	-.020935
H	3.232859	4.090494	-.453953
H	3.838451	1.903934	-1.076928
H	2.485423	-.501162	.246669
H	2.610747	.361119	-2.680137
H	1.653365	-.958366	-2.006478
H	.090165	.330834	-.774484
H	.238519	1.107602	-2.460231
H	-.348630	3.310169	-2.028451
H	1.824298	5.830000	.562917
H	.966011	4.657134	1.544406
H	4.146464	1.128287	1.869578
H	4.904785	2.476160	1.043048
H	6.266932	.975029	-.345866
H	3.950068	-1.052245	1.941396
H	1.122124	.788901	1.425266
H	.629925	2.433249	1.790874



H	6.945816	-1.172564	-1.185659
H	6.047510	-3.166576	-2.140954
H	5.524470	-3.783712	-.580883
H	3.387167	-2.819854	-.827766
H	3.819888	-2.341999	-2.466415
H	4.766704	-.260232	-1.754895
H	5.586223	-1.645310	2.230215
H	4.436799	-2.607148	1.276936
H	2.192807	1.848558	2.378319
H	3.285243	3.874580	1.294994
H	6.488811	.562279	1.354136
H	7.045225	-2.958150	1.019561
H	-4.894437	-1.519822	-.809519
H	-1.712331	-5.044342	1.140201
H	-2.579949	-1.699908	-4.238253
H	-2.936522	3.698534	-.818623
H	-1.981708	.356859	4.543261
H	-1.889567	-5.667065	-1.414165
H	-2.240401	-4.245383	-3.690684
H	-3.007142	.843932	-4.839613
H	-3.191732	3.121198	-3.385975
H	-2.777829	4.317204	1.716008
H	-2.377188	2.909523	3.998430
H	-1.590101	-2.175926	5.139719
H	-1.482327	-4.465746	3.701167

## Frequencies:

-1665.0271	7.5950	13.4269
18.0282	33.5547	36.7504
40.5094	54.1871	57.5063
58.4635	70.8818	94.8375
101.1233	104.2269	115.4226
131.3061	144.6713	154.1349
156.1974	159.7130	164.6963
183.4088	197.2796	207.2713
210.6078	218.7089	223.6947
224.9688	233.4147	235.2468
244.4968	264.8096	271.1769
276.0281	278.8336	283.9876
288.0948	288.5345	298.1317
302.0418	314.7688	324.1588
329.0297	335.0930	341.6068
363.3757	367.9936	372.5566
373.9293	379.0160	384.1091
398.5842	418.4362	423.7898
425.5001	435.9931	436.9383
439.5529	442.2574	444.0609
461.8352	474.5014	486.4815
504.5531	519.3157	526.3499
559.3568	560.3055	576.7792
585.8365	617.6751	627.5281
656.0286	662.9416	679.2429
680.3280	683.1612	691.0726
694.9990	704.5373	722.2669
724.7442	730.1254	734.9223
736.6002	740.5734	761.3601
764.6606	765.8240	766.0889
799.6692	800.5952	810.3781
811.6172	820.3218	828.0103
828.1860	833.3502	834.0777
848.8687	851.8702	852.8656
862.9458	884.7262	900.2377
902.5088	912.7882	914.8452
929.8152	933.4092	936.3077
940.7413	950.4646	950.5053
952.5053	955.9230	968.5341
974.3878	984.7337	992.4382
1002.9872	1019.2649	1022.1915
1023.7287	1026.0297	1028.8005
1033.1071	1038.6430	1049.3400
1050.1808	1059.5787	1060.6907

1061.7459	1063.4086	1076.8925
1078.6337	1086.8159	1100.8115
1116.7550	1116.9734	1119.3978
1122.7218	1128.0278	1136.0354
1150.7926	1165.6856	1171.5633
1172.4049	1175.6608	1189.1004
1191.8515	1200.5839	1212.1952
1216.0176	1217.0617	1237.1794
1242.7940	1244.5963	1255.6782
1263.9100	1274.4368	1278.6170
1294.8724	1295.5227	1297.5222
1307.0078	1316.2028	1320.8721
1326.8728	1332.3590	1338.2277
1339.5471	1345.4829	1352.9128
1353.4276	1357.6440	1363.1700
1377.9480	1379.2345	1387.2948
1388.2179	1389.8345	1395.1760
1398.3688	1400.7277	1409.3618
1412.0366	1416.3160	1420.3765
1424.3102	1429.5728	1433.0164
1436.5154	1437.3076	1452.5794
1462.6419	1500.5254	1501.7714
1505.3737	1509.9743	1524.7567
1529.5969	1533.8436	1536.2947
1539.2766	1540.1654	1545.3090
1550.4692	1556.1229	1558.7248
1562.3208	1564.5693	1579.5935
1592.3757	1594.2895	1617.1145
1628.2111	1638.1204	1642.6807
1644.1118	1714.7197	2505.6336
2953.4375	2964.9439	2977.2606
3019.7270	3033.0922	3041.9575
3043.9928	3047.9518	3053.4121
3054.8155	3061.3947	3062.0017
3075.1582	3079.3566	3081.2019
3094.8169	3097.9596	3099.3748
3104.2857	3111.4085	3112.6274
3119.8550	3131.0241	3143.6973
3151.3593	3210.8203	3212.1880
3214.5089	3214.6383	3222.8538
3263.0753	3263.4375	3264.7315
3266.3618	3286.1551	3286.8038
3287.7095	3289.3269	3630.7992

II.C.7. QM frequencies for the transition structure with 6 $\beta$ -d<sub>1</sub>-tetsosterone of the <sup>4</sup>A state

Frequencies:		
-1260.5064	7.5957	13.4204
18.0187	33.5540	36.7371
40.4929	54.1745	57.5014
58.4635	70.8531	94.7147
101.1017	104.1902	115.4026
131.1764	144.4556	154.1100
156.1360	159.7367	164.5154
183.0703	197.0411	207.2391
210.5482	218.6346	223.4672
224.5986	232.2273	235.0140
244.2237	264.7724	271.1221
275.6474	278.6873	283.9839
287.9706	288.2247	297.8494
302.0310	314.5955	322.4078
328.8987	334.8598	341.5798
363.3140	367.8897	372.5232
373.6760	378.7250	383.8426
398.4854	417.4950	423.3913
424.1304	435.9926	436.9313
439.4068	442.2293	443.2584
459.8987	472.3072	486.4811
504.4479	518.9011	524.2825
553.6248	560.1388	575.8537
585.3516	602.8514	621.2184
644.6903	656.5465	679.2374
680.3199	683.0900	691.0691
694.9966	700.9484	719.4646
724.6316	727.9197	728.8978
735.0381	737.8927	761.0897
761.4602	765.4166	766.0223
790.4151	799.8157	810.3018
811.5622	813.6281	820.3421
828.0128	833.2716	834.0691
846.1339	849.3643	851.8846
853.5434	855.0751	877.8173
900.2794	908.3842	912.7883
914.7766	918.6055	929.8161
934.1319	940.7423	950.4498
950.5025	951.7246	955.8659
961.4312	973.4307	982.0024
989.3984	998.2492	1015.1405
1019.2646	1022.3824	1023.8577
1028.7976	1033.1001	1037.9078
1047.3363	1049.6773	1059.5919
1059.8707	1060.6903	1062.5189
1076.6448	1078.6397	1085.5974
1100.6345	1116.7204	1117.0165
1119.3940	1122.5397	1123.0842
1134.2976	1146.8668	1151.9447
1171.4034	1171.8324	1175.7083
1189.0565	1191.8151	1197.8594
1202.8702	1214.5641	1217.1345
1235.4434	1242.6450	1244.5957
1255.5685	1262.3449	1272.2831
1278.4431	1294.8008	1295.4655
1297.6962	1306.9938	1315.4613
1321.7138	1331.6335	1336.7764
1339.5339	1345.4616	1352.9181
1353.4126	1357.6376	1362.7365
1376.2500	1378.6098	1387.1306
1387.9809	1389.3659	1395.0731
1398.3692	1400.6798	1409.1547
1412.0368	1416.1915	1420.2947
1424.2031	1429.5788	1431.5807
1436.4428	1437.1798	1452.5785
1462.3693	1500.4818	1501.7691
1505.3681	1509.9322	1524.6424

1529.5958	1533.7298	1536.2802
1539.2743	1540.0975	1545.2647
1550.4599	1556.0035	1558.7090
1562.3081	1564.5669	1575.0397
1592.3650	1594.2708	1617.0813
1628.2103	1638.1093	1642.6658
1644.1129	1714.7154	2505.8020
2953.4366	2964.9448	2977.2232
3019.7261	3033.0902	3041.9561
3043.9904	3047.9531	3053.4130
3054.8108	3061.3967	3062.0013
3075.1578	3079.3620	3081.1915
3094.8172	3097.9558	3099.3748
3104.2860	3111.2533	3112.6290
3119.8548	3131.0236	3143.6961
3151.3600	3210.8126	3212.1911
3214.5093	3214.6378	3222.8725
3263.0736	3263.4381	3264.7226
3266.3576	3286.1542	3286.8025
3287.7090	3289.3281	3630.8026

III. Input geometries (in Å), absolute energy (in a.u.), and frequencies ( $\text{cm}^{-1}$ ) of the supplementary Shepard points in the MCMM calculations for  $6\beta$ -H abstraction for testosterone (and  $6\beta$ -D abstraction of  $6\beta$ - $d_1$ -testosterone) by Compound I. The QM level of theory was B3LYP/6-31G

Note: For each reaction, the MCMM surface was constructed by using the MM reactant-complex, MM product-complex, the saddle point (P0), and 17 supplementary Shepard points (P1 – P17).

The points (P1 – P17) were located according to the following protocol, where MCMM- $\alpha$  referred to the MCMM calculation using the Shepard points P0 – P $\alpha$ . ( $\alpha = 0, 1, 2, \dots$ )

P0 is the saddle point ( $s = 0$  where the barrier height is  $V_a^\ddagger$ ).

P1 is at the  $(7/8)V_a^\ddagger$  position along the MCMM-0 MEP down towards the reactant.

P2 is at the  $(7/8)V_a^\ddagger$  position along the MCMM-1 MEP down towards the product.

P3 is at the  $(6/8)V_a^\ddagger$  position along the MCMM-2 MEP down towards the reactant.

P4 is at the  $(6/8)V_a^\ddagger$  position along the MCMM-3 MEP down towards the product.

P5 is at the  $(4/8)V_a^\ddagger$  position along the MCMM-4 MEP down towards the reactant.

P6 is at the  $(4/8)V_a^\ddagger$  position along the MCMM-4 MEP down towards the product.

P7 is at the  $(2/8)V_a^\ddagger$  position along the MCMM-6 MEP down towards the reactant.

P8 is at the  $(2/8)V_a^\ddagger$  position along the MCMM-6 MEP down towards the product.

P9 is at the  $V_a^G$  peak in the MCMM-8 calculation.

P10 is added to smooth the MCMM-9  $V_a^G$  profile.

P11 – P14 are added to smooth the MCMM-10  $V_a^G$  profile.

P15 – P17 are at the concave side of the potential energy surface (for performing the LCT calculations). Their locations are determined by the MCMM-10  $V_a^G$  profile through the assistant points (P15<sub>H</sub>/P15<sub>L</sub>, P16<sub>H</sub>/P16<sub>L</sub>, and P17<sub>H</sub>/P17<sub>L</sub>), which are located on the MCMM-10 MEP.

- P15 is at the midpoint of the line connecting P15<sub>H</sub> and P15<sub>L</sub>, where  
P15<sub>H</sub>:  $V_a^G(s) = 0.50 V_a^{\text{RG}} + 0.50 V_a^{\ddagger\text{G}}$  and P15<sub>L</sub>:  $V_a^G(s) = 0.50 V_a^{\text{PG}} + 0.50 V_a^{\ddagger\text{G}}$
- P16 is on the line connecting P16<sub>H</sub> and P16<sub>L</sub> and is  $1/4$  of the way starting from P16<sub>H</sub>, where  
P16<sub>H</sub>:  $V_a^G(s) = 0.75 V_a^{\text{RG}} + 0.25 V_a^{\ddagger\text{G}}$  and P16<sub>L</sub>:  $V_a^G(s) = 0.75 V_a^{\text{PG}} + 0.25 V_a^{\ddagger\text{G}}$
- P17 is on the line connecting P17<sub>H</sub> and P17<sub>L</sub> and is  $3/4$  of the way starting from P17<sub>H</sub>, where  
P17<sub>H</sub>:  $V_a^G(s) = 0.75 V_a^{\text{RG}} + 0.25 V_a^{\ddagger\text{G}}$  and P17<sub>L</sub>:  $V_a^G(s) = 0.75 V_a^{\text{PG}} + 0.25 V_a^{\ddagger\text{G}}$

Here,  $V_a^{\text{RG}}$ ,  $V_a^{\text{PG}}$ , and  $V_a^{\ddagger\text{G}}$  denote the corresponding  $V_a^G(s)$  values on the reactants, products, and saddle point, respectively.

The reaction coordinate values ( $s$ ) along the MEP for P1 – P14, P15<sub>H</sub>, P15<sub>L</sub>, P16<sub>H</sub>, P16<sub>L</sub>, P17<sub>H</sub>, and P17<sub>L</sub> are tabulated in Section III.A.

III.A. Mass-scaled reactant coordinate ( $s$ , in a.u.) of the supplementary Shepard points in the MCOMM calculations for the testosterone H abstraction by the Cpd 1.

	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10
(H; $^2A$ ) <sup>a</sup>	-0.200	0.165	-0.415	0.275	-0.830	0.445	-1.505	0.490	-0.500	-1.150
(D; $^2A$ ) <sup>b</sup>	-0.260	0.220	-0.500	0.365	-0.905	0.560	-1.655	0.650	-0.050	-1.250
(H; $^4A$ ) <sup>c</sup>	-0.200	0.160	-0.350	0.265	-0.710	0.410	-1.315	0.640	-0.450	-1.000
(D; $^4A$ ) <sup>d</sup>	-0.250	0.215	-0.450	0.350	-0.805	0.530	-1.415	0.755	-0.050	-1.100

	P11	P12	P13	P14	P15 <sub>H</sub>	P15 <sub>L</sub>	P16 <sub>H</sub>	P16 <sub>L</sub>	P17 <sub>H</sub>	P17 <sub>L</sub>
(H; $^2A$ ) <sup>a</sup>	-0.290	-0.100	-0.510	-0.560	-1.970	0.470	-2.350	0.490	-2.350	-0.490
(D; $^2A$ ) <sup>b</sup>	-0.120	-0.250	-0.460	-0.670	-2.000	0.650	-2.300	0.650	-2.300	0.650
(H; $^4A$ ) <sup>c</sup>	-0.540	-0.580	-0.480	-0.320	-1.620	0.700	-1.840	0.750	-1.840	0.750
(D; $^4A$ ) <sup>d</sup>	-0.260	-0.110	-0.470	-0.600	-1.600	0.900	-1.910	0.950	-1.910	0.950

<sup>a</sup> H abstraction at 6 $\beta$  position of testosterone by Cpd 1 of the  $^2A$  state.

<sup>b</sup> D abstraction at 6 $\beta$  position of 6 $\beta$ - $d_1$ -testosterone by Cpd 1 of the  $^2A$  state.

<sup>c</sup> H abstraction at 6 $\beta$  position of testosterone by Cpd 1 of the  $^4A$  state.

<sup>d</sup> D abstraction at 6 $\beta$  position of 6 $\beta$ - $d_1$ -testosterone by Cpd 1 of the  $^4A$  state.

### III.B. Geometries, QM energy, and QM frequencies of the supplementary Shepard points in the MCMM calculations for testosterone H-abstraction by Cpd I of the $^2A$ state

#### III.B.1. Point P1

Absolute energy: -2476.5986404			
Geometry:			
C	.465061	3.336803	-1.228043
C	.494819	4.608973	-.528253
C	1.552718	4.785372	.548010
C	5.447123	-.855850	.191526
O	-.352053	5.506841	-.763778
C	2.723354	3.799717	.396278
C	2.276966	2.317015	.226523
C	3.524035	1.438541	-.182614
C	3.122627	-.017181	-.582844
C	2.142764	.016366	-1.770977
C	.966718	.959397	-1.548318
C	1.226314	2.250383	-.895626
C	4.668183	1.472241	.870396
C	5.882498	.587793	.496397
C	4.389008	-.809591	-.943929
C	4.945111	-1.558435	1.475102
C	1.619042	1.807017	1.543085
C	6.522819	-1.747449	-.492240
C	5.701133	-2.863695	-1.208703
C	4.265448	-2.281815	-1.413884
O	7.578374	-2.243992	.371009
S	-4.528971	-.892406	.693537
Fe	-2.125056	-.636919	.107095
C	-2.561103	-1.394888	-3.199822
C	-2.715591	2.689703	-.573782
C	-1.853613	.102645	3.446885
C	-1.749202	-3.976943	.831332
N	-2.544929	.431480	-1.544947
C	-2.665788	-.060104	-2.836436
C	-2.935945	1.023016	-3.754727
C	-2.983636	2.171316	-3.016092
C	-2.744858	1.797919	-1.640263
N	-2.319731	1.043538	1.213029
C	-2.521713	2.337140	.752520
C	-2.477159	3.268093	1.856989
C	-2.238068	2.537198	2.985674
C	-2.129679	1.151911	2.584871
N	-1.863685	-1.725351	1.803707
C	-1.739536	-1.233301	3.087125
C	-1.488594	-2.320235	4.011685
C	-1.465712	-3.470293	3.278463
C	-1.696800	-3.095716	1.898776
N	-2.164256	-2.342890	-.965298
C	-1.962564	-3.625612	-.497341
C	-2.004229	-4.564845	-1.595898
C	-2.229969	-3.839911	-2.731422
C	-2.328176	-2.453943	-2.332121
O	-.383427	-.521964	.014465
H	3.317201	4.084983	-.485369
H	3.928360	1.902047	-1.101878
H	2.618177	-.505405	.263176
H	2.694147	.336047	-2.673105
H	1.760694	-.992010	-1.976474
H	.255590	.338574	-.783164
H	.322129	1.054711	-2.429293
H	-.266849	3.257861	-2.027491
H	1.903235	5.824908	.520967
H	1.059753	4.656827	1.523681
H	4.283520	1.154962	1.848236
H	5.017444	2.504584	.999451
H	6.376432	1.005144	-.395455

H	4.110332	-1.026542	1.941250
H	1.245575	.783689	1.440523
H	.759168	2.431103	1.811120
H	7.062220	-1.141789	-1.230052
H	6.175192	-3.155726	-2.152639
H	5.677675	-3.763952	-.578248
H	3.527640	-2.823560	-.806969
H	3.935844	-2.354191	-2.456638
H	4.869043	-.257201	-1.773960
H	5.757406	-1.602120	2.212649
H	4.603960	-2.583204	1.281761
H	2.332089	1.845894	2.375035
H	3.383618	3.889088	1.267129
H	6.625241	.608445	1.306184
H	7.215247	-2.905594	.990150
H	-4.972754	.332745	.238169
H	-2.678784	-1.633005	-4.253552
H	-2.827785	3.746541	-.798362
H	-1.726734	.346385	4.498152
H	-1.608899	-5.032356	1.048422
H	-3.077177	.906275	-4.821344
H	-3.168900	3.181888	-3.355785
H	-2.603812	4.338352	1.760768
H	-2.139089	2.891482	4.003475
H	-1.358408	-2.203010	5.079608
H	-1.311325	-4.483816	3.624971
H	-1.878037	-5.635150	-1.497590
H	-2.325281	-4.198118	-3.748156

## Frequencies:

-779.4897	7.6375	13.9170
16.5652	30.1239	37.0823
38.1624	52.9735	57.8280
59.5040	64.8876	75.0590
91.4401	98.6653	115.3781
119.5389	135.5551	145.5381
153.5966	156.0700	166.9723
174.7779	193.0981	202.3102
208.0862	214.8899	219.4883
225.4123	231.5671	235.6027
245.6356	267.6527	270.5622
274.8422	280.0804	281.2960
283.2003	286.9367	298.8396
300.2603	304.4786	306.7671
316.6138	319.9516	334.6561
360.4568	369.8397	370.6491
374.1124	381.7998	384.7087
400.9363	411.9984	416.0302
424.2483	434.5460	436.6130
438.6338	440.2605	444.5920
457.6542	472.8915	486.4617
501.5920	515.4964	519.8097
546.0379	560.1767	562.6351
577.5010	604.7817	623.6440
650.8078	661.4842	679.3748
680.0926	689.8561	690.0249
691.1160	704.9622	727.1991
728.1514	731.7305	736.9597
743.7000	762.4033	766.7654
768.0559	768.3783	802.0789
809.2258	817.7748	819.0453
820.1777	824.7883	828.7104
835.2358	836.1079	851.8721
853.1472	856.5386	860.8310
882.6918	910.5464	913.1944
924.7589	927.1518	931.2449
936.1379	942.2396	949.7042
954.1944	959.9372	960.3353
965.7337	968.3823	974.1013
984.6136	988.2864	997.8340
1012.0528	1020.7721	1023.2455



1025.7886	1026.9277	1035.9644
1039.3419	1042.7437	1050.7215
1055.6464	1060.8704	1061.4221
1064.2616	1070.7024	1078.4755
1079.9830	1087.8030	1103.3717
1121.8825	1122.3615	1124.3369
1128.0088	1130.2141	1137.7666
1151.4880	1160.3964	1174.0507
1176.9858	1182.9937	1195.3175
1196.8294	1202.6591	1216.9736
1220.4192	1236.2280	1243.5770
1249.1270	1250.9358	1258.7475
1269.0229	1282.2095	1295.1990
1298.3864	1300.9480	1304.2742
1308.4576	1311.3871	1322.3911
1327.0131	1334.9079	1344.6499
1347.2317	1351.4804	1353.2092
1359.1285	1364.2598	1375.6140
1380.4789	1389.6860	1390.6584
1392.0667	1395.8841	1400.1807
1401.6398	1410.8343	1415.9975
1416.2276	1420.1748	1422.8373
1426.7316	1431.4631	1437.9508
1439.3629	1440.0048	1455.8677
1465.6059	1499.9823	1501.4527
1503.8747	1511.3783	1530.1425
1530.9365	1535.7938	1536.2369
1537.8679	1542.0911	1546.8645
1551.7179	1558.4422	1560.3937
1563.2317	1566.1332	1592.2247
1593.7239	1606.5888	1616.1009
1632.6370	1644.3105	1646.8982
1657.2409	1715.6076	2518.5246
2948.5635	2959.1076	2979.4579
3011.0794	3023.3323	3031.8771
3033.4546	3037.9706	3042.6722
3044.9661	3050.3087	3051.0645
3063.4495	3066.9043	3069.8713
3082.3185	3085.0939	3086.9447
3088.8022	3091.6119	3101.5994
3107.4829	3118.8798	3132.0376
3140.0787	3193.3247	3197.2210
3197.5214	3198.4857	3208.5772
3245.0241	3245.1602	3246.6386
3247.6830	3268.2033	3268.4906
3269.5947	3270.7196	3662.0541

## III.B.2. Point P2

Absolute energy: -2476.5986503

Geometry:

C	.463173	3.337137	-1.228742
C	.495516	4.609270	-.527757
C	1.552699	4.785385	.548065
C	5.447086	-.855740	.191557
O	-.352381	5.507111	-.763989
C	2.723353	3.799728	.396018
C	2.277214	2.316682	.226704
C	3.524134	1.438616	-.182561
C	3.122813	-.017229	-.582647
C	2.140238	.015262	-1.768283
C	.974015	.967348	-1.553159
C	1.225615	2.244438	-.895140
C	4.668211	1.472244	.870456
C	5.882572	.587810	.496400
C	4.388962	-.809614	-.944087
C	4.945066	-1.558479	1.475148
C	1.619043	1.807002	1.543213
C	6.522623	-1.747481	-.492339
C	5.701081	-2.863693	-1.208783
C	4.265363	-2.281909	-1.413952
O	7.578517	-2.243967	.371025
S	-4.528825	-.892439	.693604
Fe	-2.127454	-.636900	.107061
C	-2.561134	-1.395038	-3.200276
C	-2.715565	2.690237	-.573886
C	-1.853475	.102718	3.447301
C	-1.749117	-3.977317	.831504
N	-2.543752	.431296	-1.544437
C	-2.665782	-.060240	-2.836813
C	-2.936081	1.023375	-3.755475
C	-2.983760	2.171855	-3.016769
C	-2.744920	1.798278	-1.640332
N	-2.319375	1.043126	1.212412
C	-2.521832	2.337507	.752425
C	-2.477157	3.268816	1.857360
C	-2.238041	2.537775	2.986148
C	-2.129635	1.151813	2.585240
N	-1.862920	-1.725012	1.803117
C	-1.739453	-1.233282	3.087148
C	-1.488440	-2.320780	4.012478
C	-1.465558	-3.470789	3.279284
C	-1.696712	-3.095827	1.898758
N	-2.163761	-2.342349	-.965009
C	-1.962515	-3.625733	-.497241
C	-2.004192	-4.565540	-1.596297
C	-2.229959	-3.840592	-2.731926
C	-2.328218	-2.453950	-2.332406
O	-.372206	-.516686	.009511
H	3.317353	4.085083	-.485212
H	3.928358	1.902206	-1.101670
H	2.617881	-.505341	.262356
H	2.687861	.338049	-2.673229
H	1.760117	-.992636	-1.976537
H	.161591	.240843	-.686373
H	.303377	1.042884	-2.414092
H	-.268995	3.258027	-2.027021
H	1.902768	5.824617	.520888
H	1.059721	4.656876	1.523298
H	4.283503	1.155038	1.847859
H	5.017150	2.504316	.999223
H	6.376374	1.004901	-.395300
H	4.110587	-1.026804	1.941214
H	1.244733	.784300	1.440062
H	.759124	2.430683	1.810909
H	7.063050	-1.142104	-1.229065

H	6.175091	-3.155790	-2.152199
H	5.677871	-3.763502	-.578364
H	3.527774	-2.823360	-.807283
H	3.935927	-2.354530	-2.456395
H	4.869424	-.257141	-1.773728
H	5.757464	-1.601897	2.212027
H	4.603988	-2.582838	1.281728
H	2.331988	1.846449	2.374702
H	3.383111	3.888530	1.266571
H	6.624923	.608546	1.305955
H	7.215406	-2.906044	.990730
H	-4.972910	.333516	.237685
H	-2.679055	-1.633102	-4.253638
H	-2.828714	3.746609	-.798325
H	-1.726904	.346400	4.498260
H	-1.609031	-5.032449	1.048408
H	-3.077556	.906064	-4.821496
H	-3.169518	3.182054	-3.355767
H	-2.604298	4.338481	1.760769
H	-2.139338	2.891274	4.003715
H	-1.358496	-2.203018	5.079860
H	-1.311436	-4.484047	3.625088
H	-1.878120	-5.635283	-1.497392
H	-2.325435	-4.198090	-3.748358

## Frequencies:

-1493.5397	10.2967	13.7796
19.7918	37.0740	38.6134
45.4695	53.3138	58.5477
60.0136	72.8856	74.6508
92.0199	100.4791	115.3050
125.6629	134.8911	139.3734
151.6876	155.1749	164.3220
174.4056	193.4857	202.0813
210.5227	214.0755	219.3841
226.1330	230.7205	234.9508
247.6902	269.8705	270.0270
275.0724	279.8226	281.9869
283.0325	288.0421	296.1500
297.9468	304.5282	312.0505
317.7469	324.6606	334.5375
361.8996	368.8339	369.9942
373.0902	381.2455	384.6798
400.0078	410.5225	417.5319
424.2710	433.6776	436.3159
438.8199	440.4503	443.0858
464.0391	477.2409	486.8005
508.3900	520.1363	545.1821
554.5886	561.8934	565.1033
581.2132	621.2699	635.4004
662.2954	666.9683	679.3271
680.0779	684.5512	690.0641
690.4619	691.3650	704.2073
727.5431	727.9561	731.8956
736.8682	742.7882	761.9925
767.3094	767.8388	768.2524
803.2443	806.7932	815.5003
817.4138	819.4222	825.8646
828.1922	834.7849	835.6073
851.3422	852.9705	855.8154
863.7105	890.8019	904.8082
910.3378	921.6473	924.3054
934.8889	937.6647	939.6183
946.0516	953.6921	956.7389
957.0490	962.5219	968.7978
975.7695	986.1971	994.6592
1003.7769	1018.6983	1021.7874
1023.7008	1025.1502	1027.3851
1034.5140	1038.7628	1048.5609
1050.4839	1058.4040	1059.5182
1061.7261	1063.4427	1072.6372

1078.1856	1085.1214	1096.0896
1102.9809	1119.7620	1120.3452
1122.4253	1125.9913	1129.3010
1142.5312	1151.6974	1159.5804
1172.9554	1176.2388	1192.5354
1194.0801	1196.7133	1199.7046
1213.0359	1218.3072	1230.2505
1243.5412	1247.0765	1253.9986
1262.7909	1271.0201	1278.7121
1295.9731	1298.5171	1301.8955
1307.9490	1309.2625	1313.7169
1316.3115	1323.4138	1333.3454
1338.3174	1346.7154	1350.0476
1351.6670	1359.1006	1363.9622
1378.1238	1380.0979	1388.7517
1390.1349	1390.5162	1395.7009
1399.5100	1401.3878	1410.6692
1414.2601	1417.5671	1420.9697
1425.1625	1429.2650	1431.1128
1438.3172	1438.9293	1455.6756
1466.2832	1499.2890	1500.6005
1503.0685	1510.9607	1518.4855
1530.6577	1534.9502	1535.2886
1537.5451	1541.5967	1546.5182
1551.5567	1557.9541	1559.3250
1563.0025	1565.8598	1583.8466
1591.5257	1593.1707	1608.5857
1616.0080	1637.9248	1643.8138
1646.2256	1714.7442	2511.5928
2948.7188	2959.2557	2967.1391
3013.8841	3025.7849	3036.0123
3037.4939	3041.5726	3046.2587
3051.1324	3054.1099	3055.7609
3067.5105	3070.6892	3075.5109
3087.2537	3088.7776	3091.1891
3096.5973	3105.6219	3111.3698
3115.5461	3122.3061	3135.7115
3143.0248	3199.7780	3200.1744
3201.1188	3201.6609	3211.3244
3249.2318	3249.4012	3250.5983
3251.7945	3272.5805	3272.8248
3273.6439	3274.8844	3653.5752

## III.B.3. Point P3

Absolute energy: -2476.6009496

Geometry:

C	.466712	3.337480	-1.227758
C	.494378	4.608704	-.528472
C	1.552727	4.785394	.547981
C	5.447202	-.855928	.191506
O	-.351972	5.506767	-.763577
C	2.723498	3.799816	.396726
C	2.276830	2.317630	.226375
C	3.523920	1.438482	-.182653
C	3.122508	-.017112	-.583164
C	2.145966	.017619	-1.774105
C	.965483	.957413	-1.549802
C	1.228392	2.255800	-.896807
C	4.668145	1.472271	.870368
C	5.882461	.587775	.496414
C	4.389062	-.809572	-.943676
C	4.945151	-1.558428	1.475101
C	1.618994	1.807010	1.542910
C	6.522914	-1.747403	-.492210
C	5.701181	-2.863732	-1.208651
C	4.265523	-2.281733	-1.413812
O	7.578289	-2.243994	.370972
S	-4.529257	-.892321	.693500
Fe	-2.121990	-.637155	.107256
C	-2.561100	-1.394764	-3.199417
C	-2.715685	2.689217	-.573605
C	-1.853708	.102629	3.446559
C	-1.749272	-3.976633	.831209
N	-2.546041	.431429	-1.545142
C	-2.665819	-.060090	-2.836106
C	-2.935837	1.022727	-3.754182
C	-2.983533	2.170937	-3.015549
C	-2.744823	1.797587	-1.640116
N	-2.320166	1.043451	1.213469
C	-2.521706	2.336932	.752407
C	-2.477161	3.267578	1.856690
C	-2.238091	2.536812	2.985340
C	-2.129716	1.151899	2.584742
N	-1.865012	-1.725561	1.804117
C	-1.739746	-1.233165	3.087146
C	-1.488686	-2.319800	4.011092
C	-1.465802	-3.469904	3.277818
C	-1.697030	-3.095696	1.898659
N	-2.164793	-2.343149	-.965379
C	-1.962642	-3.625454	-.497359
C	-2.004250	-4.564375	-1.595628
C	-2.229968	-3.839419	-2.731086
C	-2.328187	-2.453811	-2.331912
O	-.398224	-.528807	.020972
H	3.316982	4.084772	-.485195
H	3.928210	1.901843	-1.101947
H	2.617912	-.505276	.262989
H	2.701439	.334302	-2.673875
H	1.762362	-.990809	-1.977258
H	.287098	.383364	-.822763
H	.342872	1.067686	-2.445551
H	-.264224	3.257806	-2.027961
H	1.903321	5.824882	.520909
H	1.059852	4.656931	1.523738
H	4.283642	1.154993	1.848301
H	5.017546	2.504529	.999610
H	6.376327	1.005167	-.395426
H	4.110351	-1.026433	1.941008
H	1.246278	.783449	1.440224
H	.759352	2.431197	1.811194
H	7.061706	-1.141735	-1.230393

H	6.175181	-3.155645	-2.152627
H	5.677701	-3.764085	-.578318
H	3.527720	-2.823547	-.806945
H	3.935794	-2.353823	-2.456459
H	4.868775	-.257257	-1.773864
H	5.757200	-1.602229	2.212924
H	4.603991	-2.583203	1.281774
H	2.332085	1.845362	2.374860
H	3.383974	3.889735	1.267429
H	6.625289	.608410	1.306131
H	7.214834	-2.905660	.990077
H	-4.973606	.332748	.238730
H	-2.678363	-1.632788	-4.253110
H	-2.826471	3.746083	-.798324
H	-1.726448	.346378	4.497665
H	-1.608652	-5.031902	1.048296
H	-3.076599	.906330	-4.820754
H	-3.168065	3.181415	-3.355437
H	-2.603195	4.337769	1.760543
H	-2.138801	2.891377	4.002863
H	-1.358243	-2.202843	5.078872
H	-1.311168	-4.483189	3.624492
H	-1.877938	-5.634558	-1.497639
H	-2.325067	-4.197792	-3.747632

## Frequencies:

-123.6943	-18.8232	8.5611
11.1322	19.8139	34.5529
36.0186	52.4466	55.6406
57.9940	59.1924	80.0841
92.2242	96.8777	114.8480
121.2589	132.6494	145.5633
153.1612	160.9206	169.9394
189.3701	201.3996	201.8283
210.6981	215.4153	219.3862
224.0432	230.8393	240.5586
251.9629	268.3014	272.2218
277.4663	279.6671	281.3349
284.7877	288.4640	298.2661
301.0622	307.0108	308.2624
315.6719	334.4150	342.4849
360.6851	370.9849	374.4892
374.8320	382.1641	385.4731
400.6423	412.5814	418.2346
424.3897	434.6387	436.7697
439.2143	440.4362	446.6074
455.0731	470.7272	486.1806
496.1385	510.0540	519.1979
540.8230	556.4712	562.1574
577.1454	589.3752	623.1031
647.7905	661.2924	679.0553
679.8057	689.4976	689.6230
690.6757	702.3864	727.2854
727.7754	731.5081	737.0391
743.6394	762.5251	766.2246
768.2010	768.4977	801.0116
809.0605	817.7110	818.8696
820.0996	824.1543	828.5860
835.5025	836.3680	851.8645
853.2193	856.3745	858.5382
883.8219	910.2821	913.2987
924.9870	927.5477	932.7648
936.1012	942.8226	949.8292
954.5311	960.1443	960.5982
966.3825	969.0263	976.5372
987.2514	994.2569	1004.4986
1021.6792	1023.7411	1026.5384
1027.7355	1030.8582	1037.0144
1039.6090	1050.1347	1052.1733
1061.8128	1062.2629	1064.0327
1066.9422	1077.9136	1080.8314

1087.7722	1102.8932	1122.0303
1122.4741	1124.3857	1128.1171
1130.3191	1137.7454	1150.8360
1160.5406	1170.5569	1176.8846
1182.1954	1196.4127	1197.6907
1200.4350	1215.1367	1221.2485
1237.7025	1240.4882	1244.1582
1249.8221	1258.4596	1266.9431
1283.0891	1292.0767	1296.4376
1301.8703	1304.8303	1307.8890
1310.4380	1321.5305	1327.5499
1333.7859	1337.8230	1346.9629
1352.1559	1353.8625	1358.9016
1364.6951	1377.6293	1379.9612
1389.9546	1391.4702	1393.3045
1395.6884	1400.0670	1401.9837
1410.8800	1416.3830	1416.7352
1420.1249	1427.2273	1428.8624
1431.9090	1433.8641	1438.8909
1441.1331	1455.6473	1464.5773
1500.5486	1502.0319	1504.2956
1511.3796	1530.7828	1532.6681
1535.8469	1537.0199	1537.8367
1542.0816	1546.7693	1551.6107
1558.2315	1560.6833	1563.1767
1566.0826	1592.7199	1594.1165
1606.1741	1616.4137	1627.8074
1645.2477	1647.6771	1662.2011
1716.5822	2049.2509	2519.4486
2949.1882	2959.7248	2986.3482
3011.2078	3023.5622	3031.4402
3033.2606	3037.8328	3042.5369
3043.1521	3050.3306	3050.8840
3063.3647	3067.1083	3068.5864
3078.5867	3081.8390	3085.5171
3086.8325	3091.1436	3101.4470
3107.6611	3119.0558	3132.2350
3140.0182	3192.6156	3198.3882
3198.7054	3199.5841	3209.6584
3246.5204	3246.6596	3248.2602
3249.2518	3269.6244	3269.9090
3271.1687	3272.2519	3660.1051

## III.B.4. Point P4

Absolute energy: -2476.6009357

Geometry:

C	.462361	3.337259	-1.229139
C	.495939	4.609379	-.527414
C	1.552703	4.785420	.548101
C	5.447091	-.855670	.191563
O	-.352649	5.507359	-.764095
C	2.723413	3.799764	.395949
C	2.277331	2.316608	.226759
C	3.524192	1.438637	-.182537
C	3.122885	-.017266	-.582592
C	2.139356	.014842	-1.767369
C	.977507	.971119	-1.555752
C	1.225524	2.242044	-.895067
C	4.668222	1.472286	.870521
C	5.882652	.587823	.496413
C	4.388935	-.809614	-.944142
C	4.945028	-1.558532	1.475222
C	1.619008	1.806963	1.543332
C	6.522459	-1.747472	-.492444
C	5.701059	-2.863730	-1.208845
C	4.265298	-2.281975	-1.414008
O	7.578654	-2.243917	.371006
S	-4.528762	-.892456	.693634
Fe	-2.128310	-.636946	.107090
C	-2.561165	-1.395129	-3.200557
C	-2.715587	2.690555	-.573910
C	-1.853390	.102775	3.447562
C	-1.749064	-3.977561	.831617
N	-2.543160	.431071	-1.544003
C	-2.665779	-.060405	-2.837055
C	-2.936182	1.023611	-3.755997
C	-2.983860	2.172238	-3.017215
C	-2.744957	1.798538	-1.640317
N	-2.319184	1.042663	1.211991
C	-2.521932	2.337806	.752236
C	-2.477171	3.269333	1.857614
C	-2.238029	2.538197	2.986495
C	-2.129594	1.151698	2.585562
N	-1.862693	-1.724713	1.802618
C	-1.739443	-1.233138	3.087263
C	-1.488332	-2.321101	4.013017
C	-1.465448	-3.471143	3.279801
C	-1.696695	-3.096030	1.898672
N	-2.163508	-2.341874	-.964710
C	-1.962482	-3.625860	-.497106
C	-2.004163	-4.566052	-1.596559
C	-2.229953	-3.841054	-2.732297
C	-2.328265	-2.453882	-2.332656
O	-.369223	-.515774	.008604
H	3.317159	4.084895	-.484842
H	3.928129	1.902160	-1.101386
H	2.617865	-.505124	.261719
H	2.685677	.338431	-2.672946
H	1.759937	-.992351	-1.976324
H	.129279	.212302	-.656071
H	.296894	1.038754	-2.408126
H	-.269367	3.258290	-2.026645
H	1.902249	5.824072	.520816
H	1.059794	4.656971	1.522781
H	4.283630	1.155180	1.847349
H	5.016848	2.503785	.999076
H	6.376163	1.004574	-.394988
H	4.111070	-1.027113	1.940910
H	1.244588	.784999	1.439673
H	.759501	2.430316	1.810580
H	7.063611	-1.142561	-1.227981



H	6.174869	-3.155754	-2.151497
H	5.678135	-3.762963	-.578634
H	3.528090	-2.823038	-.807723
H	3.936041	-2.354635	-2.455728
H	4.869511	-.257193	-1.773332
H	5.757284	-1.601718	2.211367
H	4.604105	-2.582268	1.281697
H	2.331787	1.846711	2.374144
H	3.382653	3.888240	1.265981
H	6.624495	.608622	1.305543
H	7.215110	-2.906911	.991610
H	-4.973459	.334589	.237275
H	-2.679077	-1.633007	-4.253150
H	-2.828821	3.746105	-.798197
H	-1.727000	.346308	4.497759
H	-1.609127	-5.031950	1.048276
H	-3.077567	.905885	-4.820872
H	-3.169584	3.181550	-3.355364
H	-2.604381	4.337835	1.760621
H	-2.139477	2.890800	4.003227
H	-1.358602	-2.202920	5.079263
H	-1.311575	-4.483555	3.624740
H	-1.878211	-5.634653	-1.497211
H	-2.325453	-4.197685	-3.747857

## Frequencies:

-870.9214	6.8708	11.0287
18.6746	35.8171	38.0659
44.8304	52.8433	57.3141
59.5057	72.0012	80.5787
92.3960	100.3884	114.6108
129.4135	132.5078	138.8752
154.9128	156.3856	165.1991
171.8977	191.3404	202.1311
209.4931	211.9235	218.6410
224.5132	229.9314	233.5167
246.9881	266.8477	271.0977
274.7688	279.3584	282.0109
282.8577	288.5645	295.3509
297.3088	304.1749	316.3609
327.5716	328.1073	337.3937
361.9711	368.7352	369.7870
372.1795	380.3036	384.3501
398.7759	410.1964	419.6099
424.6846	432.9479	435.9919
439.1468	440.1336	442.8610
463.4182	478.0723	486.4901
508.9253	519.6216	554.5990
557.4892	560.6965	572.8884
600.1531	621.7180	638.6031
662.9898	677.0096	678.9108
679.4171	688.3291	689.6782
690.2124	691.2488	704.0335
725.8232	726.2186	731.0410
735.9694	740.8565	761.3277
766.6774	767.2867	768.0342
802.6636	803.4902	811.5499
813.3457	818.7634	821.6779
826.5568	834.4632	835.2720
850.1989	852.5959	854.1875
861.7025	892.8011	900.7298
906.5059	917.9082	920.5156
932.6188	936.5387	937.7036
941.3026	951.8759	952.5896
953.1835	958.4961	965.0568
975.1447	983.3655	989.0393
995.3363	1006.5590	1017.0251
1020.5394	1022.0541	1024.3016
1033.1633	1035.4237	1039.5364
1050.0249	1054.1868	1056.7692
1057.9805	1062.7120	1066.8185

1076.8649	1078.9517	1087.5841
1101.9896	1117.0328	1117.6479
1119.7208	1123.2943	1127.8152
1140.3666	1151.5446	1156.7160
1171.7662	1175.4962	1185.4507
1190.0138	1191.6169	1197.8136
1209.2307	1216.4072	1223.8086
1242.7975	1245.0159	1252.4926
1261.3547	1269.7171	1277.3668
1295.2804	1296.6790	1300.3676
1307.6484	1312.2620	1314.2871
1321.8369	1330.9523	1336.7813
1345.6735	1348.1471	1349.7620
1358.2399	1361.0861	1372.0808
1379.0889	1386.6322	1388.0709
1389.1390	1394.9081	1398.5457
1400.6336	1408.4642	1411.9305
1416.6536	1420.6342	1422.4806
1425.6500	1428.0928	1436.5881
1438.5315	1448.4469	1454.5634
1465.6015	1498.3485	1499.7472
1502.0567	1510.4444	1515.8698
1530.0824	1533.7578	1534.6946
1536.9754	1541.0327	1545.9437
1550.9814	1557.4647	1558.1801
1562.4785	1565.2927	1587.6043
1590.6661	1592.1521	1607.8665
1615.3900	1630.1546	1643.4455
1645.8334	1714.4218	2503.0276
2951.4739	2961.2425	2966.7349
3018.5934	3030.7813	3041.1497
3043.2094	3047.0085	3051.7127
3056.7988	3060.1029	3061.7363
3073.6070	3077.1263	3082.3300
3093.6001	3095.5583	3097.4065
3103.1178	3111.6140	3117.9221
3127.6589	3128.1045	3142.0301
3148.8665	3206.9920	3207.4338
3208.3798	3210.3528	3218.8039
3259.5567	3259.7434	3260.8752
3262.0743	3282.8755	3283.1092
3283.8739	3285.1311	3636.1646

## III.B.5. Point P5

Absolute energy: -2476.6039399

Geometry:

C	.470396	3.341730	-1.228153
C	.493564	4.608769	-.528689
C	1.552655	4.785646	.548172
C	5.447446	-.856173	.191648
O	-.352024	5.506698	-.762873
C	2.724183	3.800573	.398171
C	2.277386	2.319345	.226133
C	3.523817	1.438672	-.182606
C	3.122664	-.016677	-.584243
C	2.154074	.020880	-1.781060
C	.971473	.961925	-1.561627
C	1.235286	2.264705	-.901115
C	4.668059	1.472229	.870301
C	5.882340	.587743	.496451
C	4.389429	-.809570	-.942892
C	4.945273	-1.558379	1.475083
C	1.618751	1.807151	1.541745
C	6.523358	-1.747331	-.492073
C	5.701345	-2.863765	-1.208466
C	4.265741	-2.281469	-1.413499
O	7.577950	-2.244051	.370877
S	-4.530507	-.891983	.693477
Fe	-2.115260	-.638389	.108115
C	-2.561063	-1.394470	-3.198263
C	-2.715777	2.687785	-.573167
C	-1.853948	.102621	3.445755
C	-1.749494	-3.975638	.830797
N	-2.548671	.431205	-1.545575
C	-2.666100	-.060088	-2.835112
C	-2.935359	1.021647	-3.752291
C	-2.982993	2.169628	-3.013596
C	-2.744859	1.796429	-1.639548
N	-2.321497	1.043590	1.214856
C	-2.521742	2.335787	.752449
C	-2.477056	3.265821	1.855609
C	-2.238098	2.535515	2.984226
C	-2.129975	1.151875	2.584242
N	-1.870046	-1.726665	1.806150
C	-1.740856	-1.233076	3.086844
C	-1.488832	-2.318536	4.009196
C	-1.465974	-3.468576	3.275859
C	-1.698230	-3.095118	1.898418
N	-2.166411	-2.344361	-.965940
C	-1.963004	-3.624714	-.497552
C	-2.004304	-4.562744	-1.594826
C	-2.229924	-3.837834	-2.729998
C	-2.328323	-2.453518	-2.331068
O	-.432004	-.545560	.037243
H	3.317683	4.085684	-.484126
H	3.928765	1.901889	-1.101949
H	2.615096	-.505277	.260466
H	2.717630	.333407	-2.676981
H	1.768482	-.987505	-1.984048
H	.292226	.420334	-.867646
H	.382313	1.093338	-2.478185
H	-.258813	3.260012	-2.030333
H	1.903875	5.825384	.520832
H	1.060112	4.657530	1.524536
H	4.283703	1.154965	1.848735
H	5.017896	2.504759	.999826
H	6.376300	1.005524	-.395553
H	4.109944	-1.026120	1.940744
H	1.247164	.782722	1.438533

H	.758842	2.430996	1.811515
H	7.060325	-1.141318	-1.231952
H	6.175250	-3.155417	-2.153135
H	5.677331	-3.764694	-.578308
H	3.527700	-2.823741	-.806564
H	3.935938	-2.352978	-2.456621
H	4.868949	-.257475	-1.773618
H	5.756761	-1.602532	2.214089
H	4.603973	-2.583569	1.281964
H	2.331770	1.843939	2.374384
H	3.384891	3.891716	1.269200
H	6.625617	.608344	1.306334
H	7.214252	-2.905085	.989301
H	-4.975912	.332610	.241659
H	-2.677306	-1.632436	-4.252503
H	-2.824296	3.745264	-.798265
H	-1.725272	.346547	4.497074
H	-1.607571	-5.031163	1.047940
H	-3.075298	.906527	-4.819671
H	-3.166295	3.180506	-3.354721
H	-2.602004	4.336771	1.760155
H	-2.138116	2.891611	4.001730
H	-1.357163	-2.202646	5.077503
H	-1.310122	-4.481892	3.623649
H	-1.877670	-5.633552	-1.497949
H	-2.324570	-4.197320	-3.746782

## Frequencies:

-32.9106	-27.9748	-14.2910
-4.5885	11.9141	30.4743
34.6948	47.5659	52.8354
54.9367	62.2335	88.2013
90.5896	102.7714	108.8164
125.6238	130.2122	142.2428
151.1202	159.3340	168.2573
189.5285	196.6463	200.0830
211.6467	215.7614	218.1179
223.6125	231.5135	235.3021
257.3174	264.8811	273.5656
279.3143	279.5360	281.2880
283.1565	291.6696	297.3628
301.0479	303.5205	308.0136
315.1783	334.5377	353.5921
360.2379	371.5496	374.6530
380.9592	382.6780	386.6109
401.7936	412.4304	418.1964
420.9432	434.9401	437.1717
439.6565	440.5959	444.0886
469.9809	479.5794	486.1857
509.0522	518.7789	526.8088
552.1487	562.4523	577.3842
583.5793	623.7440	646.8168
661.1038	662.5129	679.2840
680.0890	689.4541	690.1643
691.6163	700.6616	728.3564
728.8434	732.2128	738.5982
744.9513	763.4870	766.6164
769.4041	769.5654	801.3003
811.2188	819.9929	821.0805
822.5772	823.3334	831.1269
836.3560	837.0405	852.7141
853.8683	857.4224	858.0469
883.3029	911.4355	915.5183
927.2031	929.8914	932.5316
936.9143	944.8199	952.7571
954.5358	962.6087	963.3485
968.9721	969.6957	977.3547
988.0038	994.8305	1004.8134
1025.0396	1026.8195	1030.6592
1030.9025	1032.0187	1039.8007
1040.5951	1050.0568	1052.8753

1064.8037	1064.8778	1065.6771
1068.2608	1078.4996	1083.8839
1088.1326	1103.4447	1123.9013
1124.3668	1126.1802	1129.9758
1130.8555	1138.4145	1150.2843
1166.6412	1171.8733	1177.2541
1184.5175	1200.0152	1200.8274
1201.9399	1215.0294	1224.7550
1239.9160	1243.4098	1247.9325
1252.7813	1259.5001	1268.6458
1284.8619	1295.8383	1302.2034
1305.7848	1308.1605	1308.4962
1314.4444	1323.2247	1335.3140
1336.8306	1341.4370	1347.8377
1355.9271	1357.2487	1359.4241
1365.7590	1378.9760	1380.6161
1390.7406	1395.7421	1396.5651
1397.9632	1400.8858	1403.7847
1411.6380	1417.3770	1419.0793
1420.8293	1430.4057	1432.2272
1435.1333	1438.5319	1444.0954
1456.1734	1459.1060	1470.8696
1502.6599	1504.7750	1506.5021
1511.8498	1531.1256	1535.9560
1536.0877	1538.1608	1540.5485
1542.3293	1547.0104	1551.9118
1558.0325	1562.3424	1563.4790
1566.4025	1595.1429	1596.4308
1609.4039	1618.6947	1645.4875
1647.5809	1649.4534	1672.9330
1718.8106	2526.7128	2615.0462
2947.1675	2957.7163	2988.3118
3008.1290	3020.1657	3027.8599
3029.5250	3034.2831	3038.4964
3038.8608	3046.4692	3047.2121
3059.3405	3062.4580	3063.3400
3066.6334	3077.4331	3081.3410
3082.7507	3086.7959	3097.4808
3103.5479	3115.3033	3128.1844
3135.2609	3187.3135	3194.6921
3194.9444	3195.6876	3205.6423
3241.3560	3241.4996	3243.1854
3244.1327	3264.4566	3264.7138
3266.0816	3267.1108	3669.9862

## III.B.6. Point P6

Absolute energy: -2476.6044811

Geometry:

C	.461017	3.338163	-1.229072
C	.496212	4.609025	-.527462
C	1.552647	4.785342	.548110
C	5.447070	-.855671	.191573
O	-.352737	5.507396	-.764259
C	2.723349	3.799701	.395761
C	2.277510	2.316278	.226819
C	3.524226	1.438720	-.182489
C	3.122998	-.017286	-.582420
C	2.137737	.014250	-1.765651
C	.984666	.978661	-1.560830
C	1.225189	2.238044	-.895082
C	4.668237	1.472222	.870506
C	5.882636	.587824	.496399
C	4.388945	-.809617	-.944233
C	4.945008	-1.558515	1.475195
C	1.619086	1.807030	1.543303
C	6.522517	-1.747489	-.492427
C	5.701070	-2.863715	-1.208830
C	4.265298	-2.281974	-1.413991
O	7.578575	-2.243904	.370999
S	-4.528729	-.892405	.693646
Fe	-2.129277	-.637046	.107171
C	-2.561150	-1.395166	-3.200414
C	-2.715578	2.690446	-.573830
C	-1.853366	.102688	3.447409
C	-1.749049	-3.977355	.831646
N	-2.542958	.431297	-1.544298
C	-2.665764	-.060220	-2.836999
C	-2.936160	1.023542	-3.755926
C	-2.983818	2.172221	-3.017134
C	-2.744954	1.798430	-1.640469
N	-2.319278	1.042832	1.212057
C	-2.521971	2.337841	.752339
C	-2.477150	3.269243	1.857538
C	-2.238020	2.538067	2.986409
C	-2.129603	1.151753	2.585437
N	-1.862788	-1.724855	1.802816
C	-1.739451	-1.233329	3.087044
C	-1.488338	-2.321150	4.012978
C	-1.465448	-3.471094	3.279819
C	-1.696719	-3.095755	1.898747
N	-2.163577	-2.342127	-.964784
C	-1.962521	-3.625656	-.497268
C	-2.004161	-4.565946	-1.596522
C	-2.229950	-3.840997	-2.732241
C	-2.328252	-2.453963	-2.332530
O	-.364655	-.515375	.007972
H	3.317381	4.085194	-.484961
H	3.928290	1.902353	-1.101367
H	2.617684	-.505295	.261672
H	2.682271	.338579	-2.672995
H	1.758761	-.992951	-1.975846
H	.079627	.177967	-.615562
H	.284627	1.030881	-2.397923
H	-.271029	3.258752	-2.026481
H	1.902396	5.824114	.520725
H	1.059875	4.656937	1.522978
H	4.283535	1.155125	1.847425
H	5.016875	2.503896	.999027
H	6.376263	1.004677	-.395058
H	4.110889	-1.027136	1.941037
H	1.244333	.784919	1.439469

H	.759172	2.430205	1.810629
H	7.063506	-1.142463	-1.228268
H	6.174901	-3.155751	-2.151681
H	5.677977	-3.763089	-.578602
H	3.528000	-2.823080	-.807614
H	3.936102	-2.354777	-2.455962
H	4.869658	-.257161	-1.773508
H	5.757327	-1.601718	2.211483
H	4.604048	-2.582393	1.281735
H	2.331647	1.846986	2.374516
H	3.382603	3.888075	1.265950
H	6.624574	.608573	1.305641
H	7.215237	-2.906756	.991335
H	-4.973818	.334227	.237360
H	-2.679207	-1.633078	-4.253230
H	-2.829444	3.746165	-.798159
H	-1.726987	.346310	4.497837
H	-1.609068	-5.031996	1.048304
H	-3.077798	.905994	-4.821085
H	-3.169923	3.181677	-3.355597
H	-2.604577	4.338046	1.760849
H	-2.139505	2.890942	4.003360
H	-1.358522	-2.203130	5.079528
H	-1.311520	-4.483714	3.625038
H	-1.878226	-5.634854	-1.497320
H	-2.325486	-4.197923	-3.748007

## Frequencies:

-20.9041	9.6816	14.6517
28.1303	35.4290	41.1973
50.8109	53.8072	58.5232
68.9257	75.9493	88.3473
98.6119	101.8669	113.8027
119.3954	135.5592	154.6759
155.3407	163.8287	168.7403
182.1749	201.1442	208.7100
211.3499	217.1829	219.8098
227.6376	230.9467	233.7775
250.9337	267.6990	271.4220
276.3569	278.6694	282.4660
283.6023	290.5038	294.7751
297.7715	303.5471	316.8848
324.4717	335.2798	349.0671
362.3009	369.1150	371.0205
372.0488	380.6902	385.5034
398.5427	409.9408	419.7440
428.0801	432.8102	436.0024
439.9054	440.7432	448.1329
462.5335	480.0258	486.6164
510.9842	518.3062	547.6281
554.1137	561.0372	573.9808
594.7422	619.8981	630.1814
650.8295	678.8629	679.4252
688.1005	689.9682	690.2336
692.4772	700.7249	712.6332
726.1958	727.0627	731.1625
736.1366	741.3653	761.5531
766.4770	767.6127	768.0162
803.8836	805.4920	812.3048
814.1604	818.5097	822.5994
827.1826	834.5316	835.2503
849.2384	852.7653	853.8849
860.3052	881.0598	898.1385
907.4986	914.0955	918.7638
921.4206	929.5028	936.3996
937.3421	942.2141	951.6941
953.3879	954.0402	959.3099
964.3311	975.6524	983.7151
992.3651	1000.2682	1015.8264
1017.8889	1021.1468	1022.6834
1024.9428	1033.7614	1038.5098

1047.4057	1050.3741	1056.7851
1058.2584	1061.2024	1063.0705
1077.0154	1077.6726	1086.8528
1100.0100	1117.5439	1118.1917
1120.3001	1123.8780	1126.7255
1139.6531	1152.0050	1156.7015
1169.0549	1175.6108	1178.4765
1190.4415	1192.1419	1198.1550
1208.3703	1216.9225	1223.9394
1243.3225	1245.4885	1252.5339
1261.7241	1269.8553	1276.9946
1295.6404	1296.9892	1300.8893
1308.1382	1311.5310	1315.3383
1322.1398	1332.5835	1338.4298
1346.0112	1348.1688	1349.8690
1358.5845	1362.0086	1375.3605
1379.6022	1387.1530	1388.7537
1389.5874	1395.1432	1398.9781
1401.1955	1409.6181	1412.4879
1417.2803	1420.9228	1423.3732
1427.9062	1431.1226	1437.1224
1439.0075	1454.9909	1466.2750
1498.3009	1499.6652	1502.0813
1509.7874	1512.9427	1527.9524
1530.3629	1533.7860	1534.9391
1537.4253	1541.8764	1546.7086
1551.1827	1557.8134	1558.4924
1562.6652	1565.4584	1590.6896
1592.2376	1607.2435	1615.3392
1622.0880	1643.4184	1645.6755
1714.2840	2407.0374	2504.7465
2950.0223	2955.4749	2963.3134
3017.3557	3029.1281	3040.0988
3042.0353	3045.8163	3050.2934
3055.6021	3058.8309	3061.3275
3072.1946	3075.4693	3081.6699
3092.3584	3093.7309	3095.8959
3101.9499	3110.2920	3116.3048
3126.0286	3133.4875	3140.5557
3146.6783	3204.7030	3205.1237
3206.0132	3209.1386	3216.4695
3256.6561	3256.8715	3257.9698
3259.1998	3280.0489	3280.2735
3280.9963	3282.2732	3640.6083



## III.B.7. Point P7

Absolute energy: -2476.6067008

Geometry:

C	.481184	3.351984	-1.233652
C	.494582	4.612147	-.527540
C	1.552886	4.787809	.550481
C	5.448404	-.856626	.192740
O	-.353284	5.507666	-.759772
C	2.726534	3.803944	.402366
C	2.280721	2.323070	.223975
C	3.525893	1.440250	-.182320
C	3.124436	-.014169	-.588079
C	2.173624	.030895	-1.797907
C	.990216	.977623	-1.596580
C	1.249398	2.277221	-.912804
C	4.668594	1.472057	.871195
C	5.882673	.587621	.497040
C	4.391199	-.809480	-.941113
C	4.945402	-1.558463	1.475730
C	1.617194	1.807446	1.535993
C	6.524142	-1.747269	-.491812
C	5.701805	-2.863842	-1.207975
C	4.266371	-2.280851	-1.412495
O	7.577569	-2.244227	.370638
S	-4.536595	-.890979	.693980
Fe	-2.112098	-.644035	.112344
C	-2.561114	-1.394338	-3.196033
C	-2.715523	2.684078	-.571820
C	-1.855026	.102536	3.444862
C	-1.750654	-3.973350	.830112
N	-2.552229	.428748	-1.543831
C	-2.667090	-.061459	-2.832378
C	-2.934050	1.019233	-3.748133
C	-2.981296	2.166683	-3.009091
C	-2.744946	1.793281	-1.636964
N	-2.324917	1.041941	1.217075
C	-2.522287	2.332473	.752498
C	-2.476572	3.262341	1.853413
C	-2.237717	2.533397	2.982408
C	-2.131255	1.151058	2.584176
N	-1.887584	-1.729058	1.810552
C	-1.747100	-1.232814	3.087190
C	-1.488151	-2.316402	4.006161
C	-1.465472	-3.466203	3.272572
C	-1.704765	-3.094436	1.898276
N	-2.170743	-2.345935	-.966064
C	-1.964590	-3.623612	-.497462
C	-2.004129	-4.560102	-1.593698
C	-2.229721	-3.835197	-2.728438
C	-2.329542	-2.452782	-2.329756
O	-.461042	-.572574	.064669
H	3.322172	4.091441	-.477284
H	3.933278	1.903667	-1.100267
H	2.607010	-.503553	.249805
H	2.753762	.342459	-2.682887
H	1.787407	-.975028	-2.009581
H	.279413	.450580	-.949743
H	.450049	1.139622	-2.538380
H	-.243460	3.272279	-2.039697
H	1.904201	5.827104	.523447
H	1.060221	4.659821	1.526449
H	4.283915	1.154596	1.849118
H	5.018851	2.503976	1.001456
H	6.376036	1.005494	-.394913
H	4.109346	-1.026346	1.939357
H	1.246763	.783368	1.429057

H	.757173	2.430294	1.805981
H	7.059516	-1.141416	-1.232396
H	6.174985	-3.154841	-2.152704
H	5.677336	-3.764919	-.578624
H	3.528266	-2.823088	-.806260
H	3.936959	-2.351315	-2.455309
H	4.872259	-.258706	-1.771581
H	5.755168	-1.602302	2.216181
H	4.604659	-2.583485	1.282697
H	2.327942	1.841015	2.370317
H	3.384196	3.894454	1.275347
H	6.626035	.608510	1.306342
H	7.212728	-2.905562	.989452
H	-4.981494	.338395	.252955
H	-2.674702	-1.631541	-4.250101
H	-2.822259	3.741036	-.797286
H	-1.720498	.346901	4.494710
H	-1.602695	-5.027579	1.046574
H	-3.072338	.905810	-4.815066
H	-3.162408	3.176909	-3.350667
H	-2.600199	4.332615	1.757949
H	-2.136560	2.891165	3.998320
H	-1.350653	-2.201476	5.072979
H	-1.303904	-4.477777	3.620216
H	-1.876710	-5.630091	-1.498161
H	-2.323241	-4.195074	-3.744289

## Frequencies:

-26.9317	-18.9802	-14.8099
-9.2738	17.5434	24.2153
32.6231	43.1220	48.2850
52.1935	63.1872	86.7088
88.3425	103.5091	113.7606
124.4927	129.4576	139.7945
146.9276	155.1693	165.5885
181.7125	190.2089	198.0367
206.4893	213.8818	217.0902
220.8354	231.4206	240.0923
256.1860	265.9672	270.9235
278.0101	278.2787	279.7487
280.1533	289.3057	296.1607
299.1115	306.2878	307.1368
314.6545	334.5057	345.1370
358.9858	371.6329	373.3013
380.3767	382.6422	385.3474
401.5305	411.6214	415.2675
420.9237	434.1528	437.5172
438.7896	439.9208	443.3471
470.0393	476.8632	485.4519
508.6560	518.1206	520.0254
547.7550	561.8825	577.5812
581.6148	623.6510	645.8303
659.9409	678.3313	679.0718
687.9397	688.8477	690.1484
698.5291	726.5397	727.0709
732.1015	737.3547	743.8794
764.3371	765.9975	770.6474
770.8232	800.0345	808.4899
817.0086	819.7004	820.0162
823.6793	828.2306	831.0208
837.5642	838.3069	852.3163
854.5987	857.0398	857.8138
881.8838	910.7864	913.3476
925.1758	928.0474	931.8184
936.9296	943.3743	950.4237
953.7192	960.5970	961.3657
967.6097	969.2665	977.2710
987.9183	994.4187	1004.5529
1028.2149	1031.1235	1031.5500
1034.9645	1036.1323	1039.8484
1045.7968	1049.0540	1054.1543

1065.2807	1068.2187	1068.4578
1069.4326	1079.2873	1087.6488
1088.8001	1103.3115	1122.9353
1123.5606	1125.1326	1129.0795
1130.4058	1139.3610	1149.0852
1172.2122	1173.5802	1177.1598
1185.3635	1199.7356	1204.6514
1205.9519	1214.8851	1228.4229
1238.5619	1243.7261	1251.1549
1255.1861	1259.8420	1269.0044
1285.0827	1295.4803	1304.9514
1308.6265	1310.3731	1312.3896
1320.7831	1323.5755	1335.5865
1341.4324	1346.3766	1351.3999
1359.0561	1360.3586	1361.3758
1366.2901	1379.8277	1380.1311
1390.5008	1397.4193	1400.8337
1400.9642	1403.1874	1405.5692
1411.0650	1417.1228	1420.4175
1420.7557	1432.5892	1433.6037
1438.1311	1438.8203	1447.8240
1455.6171	1461.1004	1492.8291
1506.1743	1508.6012	1509.6540
1511.3642	1530.7495	1535.2137
1537.4132	1538.5501	1541.7668
1546.2237	1546.5780	1551.5135
1557.0751	1563.2727	1563.8813
1565.9324	1598.6880	1600.1523
1616.2593	1622.3805	1651.9893
1652.7335	1654.0434	1680.3616
1724.3231	2523.1661	2911.7470
2948.3178	2959.0682	2993.3946
3010.6546	3023.2174	3030.7093
3032.6024	3037.1956	3041.4011
3041.6849	3049.9035	3050.4056
3062.4771	3062.8514	3066.4357
3067.5526	3080.4198	3085.4669
3086.0453	3089.6092	3100.5602
3107.3702	3118.8588	3131.4803
3138.4564	3189.3952	3200.2854
3200.5372	3201.0105	3211.1680
3249.2554	3249.4083	3250.9972
3251.9104	3272.2670	3272.5102
3273.8288	3274.7949	3658.4870

### III.B.8. Point P8

Absolute energy: -2476.6050455

Geometry:

C	.460773	3.338399	-1.228958
C	.496224	4.608879	-.527527
C	1.552635	4.785303	.548099
C	5.447065	-.855680	.191573
O	-.352743	5.507402	-.764290
C	2.723306	3.799671	.395712
C	2.277561	2.316200	.226817
C	3.524226	1.438733	-.182464
C	3.123024	-.017278	-.582394
C	2.137379	.014150	-1.765271
C	.986655	.980820	-1.562220
C	1.225031	2.237022	-.895187
C	4.668241	1.472188	.870478
C	5.882609	.587818	.496393
C	4.388946	-.809620	-.944244
C	4.945016	-1.558497	1.475163

C	1.619122	1.807065	1.543268
C	6.522533	-1.747506	-.492397
C	5.701059	-2.863686	-1.208811
C	4.265323	-2.281957	-1.413972
O	7.578527	-2.243940	.371033
S	-4.528700	-.892373	.693632
Fe	-2.129526	-.637088	.107211
C	-2.561142	-1.395171	-3.200335
C	-2.715576	2.690372	-.573801
C	-1.853367	.102650	3.447328
C	-1.749051	-3.977261	.831641
N	-2.542950	.431385	-1.544433
C	-2.665756	-.060138	-2.836958
C	-2.936142	1.023507	-3.755815
C	-2.983793	2.172141	-3.017057
C	-2.744946	1.798375	-1.640525
N	-2.319303	1.042922	1.212115
C	-2.521969	2.337829	.752393
C	-2.477140	3.269132	1.857502
C	-2.238026	2.537984	2.986312
C	-2.129609	1.151792	2.585360
N	-1.862850	-1.724922	1.802907
C	-1.739453	-1.233398	3.086980
C	-1.488355	-2.321138	4.012874
C	-1.465464	-3.471010	3.279762
C	-1.696725	-3.095666	1.898785
N	-2.163609	-2.342242	-.964823
C	-1.962532	-3.625590	-.497337
C	-2.004169	-4.565831	-1.596495
C	-2.229946	-3.840928	-2.732151
C	-2.328240	-2.453999	-2.332472
O	-.363790	-.515689	.008177
H	3.317548	4.085338	-.485192
H	3.928389	1.902454	-1.101481
H	2.617579	-.505450	.261917
H	2.681815	.338342	-2.673081
H	1.758253	-.993318	-1.975647
H	.069198	.173654	-.608433
H	.281834	1.029347	-2.395949
H	-.271623	3.258863	-2.026757
H	1.902581	5.824426	.520703
H	1.059825	4.656888	1.523255
H	4.283428	1.155032	1.847678
H	5.016989	2.504203	.999057
H	6.376379	1.004805	-.395248
H	4.110607	-1.026979	1.941200
H	1.244257	.784596	1.439435
H	.758879	2.430372	1.810723
H	7.063532	-1.142249	-1.228630
H	6.175049	-3.155819	-2.152045
H	5.677903	-3.763338	-.578434
H	3.527798	-2.823238	-.807402
H	3.936027	-2.354808	-2.456352
H	4.869719	-.257099	-1.773679
H	5.757512	-1.601751	2.211720
H	4.603960	-2.582688	1.281703
H	2.331760	1.847027	2.374862
H	3.382800	3.888081	1.266214
H	6.624802	.608551	1.305879
H	7.215565	-2.906102	.990691
H	-4.973844	.333780	.237511
H	-2.679277	-1.633180	-4.253619
H	-2.829601	3.746573	-.798231
H	-1.726932	.346389	4.498229
H	-1.608997	-5.032377	1.048394
H	-3.077917	.905992	-4.821679
H	-3.170081	3.182215	-3.355853
H	-2.604663	4.338653	1.760882
H	-2.139456	2.891192	4.003894
H	-1.358426	-2.203142	5.080135
H	-1.311417	-4.484260	3.625307

H	-1.878164	-5.635452	-1.497327
H	-2.325533	-4.198193	-3.748554

## Frequencies:

-27.1723	10.2280	14.6269
30.8435	35.1488	40.2922
51.3680	55.7316	58.4709
69.8009	75.8428	88.9622
97.7521	106.1811	107.4375
121.5359	136.7459	154.1672
154.8746	161.8334	168.4863
185.8032	201.4201	208.8163
212.7049	217.9160	219.9891
227.7964	230.8331	242.5848
257.0560	269.5258	270.0224
276.8256	278.7535	282.6290
284.5382	291.2123	294.4382
298.2090	303.5325	311.7618
318.2339	333.6516	353.7769
362.5408	369.2480	370.9337
373.4021	381.1696	386.4189
398.8021	410.0020	419.2384
428.2338	433.1353	436.1767
440.1387	440.9791	448.0403
461.7074	480.2776	486.8167
509.6393	512.9750	527.8467
552.1973	561.5004	568.6048
579.3272	620.0448	630.6864
651.2375	679.3745	679.9285
688.0763	690.2010	690.5286
692.8396	700.7916	704.7721
727.1979	727.9564	731.5986
736.5864	742.4210	761.8341
766.6610	767.8077	768.0792
805.4196	806.3142	814.6519
816.6052	818.5682	825.1639
826.5992	834.6076	835.3112
849.7570	852.9281	854.7722
860.3468	878.3990	898.2256
909.7217	911.1863	920.9031
923.0222	923.8237	935.9331
939.0512	944.9681	952.0754
955.7534	956.3311	961.5942
963.3091	975.9267	982.0594
989.7695	999.1486	1014.6142
1017.9047	1021.5260	1022.8100
1025.1629	1034.0511	1038.5222
1047.2261	1050.6653	1057.1840
1058.7016	1061.2397	1063.3613
1077.2743	1077.9585	1086.8911
1100.0976	1119.1068	1119.7512
1121.9050	1125.4485	1127.1605
1139.7266	1152.3913	1157.3746
1169.4593	1176.0004	1179.0502
1191.2537	1192.9757	1199.0991
1208.6430	1217.5753	1224.3506
1243.9037	1246.3989	1252.8698
1262.1991	1270.3443	1277.3922
1296.0643	1297.4527	1301.3900
1308.5649	1311.8278	1316.0618
1322.6093	1333.1216	1339.4923
1346.5036	1348.8175	1350.5153
1359.0629	1362.4374	1375.9900
1380.1564	1387.8262	1389.0877
1389.9960	1395.5590	1399.4478
1401.6843	1410.2321	1413.6702
1417.8751	1421.1166	1423.9407
1428.6016	1432.3729	1437.6629
1439.3351	1455.6356	1466.9595
1498.6890	1500.0356	1502.5399
1509.8319	1513.0572	1525.5933

1530.6306	1534.1144	1535.2797
1537.7048	1542.1319	1547.0109
1551.5218	1558.2303	1559.0108
1562.9659	1565.7676	1591.1084
1592.6447	1607.4029	1615.7465
1620.6449	1643.6305	1645.8310
1714.3953	2507.7532	2602.4159
2948.3260	2952.7872	2961.4472
3014.8581	3026.3398	3037.4207
3039.0623	3042.9691	3047.3072
3052.6077	3055.6413	3058.5417
3068.8951	3071.9121	3078.7326
3089.0339	3089.9587	3092.5266
3098.5678	3107.1638	3112.7372
3122.6853	3130.6996	3137.1836
3143.2821	3200.1868	3200.5429
3201.4418	3204.2105	3211.7344
3249.8811	3250.0964	3251.2171
3252.4514	3273.3369	3273.5669
3274.2969	3275.5670	3654.0209

## III.B.9. Point P9

Absolute energy: -2476.6018898

Geometry:

C	.467280	3.336953	-1.228626
C	.494737	4.609388	-.527643
C	1.552863	4.785612	.548058
C	5.447245	-.855775	.191502
O	-.352589	5.507470	-.763463
C	2.723791	3.800062	.397039
C	2.276906	2.318201	.226335
C	3.523988	1.438376	-.182606
C	3.122502	-.017122	-.583493
C	2.147545	.018084	-1.775666
C	.966140	.957738	-1.552253
C	1.229958	2.257624	-.897526
C	4.668143	1.472447	.870483
C	5.882620	.587785	.496482
C	4.388992	-.809577	-.943518
C	4.945145	-1.558564	1.475267
C	1.618778	1.806853	1.543081
C	6.522374	-1.747372	-.492436
C	5.701081	-2.863788	-1.208814
C	4.265430	-2.281857	-1.413936
O	7.578771	-2.244003	.371028
S	-4.529295	-.892308	.693542
Fe	-2.121547	-.637414	.107405
C	-2.561240	-1.394954	-3.200353
C	-2.715877	2.690185	-.573724
C	-1.853504	.102924	3.447510
C	-1.749164	-3.977591	.831436
N	-2.545100	.430481	-1.543642
C	-2.665802	-.060685	-2.836731
C	-2.936111	1.023384	-3.755450
C	-2.983834	2.171794	-3.016669
C	-2.744863	1.798274	-1.639886
N	-2.319648	1.041844	1.212448
C	-2.521893	2.337651	.751770
C	-2.477234	3.268884	1.857438
C	-2.238102	2.538049	2.986224
C	-2.129606	1.151625	2.585695
N	-1.865066	-1.724652	1.802701
C	-1.739787	-1.232527	3.087801
C	-1.488408	-2.320477	4.012345
C	-1.465529	-3.470726	3.278972
C	-1.697053	-3.096619	1.898358
N	-2.164171	-2.341610	-.964503
C	-1.962512	-3.625991	-.496875
C	-2.004198	-4.565703	-1.596365
C	-2.229948	-3.840619	-2.731996
C	-2.328290	-2.453539	-2.332651
O	-.406045	-.532721	.024896
H	3.316454	4.083985	-.484534
H	3.927477	1.901554	-1.101600
H	2.617693	-.504712	.261822
H	2.705130	.332905	-2.673554
H	1.762944	-.989046	-1.977404
H	.293097	.396160	-.834335
H	.353123	1.074793	-2.452572
H	-.262034	3.258081	-2.028635
H	1.902120	5.824315	.520886
H	1.059764	4.657188	1.522787
H	4.283932	1.155239	1.847547
H	5.017036	2.503760	.999457
H	6.375856	1.004417	-.395019
H	4.111265	-1.026689	1.940319
H	1.246454	.784448	1.439323

H	.760292	2.431019	1.810549
H	7.063437	-1.142546	-1.227908
H	6.174964	-3.155762	-2.151390
H	5.678633	-3.763064	-.578560
H	3.528173	-2.823061	-.807743
H	3.935706	-2.353742	-2.455253
H	4.868795	-.257265	-1.772850
H	5.757194	-1.601889	2.211644
H	4.604187	-2.582268	1.281512
H	2.332171	1.845252	2.373419
H	3.383604	3.889722	1.266848
H	6.624654	.608681	1.305486
H	7.214453	-2.906853	.991709
H	-4.974963	.334779	.238444
H	-2.678211	-1.632649	-4.252773
H	-2.825233	3.745813	-.798341
H	-1.726386	.346389	4.497304
H	-1.608710	-5.031580	1.048121
H	-3.076249	.905593	-4.820174
H	-3.167631	3.181227	-3.354441
H	-2.603018	4.337172	1.759652
H	-2.138911	2.890509	4.002633
H	-1.358282	-2.202088	5.078223
H	-1.311252	-4.482908	3.623542
H	-1.877932	-5.633981	-1.496937
H	-2.325100	-4.196857	-3.747414

## Frequencies:

-53.1814	-19.7125	9.6964
12.6992	17.5852	34.0167
35.9760	52.5676	55.1513
58.9096	75.4186	84.8254
94.4627	98.7303	119.8334
128.4621	138.6515	148.3563
153.5435	157.3509	171.1284
183.3355	199.0281	201.9911
209.5313	216.1803	219.7242
220.5789	231.5057	241.7791
254.2376	267.3409	271.0988
278.4039	280.0946	281.7672
283.0863	291.9144	296.9238
301.5577	308.9553	313.5876
327.9105	338.6813	351.5681
360.7858	370.9888	374.3708
377.4663	381.7493	385.8482
399.1193	412.9727	419.1393
423.1008	434.1615	436.4105
438.7326	439.7085	444.5848
469.1781	470.7746	485.5118
507.2630	509.7718	518.5581
548.0843	553.7427	560.6823
576.4524	584.8848	621.7912
646.6304	660.7786	677.9562
678.7411	687.4613	689.0653
689.5506	700.6451	724.7431
725.1587	729.8686	735.0711
740.6025	760.9248	764.7922
766.5515	766.7456	798.7107
803.2980	812.1509	813.9427
816.9523	821.7166	822.3378
834.6798	835.5350	849.8801
852.2110	853.1373	856.1971
881.3451	906.8875	907.4171
919.3592	921.8435	930.3707
934.6018	938.2622	942.8341
952.4796	954.2076	954.4632
960.5688	967.5573	975.4523
985.9624	992.5319	1003.6404
1017.5342	1020.0258	1022.5801
1024.4888	1030.0731	1033.3636
1039.0221	1049.0127	1051.8393



1058.2088	1058.7794	1062.9008
1065.8406	1076.9635	1077.8294
1087.4540	1102.0028	1117.8838
1118.3159	1120.2279	1123.9417
1129.0245	1137.4866	1150.1758
1154.1381	1169.6923	1175.8477
1181.4794	1191.1301	1192.4222
1199.5402	1214.8419	1216.8085
1238.0144	1240.3709	1243.4817
1245.7423	1257.4683	1265.6908
1281.5231	1292.9938	1296.2804
1297.9479	1300.4612	1306.5228
1307.8358	1320.5095	1327.8336
1332.8726	1336.5294	1345.5437
1348.6710	1350.3290	1357.2901
1363.4235	1376.7627	1378.5516
1386.3363	1388.5994	1389.3519
1394.5459	1398.8508	1400.8160
1409.2476	1412.0462	1415.3240
1419.5895	1423.5723	1428.0119
1429.5691	1436.2186	1437.2847
1442.1931	1453.3919	1462.3313
1498.8697	1499.9848	1501.9889
1510.2460	1529.8159	1532.5512
1534.2192	1534.6775	1536.8354
1540.9680	1545.6730	1550.5711
1557.0616	1558.6102	1562.2191
1565.0748	1590.5771	1591.9536
1604.6839	1614.4759	1634.6928
1644.5728	1647.0604	1660.5111
1716.0550	2266.9345	2504.4400
2954.6956	2965.3618	2995.4468
3019.0569	3032.2421	3039.3691
3042.2184	3046.4119	3050.6267
3051.3387	3059.7078	3060.1762
3073.0758	3077.7801	3078.4070
3086.5967	3091.6239	3096.7721
3096.8969	3100.8809	3111.0428
3118.4572	3129.2520	3142.5459
3150.3990	3204.6314	3210.8816
3211.2851	3212.1314	3222.4648
3263.2918	3263.4230	3265.0267
3265.9416	3286.2676	3286.5474
3287.8333	3288.8759	3632.7101

## III.B.10. Point P10

Absolute energy: -2476.6059702

Geometry:

C	.475086	3.344790	-1.231617
C	.494043	4.611369	-.527140
C	1.552982	4.786968	.549188
C	5.447732	-.856076	.192075
O	-.353713	5.508624	-.761386
C	2.725555	3.802356	.400116
C	2.278917	2.321498	.225562
C	3.524600	1.439015	-.182237
C	3.123236	-.015905	-.586053
C	2.162964	.024740	-1.788798
C	.979816	.968650	-1.577917
C	1.242603	2.269927	-.906450
C	4.668261	1.472438	.870648
C	5.882636	.587781	.496721
C	4.389854	-.809648	-.941930
C	4.945447	-1.558588	1.475443
C	1.617918	1.807110	1.540020
C	6.522898	-1.747349	-.492153
C	5.701271	-2.863776	-1.208649
C	4.265732	-2.281494	-1.413427
O	7.578765	-2.244284	.371010
S	-4.532449	-.891544	.693768
Fe	-2.114154	-.640881	.109752
C	-2.561368	-1.394968	-3.199967
C	-2.715998	2.689122	-.573173
C	-1.853668	.103316	3.447906
C	-1.749501	-3.977268	.831033
N	-2.547685	.429107	-1.542916
C	-2.666271	-.061257	-2.835660
C	-2.935492	1.022123	-3.753389
C	-2.983053	2.170274	-3.014286
C	-2.744809	1.796791	-1.638656
N	-2.321352	1.040957	1.214172
C	-2.522035	2.336141	.751736
C	-2.477062	3.267259	1.856375
C	-2.238085	2.537301	2.985394
C	-2.130053	1.151611	2.585929
N	-1.875935	-1.726310	1.805907
C	-1.742608	-1.232199	3.088244
C	-1.488023	-2.319188	4.010656
C	-1.465254	-3.469416	3.277078
C	-1.700094	-3.096503	1.898225
N	-2.166076	-2.342783	-.965008
C	-1.962992	-3.625455	-.497034
C	-2.004219	-4.564441	-1.595947
C	-2.229851	-3.839367	-2.731258
C	-2.328609	-2.453204	-2.332064
O	-.455370	-.560018	.052366
H	3.319088	4.087093	-.481188
H	3.929429	1.902120	-1.101077
H	2.611332	-.504356	.255214
H	2.735313	.334326	-2.679066
H	1.775966	-.981651	-1.993874
H	.287918	.433184	-.907411
H	.417153	1.118183	-2.507486
H	-.250378	3.264813	-2.035979
H	1.902659	5.826162	.521932
H	1.060097	4.658809	1.524562
H	4.284124	1.155247	1.848323
H	5.017611	2.504151	.999943
H	6.375803	1.004680	-.395223
H	4.110879	-1.026247	1.940040

H	1.246913	.783805	1.433998
H	.759096	2.430769	1.809508
H	7.062437	-1.142023	-1.229161
H	6.175133	-3.155590	-2.152007
H	5.678463	-3.763646	-.578392
H	3.528047	-2.823390	-.807377
H	3.935891	-2.352274	-2.455392
H	4.870179	-.257815	-1.771683
H	5.756909	-1.602335	2.213206
H	4.604241	-2.582749	1.281733
H	2.330995	1.842432	2.371507
H	3.384690	3.893187	1.271132
H	6.625373	.608876	1.305813
H	7.214215	-2.905792	.991425
H	-4.980070	.336291	.246429
H	-2.676682	-1.632514	-4.253166
H	-2.821905	3.745591	-.798415
H	-1.723340	.347087	4.497797
H	-1.606082	-5.031470	1.047582
H	-3.074342	.905500	-4.819235
H	-3.164994	3.180609	-3.352974
H	-2.601510	4.336545	1.758554
H	-2.138036	2.891444	4.001977
H	-1.354910	-2.201554	5.077058
H	-1.308061	-4.481750	3.622395
H	-1.877480	-5.633557	-1.497312
H	-2.324538	-4.196404	-3.747288

## Frequencies:

-29.6060	-15.3492	-8.2186
9.4940	30.9524	34.2285
50.0888	52.0416	56.1083
59.0418	63.2688	89.7916
92.4960	107.7152	119.4834
127.4316	130.8972	144.1439
150.6140	156.0109	167.1517
182.3575	191.9000	200.2473
207.8373	213.6275	218.7559
220.4910	232.4212	242.4450
257.8676	266.6258	272.0634
279.8969	280.5078	281.0125
282.6009	291.9784	295.8872
301.9538	307.7963	313.3686
318.3314	334.5211	349.3899
359.5556	371.7046	374.1024
379.6827	382.7163	385.7421
400.5646	412.4511	416.6378
420.3184	434.8643	436.9713
439.3703	440.3875	443.2279
469.4473	477.9215	485.7868
507.5933	518.0807	529.8692
548.9760	561.1378	576.8146
581.5677	622.7465	646.0566
660.3462	678.7061	679.4860
687.6872	689.6969	690.4107
699.2250	725.3673	726.4620
730.9439	734.8680	741.7600
761.4127	764.9540	767.4275
767.5682	785.7304	800.1122
806.0263	815.5787	817.2278
819.4190	822.3110	825.8499
835.3851	836.0087	851.0811
852.7679	854.9593	856.7451
881.4246	908.8549	910.0607
922.0295	924.7399	931.0000
935.7237	940.4929	946.6373
952.8085	957.2068	957.8573
964.0784	968.5010	976.4575
986.9039	993.2664	1004.0970
1020.9418	1021.9086	1025.5588
1027.5681	1030.9837	1036.3177

1039.3835	1048.6704	1052.3423
1060.4170	1061.6222	1064.1959
1067.2164	1078.2898	1080.2586
1088.2719	1102.7155	1120.1440
1120.6743	1122.4838	1126.2300
1129.6834	1138.7936	1149.5758
1160.1696	1171.2597	1176.5054
1184.7325	1194.7593	1195.8925
1199.7605	1214.7858	1219.5282
1238.4710	1242.6836	1248.3669
1250.1444	1258.9391	1267.8552
1283.3687	1294.6358	1300.6395
1302.7296	1303.9842	1307.6939
1312.9150	1322.4965	1334.4701
1336.8452	1345.0832	1348.8532
1352.3620	1353.4899	1358.0363
1365.0717	1378.8656	1379.2015
1389.7073	1389.8167	1392.4488
1396.2639	1400.0716	1403.3294
1410.0941	1414.6840	1416.2164
1420.2302	1426.2560	1430.5751
1431.4926	1438.1706	1440.0899
1454.2439	1458.8531	1482.9736
1501.1017	1502.4898	1503.7435
1510.7164	1530.2729	1534.7246
1536.4178	1537.3700	1537.4750
1541.2163	1545.9761	1550.9966
1556.7057	1560.1570	1562.6382
1565.4609	1592.7098	1594.0789
1608.4810	1616.6498	1646.1126
1646.5196	1648.1615	1671.1313
1717.6698	2512.9947	2798.4680
2951.5953	2962.1870	2996.3260
3015.0149	3027.8648	3034.8321
3037.4553	3041.8003	3045.1357
3046.4980	3054.9709	3055.2291
3067.9362	3070.2086	3072.4828
3073.0291	3085.9953	3091.3169
3091.4854	3095.2078	3106.0548
3113.1223	3124.5931	3137.2684
3144.4656	3196.6072	3205.9216
3206.3354	3206.9640	3216.9842
3255.7363	3255.9170	3257.4521
3258.3694	3278.7374	3279.0372
3280.2658	3281.2558	3645.4134

## III.B.11. Point P11

Absolute energy: -2476.5998728

Geometry:

C	0.465516	3.336258	-1.228452
C	0.495049	4.609261	-0.527777
C	1.552794	4.785481	0.548036
C	5.447160	-0.855760	0.191509
O	-0.352395	5.507227	-0.763745
C	2.723508	3.799827	0.396445
C	2.276942	2.317321	0.226478
C	3.524074	1.438464	-0.182601
C	3.122579	-0.017207	-0.583006
C	2.143807	0.016694	-1.772114
C	0.965755	0.958230	-1.548612
C	1.227078	2.252164	-0.895976
C	4.668183	1.472358	0.870480
C	5.882604	0.587798	0.496437
C	4.388960	-0.809584	-0.943855
C	4.945091	-1.558527	1.475221
C	1.618923	1.806898	1.543250
C	6.522491	-1.747416	-0.492399
C	5.701086	-2.863754	-1.208799
C	4.265388	-2.281889	-1.413963
O	7.578644	-2.243960	0.371015
S	-4.528978	-0.892421	0.693550
Fe	-2.124619	-0.637036	0.107173
C	-2.561172	-1.394977	-3.200281
C	-2.715690	2.690175	-0.573821
C	-1.853517	0.102795	3.447338
C	-1.749147	-3.977417	0.831459
N	-2.544457	0.430922	-1.544080
C	-2.665782	-0.060484	-2.836778
C	-2.936105	1.023394	-3.755451
C	-2.983812	2.171811	-3.016730
C	-2.744893	1.798327	-1.640105
N	-2.319447	1.042573	1.212420
C	-2.521839	2.337583	0.752089
C	-2.477204	3.268836	1.857406
C	-2.238072	2.537886	2.986177
C	-2.129612	1.151710	2.585447
N	-1.863661	-1.724786	1.802801
C	-1.739562	-1.232867	3.087543
C	-1.488446	-2.320596	4.012392
C	-1.465565	-3.470765	3.279094
C	-1.696809	-3.096308	1.898564
N	-2.163936	-2.341952	-0.964747
C	-1.962494	-3.625953	-0.497017
C	-2.004195	-4.565605	-1.596291
C	-2.229961	-3.840572	-2.731943
C	-2.328253	-2.453744	-2.332582
O	-0.388778	-0.524782	0.017201
H	3.316684	4.084360	-0.484855
H	3.927802	1.901794	-1.101579
H	2.618292	-0.504969	0.262565
H	2.696733	0.334921	-2.672661
H	1.761003	-0.990704	-1.976146
H	0.276818	0.364452	-0.806328
H	0.330144	1.060084	-2.434744
H	-0.265241	3.258007	-2.027556
H	1.902416	5.824294	0.520919
H	1.059762	4.656982	1.522921
H	4.283769	1.155159	1.847614
H	5.017076	2.503892	0.999366
H	6.376051	1.004606	-0.395068
H	4.111049	-1.026804	1.940682

H	1.245861	0.784493	1.439963
H	0.759970	2.430925	1.810585
H	7.063204	-1.142429	-1.228350
H	6.174953	-3.155725	-2.151652
H	5.678278	-3.763221	-0.578552
H	3.528058	-2.823143	-0.807586
H	3.935844	-2.354111	-2.455616
H	4.868959	-0.257266	-1.773255
H	5.757242	-1.601899	2.211740
H	4.604137	-2.582443	1.281605
H	2.332038	1.845868	2.374034
H	3.383248	3.888972	1.266565
H	6.624706	0.608597	1.305628
H	7.214781	-2.906686	0.991341
H	-4.973621	0.334327	0.237775
H	-2.678634	-1.632820	-4.252931
H	-2.826928	3.745952	-0.798267
H	-1.726751	0.346298	4.497492
H	-1.608976	-5.031738	1.048241
H	-3.076879	0.905849	-4.820509
H	-3.168515	3.181335	-3.354985
H	-2.603603	4.337492	1.760199
H	-2.139140	2.890733	4.002883
H	-1.358517	-2.202535	5.078719
H	-1.311467	-4.483207	3.624164
H	-1.878077	-5.634309	-1.497159
H	-2.325263	-4.197337	-3.747571

## Frequencies:

-323.7523	-9.9857	11.5609
13.7678	24.0607	35.1824
37.0239	52.9257	56.5973
58.6292	74.7864	79.4507
92.8345	98.7443	118.5277
130.4026	136.0060	147.8060
153.9320	159.3383	168.7090
181.6384	190.9732	202.3965
205.7338	211.7844	219.5673
222.6839	231.0247	236.2397
248.2782	268.6808	271.1843
273.0623	279.7376	281.4608
283.2885	286.6045	298.0694
300.8825	306.2574	314.5953
324.0909	325.3832	335.7794
360.0083	370.6059	370.9166
373.9622	380.6405	384.0988
399.4397	412.4636	416.6619
423.8702	434.0706	436.2853
437.9083	439.6877	443.8261
451.0023	471.1197	485.7834
493.8991	510.2685	519.0211
551.2113	556.7546	561.0783
576.6768	594.0646	622.1503
648.3135	660.9003	678.2669
679.0204	688.1345	689.3780
689.6970	702.9538	725.1277
725.8357	730.2826	735.5879
741.1157	761.3021	765.3879
766.9091	767.1841	799.9435
804.3603	813.1252	814.9946
817.3696	823.3851	823.6566
834.7619	835.6704	850.2644
852.4591	853.8523	858.6593
882.8239	907.7756	908.4519
920.2996	922.7372	932.0777
934.8366	938.8606	944.0025
953.3268	955.1928	955.4044
961.3227	968.1081	975.4560
986.1230	992.8635	1003.6274
1018.1119	1020.8798	1023.0304
1024.8992	1028.7494	1033.8810

1039.1872	1049.4969	1051.5067
1058.7137	1059.1955	1062.9693
1065.2101	1077.3365	1078.1634
1087.4812	1102.0582	1118.5447
1119.0147	1120.9537	1124.6510
1129.1689	1137.4226	1150.8822
1155.5062	1167.6719	1176.1288
1179.8203	1191.7936	1193.2128
1199.8848	1213.7740	1217.5092
1228.3366	1238.9601	1242.6695
1246.3421	1257.2834	1264.3159
1280.3992	1283.6842	1295.0335
1298.2635	1301.2235	1306.8243
1308.4816	1318.4919	1323.8734
1331.4170	1335.7810	1345.7294
1348.9648	1350.7277	1357.7000
1363.3828	1375.9331	1378.4245
1387.2459	1387.5067	1389.8225
1393.3963	1398.0613	1400.7440
1404.5773	1410.3992	1412.8027
1416.1769	1420.5828	1424.1427
1429.1904	1430.3841	1437.6219
1437.9622	1453.9677	1462.8795
1498.8714	1500.0463	1502.3017
1510.4407	1529.1770	1530.1351
1534.3893	1534.9099	1537.0361
1541.2269	1545.9716	1550.8309
1557.5694	1558.8869	1562.4389
1565.3045	1584.3010	1591.0057
1592.2665	1604.9060	1614.6893
1644.0310	1646.7470	1653.6845
1715.5092	1731.3782	2506.8076
2953.4308	2964.0306	2988.1618
3017.6012	3030.6102	3038.3082
3040.7766	3045.0217	3049.8972
3050.6664	3058.0644	3058.5878
3071.4476	3075.8349	3077.8195
3090.2403	3091.0852	3094.5724
3095.1299	3099.5019	3109.4306
3116.3907	3127.1748	3140.5719
3148.6628	3203.0201	3207.8722
3208.2538	3209.1828	3219.5063
3259.5385	3259.6668	3261.1720
3262.1626	3282.5774	3282.8566
3284.0227	3285.1310	3638.9190

## III.B.12. Point P12

Absolute energy: -2476.5977899

Geometry:

C	0.464336	3.336340	-1.228743
C	0.495343	4.609440	-0.527642
C	1.552775	4.785476	0.548066
C	5.447112	-0.855716	0.191535
O	-0.352469	5.507280	-0.763858
C	2.723445	3.799797	0.396208
C	2.277082	2.316989	0.226605
C	3.524132	1.438525	-0.182570
C	3.122693	-0.017232	-0.582834
C	2.141858	0.015900	-1.770089
C	0.968774	0.961697	-1.549761
C	1.226149	2.248171	-0.895428
C	4.668204	1.472329	0.870490
C	5.882620	0.587811	0.496426
C	4.388937	-0.809602	-0.943988
C	4.945076	-1.558524	1.475208
C	1.618955	1.806921	1.543295
C	6.522459	-1.747450	-0.492403
C	5.701059	-2.863725	-1.208827
C	4.265345	-2.281932	-1.413994
O	7.578681	-2.243969	0.371039
S	-4.528848	-0.892449	0.693580
Fe	-2.126468	-0.636946	0.107109
C	-2.561175	-1.395058	-3.200530
C	-2.715633	2.690474	-0.573931
C	-1.853449	0.102814	3.447559
C	-1.749103	-3.977613	0.831534
N	-2.543760	0.430973	-1.544001
C	-2.665773	-0.060449	-2.836957
C	-2.936156	1.023542	-3.755752
C	-2.983856	2.172026	-3.017021
C	-2.744920	1.798477	-1.640216
N	-2.319204	1.042661	1.212188
C	-2.521848	2.337674	0.752209
C	-2.477195	3.269122	1.857554
C	-2.238057	2.538093	2.986363
C	-2.129602	1.151745	2.585495
N	-1.862966	-1.724721	1.802658
C	-1.739460	-1.233007	3.087467
C	-1.488388	-2.320853	4.012728
C	-1.465508	-3.470978	3.279468
C	-1.696703	-3.096237	1.898658
N	-2.163617	-2.341870	-0.964741
C	-1.962461	-3.625990	-0.497057
C	-2.004183	-4.565861	-1.596448
C	-2.229959	-3.840847	-2.732133
C	-2.328241	-2.453846	-2.332651
O	-0.379829	-0.520569	0.013219
H	3.316951	4.084623	-0.484967
H	3.927992	1.901972	-1.101562
H	2.618156	-0.505098	0.262406
H	2.691986	0.336495	-2.672707
H	1.760455	-0.991573	-1.976234
H	0.232653	0.314231	-0.759063
H	0.316062	1.051152	-2.423827
H	-0.267038	3.258047	-2.027345
H	1.902427	5.824395	0.520950
H	1.059715	4.656939	1.522973
H	4.283667	1.155129	1.847625
H	5.017031	2.504005	0.999253
H	6.376157	1.004645	-0.395131
H	4.110965	-1.026853	1.940900
H	1.245273	0.784574	1.440023



H	0.759700	2.430803	1.810655
H	7.063447	-1.142393	-1.228292
H	6.174985	-3.155782	-2.151759
H	5.678204	-3.763192	-0.578470
H	3.527968	-2.823196	-0.807547
H	3.935879	-2.354348	-2.455857
H	4.869212	-0.257214	-1.773358
H	5.757396	-1.601851	2.211653
H	4.604092	-2.582513	1.281621
H	2.332033	1.846181	2.374193
H	3.383082	3.888635	1.266456
H	6.624733	0.608614	1.305709
H	7.215115	-2.906541	0.991321
H	-4.973172	0.334140	0.237587
H	-2.678908	-1.632982	-4.253333
H	-2.827805	3.746352	-0.798318
H	-1.726885	0.346346	4.497936
H	-1.609085	-5.032153	1.048331
H	-3.077257	0.905852	-4.821005
H	-3.169074	3.181732	-3.355289
H	-2.604008	4.337990	1.760398
H	-2.139311	2.890906	4.003360
H	-1.358559	-2.202696	5.079306
H	-1.311507	-4.483684	3.624566
H	-1.878125	-5.634806	-1.497174
H	-2.325395	-4.197633	-3.748005

## Frequencies:

-1295.7857	10.0415	15.5593
18.8606	35.6476	36.5283
40.8263	53.5505	58.7587
59.1925	73.8629	78.9954
92.4672	100.4163	116.7080
131.2911	135.7424	143.9882
153.4967	155.6565	165.4047
174.5341	190.4246	202.8794
208.4121	212.3088	219.6601
224.5706	232.0091	235.3037
247.9558	268.1189	270.2135
273.6745	279.8808	281.5563
282.9228	287.3015	298.1431
299.6533	304.4093	315.2023
320.3652	322.6556	335.2753
360.6036	369.2368	370.3628
373.6546	380.6200	384.3266
399.7955	411.6677	416.0794
423.9441	433.9870	436.2551
438.3443	439.8032	444.3063
461.3847	473.9500	486.1830
504.9597	519.6282	523.0693
553.8484	560.0664	562.0978
577.5094	613.0389	624.1752
652.9177	661.5585	678.7049
679.4198	688.7838	689.8813
690.2222	704.9563	724.1633
726.4083	730.7509	735.5463
741.0848	760.8507	762.8937
766.6820	767.0454	768.4528
801.7223	804.8169	813.7294
815.4787	818.2014	823.8674
830.1583	834.6074	835.5651
850.5439	852.5316	854.3687
863.4737	889.9097	907.8619
908.6182	920.3010	922.8065
934.8938	937.4862	938.8456
944.2023	954.1726	955.3220
955.4926	961.2611	969.3042
975.9660	986.2959	993.6391
1004.8790	1017.8323	1020.7341
1022.8192	1024.4985	1030.3970
1033.4764	1039.3268	1049.9823

1051.5516	1058.1345	1058.8241
1063.1151	1065.0437	1077.5462
1077.8575	1087.4464	1102.2016
1118.6137	1119.1304	1121.1353
1124.7667	1129.0547	1137.0018
1151.3724	1156.7410	1171.5411
1175.7026	1177.4528	1191.3622
1192.8921	1201.5122	1216.1264
1217.1431	1226.8558	1241.9397
1243.7401	1246.0498	1257.1667
1265.9765	1279.6213	1284.9185
1295.4392	1297.7682	1300.9032
1307.4554	1310.7986	1319.5572
1323.4100	1333.3543	1339.0615
1345.9727	1348.9358	1350.5890
1358.1095	1360.4980	1366.8812
1379.2131	1383.5977	1387.1314
1389.4069	1392.1310	1396.0146
1399.5509	1401.6884	1410.3423
1412.8313	1416.7635	1420.5232
1424.0468	1428.5880	1432.4588
1437.3411	1438.0913	1454.4312
1464.1615	1498.6274	1499.8888
1502.2170	1510.5463	1526.5487
1530.2101	1534.1263	1534.8820
1537.1357	1541.2539	1546.1084
1551.0342	1557.6942	1558.8018
1562.5720	1565.4350	1590.6131
1592.1968	1606.3490	1614.7404
1616.5714	1643.3960	1646.1049
1649.3793	1714.7817	2507.5768
2952.0602	2962.7342	2979.0837
3016.8471	3029.5387	3038.1569
3040.3200	3044.4868	3049.3424
3052.0952	3057.3408	3058.0524
3070.8290	3074.7545	3078.1720
3090.0396	3093.2524	3094.4830
3099.3250	3102.7264	3108.8569
3115.3527	3126.1934	3139.5627
3147.5520	3203.7475	3205.7596
3206.1611	3207.1275	3217.4571
3256.9499	3257.0810	3258.4484
3259.5221	3280.0848	3280.3650
3281.3603	3282.5331	3642.1706

## III.B.13. Point P13

Absolute energy: -2476.6019793

Geometry:

C	0.467351	3.336972	-1.228668
C	0.494754	4.609422	-0.527597
C	1.552863	4.785621	0.548060
C	5.447255	-0.855771	0.191499
O	-0.352611	5.507486	-0.763459
C	2.723821	3.800080	0.397074
C	2.276913	2.318257	0.226321
C	3.523991	1.438373	-0.182607
C	3.122502	-0.017118	-0.583518
C	2.147739	0.018151	-1.775845
C	0.966154	0.957721	-1.552454
C	1.230122	2.257872	-0.897593
C	4.668139	1.472457	0.870493
C	5.882631	0.587783	0.496483
C	4.388996	-0.809571	-0.943501
C	4.945141	-1.558576	1.475281
C	1.618762	1.806843	1.543085
C	6.522337	-1.747362	-0.492459
C	5.701081	-2.863795	-1.208820
C	4.265425	-2.281860	-1.413937
O	7.578792	-2.243997	0.371031
S	-4.529318	-0.892306	0.693542
Fe	-2.121410	-0.637438	0.107417
C	-2.561245	-1.394954	-3.200363
C	-2.715891	2.690190	-0.573717
C	-1.853500	0.102935	3.447526
C	-1.749162	-3.977604	0.831440
N	-2.545126	0.430416	-1.543561
C	-2.665813	-0.060711	-2.836737
C	-2.936112	1.023389	-3.755465
C	-2.983835	2.171804	-3.016674
C	-2.744870	1.798278	-1.639866
N	-2.319664	1.041748	1.212418
C	-2.521906	2.337657	0.751742
C	-2.477234	3.268900	1.857447
C	-2.238099	2.538071	2.986236
C	-2.129612	1.151609	2.585725
N	-1.865177	-1.724617	1.802653
C	-1.739817	-1.232497	3.087818
C	-1.488399	-2.320478	4.012357
C	-1.465521	-3.470731	3.278978
C	-1.697083	-3.096643	1.898337
N	-2.164188	-2.341542	-0.964455
C	-1.962518	-3.625994	-0.496855
C	-2.004196	-4.565724	-1.596376
C	-2.229947	-3.840635	-2.732009
C	-2.328302	-2.453521	-2.332661
O	-0.406805	-0.533139	0.025311
H	3.316403	4.083933	-0.484465
H	3.927424	1.901528	-1.101571
H	2.617669	-0.504668	0.261716
H	2.705518	0.332839	-2.673515
H	1.763082	-0.988872	-1.977486
H	0.294503	0.398386	-0.836694
H	0.354226	1.075514	-2.453308
H	-0.261813	3.258143	-2.028637
H	1.902045	5.824247	0.520875
H	1.059771	4.657204	1.522718
H	4.283960	1.155246	1.847478
H	5.017005	2.503679	0.999441
H	6.375808	1.004369	-0.394980
H	4.111335	-1.026712	1.940243
H	1.246515	0.784524	1.439263

H	0.760372	2.430982	1.810500
H	7.063574	-1.142626	-1.227725
H	6.174932	-3.155736	-2.151297
H	5.678680	-3.762988	-0.578592
H	3.528227	-2.823012	-0.807791
H	3.935726	-2.353713	-2.455143
H	4.868783	-0.257273	-1.772778
H	5.757163	-1.601874	2.211556
H	4.604208	-2.582187	1.281490
H	2.332171	1.845238	2.373286
H	3.383560	3.889747	1.266812
H	6.624590	0.608692	1.305428
H	7.214379	-2.906972	0.991777
H	-4.975088	0.334908	0.238493
H	-2.678167	-1.632616	-4.252661
H	-2.825117	3.745698	-0.798322
H	-1.726368	0.346374	4.497187
H	-1.608698	-5.031463	1.048088
H	-3.076193	0.905543	-4.820016
H	-3.167554	3.181110	-3.354314
H	-2.602967	4.337012	1.759577
H	-2.138907	2.890401	4.002508
H	-1.358283	-2.202028	5.078054
H	-1.311259	-4.482776	3.623413
H	-1.877940	-5.633822	-1.496885
H	-2.325092	-4.196735	-3.747291

## Frequencies:

-45.0088	-18.8576	8.9098
15.7627	17.0211	33.8561
35.9174	52.2347	55.0334
58.8659	75.7330	85.2812
94.5925	98.9274	119.5389
128.1030	139.4643	148.4056
153.6409	156.9424	171.2132
182.4620	198.3087	201.9580
209.1202	216.2680	219.5152
220.2423	231.5558	241.4529
254.1318	266.7943	270.7109
278.5195	280.0835	281.7356
282.8643	292.2525	296.7073
301.4871	309.0332	313.4280
328.5854	340.3038	352.3096
360.7896	370.9877	374.3453
377.6587	381.8016	385.9372
399.0014	412.9936	419.1543
422.8214	434.0801	436.3733
438.6663	439.6089	444.1826
469.3346	472.0466	485.4396
507.2573	512.6110	518.5601
548.3231	553.3491	560.5388
576.3898	584.0350	621.6617
646.4356	660.7205	677.8106
678.5977	687.1981	688.9168
689.4926	700.3267	724.4700
724.8740	729.7152	734.8820
740.3515	760.8385	764.6314
766.4710	766.6585	798.4348
802.7591	811.5905	813.3684
816.8851	821.3003	821.7421
834.6572	835.5097	849.6951
852.1590	852.8523	855.7668
880.9925	906.4621	906.8980
918.8204	921.3011	929.9361
934.4687	937.8346	942.1788
952.2471	953.6592	953.8969
960.0343	967.3539	975.3474
985.8432	992.3837	1003.5470
1017.3658	1019.8935	1022.4618
1024.3964	1030.0392	1033.2672
1038.9452	1048.8982	1051.8101

1058.0590	1058.6438	1062.7988
1065.7678	1076.8095	1077.7282
1087.3997	1101.9155	1117.5135
1117.9440	1119.8479	1123.5692
1128.9059	1137.3960	1150.0949
1153.8466	1169.5132	1175.7522
1181.1619	1190.8830	1192.1703
1199.3705	1214.7934	1216.6192
1237.9932	1240.1779	1243.3526
1245.5110	1257.3754	1265.5698
1281.4035	1292.9900	1296.3023
1297.8437	1300.3006	1306.3888
1307.6709	1320.3868	1327.7659
1332.8199	1336.3693	1345.4224
1348.4856	1350.1401	1357.1415
1363.3124	1376.6499	1378.4389
1386.1127	1388.4965	1389.2429
1394.4448	1398.7215	1400.6891
1409.0953	1411.7454	1415.1614
1419.5430	1423.3873	1427.8674
1429.3131	1436.2878	1437.1564
1442.8561	1453.1932	1462.1613
1498.8044	1499.9139	1501.8948
1510.1517	1529.7220	1532.6066
1534.1251	1534.5624	1536.7395
1540.8614	1545.5667	1550.4710
1556.9499	1558.4936	1562.1303
1564.9814	1590.4910	1591.8597
1604.6072	1614.3955	1635.5453
1644.5697	1647.0541	1660.7776
1716.0645	2310.6839	2503.6128
2955.2002	2965.8692	2996.5191
3019.7501	3033.0062	3040.0327
3043.0020	3047.1802	3051.2660
3052.1308	3060.5344	3061.0189
3073.9325	3078.7029	3079.3059
3087.2682	3092.4841	3097.6335
3097.8841	3101.7519	3111.8930
3119.4227	3130.1880	3143.4660
3151.3269	3205.8556	3212.1087
3212.5278	3213.3700	3223.7059
3264.9482	3265.0793	3266.6746
3267.5786	3287.9106	3288.1884
3289.4694	3290.5041	3630.6332

## III.B.14. Point P14

Absolute energy: -2476.6024028

Geometry:

C	0.467791	3.337355	-1.228782
C	0.494675	4.609501	-0.527553
C	1.552876	4.785672	0.548082
C	5.447277	-0.855779	0.191509
O	-0.352681	5.507566	-0.763365
C	2.723917	3.800177	0.397255
C	2.276960	2.318508	0.226297
C	3.523975	1.438370	-0.182596
C	3.122510	-0.017079	-0.583670
C	2.148741	0.018526	-1.776732
C	0.966835	0.958202	-1.553901
C	1.231011	2.258979	-0.898103
C	4.668129	1.472473	0.870489
C	5.882631	0.587781	0.496494
C	4.389016	-0.809573	-0.943398
C	4.945160	-1.558583	1.475286
C	1.618717	1.806843	1.542991
C	6.522316	-1.747354	-0.492461
C	5.701081	-2.863794	-1.208823
C	4.265437	-2.281848	-1.413922
O	7.578818	-2.244020	0.371043
S	-4.529434	-0.892264	0.693544
Fe	-2.120650	-0.637580	0.107505
C	-2.561264	-1.394955	-3.200398
C	-2.715934	2.690205	-0.573701
C	-1.853490	0.102978	3.447599
C	-1.749166	-3.977662	0.831430
N	-2.545276	0.430293	-1.543444
C	-2.665830	-0.060753	-2.836722
C	-2.936103	1.023368	-3.755435
C	-2.983826	2.171778	-3.016626
C	-2.744867	1.798244	-1.639809
N	-2.319723	1.041583	1.212446
C	-2.521919	2.337637	0.751695
C	-2.477236	3.268890	1.857440
C	-2.238105	2.538101	2.986234
C	-2.129622	1.151601	2.585775
N	-1.865648	-1.724623	1.802697
C	-1.739905	-1.232435	3.087863
C	-1.488383	-2.320440	4.012323
C	-1.465508	-3.470701	3.278931
C	-1.697179	-3.096689	1.898297
N	-2.164251	-2.341490	-0.964418
C	-1.962530	-3.625984	-0.496839
C	-2.004198	-4.565726	-1.596393
C	-2.229940	-3.840632	-2.732009
C	-2.328311	-2.453482	-2.332656
O	-0.411308	-0.535259	0.027397
H	3.316443	4.083941	-0.484371
H	3.927408	1.901505	-1.101586
H	2.617337	-0.504644	0.261397
H	2.707632	0.332548	-2.673886
H	1.763782	-0.988479	-1.978184
H	0.294598	0.402404	-0.841379
H	0.359447	1.078949	-2.457541
H	-0.261043	3.258299	-2.029068
H	1.902016	5.824336	0.520882
H	1.059770	4.657273	1.522763
H	4.283978	1.155252	1.847512
H	5.017013	2.503713	0.999455
H	6.375787	1.004355	-0.395008
H	4.111336	-1.026658	1.940200
H	1.246609	0.784456	1.439039

H	0.760361	2.430998	1.810543
H	7.063638	-1.142611	-1.227691
H	6.174959	-3.155751	-2.151313
H	5.678739	-3.762991	-0.578555
H	3.528216	-2.823032	-0.807785
H	3.935693	-2.353617	-2.455142
H	4.868798	-0.257270	-1.772691
H	5.757189	-1.601888	2.211586
H	4.604202	-2.582205	1.281469
H	2.332219	1.845061	2.373154
H	3.383693	3.889983	1.266989
H	6.624627	0.608714	1.305441
H	7.214374	-2.906905	0.991786
H	-4.975444	0.334936	0.238818
H	-2.678069	-1.632604	-4.252735
H	-2.824729	3.745773	-0.798367
H	-1.726235	0.346427	4.497265
H	-1.608598	-5.031534	1.048070
H	-3.076050	0.905480	-4.820043
H	-3.167354	3.181181	-3.354216
H	-2.602837	4.337049	1.759449
H	-2.138847	2.890414	4.002550
H	-1.358169	-2.201926	5.078044
H	-1.311151	-4.482794	3.623313
H	-1.877897	-5.633859	-1.496840
H	-2.325064	-4.196669	-3.747360

## Frequencies:

-33.5561	-15.2441	8.0037
16.4698	25.5040	34.3494
36.7271	52.3221	55.1466
59.0743	75.1791	86.6706
94.7603	99.8584	119.8620
128.0749	139.0640	148.1646
153.5194	156.8522	171.1860
182.3809	197.7792	201.8542
209.1078	216.3689	219.3022
220.2171	231.7639	241.6716
255.0972	266.7644	270.7809
278.9772	280.2291	281.7845
282.7828	292.7909	296.5540
301.6814	309.1658	313.3700
328.3555	339.7469	353.3468
360.7866	371.0861	374.4464
378.1550	381.9410	386.2704
399.1431	413.0552	419.3168
422.2497	434.1713	436.4130
438.7356	439.6452	444.0473
469.3987	475.2296	485.4473
507.2533	518.1790	531.7225
547.2428	554.0134	560.7511
576.4172	583.5521	621.7106
646.3706	660.7165	677.8691
678.6615	687.2558	689.0042
689.5260	700.1826	724.6152
724.9527	729.7545	734.9167
740.4396	760.8064	764.6637
766.4514	766.6155	798.4432
802.9118	811.7909	813.5641
816.9317	821.2760	821.9504
834.6554	835.4818	849.7538
852.1398	852.9143	855.7702
880.9705	906.5615	907.0227
918.9638	921.4645	929.9765
934.5161	937.9621	942.3875
952.2359	953.8156	954.0835
960.2376	967.4328	975.4136
985.8952	992.3764	1003.5574
1017.3687	1019.7718	1022.4267
1024.3804	1030.1206	1033.2103
1038.9612	1048.8515	1051.8092

1058.0054	1058.6473	1062.8547
1065.8582	1076.8939	1077.7028
1087.4446	1101.9581	1117.6305
1118.0569	1119.9597	1123.6776
1128.9404	1137.5114	1150.0200
1153.8893	1169.7191	1175.7683
1181.6360	1190.8840	1192.1372
1199.3149	1214.7354	1216.5695
1238.0671	1240.7456	1243.9516
1245.5306	1257.4573	1265.7545
1281.5469	1293.3421	1296.8434
1298.1521	1300.1864	1306.4276
1307.8561	1320.6078	1328.8615
1333.0095	1336.6503	1345.4836
1348.5902	1350.1883	1357.1583
1363.3968	1376.7849	1378.4681
1386.0545	1388.5339	1389.2190
1394.5822	1398.8360	1400.8297
1409.1355	1411.7894	1415.2030
1419.6112	1423.3918	1427.9390
1429.3973	1436.6770	1437.1851
1446.0741	1453.2285	1462.4801
1498.8765	1499.9740	1501.8981
1510.1726	1529.7420	1532.9435
1534.1553	1534.5595	1536.7528
1540.8601	1545.5664	1550.4817
1556.8881	1558.5308	1562.1402
1564.9905	1590.5277	1591.8769
1604.7396	1614.4338	1637.4288
1644.6658	1647.0623	1661.7796
1716.1029	2369.5620	2503.9357
2955.0714	2965.7454	2996.9328
3019.5713	3032.8105	3039.7849
3042.7626	3046.9525	3050.8917
3051.8882	3060.3204	3060.7756
3073.6843	3078.3265	3078.9654
3086.1376	3092.2080	3097.3937
3097.6612	3101.4721	3111.6724
3119.1913	3130.0139	3143.2463
3151.0400	3205.4626	3211.9173
3212.3418	3213.1601	3223.4701
3264.5543	3264.6921	3266.2927
3267.2004	3287.5135	3287.8045
3289.0879	3290.1282	3631.2920



## III.B.15. Point P15

Absolute energy: -2476.5962902

Geometry:

C	0.477841	3.349120	-1.237791
C	0.497781	4.614387	-0.526265
C	1.553656	4.788708	0.551463
C	5.448165	-0.856010	0.193118
O	-0.354882	5.509645	-0.758509
C	2.726332	3.803899	0.401282
C	2.280879	2.321601	0.223087
C	3.527409	1.440824	-0.182496
C	3.125306	-0.013400	-0.588987
C	2.165747	0.029053	-1.791907
C	0.994021	0.982742	-1.593692
C	1.242618	2.259920	-0.910349
C	4.669268	1.472338	0.872127
C	5.883530	0.587655	0.497761
C	4.391195	-0.809335	-0.942067
C	4.945371	-1.558784	1.476236
C	1.616162	1.806901	1.535084
C	6.523102	-1.747612	-0.491607
C	5.701456	-2.863698	-1.208387
C	4.265973	-2.281303	-1.412981
O	7.579453	-2.244671	0.371221
S	-4.536939	-0.890935	0.694616
Fe	-2.124980	-0.644059	0.112127
C	-2.561598	-1.395876	-3.200519
C	-2.715390	2.688636	-0.572643
C	-1.854582	0.102943	3.449693
C	-1.750644	-3.978055	0.831794
N	-2.545173	0.427638	-1.541428
C	-2.666175	-0.062128	-2.835431
C	-2.935293	1.022175	-3.753780
C	-2.982436	2.170368	-3.014378
C	-2.744213	1.795931	-1.637964
N	-2.322362	1.039500	1.214568
C	-2.522502	2.335589	0.752546
C	-2.476642	3.268034	1.857044
C	-2.237533	2.538337	2.986598
C	-2.130861	1.151257	2.587484
N	-1.882969	-1.727203	1.807068
C	-1.747100	-1.233124	3.089859
C	-1.486861	-2.320520	4.012633
C	-1.464282	-3.470625	3.279027
C	-1.704870	-3.097467	1.899629
N	-2.167156	-2.343117	-0.964148
C	-1.963864	-3.626578	-0.496799
C	-2.003661	-4.566194	-1.596760
C	-2.229603	-3.840997	-2.732237
C	-2.329427	-2.454078	-2.332469
O	-0.414218	-0.547797	0.041917
H	3.322783	4.091720	-0.476581
H	3.934528	1.904871	-1.099596
H	2.608002	-0.501984	0.247582
H	2.735355	0.350433	-2.681380
H	1.785867	-0.976250	-2.009628
H	0.177010	0.304955	-0.799743
H	0.385392	1.098705	-2.486475
H	-0.246939	3.273414	-2.042148
H	1.902923	5.827483	0.525945
H	1.059453	4.659311	1.525359
H	4.283874	1.154428	1.848425
H	5.018432	2.503425	1.002274
H	6.376242	1.004266	-0.394072
H	4.110539	-1.027164	1.939983
H	1.241903	0.785634	1.425518

H	0.757464	2.430808	1.802830
H	7.063815	-1.142473	-1.227088
H	6.175121	-3.155344	-2.151146
H	5.678823	-3.763127	-0.578484
H	3.528430	-2.822351	-0.807112
H	3.936482	-2.352545	-2.454493
H	4.874270	-0.258749	-1.770881
H	5.756427	-1.601696	2.213692
H	4.604919	-2.582576	1.282315
H	2.327027	1.841049	2.367803
H	3.382163	3.890694	1.274179
H	6.625961	0.608719	1.306304
H	7.214993	-2.906433	0.992969
H	-4.981248	0.341472	0.252653
H	-2.677229	-1.632983	-4.253255
H	-2.823900	3.744283	-0.797684
H	-1.721237	0.346966	4.498615
H	-1.603845	-5.031387	1.047776
H	-3.074986	0.904956	-4.818677
H	-3.165518	3.180137	-3.351722
H	-2.601666	4.336369	1.758148
H	-2.137515	2.891985	4.002549
H	-1.349719	-2.201980	5.077627
H	-1.303282	-4.482025	3.622842
H	-1.876567	-5.634436	-1.497698
H	-2.324041	-4.197006	-3.747835

## Frequencies:

-1657.7204	10.8424	14.4218
19.3832	35.7107	37.3336
41.8917	52.8791	58.3578
58.6786	72.2810	77.6228
92.9376	100.3109	115.4367
130.9820	139.7327	143.9149
153.8397	157.0639	163.2734
177.6195	188.5347	201.0967
206.5203	211.1821	219.2446
224.1375	232.0933	232.6736
245.4706	265.9240	270.9860
273.9069	280.0605	281.5124
282.3471	287.8187	297.0107
301.9983	303.7351	314.8325
319.1847	328.8605	338.8787
359.6476	369.5169	370.8511
374.3984	379.9135	384.1602
399.7649	411.5570	414.9023
422.6915	434.0253	436.3079
437.3187	439.7660	442.2649
462.5329	473.9408	485.9444
500.9306	518.1496	520.4030
548.5036	559.9132	561.0555
577.4502	616.8116	626.3100
655.3811	662.4008	678.4474
679.1768	687.5626	689.9298
690.3469	705.5927	721.5015
725.5837	730.2362	732.9888
737.8516	748.9420	761.1538
766.4777	766.9144	767.0782
801.4312	802.9450	811.9533
813.7189	819.2654	822.1051
829.6293	834.8043	835.4796
850.0833	852.4229	853.7875
864.9358	888.9998	906.1839
906.5860	918.4086	921.0024
934.6357	937.0922	939.9517
942.1714	953.2827	953.5934
953.9940	959.7501	971.0016
975.4625	986.0355	992.6418
1004.0827	1018.1090	1019.5642
1022.9555	1025.0132	1027.4235
1033.7387	1039.4643	1048.6500

1051.2515	1058.1756	1058.6423
1063.4651	1064.1875	1077.9232
1079.1631	1088.2258	1102.2205
1117.4452	1118.0002	1119.9528
1123.5997	1128.3343	1139.0566
1150.5548	1157.8133	1172.0986
1176.2356	1183.2864	1191.0467
1192.5504	1201.4508	1214.9409
1216.5422	1233.6324	1242.0274
1245.5727	1247.0540	1256.8131
1266.3336	1279.8978	1288.2744
1295.7292	1297.7671	1300.2872
1307.3233	1313.5305	1321.4387
1327.9048	1333.5906	1342.7969
1345.6415	1349.7719	1350.9943
1357.6509	1363.3944	1368.0110
1378.4617	1384.3643	1387.0866
1389.3754	1391.8666	1395.9593
1399.4053	1401.9986	1409.5191
1412.0768	1415.8504	1420.5755
1423.8123	1427.8339	1428.4067
1437.4573	1438.6024	1453.7357
1462.8343	1499.4016	1500.5285
1502.1955	1510.1119	1527.3094
1529.9158	1534.0989	1535.1745
1536.7505	1540.7441	1545.7158
1550.6882	1557.1670	1558.6044
1562.3706	1564.9605	1591.1517
1592.5421	1608.7789	1609.6127
1615.2439	1644.7460	1646.6619
1647.1074	1715.8292	2503.6177
2952.4536	2963.6009	2983.2804
3019.0397	3032.0790	3040.5999
3043.0647	3046.9059	3051.6442
3055.4725	3060.1324	3060.9411
3073.6653	3078.0552	3080.4557
3092.6595	3096.8131	3097.0050
3101.9695	3111.5442	3118.6602
3129.0500	3142.2176	3149.8640
3175.8164	3206.3447	3210.2238
3210.7443	3211.2477	3221.8638
3262.7444	3262.9432	3264.1186
3265.1827	3285.7877	3286.1685
3286.9878	3288.1176	3632.9137

## III.B.16. Point P16

Absolute energy: -2476.6034355

Geometry:

C	0.493814	3.360961	-1.248232
C	0.501409	4.619143	-0.526330
C	1.555070	4.791127	0.555122
C	5.449514	-0.856305	0.194958
O	-0.355672	5.510640	-0.751698
C	2.729117	3.807251	0.406363
C	2.284441	2.326080	0.217441
C	3.532145	1.444311	-0.183649
C	3.129628	-0.007680	-0.598203
C	2.191648	0.046751	-1.817421
C	1.005368	0.988845	-1.620401
C	1.257020	2.276114	-0.925652
C	4.670474	1.472086	0.874490
C	5.884748	0.587342	0.500216
C	4.394970	-0.808316	-0.941446
C	4.945149	-1.558919	1.477266
C	1.612084	1.806245	1.523529
C	6.524393	-1.747878	-0.490074
C	5.702231	-2.863652	-1.207250
C	4.267292	-2.280118	-1.411681
O	7.580045	-2.245683	0.371867
S	-4.547538	-0.889164	0.695888
Fe	-2.122842	-0.650599	0.117275
C	-2.562129	-1.396954	-3.198662
C	-2.714611	2.684516	-0.570698
C	-1.857916	0.101889	3.451281
C	-1.754197	-3.978005	0.832464
N	-2.548151	0.423951	-1.538998
C	-2.666779	-0.064271	-2.832419
C	-2.933662	1.019661	-3.749876
C	-2.979973	2.167155	-3.010037
C	-2.743306	1.791790	-1.634949
N	-2.327248	1.036472	1.218142
C	-2.523344	2.331633	0.753846
C	-2.475409	3.264863	1.856103
C	-2.236600	2.536662	2.986259
C	-2.133535	1.149908	2.589136
N	-1.902672	-1.730494	1.812189
C	-1.756453	-1.234299	3.092279
C	-1.486167	-2.319886	4.011607
C	-1.463907	-3.469893	3.277722
C	-1.714709	-3.098640	1.901317
N	-2.172867	-2.345703	-0.963166
C	-1.966859	-3.627492	-0.496011
C	-2.002891	-4.565635	-1.595861
C	-2.228880	-3.840242	-2.730928
C	-2.331415	-2.454873	-2.330889
O	-0.439994	-0.563830	0.058977
H	3.329825	4.099557	-0.467500
H	3.944297	1.910395	-1.097730
H	2.599526	-0.497518	0.230274
H	2.778615	0.376402	-2.691290
H	1.816267	-0.957519	-2.050206
H	0.236089	0.370854	-0.906528
H	0.445555	1.139691	-2.543717
H	-0.226497	3.289254	-2.058016
H	1.904669	5.830434	0.532807
H	1.058427	4.659793	1.527935
H	4.282578	1.152191	1.849652
H	5.020564	2.502939	1.008120
H	6.377660	1.004631	-0.391625
H	4.107988	-1.027737	1.938517
H	1.236855	0.785613	1.407965

H	0.753554	2.431068	1.791137
H	7.063689	-1.142199	-1.226861
H	6.175865	-3.154890	-2.150782
H	5.678943	-3.763872	-0.577749
H	3.528956	-2.820295	-0.805098
H	3.937442	-2.351210	-2.453552
H	4.882258	-0.260733	-1.770038
H	5.754347	-1.600677	2.217513
H	4.606324	-2.583735	1.283364
H	2.319611	1.834192	2.359939
H	3.380964	3.890496	1.283338
H	6.627559	0.608045	1.309068
H	7.215186	-2.905875	0.993548
H	-4.986136	0.349094	0.268069
H	-2.675168	-1.633386	-4.252274
H	-2.819732	3.740850	-0.796465
H	-1.717317	0.346582	4.499548
H	-1.599925	-5.030825	1.048029
H	-3.072024	0.903757	-4.815760
H	-3.160756	3.177939	-3.347692
H	-2.597581	4.334105	1.756037
H	-2.134331	2.892602	4.001887
H	-1.340032	-2.201552	5.076091
H	-1.294131	-4.480668	3.621245
H	-1.873676	-5.634427	-1.498133
H	-2.321107	-4.196667	-3.747291

## Frequencies:

-130.6533	3.5608	9.6430
13.1546	24.7761	34.7271
35.8814	52.2765	55.0169
57.8548	67.5137	80.4665
92.4293	98.4880	120.3925
131.9193	135.8160	148.3180
151.9951	161.0116	174.8594
184.5350	193.9509	199.4521
203.2461	211.9215	219.2726
222.2096	232.1306	240.5520
256.7162	267.9286	274.3759
279.1406	280.6166	280.8608
283.3928	288.1632	298.2802
303.8167	308.5298	314.8170
318.2236	328.3543	335.4879
359.0912	371.8217	373.0147
377.3905	380.9819	384.9816
400.7361	413.0415	417.6900
424.1194	434.6618	437.0896
438.9873	440.0590	450.2097
471.5477	472.4392	485.5597
510.6788	518.5369	535.1737
556.1790	560.8414	576.9276
592.0793	622.1967	635.6594
652.6723	658.9967	678.5821
679.3077	688.4257	689.6037
690.3457	705.6049	726.1233
726.4161	731.1236	736.3522
742.3011	761.8217	766.0782
767.6120	767.9095	799.9566
805.5841	814.8807	816.8289
819.8212	825.3124	826.7855
835.7227	836.1491	850.7921
852.9129	855.1108	863.2218
882.9295	908.4493	909.7167
921.6717	924.4724	935.3194
936.1838	940.2404	946.2053
954.4987	956.9144	957.3886
963.7105	970.9262	975.5729
986.3872	992.2806	1002.7533
1020.7388	1022.0083	1025.2017
1026.0536	1028.4651	1036.9553
1039.7619	1048.1425	1051.4148

1060.8213	1061.8918	1064.6152
1064.9864	1080.1739	1080.7968
1089.0314	1102.6863	1119.9279
1120.4459	1122.2730	1126.0237
1129.0449	1139.7266	1149.6221
1160.7480	1171.9774	1176.4970
1187.1021	1194.7267	1196.4734
1202.4488	1213.4894	1219.7022
1232.2249	1242.7467	1248.6451
1255.8033	1258.6017	1268.5678
1281.0734	1293.4880	1300.7088
1301.5932	1303.3091	1307.9738
1313.8300	1322.7210	1333.2919
1335.5685	1346.1580	1352.9811
1353.6863	1358.0197	1358.7659
1365.3971	1378.1141	1383.0286
1389.4460	1390.5935	1392.8191
1397.0631	1400.1734	1403.7947
1409.3770	1414.7458	1416.7542
1420.5432	1426.3913	1430.0603
1432.5088	1438.8454	1440.1766
1453.9986	1460.0573	1481.7665
1501.8875	1502.8933	1504.1874
1510.2907	1529.5910	1530.5200
1534.4368	1537.1244	1538.4573
1540.9999	1545.8096	1550.7489
1553.4592	1557.8107	1560.4859
1562.9422	1565.0761	1593.4362
1594.9215	1609.8840	1617.2677
1647.7004	1649.3287	1650.7103
1677.1067	1719.1497	2510.9610
2950.4928	2961.6554	2992.0892
3015.5419	3028.9529	3036.5664
3038.6578	3042.6702	3047.4265
3049.6014	3055.9730	3056.4430
3069.0201	3073.4467	3075.1630
3087.3901	3091.9675	3092.4315
3096.5350	3106.8683	3114.0835
3125.0097	3135.1154	3137.2797
3145.7424	3196.3335	3206.6581
3207.0864	3207.2842	3217.8646
3256.7424	3257.0818	3258.2547
3259.2594	3279.7295	3280.2014
3281.1103	3282.1406	3644.9876

## III.B.17. Point P17

Absolute energy: -2476.597926

Geometry:

C	0.471801	3.345926	-1.235371
C	0.497943	4.612296	-0.527138
C	1.553446	4.787242	0.550439
C	5.447881	-0.855890	0.192702
O	-0.353712	5.508471	-0.760093
C	2.725241	3.802196	0.399263
C	2.279853	2.319496	0.223690
C	3.526864	1.440592	-0.182860
C	3.125224	-0.014077	-0.587665
C	2.155482	0.025024	-1.782666
C	0.992849	0.983457	-1.581572
C	1.235691	2.250077	-0.905346
C	4.668985	1.472151	0.871813
C	5.883318	0.587659	0.497666
C	4.390955	-0.809185	-0.943309
C	4.945061	-1.558638	1.475860
C	1.616779	1.806792	1.536684
C	6.523160	-1.747630	-0.491619
C	5.701454	-2.863673	-1.208289
C	4.265981	-2.281341	-1.413206
O	7.579026	-2.244521	0.371314
S	-4.534981	-0.891303	0.694381
Fe	-2.127276	-0.641590	0.110564
C	-2.561469	-1.395762	-3.199763
C	-2.715253	2.688404	-0.572764
C	-1.854887	0.102394	3.448632
C	-1.750769	-3.977496	0.831912
N	-2.544704	0.428914	-1.542637
C	-2.666098	-0.061510	-2.835436
C	-2.935311	1.022215	-3.753815
C	-2.982514	2.170464	-3.014698
C	-2.744398	1.796169	-1.638666
N	-2.321963	1.040787	1.214139
C	-2.522425	2.335753	0.752884
C	-2.476561	3.267689	1.857025
C	-2.237551	2.537525	2.986280
C	-2.130921	1.151166	2.586607
N	-1.876136	-1.726789	1.806020
C	-1.745122	-1.233704	3.088740
C	-1.487630	-2.320709	4.012431
C	-1.464949	-3.470622	3.279063
C	-1.702723	-3.096646	1.899631
N	-2.166707	-2.343414	-0.964280
C	-1.963976	-3.626217	-0.496899
C	-2.003744	-4.565745	-1.596274
C	-2.229591	-3.840681	-2.731728
C	-2.329296	-2.454293	-2.331934
O	-0.389212	-0.531720	0.025096
H	3.321651	4.090087	-0.479307
H	3.933702	1.905104	-1.100240
H	2.611556	-0.502815	0.251387
H	2.714106	0.351043	-2.679161
H	1.777603	-0.981405	-2.000516
H	0.124884	0.239316	-0.707799
H	0.336468	1.066167	-2.445284
H	-0.256592	3.268988	-2.037186
H	1.903296	5.826447	0.524741
H	1.059356	4.657850	1.524834
H	4.283140	1.154077	1.848355
H	5.018192	2.503801	1.002083
H	6.376813	1.004758	-0.394055
H	4.109715	-1.027223	1.940319

H	1.241789	0.784910	1.428952
H	0.757090	2.430614	1.804211
H	7.063571	-1.142216	-1.228079
H	6.175328	-3.155505	-2.151654
H	5.678242	-3.763540	-0.578203
H	3.528171	-2.822269	-0.806619
H	3.936497	-2.353604	-2.455445
H	4.873898	-0.258308	-1.772479
H	5.756464	-1.601406	2.213670
H	4.604740	-2.583057	1.282250
H	2.327724	1.842739	2.369906
H	3.382203	3.888893	1.271944
H	6.625738	0.608379	1.306955
H	7.215456	-2.906006	0.991583
H	-4.977921	0.338859	0.247730
H	-2.677910	-1.633252	-4.253186
H	-2.826313	3.744682	-0.797646
H	-1.723720	0.346459	4.498686
H	-1.605970	-5.031876	1.048278
H	-3.075959	0.905253	-4.819731
H	-3.166975	3.180812	-3.353145
H	-2.602298	4.337164	1.759274
H	-2.137736	2.891677	4.003245
H	-1.352286	-2.202616	5.078812
H	-1.305648	-4.483083	3.623966
H	-1.876669	-5.635138	-1.497601
H	-2.324064	-4.197698	-3.748154

## Frequencies:

-1710.2561	7.7148	13.6607
19.3029	36.8663	38.8199
46.2718	52.6074	58.1129
59.7589	71.8073	74.2198
92.2873	99.9680	114.8867
130.1023	135.7011	138.8931
153.3063	154.3730	164.8558
174.7617	192.5027	200.3853
209.8828	213.4012	218.9058
225.0013	230.7046	233.7870
246.2775	268.9704	270.2762
274.7941	279.8050	281.7416
282.5938	287.7035	296.6406
297.9268	303.8918	312.6163
317.6633	324.0669	334.3757
361.6887	369.0566	370.0770
373.3153	380.8065	384.5063
399.9180	410.3919	416.9050
423.5693	433.5464	436.4045
437.8480	440.4195	442.0654
464.3181	477.2988	486.6731
506.4878	520.0211	533.4294
548.1430	561.7834	562.3794
578.9879	620.6764	634.3292
659.0327	673.6646	679.4589
680.0607	689.8604	690.3591
691.2854	703.9094	709.7984
727.5728	728.2398	731.9451
737.0600	743.0232	761.9890
767.3244	767.9062	768.1665
803.3056	805.9120	814.6708
816.6148	820.1996	825.0771
827.8651	834.9935	835.6808
851.1581	853.0278	855.5942
863.8809	888.6507	903.3607
909.3272	920.6610	923.4424
935.0359	937.5738	938.8439
945.0661	952.9802	955.8198
956.1704	961.8179	969.1946
975.3857	985.9667	994.0475
1003.0755	1019.1590	1021.5013
1024.4473	1025.1432	1026.7043



1035.0237	1039.0758	1049.9050
1050.0881	1058.7857	1059.5323
1063.0306	1063.9397	1076.8509
1078.6955	1086.9303	1101.5304
1116.6979	1119.2675	1119.8824
1121.9156	1125.4955	1129.1637
1144.5078	1151.7303	1160.6218
1172.7361	1176.5928	1192.6645
1194.3194	1198.5040	1200.4427
1213.4738	1218.3801	1232.8917
1243.6127	1247.1267	1255.2645
1263.7505	1272.4710	1279.0566
1295.8189	1298.7825	1301.5449
1306.0606	1308.5004	1315.6510
1316.3446	1323.3458	1333.2752
1338.4965	1346.5416	1350.7816
1352.3804	1358.9204	1363.6727
1377.2011	1379.8335	1389.2087
1390.0635	1390.5613	1396.1627
1399.6033	1401.8284	1410.2544
1414.0945	1416.8315	1421.0353
1425.2442	1427.0813	1429.8175
1438.7400	1439.3242	1455.3178
1465.9540	1500.1167	1501.3041
1503.4623	1510.7206	1518.3494
1530.5278	1534.8248	1536.0897
1537.3655	1541.3152	1546.3168
1551.3865	1557.6976	1559.4318
1562.9548	1565.5687	1571.6388
1592.2594	1593.7411	1610.6106
1616.7270	1633.4048	1645.2176
1647.2137	1715.8984	2509.4401
2949.0576	2960.1548	2970.2829
3014.9796	3027.2236	3037.2849
3038.8801	3042.7899	3047.3789
3052.6988	3055.6343	3057.7761
3068.8867	3072.1952	3077.9993
3088.5351	3090.5466	3092.3728
3097.9242	3107.0141	3112.9619
3123.5744	3137.0267	3144.2039
3171.4492	3201.8332	3202.3707
3202.3792	3203.0717	3213.2396
3251.6893	3251.9448	3252.9123
3254.1125	3274.9459	3275.4356
3275.9662	3277.1951	3651.9130

### III.C. Geometries, QM energy, and QM frequencies of the supplementary Shepard points in the MCOMM calculations for D-abstraction of 6 $\beta$ -d<sub>1</sub>-testosterone by Cpd I of the <sup>2</sup>A state

#### III.C.1. Point P1

Absolute energy: -2476.5986301

Geometry:

C	.465157	3.336705	-1.226836
C	.494406	4.608387	-.527438
C	1.552384	4.784921	.549044
C	5.446853	-.856316	.192572
O	-.352191	5.506222	-.762697
C	2.723063	3.799303	.397412
C	2.276626	2.316701	.227519
C	3.523684	1.438148	-.181600
C	3.122324	-.017562	-.581844
C	2.142903	.016201	-1.770334
C	.964776	.957398	-1.545778
C	1.226062	2.250611	-.894637
C	4.667868	1.471807	.871422
C	5.882165	.587376	.497433
C	4.388761	-.809989	-.942835
C	4.944819	-1.558824	1.476125
C	1.618781	1.806641	1.544039
C	6.522676	-1.747844	-.491149
C	5.700879	-2.864116	-1.207603
C	4.265191	-2.282170	-1.412779
O	7.577929	-2.244376	.372021
S	-4.529348	-.892808	.694555
Fe	-2.124470	-.637354	.108161
C	-2.561360	-1.395200	-3.198391
C	-2.715864	2.688868	-.572647
C	-1.854002	.102165	3.447579
C	-1.749552	-3.976998	.832279
N	-2.545854	.431210	-1.544205
C	-2.666123	-.060446	-2.835135
C	-2.936134	1.022338	-3.753191
C	-2.983818	2.170577	-3.014574
C	-2.745152	1.797257	-1.639151
N	-2.320333	1.043432	1.214435
C	-2.521971	2.336454	.753640
C	-2.477435	3.267199	1.857746
C	-2.238363	2.536360	2.986410
C	-2.130020	1.151503	2.585678
N	-1.864522	-1.726032	1.805217
C	-1.739934	-1.233763	3.088015
C	-1.488979	-2.320331	4.012239
C	-1.466099	-3.470374	3.279015
C	-1.697204	-3.095902	1.899799
N	-2.164943	-2.343713	-.964451
C	-1.962926	-3.625841	-.496350
C	-2.004543	-4.564786	-1.594577
C	-2.230270	-3.839865	-2.730051
C	-2.328477	-2.454325	-2.330836
O	-.386946	-.524199	.017227
H	3.316923	4.084672	-.484287
H	3.928155	1.901614	-1.100872
H	2.617871	-.505860	.264238
H	2.694454	.336421	-2.672165
H	1.761487	-.992502	-1.976133
H(iso=2)	.249992	.332414	-.777369
H	.324251	1.055188	-2.429704
H	-.266870	3.257381	-2.026229
H	1.903142	5.824458	.521982
H	1.059517	4.656425	1.524841
H	4.283229	1.154537	1.849356
H	5.017235	2.504188	1.000556
H	6.376152	1.004857	-.394408

H	4.109940	-1.026941	1.942296
H	1.245577	.783107	1.441770
H	.758809	2.430625	1.812308
H	7.061378	-1.142097	-1.229526
H	6.174869	-3.156033	-2.151715
H	5.677199	-3.764543	-.577272
H	3.527354	-2.823996	-.805827
H	3.935614	-2.354499	-2.455633
H	4.868675	-.257655	-1.773033
H	5.756946	-1.602626	2.213968
H	4.603657	-2.583693	1.282874
H	2.331732	1.845389	2.376191
H	3.383409	3.888882	1.268293
H	6.624992	.607973	1.307258
H	7.214771	-2.906026	.990935
H	-4.973049	.332201	.239463
H	-2.678912	-1.633313	-4.252213
H	-2.827930	3.745794	-.797247
H	-1.726954	.345935	4.498897
H	-1.609099	-5.032461	1.049412
H	-3.077320	.906028	-4.819941
H	-3.168960	3.181113	-3.354694
H	-2.603912	4.337594	1.761907
H	-2.139266	2.891093	4.004127
H	-1.358657	-2.203518	5.080273
H	-1.311572	-4.483825	3.625929
H	-1.878337	-5.635209	-1.496696
H	-2.325491	-4.198481	-3.746735

## Frequencies:

-706.3034	7.0764	12.8058
16.2350	29.7793	36.5545
37.9183	52.2965	57.0962
59.0368	61.0638	74.7473
91.0820	97.9138	113.1294
119.0684	135.6105	144.7505
152.8059	155.2995	166.6755
174.0921	193.0660	201.8784
207.5833	215.0242	219.2845
225.1127	231.2061	233.9199
244.4867	267.3057	270.2625
274.8822	279.8507	281.0422
282.9474	286.2796	298.5285
299.8714	303.9588	306.2457
316.4366	318.2399	334.6234
360.3429	369.6793	370.6223
373.9039	381.5382	384.2838
400.8213	411.7862	415.1594
421.8711	434.4746	436.6233
438.2369	440.1955	443.9809
450.4428	470.7304	486.4730
501.4553	512.8141	519.2475
544.1753	551.6388	562.1697
576.3351	586.4366	622.8975
645.1075	656.7552	679.3567
680.0797	689.8088	690.0259
691.1330	700.3529	727.1564
728.2195	730.4333	737.2041
743.8373	762.3895	763.2502
768.3781	768.7395	795.3246
808.5589	809.4958	818.1817
819.5723	820.4700	829.0261
835.4735	836.0192	841.0689
851.0927	853.3861	853.8683
857.5327	874.7813	904.1716
913.5761	916.9997	925.1223
927.7188	936.2744	942.7766
950.1439	951.9422	957.4219
960.4235	960.7423	965.9915
966.5128	977.0209	986.5590
992.7871	1001.9333	1020.9339

1021.8779	1024.1832	1026.9112
1027.9363	1037.1807	1039.0379
1049.5556	1051.4165	1061.8322
1062.3544	1062.9878	1064.1396
1080.4879	1080.8468	1087.1244
1102.6535	1122.1856	1122.6770
1124.6283	1128.3273	1128.9606
1139.6134	1151.0866	1162.2532
1173.3647	1176.7971	1188.5884
1196.5605	1197.9872	1200.7386
1216.3699	1221.3939	1223.5479
1243.1383	1244.8532	1249.9395
1258.3337	1265.7915	1277.5881
1284.2200	1296.1502	1301.9242
1305.1431	1308.1842	1312.5315
1316.9658	1323.8669	1333.5837
1337.9774	1347.0727	1352.4039
1354.1257	1359.2419	1364.7014
1377.8071	1380.2650	1390.7348
1391.9675	1393.5243	1396.3922
1400.4664	1402.4362	1411.1825
1416.6797	1417.4820	1420.8264
1427.5103	1430.5942	1432.3604
1438.3931	1440.8425	1456.0762
1465.0864	1500.5195	1502.1043
1504.5164	1511.4147	1529.5462
1530.9830	1535.7944	1537.1940
1537.9165	1542.1072	1546.9011
1551.7837	1558.2793	1560.7734
1563.2876	1566.2140	1592.8644
1594.3566	1607.5585	1616.6823
1624.5619	1644.8431	1647.3859
1657.7879	1716.1816	2520.1178
2948.1348	2958.7193	2979.4467
3010.4786	3022.6452	3031.2831
3032.7650	3037.3080	3042.0064
3044.1929	3049.5939	3050.3624
3062.6806	3066.0907	3068.6711
3081.5501	3084.2859	3086.2454
3086.7004	3090.8404	3100.8087
3106.6990	3118.1157	3131.2640
3139.2945	3192.5776	3196.5095
3196.7955	3197.7547	3207.8398
3244.2392	3244.3759	3245.8729
3246.9182	3267.4243	3267.6940
3268.8283	3269.9505	3663.3330

## III.C.2. Point P2

Absolute energy: -2476.5986311

Geometry:

C	.462551	3.336984	-1.227400
C	.495134	4.608623	-.526879
C	1.552357	4.784898	.549093
C	5.446784	-.856192	.192606
O	-.352520	5.506513	-.763015
C	2.722990	3.799248	.396976
C	2.276939	2.316099	.227758
C	3.523831	1.438243	-.181519
C	3.122527	-.017635	-.581477
C	2.139563	.014734	-1.766802
C	.975574	.968892	-1.553461
C	1.225141	2.243462	-.894100
C	4.667917	1.471783	.871483
C	5.882239	.587397	.497427
C	4.388691	-.810021	-.943082
C	4.944759	-1.558860	1.476157
C	1.618800	1.806633	1.544210
C	6.522485	-1.747894	-.491240
C	5.700821	-2.864100	-1.207691
C	4.265088	-2.282284	-1.412864
O	7.578067	-2.244347	.372045
S	-4.529126	-.892847	.694648
Fe	-2.127733	-.637254	.108062
C	-2.561391	-1.395392	-3.198897
C	-2.715821	2.689492	-.572770
C	-1.853832	.102210	3.448022
C	-1.749447	-3.977381	.832487
N	-2.544385	.431153	-1.543821
C	-2.666084	-.060501	-2.835568
C	-2.936293	1.022759	-3.754062
C	-2.983961	2.171208	-3.015378
C	-2.745203	1.797654	-1.639328
N	-2.319908	1.043122	1.213763
C	-2.522101	2.336891	.753614
C	-2.477430	3.268025	1.858179
C	-2.238327	2.536994	2.986937
C	-2.129969	1.151442	2.586024
N	-1.863375	-1.725678	1.804585
C	-1.739773	-1.233847	3.087992
C	-1.488812	-2.320987	4.013165
C	-1.465929	-3.470958	3.279989
C	-1.697040	-3.095954	1.899857
N	-2.164302	-2.343197	-.964190
C	-1.962861	-3.625947	-.496308
C	-2.004500	-4.565564	-1.595029
C	-2.230260	-3.840649	-2.730619
C	-2.328497	-2.454404	-2.331136
O	-.369795	-.515415	.008897
H	3.317158	4.084859	-.484253
H	3.928240	1.901860	-1.100654
H	2.617630	-.505853	.263627
H	2.686879	.337260	-2.672273
H	1.759049	-.993143	-1.975118
H(iso=2)	.165630	.244768	-.689159
H	.300373	1.040794	-2.411211
H	-.269850	3.257683	-2.025711
H	1.902739	5.824204	.521901
H	1.059491	4.656403	1.524519
H	4.283157	1.154579	1.849017
H	5.016953	2.503990	1.000306
H	6.376163	1.004654	-.394291
H	4.110118	-1.027225	1.942377
H	1.244370	.783761	1.441263

H	.758652	2.430232	1.812083
H	7.062225	-1.142369	-1.228617
H	6.174789	-3.156118	-2.151369
H	5.677326	-3.764132	-.577351
H	3.527427	-2.823837	-.806091
H	3.935699	-2.354956	-2.455528
H	4.869091	-.257568	-1.772898
H	5.757073	-1.602400	2.213350
H	4.603660	-2.583398	1.282846
H	2.331596	1.846086	2.376038
H	3.382830	3.888102	1.267676
H	6.624717	.608057	1.307087
H	7.215083	-2.906403	.991429
H	-4.973042	.332760	.238840
H	-2.679359	-1.633497	-4.252448
H	-2.829369	3.746027	-.797209
H	-1.727189	.345941	4.499165
H	-1.609290	-5.032696	1.049452
H	-3.077922	.905869	-4.820350
H	-3.169893	3.181463	-3.354877
H	-2.604606	4.337971	1.762074
H	-2.139585	2.890989	4.004579
H	-1.358774	-2.203646	5.080823
H	-1.311717	-4.484289	3.626281
H	-1.878449	-5.635590	-1.496538
H	-2.325714	-4.198646	-3.747132

## Frequencies:

-1156.2960	9.9105	13.6999
19.6944	37.1599	38.1856
45.3981	52.8482	58.2401
60.0164	71.6428	72.9541
91.6712	99.9414	115.1223
122.6407	134.9569	139.4544
150.5706	154.8268	163.8868
174.9536	193.9257	202.0055
210.5862	214.5365	219.4008
225.6678	230.3761	233.5833
247.2457	268.9303	270.5809
275.0162	279.4720	281.8894
283.0178	287.4325	295.9964
297.8772	304.1796	309.9489
317.5436	322.4052	334.4737
361.8416	368.7147	369.9115
372.5867	381.2725	384.5347
400.2151	410.4650	416.8695
422.8367	433.6834	436.3610
438.6860	440.4609	442.3207
463.5543	475.7728	486.8661
508.3333	519.7817	541.5247
552.0701	558.7652	564.1645
579.4971	612.7983	623.8581
642.6374	659.1707	672.7594
679.7601	680.3364	690.0915
690.5151	691.4734	701.3040
727.6545	728.0488	731.3752
737.1757	743.1133	762.3632
764.4082	767.9309	768.5569
785.5451	807.4290	813.1283
815.7204	817.0935	819.6994
819.9821	826.8384	835.0241
835.8525	846.2897	851.9301
853.2252	856.4535	872.3053
907.0833	911.2451	914.8837
922.5112	925.1775	935.8495
940.2736	947.0890	952.7376
957.6521	957.9304	959.6752
963.4282	975.2852	980.6853
989.4112	997.9532	1013.3781
1019.8492	1022.7788	1024.9024
1026.5119	1035.5360	1038.3308

1046.3583	1050.8361	1059.4107
1060.1538	1060.5041	1063.4635
1076.0742	1078.9698	1085.7158
1101.1449	1111.8636	1120.3982
1121.0012	1123.0452	1126.6389
1132.0735	1143.3470	1151.9943
1161.1469	1172.9318	1176.7024
1193.8688	1195.4097	1199.0625
1201.3140	1214.9020	1219.4673
1238.3476	1243.8179	1247.9815
1256.3862	1263.9828	1273.0505
1280.4023	1296.2227	1299.6030
1303.1537	1308.5038	1314.2320
1316.0718	1323.1943	1332.9741
1338.4071	1346.8533	1350.8629
1352.4967	1359.3392	1363.6941
1376.8754	1380.2170	1390.0637
1390.3391	1391.1962	1395.9354
1399.8190	1401.7035	1410.8748
1415.1015	1417.8323	1421.0315
1425.9855	1430.1207	1431.7134
1438.9933	1439.2196	1456.0580
1466.5920	1499.6989	1501.0664
1503.6162	1511.1054	1518.6293
1530.7998	1535.2446	1535.8345
1537.6769	1541.7012	1546.6287
1551.7109	1558.1003	1559.7251
1563.1407	1566.0152	1576.8945
1592.0568	1593.6832	1608.8999
1616.4660	1638.6442	1644.1111
1646.4995	1715.0276	2514.1859
2947.8725	2958.1882	2965.3848
3012.6671	3024.4246	3034.8413
3036.1240	3040.2526	3044.9050
3049.8929	3052.6486	3054.5966
3065.9767	3069.0487	3074.4218
3085.7685	3087.0472	3089.7251
3095.0884	3104.0957	3109.7429
3114.8267	3120.6711	3134.1377
3141.3153	3197.9488	3198.3465
3199.2754	3199.8649	3209.4687
3246.9739	3247.1326	3248.3363
3249.5450	3270.3213	3270.5781
3271.3873	3272.6383	3656.9823

## III.C.3. Point P3

Absolute energy: -2476.6010733

Geometry:

C	.466895	3.337307	-1.227026
C	.494212	4.608389	-.527455
C	1.552435	4.785016	.549064
C	5.446943	-.856341	.192571
O	-.352331	5.506359	-.762451
C	2.723288	3.799500	.397938
C	2.276555	2.317448	.227390
C	3.523594	1.438084	-.181612
C	3.122261	-.017480	-.582303
C	2.146151	.017520	-1.773493
C	.962999	.954764	-1.546458
C	1.228164	2.255214	-.895769
C	4.667829	1.471873	.871418
C	5.882165	.587366	.497472
C	4.388810	-.809976	-.942541
C	4.944863	-1.558849	1.476155
C	1.618697	1.806606	1.543878
C	6.522623	-1.747803	-.491172
C	5.700895	-2.864154	-1.207600
C	4.265249	-2.282120	-1.412734
O	7.577982	-2.244397	.372014
S	-4.529677	-.892717	.694523
Fe	-2.121617	-.637731	.108429
C	-2.561398	-1.395145	-3.198320
C	-2.715983	2.688719	-.572534
C	-1.854033	.102254	3.447600
C	-1.749588	-3.977022	.832226
N	-2.546576	.430822	-1.543850
C	-2.666182	-.060627	-2.834981
C	-2.936104	1.022248	-3.753029
C	-2.983793	2.170455	-3.014369
C	-2.745164	1.797112	-1.638905
N	-2.320585	1.042853	1.214521
C	-2.522029	2.336397	.753375
C	-2.477449	3.267088	1.857671
C	-2.238386	2.536362	2.986353
C	-2.130045	1.151401	2.585823
N	-1.865927	-1.725978	1.805205
C	-1.740207	-1.233456	3.088188
C	-1.488971	-2.320122	4.012040
C	-1.466093	-3.470235	3.278743
C	-1.697492	-3.096111	1.899592
N	-2.165301	-2.343491	-.964259
C	-1.962988	-3.625824	-.496223
C	-2.004548	-4.564727	-1.594546
C	-2.230259	-3.839751	-2.729999
C	-2.328544	-2.454112	-2.330826
O	-.403105	-.532047	.024798
H	3.316709	4.084399	-.483954
H	3.927885	1.901406	-1.100868
H	2.617374	-.505678	.263583
H	2.701331	.336045	-2.672806
H	1.764297	-.991261	-1.977900
H(iso=2)	.280752	.370723	-.813961
H	.343361	1.066958	-2.444001
H	-.264158	3.257430	-2.026939
H	1.902934	5.824432	.521946
H	1.059536	4.656612	1.524735
H	4.283373	1.154614	1.849294
H	5.017208	2.504047	1.000653
H	6.375972	1.004709	-.394342
H	4.110113	-1.026856	1.941946
H	1.246273	.783032	1.441196



H	.759078	2.430634	1.812247
H	7.061399	-1.142183	-1.229266
H	6.174863	-3.156033	-2.151487
H	5.677469	-3.764452	-.577323
H	3.527481	-2.823909	-.805952
H	3.935529	-2.354150	-2.455280
H	4.868554	-.257699	-1.772682
H	5.756829	-1.602636	2.213950
H	4.603709	-2.583539	1.282808
H	2.331800	1.844910	2.375716
H	3.383711	3.889478	1.268553
H	6.624945	.608036	1.307116
H	7.214427	-2.906235	.991166
H	-4.974133	.332644	.240099
H	-2.678450	-1.633117	-4.251926
H	-2.826371	3.745500	-.797263
H	-1.726602	.345997	4.498565
H	-1.608800	-5.032157	1.049274
H	-3.076692	.905845	-4.819470
H	-3.168091	3.180847	-3.354157
H	-2.603318	4.337134	1.761412
H	-2.138998	2.890861	4.003727
H	-1.358424	-2.203131	5.079649
H	-1.311353	-4.483381	3.625299
H	-1.878199	-5.634748	-1.496534
H	-2.325304	-4.197998	-3.746431

## Frequencies:

-151.1131	-18.2096	8.3054
11.2392	20.7986	34.6533
35.8677	52.3865	55.7012
58.3889	60.8729	79.3855
92.0575	96.7997	115.9932
120.9443	132.6649	145.2715
153.1066	161.0357	169.2178
188.3270	200.1034	201.2733
208.5591	214.7685	219.3300
223.4723	230.7164	239.5112
249.2991	268.6552	272.1956
276.7869	279.6238	281.2713
283.6160	287.5394	297.6507
300.8957	306.8405	308.6730
315.2474	334.2768	337.7423
360.1075	370.9831	373.8389
374.4957	381.1439	384.4821
400.0997	412.4655	415.1712
421.1400	434.6078	436.7724
438.0168	439.7675	440.3670
453.6751	469.4480	486.1204
500.3170	508.6297	518.5542
540.5064	547.4626	561.5939
575.9366	578.6393	622.6274
644.4364	657.3126	678.9820
679.7467	689.3860	689.6164
690.5436	697.6735	727.0945
727.5659	729.9739	736.9728
743.3928	761.6092	762.7120
768.1325	768.4172	794.1750
808.5028	811.9731	817.4268
818.8726	819.6126	828.0556
835.4958	836.3347	850.7256
851.9005	853.1893	856.4857
872.7398	890.9514	912.7695
916.7317	924.4925	927.0582
935.9394	942.3516	948.6879
949.2551	955.1661	959.6511
960.0848	966.0081	966.5521
977.6427	987.5300	993.3066
1002.6915	1021.6858	1022.9759
1023.6148	1026.5582	1027.6896
1036.9711	1038.9337	1049.9169

1051.6213	1061.7633	1062.1993
1063.3627	1063.9693	1080.8133
1081.5254	1087.2141	1102.5295
1121.6933	1122.1442	1124.0510
1127.7828	1128.4822	1139.9059
1149.9759	1160.7830	1172.3714
1175.8863	1193.7327	1196.2556
1197.4042	1198.2148	1214.1170
1221.0540	1236.1925	1242.5435
1246.9681	1249.6380	1259.6416
1265.8313	1280.6018	1283.6832
1295.7008	1301.7538	1304.7706
1307.4076	1311.1293	1314.8318
1323.7038	1333.5198	1336.4940
1346.7706	1352.2334	1353.7781
1358.7720	1364.5234	1377.5459
1379.5989	1390.4330	1391.3167
1393.2187	1396.2909	1400.2370
1402.7122	1409.4950	1416.1124
1416.8198	1420.0640	1421.1223
1427.1872	1430.0003	1434.4992
1438.1395	1440.8367	1455.4816
1463.3876	1500.6576	1502.1133
1504.3280	1511.2577	1530.7278
1533.9018	1535.6629	1537.2113
1537.7407	1541.9240	1546.6455
1551.5233	1557.8904	1560.6010
1563.0883	1566.0058	1592.8144
1594.1898	1606.8408	1616.5044
1642.4619	1645.5234	1647.9020
1665.4491	1716.8985	2518.2852
2949.5461	2960.1312	2986.1935
3011.8277	3024.2203	3032.1364
3034.0011	3038.5259	3043.2482
3043.6388	3051.0971	3051.5973
3064.1483	3067.9070	3068.9132
3078.7199	3082.6623	3086.4220
3087.6630	3091.9497	3102.2185
3108.5230	3119.8613	3133.0393
3140.8090	3193.7419	3199.4633
3199.7778	3200.6445	3210.7589
3247.9651	3248.1013	3249.6902
3250.6899	3271.0613	3271.3362
3272.5899	3273.6805	3657.7281

### III.C.4. Point P4

Absolute energy: -2476.6010262

Geometry:

C	.461369	3.336952	-1.227895
C	.495709	4.608796	-.526337
C	1.552384	4.784934	.549136
C	5.446779	-.856078	.192610
O	-.352930	5.506920	-.763179
C	2.723052	3.799282	.396851
C	2.277114	2.315955	.227834
C	3.523932	1.438258	-.181463
C	3.122621	-.017693	-.581391
C	2.138362	.014171	-1.765562
C	.980812	.974374	-1.557566
C	1.225070	2.240435	-.894023
C	4.667939	1.471838	.871566
C	5.882345	.587410	.497448
C	4.388638	-.810025	-.943163
C	4.944709	-1.558936	1.476252
C	1.618750	1.806569	1.544392
C	6.522194	-1.747892	-.491393
C	5.700768	-2.864136	-1.207788

C	4.265002	-2.282383	-1.412951
O	7.578284	-2.244297	.372046
S	-4.529025	-.892864	.694693
Fe	-2.129011	-.637306	.108095
C	-2.561444	-1.395537	-3.199364
C	-2.715866	2.690023	-.572821
C	-1.853694	.102300	3.448454
C	-1.749362	-3.977787	.832664
N	-2.543435	.430782	-1.543106
C	-2.666071	-.060758	-2.835962
C	-2.936461	1.023165	-3.754897
C	-2.984128	2.171806	-3.016118
C	-2.745256	1.798078	-1.639311
N	-2.319583	1.042355	1.213068
C	-2.522257	2.337370	.753323
C	-2.477453	3.268851	1.858619
C	-2.238312	2.537691	2.987479
C	-2.129906	1.151269	2.586524
N	-1.862966	-1.725158	1.803726
C	-1.739747	-1.233616	3.088204
C	-1.488641	-2.321513	4.014021
C	-1.465755	-3.471513	3.280825
C	-1.697001	-3.096306	1.899734
N	-2.163868	-2.342388	-.963689
C	-1.962803	-3.626170	-.496091
C	-2.004457	-4.566378	-1.595469
C	-2.230250	-3.841408	-2.731199
C	-2.328568	-2.454306	-2.331543
O	-.365154	-.513773	.007247
H	3.316921	4.084571	-.483869
H	3.927906	1.901826	-1.100313
H	2.617620	-.505580	.262935
H	2.684343	.336928	-2.671810
H	1.757938	-.992659	-1.974332
H(iso=2)	.136672	.218784	-.661350
H	.291874	1.035763	-2.403531
H	-.270463	3.258154	-2.025455
H	1.902005	5.823617	.521790
H	1.059523	4.656507	1.523880
H	4.283286	1.154732	1.848415
H	5.016563	2.503394	1.000120
H	6.375909	1.004202	-.393957
H	4.110686	-1.027562	1.942004
H	1.244087	.784635	1.440653
H	.759105	2.429875	1.811588
H	7.063230	-1.142939	-1.227073
H	6.174567	-3.156144	-2.150519
H	5.677765	-3.763448	-.577615
H	3.527762	-2.823455	-.806632
H	3.935777	-2.355126	-2.454747
H	4.869234	-.257588	-1.772366
H	5.756978	-1.602131	2.212455
H	4.603784	-2.582725	1.282745
H	2.331431	1.846471	2.375345
H	3.382282	3.887647	1.266968
H	6.624214	.608183	1.306619
H	7.214840	-2.907376	.992462
H	-4.973752	.334081	.238296
H	-2.679434	-1.633434	-4.252019
H	-2.829521	3.745605	-.797088
H	-1.727295	.345859	4.498717
H	-1.609399	-5.032244	1.049328
H	-3.077993	.905523	-4.819852
H	-3.170066	3.181135	-3.354391
H	-2.604780	4.337446	1.761788
H	-2.139764	2.890398	4.004270
H	-1.358889	-2.203417	5.080364
H	-1.311874	-4.483983	3.625875
H	-1.878531	-5.635076	-1.496194
H	-2.325783	-4.198168	-3.746807

## Frequencies:

-773.5193	8.4935	11.2306
18.9092	36.1086	37.9699
45.1673	52.8401	57.5375
59.4235	72.0752	80.6019
92.3071	100.3429	114.5955
130.4096	132.8067	138.5924
154.8458	156.0895	164.7782
172.5383	191.5966	202.3404
209.7944	212.0789	218.6682
223.6629	229.4988	232.6363
247.2612	267.1490	271.0005
274.5055	279.0090	281.9769
282.8232	288.0745	295.4374
297.2091	303.9200	316.4028
324.9951	326.8674	336.6714
361.8860	368.5253	369.6483
371.5989	380.1800	384.2369
398.8283	410.2654	418.8061
423.2420	432.9641	435.9968
438.8436	439.9858	441.7586
463.0693	477.0161	486.4857
508.5392	519.1402	548.0522
555.8554	559.8633	569.6412
588.6343	604.2887	622.4314
642.3279	662.1178	676.5097
679.1108	679.7069	688.9726
690.1565	690.3568	700.8686
725.6369	726.1345	730.7282
735.9464	740.7635	761.3806
762.5604	766.4000	767.5943
770.2175	803.2538	806.3654
811.1161	812.5389	815.0628
818.7869	822.0988	834.5158
835.3548	841.5912	850.5169
852.6816	854.5413	869.5054
901.3185	906.8536	907.5108
918.2507	920.8371	934.7830
936.8218	941.6832	951.6174
952.9154	953.4511	955.3351
958.8246	974.2084	977.4694
987.5402	997.0205	1010.8577
1017.2845	1020.8029	1022.3243
1024.4625	1033.4367	1038.2282
1045.3391	1050.2655	1056.9532
1058.2226	1059.5552	1062.7875
1076.3737	1077.0197	1086.0337
1099.2144	1117.1985	1117.8407
1118.4665	1119.9486	1123.5165
1134.8351	1145.0033	1151.9821
1157.0123	1172.2535	1176.0181
1190.3469	1191.9765	1199.4902
1203.2064	1216.6273	1217.0226
1243.0177	1245.2477	1246.9997
1258.4847	1265.8341	1274.7428
1281.5176	1295.4315	1296.9189
1300.6079	1307.8582	1312.2856
1315.5537	1322.2529	1332.9143
1338.4291	1345.9111	1348.3371
1350.0279	1358.3654	1362.6625
1376.7519	1379.3631	1386.9393
1388.4909	1389.6142	1395.0611
1398.9550	1401.0498	1409.8684
1412.1563	1416.9871	1420.7215
1423.5259	1427.8313	1431.4986
1436.9718	1438.6713	1454.6751
1465.6299	1498.3733	1499.7378
1502.1291	1510.3285	1515.3878
1530.1231	1533.8990	1534.6107
1536.9440	1540.8311	1545.7435
1551.0280	1556.4672	1558.0367

1560.6948	1562.6733	1565.3638
1590.6588	1592.2715	1607.8578
1615.3050	1629.2057	1643.5775
1645.9794	1714.5568	2503.4389
2951.2466	2960.3886	2965.8138
3018.2097	3030.3622	3040.8064
3042.7907	3046.5940	3051.2700
3056.4427	3059.6763	3061.5551
3073.1408	3076.5791	3082.6377
3093.1421	3094.9915	3096.9355
3102.6480	3111.1479	3117.3934
3127.4965	3128.8435	3141.5277
3148.2851	3206.3120	3206.7746
3207.7244	3209.6105	3218.1418
3258.7128	3258.9071	3260.0275
3261.2235	3282.0442	3282.2738
3283.0241	3284.2803	3637.4276

## III.C.5. Point P5

Absolute energy: -2476.6038375

Geometry:

C	.470355	3.341183	-1.227245
C	.493498	4.608213	-.528008
C	1.552339	4.785206	.549217
C	5.447176	-.856612	.192707
O	-.352191	5.506015	-.761802
C	2.723837	3.800138	.399205
C	2.277001	2.318857	.227164
C	3.523498	1.438303	-.181590
C	3.122463	-.017063	-.583312
C	2.153621	.020677	-1.779936
C	.968900	.958480	-1.556445
C	1.233938	2.263168	-.899403
C	4.667743	1.471793	.871336
C	5.882017	.587334	.497494
C	4.389219	-.809959	-.941871
C	4.944972	-1.558773	1.476116
C	1.618562	1.806773	1.542780
C	6.523163	-1.747729	-.491000
C	5.701086	-2.864172	-1.207373
C	4.265489	-2.281837	-1.412399
O	7.577548	-2.244451	.371907
S	-4.530988	-.892395	.694499
Fe	-2.115457	-.638965	.109310
C	-2.561333	-1.394823	-3.196942
C	-2.716015	2.687043	-.572047
C	-1.854340	.102162	3.446564
C	-1.749851	-3.975775	.831769
N	-2.549367	.430785	-1.544580
C	-2.666483	-.060497	-2.833803
C	-2.935553	1.020994	-3.750803
C	-2.983173	2.168917	-3.012118
C	-2.745198	1.795751	-1.638371
N	-2.322051	1.043327	1.216120
C	-2.522029	2.335075	.753572
C	-2.477318	3.265001	1.856408
C	-2.238381	2.534762	2.985018
C	-2.130358	1.151434	2.585102
N	-1.871126	-1.727296	1.807564
C	-1.741387	-1.233537	3.087741
C	-1.489166	-2.318703	4.009846
C	-1.466309	-3.468708	3.276516
C	-1.698763	-3.095320	1.899442
N	-2.167127	-2.345040	-.964994
C	-1.963421	-3.624954	-.496535
C	-2.004607	-4.562771	-1.593571
C	-2.230215	-3.837881	-2.728694
C	-2.328694	-2.453899	-2.329807
O	-.433756	-.548393	.040645
H	3.317453	4.085436	-.483072
H	3.928552	1.901560	-1.100929
H	2.614897	-.505841	.261434
H	2.715882	.336477	-2.675621
H	1.770305	-.988328	-1.984914
H(iso=2)	.297043	.410045	-.854354
H	.374931	1.087008	-2.470355
H	-.259525	3.259325	-2.028947
H	1.903750	5.825003	.521940
H	1.059731	4.657080	1.525634
H	4.283365	1.154525	1.849855
H	5.017658	2.504400	1.000899
H	6.376036	1.005222	-.394527
H	4.109523	-1.026515	1.941811
H	1.247290	.782086	1.439915

H	.758366	2.430389	1.812597
H	7.059748	-1.141637	-1.231256
H	6.174953	-3.155768	-2.152214
H	5.676908	-3.765238	-.577258
H	3.527394	-2.824164	-.805395
H	3.935728	-2.353353	-2.455657
H	4.868752	-.257937	-1.772708
H	5.756374	-1.602982	2.215355
H	4.603673	-2.584078	1.283057
H	2.331448	1.843710	2.375657
H	3.384575	3.891276	1.270346
H	6.625368	.607911	1.307447
H	7.213882	-2.905443	.990078
H	-4.976131	.332204	.243214
H	-2.677400	-1.632786	-4.251320
H	-2.824534	3.744639	-.797154
H	-1.725427	.346129	4.497963
H	-1.607657	-5.031376	1.048937
H	-3.075461	.906151	-4.818365
H	-3.166424	3.179860	-3.353548
H	-2.602170	4.336130	1.761160
H	-2.138321	2.891196	4.002552
H	-1.357274	-2.203063	5.078302
H	-1.310225	-4.482050	3.624581
H	-1.877918	-5.633748	-1.496966
H	-2.324776	-4.197655	-3.745541

## Frequencies:

-40.8862	-30.1729	-14.2442
-2.0319	11.4344	29.7516
34.6765	47.0069	52.4836
54.8470	62.1024	87.7514
90.2105	101.9152	107.6193
125.5320	130.3392	141.6368
150.8561	159.7071	167.6991
189.6671	195.2220	200.0409
211.2721	215.8031	217.9957
223.7642	231.4093	233.2346
254.2028	264.1678	274.0153
279.1363	279.2083	281.0491
282.6841	290.7373	297.0080
300.8007	303.0194	307.3735
314.7548	334.3591	350.0884
359.4345	371.5468	374.5838
379.5243	380.9849	384.6620
401.8599	412.2652	415.8839
417.9062	434.9329	437.2152
439.2101	439.9645	441.3706
468.9616	476.9598	486.2097
507.5826	517.6823	525.5646
540.8480	562.0820	575.5985
576.6094	623.5383	643.9951
657.3789	665.6683	679.3203
680.1354	689.4074	690.2280
691.7666	695.3836	728.5290
729.0418	730.9849	738.8967
745.2284	761.7195	763.9393
769.6962	769.8590	793.8831
811.4042	812.0467	820.4857
821.5986	823.1342	831.6958
836.5439	837.2198	851.1227
852.9089	854.0550	858.1695
874.8707	895.4995	916.0361
918.0193	927.7091	930.4075
937.0089	945.2270	952.9202
953.4209	962.3398	963.2304
963.9503	968.0362	969.9214
980.5500	989.0874	995.0060
1005.4827	1025.4319	1025.7915
1027.6258	1031.6113	1031.6645
1039.3014	1041.4227	1050.3558

1052.4259	1064.8188	1065.1705
1065.5910	1066.3638	1083.3525
1084.5279	1087.9595	1103.1866
1124.3165	1124.7929	1126.5882
1129.6966	1130.3999	1140.3378
1149.9084	1168.0215	1173.5157
1176.9290	1197.5854	1200.7361
1201.7369	1202.8451	1215.0363
1225.5730	1238.6547	1244.0468
1253.4426	1256.6632	1265.0514
1274.1922	1284.2066	1296.1637
1298.9793	1306.5829	1308.1741
1309.2154	1315.2873	1316.5564
1324.7424	1335.4063	1339.2180
1347.6181	1356.6667	1357.9778
1359.5499	1365.6826	1377.9185
1380.7087	1391.0419	1396.7726
1397.2302	1398.8461	1401.1744
1405.5243	1411.5254	1417.5352
1419.7021	1420.9218	1430.1777
1431.1300	1435.8496	1438.4937
1444.8521	1456.5777	1463.4098
1503.0253	1505.3303	1507.0412
1511.8788	1531.2138	1536.0244
1536.1784	1538.2400	1541.2950
1542.3976	1547.0799	1551.9927
1557.9303	1562.7087	1563.5590
1566.4983	1595.6638	1596.9463
1610.1006	1619.1788	1642.3788
1647.9656	1649.8062	1671.5606
1719.2284	1888.8283	2528.3542
2946.7189	2957.2597	2987.3539
3007.3791	3019.3418	3027.1126
3028.6569	3033.4419	3037.4132
3038.0311	3045.5277	3046.3357
3058.4028	3061.1970	3062.2522
3065.9155	3076.4933	3080.2860
3081.7833	3085.8904	3096.5429
3102.5437	3114.3143	3127.2041
3134.2047	3186.2958	3193.6185
3193.8704	3194.6165	3204.5561
3239.9413	3240.0898	3241.7798
3242.7282	3263.0493	3263.3148
3264.6815	3265.7118	3672.5855



## III.C.6. Point P6

Absolute energy: -2476.6045385

Geometry:

C	.459819	3.337740	-1.227694
C	.495948	4.608391	-.526330
C	1.552334	4.784838	.549138
C	5.446758	-.856071	.192613
O	-.353038	5.507005	-.763386
C	2.722975	3.799188	.396614
C	2.277322	2.315543	.227884
C	3.523995	1.438334	-.181395
C	3.122721	-.017729	-.581160
C	2.136719	.013567	-1.763816
C	.989045	.982891	-1.563753
C	1.224830	2.236607	-.894125
C	4.667964	1.471774	.871560
C	5.882345	.587411	.497436
C	4.388634	-.810027	-.943276
C	4.944680	-1.558925	1.476231
C	1.618824	1.806631	1.544392
C	6.522221	-1.747906	-.491392
C	5.700768	-2.864123	-1.207782
C	4.264992	-2.282394	-1.412948
O	7.578220	-2.244279	.372043
S	-4.528968	-.892810	.694708
Fe	-2.130071	-.637389	.108167
C	-2.561436	-1.395592	-3.199261
C	-2.715868	2.689970	-.572750
C	-1.853654	.102210	3.448330
C	-1.749337	-3.977604	.832709
N	-2.543144	.430996	-1.543366
C	-2.666045	-.060576	-2.835944
C	-2.936456	1.023139	-3.754907
C	-2.984106	2.171849	-3.016115
C	-2.745249	1.798009	-1.639482
N	-2.319647	1.042463	1.213070
C	-2.522314	2.337444	.753419
C	-2.477436	3.268840	1.858593
C	-2.238300	2.537623	2.987436
C	-2.129913	1.151316	2.586414
N	-1.862994	-1.725235	1.803818
C	-1.739747	-1.233801	3.088007
C	-1.488634	-2.321608	4.014058
C	-1.465741	-3.471519	3.280916
C	-1.697015	-3.096065	1.899815
N	-2.163886	-2.342559	-.963709
C	-1.962836	-3.625987	-.496243
C	-2.004450	-4.566344	-1.595470
C	-2.230245	-3.841421	-2.731194
C	-2.328560	-2.454391	-2.331449
O	-.359437	-.512524	.005743
H	3.317087	4.084815	-.484005
H	3.928033	1.902013	-1.100258
H	2.617543	-.505707	.263007
H	2.681499	.335691	-2.671849
H	1.755571	-.992909	-1.973034
H(iso=2)	.098109	.188670	-.627215
H	.280026	1.028416	-2.393397
H	-.272105	3.258794	-2.025312
H	1.902103	5.823596	.521668
H	1.059635	4.656454	1.524039
H	4.283205	1.154677	1.848449
H	5.016569	2.503454	1.000068
H	6.375988	1.004273	-.394003
H	4.110544	-1.027604	1.942098
H	1.243791	.784648	1.440406

H	.758838	2.429793	1.811536
H	7.063214	-1.142886	-1.227231
H	6.174588	-3.156144	-2.150643
H	5.677649	-3.763517	-.577587
H	3.527699	-2.823469	-.806548
H	3.935832	-2.355283	-2.454926
H	4.869348	-.257552	-1.772516
H	5.757009	-1.602110	2.212498
H	4.603743	-2.582809	1.282769
H	2.331255	1.846792	2.375701
H	3.382183	3.887395	1.266858
H	6.624267	.608135	1.306686
H	7.214951	-2.907293	.992254
H	-4.974165	.333741	.238299
H	-2.679589	-1.633514	-4.252060
H	-2.830178	3.745645	-.797039
H	-1.727283	.345835	4.498754
H	-1.609343	-5.032238	1.049357
H	-3.078242	.905595	-4.820038
H	-3.170433	3.181251	-3.354588
H	-2.604992	4.337627	1.761997
H	-2.139807	2.890486	4.004386
H	-1.358823	-2.203594	5.080603
H	-1.311835	-4.484136	3.626130
H	-1.878548	-5.635246	-1.496259
H	-2.325824	-4.198373	-3.746940

## Frequencies:

-70.8049	-6.4149	9.6803
17.7092	36.2513	40.7985
43.7193	52.3439	58.7037
61.7482	72.4358	83.4330
94.0691	99.5696	116.9855
122.2526	135.5226	154.2212
154.8499	162.2985	168.9644
170.7090	198.7776	204.5344
209.8501	213.4301	218.4175
221.9060	228.1535	231.0646
249.0339	267.7491	271.2061
275.5363	278.3865	282.3087
283.2079	289.5147	295.1336
297.3945	303.2188	316.8682
324.3957	334.8551	339.2269
362.1171	368.9307	370.3061
370.6438	380.4293	384.9427
398.4946	410.0470	418.9961
425.9895	432.8042	435.9743
439.7255	440.2135	443.0594
461.3026	478.9608	486.5570
498.1453	510.6932	522.3745
554.4905	560.8514	565.5680
577.6839	617.0064	625.7302
647.2338	661.9463	678.8722
679.4332	685.9092	689.4895
690.2330	690.6688	700.4788
725.7035	726.5626	730.8193
735.7326	738.5705	749.0088
761.6407	766.3561	767.4506
768.5911	804.2005	805.7688
812.3863	814.1594	818.4549
822.5534	826.6250	834.5466
835.4195	848.6360	852.7020
853.0562	861.2506	867.0020
898.2288	907.4889	911.7082
918.7641	921.4003	934.8594
937.3001	942.2086	951.5187
953.3622	954.0242	956.1865
959.2704	973.9258	976.4278
987.0248	997.7080	1011.4827
1017.3159	1021.1356	1022.2607
1024.7182	1033.6928	1038.5002

1046.3916	1050.4438	1056.8615
1058.3471	1060.3622	1063.1214
1077.0660	1077.6938	1086.7667
1099.3229	1117.5314	1118.1841
1120.3007	1123.8544	1126.0770
1139.5862	1152.4668	1156.7075
1166.9181	1174.8961	1176.7133
1190.5341	1192.2600	1200.4137
1208.6718	1216.9869	1222.9966
1243.6228	1245.5156	1252.6107
1261.7803	1269.7321	1276.9031
1295.7302	1297.0466	1300.9432
1308.2692	1311.3975	1316.5499
1322.2291	1332.9810	1339.6323
1346.0076	1348.1724	1349.8627
1358.5793	1361.9471	1375.3631
1379.6956	1387.2080	1388.6986
1389.5764	1395.2037	1399.1619
1401.4849	1409.6805	1412.4822
1417.4329	1420.9283	1423.4152
1428.0263	1432.2648	1437.2033
1438.9496	1454.9893	1466.1158
1498.1854	1499.5246	1501.8823
1506.5165	1512.3116	1515.9431
1530.2560	1533.7589	1534.8041
1537.2482	1541.5013	1546.3990
1551.1718	1557.8701	1558.5225
1562.6589	1565.4562	1590.6770
1592.2513	1607.1046	1615.0783
1621.1216	1643.3359	1645.5512
1650.4490	1714.3503	2504.6875
2950.1693	2954.9275	2963.3078
3017.3964	3029.1820	3040.1351
3042.0571	3045.8595	3050.3231
3055.6665	3058.8702	3061.6314
3072.2391	3075.5000	3082.6798
3092.3822	3093.7428	3095.9396
3101.9555	3110.3235	3116.3140
3126.0037	3135.0852	3140.5978
3146.7160	3204.7426	3205.1692
3206.0828	3208.9771	3216.5192
3256.7455	3256.9598	3258.0690
3259.2827	3280.1354	3280.3621
3281.0887	3282.3580	3640.5362

## III.C.7. Point P7

Absolute energy: -2476.6068656

Geometry:

C	.482242	3.352025	-1.233910
C	.495124	4.611927	-.526613
C	1.552692	4.787462	.551678
C	5.448345	-.857043	.193923
O	-.353649	5.506915	-.758516
C	2.726544	3.803856	.403921
C	2.280947	2.323176	.224756
C	3.526121	1.440146	-.181291
C	3.124962	-.014149	-.588069
C	2.175737	.032641	-1.798939
C	.991022	.976638	-1.592568
C	1.250226	2.277303	-.912601
C	4.668412	1.471596	.872486
C	5.882498	.587171	.498257
C	4.391490	-.809805	-.940106
C	4.945026	-1.558889	1.476875
C	1.616908	1.807111	1.536452
C	6.523856	-1.747674	-.490790
C	5.701615	-2.864286	-1.206811
C	4.266303	-2.281165	-1.411292
O	7.577199	-2.244658	.371692
S	-4.538151	-.891269	.695021
Fe	-2.112966	-.645511	.114348
C	-2.561465	-1.394712	-3.194387
C	-2.715763	2.682761	-.570466
C	-1.855793	.101997	3.445618
C	-1.751395	-3.973220	.831094
N	-2.552989	.427406	-1.541666
C	-2.667677	-.062406	-2.830568
C	-2.934085	1.018396	-3.746310
C	-2.981260	2.165731	-3.007224
C	-2.745414	1.792118	-1.635112
N	-2.325988	1.040559	1.218050
C	-2.522877	2.331248	.753419
C	-2.476722	3.261318	1.854087
C	-2.237857	2.532588	2.983143
C	-2.132014	1.150147	2.585207
N	-1.891395	-1.729588	1.811803
C	-1.749041	-1.233090	3.088231
C	-1.488282	-2.316531	4.006784
C	-1.465615	-3.466250	3.273166
C	-1.706712	-3.094753	1.899172
N	-2.172388	-2.346066	-.964495
C	-1.965546	-3.623772	-.496124
C	-2.004311	-4.560119	-1.592468
C	-2.229930	-3.835197	-2.727142
C	-2.330410	-2.452885	-2.328358
O	-.462033	-.578974	.071403
H	3.322522	4.091594	-.475272
H	3.933749	1.903855	-1.098889
H	2.606215	-.503799	.248758
H	2.755957	.348030	-2.682416
H	1.790954	-.972969	-2.013997
H(iso=2)	.291305	.445315	-.932501
H	.441741	1.133300	-2.529637
H	-.242563	3.272602	-2.039636
H	1.903642	5.826734	.524780
H	1.059498	4.659443	1.527252
H	4.283523	1.153947	1.850144
H	5.018642	2.503354	1.003021
H	6.375739	1.004980	-.393666
H	4.108767	-1.026859	1.939936
H	1.247310	.782905	1.429378

H	.756467	2.429435	1.805779
H	7.059706	-1.141943	-1.230924
H	6.174758	-3.155307	-2.151376
H	5.677347	-3.765261	-.577509
H	3.528137	-2.823095	-.805083
H	3.936837	-2.351691	-2.453921
H	4.873124	-.259356	-1.770352
H	5.754549	-1.602362	2.217432
H	4.604545	-2.583863	1.283789
H	2.327282	1.841284	2.370908
H	3.383657	3.894026	1.277175
H	6.625765	.608152	1.307463
H	7.212173	-2.906312	.990419
H	-4.982188	.339587	.255940
H	-2.674283	-1.631685	-4.248405
H	-2.821841	3.739583	-.795982
H	-1.719941	.346497	4.495078
H	-1.601853	-5.027085	1.047345
H	-3.071969	.904778	-4.813069
H	-3.161919	3.175964	-3.348372
H	-2.599971	4.331371	1.758013
H	-2.136353	2.890159	3.998872
H	-1.349378	-2.201222	5.073168
H	-1.302632	-4.477584	3.620201
H	-1.876436	-5.629827	-1.496743
H	-2.323041	-4.194629	-3.742970

## Frequencies:

-26.7020	-18.6001	-14.3012
-9.7414	20.3964	31.2054
38.5459	42.5767	48.0262
52.0987	62.9946	86.9040
88.0494	104.1752	115.7198
124.7571	129.2070	140.3235
146.5837	154.7455	165.6390
181.3684	187.9328	197.8504
206.5195	213.5655	217.1320
220.2550	231.5341	240.9886
250.6193	266.2665	271.2730
277.3675	278.1851	278.9309
279.6235	288.8025	295.5495
298.9967	306.3044	308.8462
313.9531	334.1591	339.7263
358.4289	371.6620	373.1557
378.4740	381.4093	384.0700
401.3740	411.8733	415.1504
416.0377	434.0391	437.5118
438.2121	439.1220	440.3714
469.0758	473.9917	485.1661
506.6793	516.9157	521.7621
536.6185	561.2428	574.1295
576.7486	623.1307	643.1332
656.9114	678.1065	678.8556
687.6059	688.7117	689.8996
693.1547	726.2373	726.7442
730.5556	737.1835	743.6742
760.6675	764.4207	770.6554
770.8631	791.7598	807.7958
809.9460	816.8214	819.2897
823.8726	827.5804	831.4023
837.6653	838.4432	851.3473
852.1918	854.5982	856.8126
874.4236	897.3508	912.7233
918.2596	924.6249	927.5085
936.7781	942.9642	949.6881
952.2217	959.9800	960.7432
965.3591	967.1721	969.2590
981.4649	989.8484	995.0538
1008.4385	1025.1731	1028.2279
1031.2526	1034.9310	1036.3346
1039.5124	1045.9615	1049.6606

1053.3723	1065.0705	1065.5769
1068.2452	1069.4471	1084.7047
1087.7729	1089.2083	1102.8030
1122.5824	1123.1951	1124.7594
1128.7042	1129.0824	1140.8038
1149.2901	1173.2246	1173.5142
1177.0482	1197.4435	1201.8548
1204.4490	1205.8365	1215.4968
1228.3688	1238.6327	1243.8176
1255.1487	1257.2165	1265.2814
1278.0054	1284.7744	1295.6897
1307.3369	1310.3995	1312.1522
1315.8928	1317.8000	1321.5039
1324.8693	1335.5790	1341.3680
1346.9723	1358.8724	1360.6761
1361.6900	1365.6016	1376.7577
1379.9807	1390.5311	1397.7300
1400.9072	1401.0040	1403.4199
1407.2340	1410.6218	1416.9166
1420.2007	1420.6561	1430.0129
1433.6125	1438.0713	1438.5502
1447.8519	1455.3346	1461.8997
1506.7416	1509.0212	1510.0842
1511.0978	1530.6471	1535.0453
1537.3678	1538.6500	1541.5720
1546.4015	1546.9804	1551.3728
1556.9428	1563.1865	1564.0115
1565.7815	1599.2159	1600.6993
1617.7361	1622.9713	1651.5964
1654.1995	1655.5132	1679.1485
1725.9774	2113.9495	2520.3660
2949.0124	2959.7411	2993.5751
3011.6137	3024.2743	3031.7444
3033.7136	3038.1991	3042.0004
3042.7463	3051.0722	3051.4804
3063.5315	3063.7074	3067.7526
3068.8400	3081.6118	3086.8275
3087.2542	3090.7684	3101.7426
3108.6720	3120.0904	3132.6421
3139.7246	3190.8818	3201.8775
3202.1337	3202.5839	3212.8259
3251.1976	3251.3553	3252.9041
3253.8397	3274.2014	3274.4527
3275.7383	3276.7277	3655.4926

### III.C.8. Point P8

Absolute energy: -2476.6058325

Geometry:

C	.459034	3.338125	-1.227507
C	.496043	4.608120	-.526327
C	1.552317	4.784774	.549128
C	5.446742	-.856063	.192610
O	-.353129	5.507105	-.763494
C	2.722922	3.799129	.396485
C	2.277450	2.315326	.227894
C	3.524033	1.438364	-.181337
C	3.122768	-.017746	-.581052
C	2.135906	.013299	-1.762967
C	.993700	.987679	-1.567319
C	1.224697	2.234654	-.894280
C	4.667983	1.471732	.871544
C	5.882334	.587406	.497433
C	4.388621	-.810031	-.943325
C	4.944674	-1.558917	1.476211

C	1.618871	1.806670	1.544386
C	6.522205	-1.747921	-.491385
C	5.700758	-2.864101	-1.207779
C	4.265000	-2.282397	-1.412945
O	7.578199	-2.244300	.372071
S	-4.528914	-.892762	.694701
Fe	-2.130697	-.637478	.108253
C	-2.561436	-1.395632	-3.199226
C	-2.715882	2.689968	-.572713
C	-1.853623	.102161	3.448282
C	-1.749319	-3.977526	.832737
N	-2.542931	.431088	-1.543475
C	-2.666021	-.060487	-2.835966
C	-2.936465	1.023154	-3.754924
C	-2.984105	2.171871	-3.016145
C	-2.745243	1.798012	-1.639581
N	-2.319627	1.042472	1.213035
C	-2.522348	2.337524	.753453
C	-2.477429	3.268854	1.858618
C	-2.238302	2.537627	2.987410
C	-2.129907	1.151344	2.586373
N	-1.863026	-1.725245	1.803796
C	-1.739745	-1.233873	3.087942
C	-1.488626	-2.321686	4.014088
C	-1.465728	-3.471522	3.280995
C	-1.697018	-3.095989	1.899856
N	-2.163859	-2.342596	-.963674
C	-1.962843	-3.625919	-.496312
C	-2.004450	-4.566342	-1.595505
C	-2.230240	-3.841467	-2.731191
C	-2.328555	-2.454432	-2.331435
O	-.357226	-.512984	.005920
H	3.317212	4.084943	-.484205
H	3.928095	1.902137	-1.100288
H	2.617497	-.505827	.263239
H	2.680573	.334371	-2.671889
H	1.753879	-.993057	-1.972050
H(iso=2)	.082081	.180153	-.615128
H	.274362	1.025168	-2.388544
H	-.273020	3.259206	-2.025510
H	1.902196	5.823765	.521585
H	1.059655	4.656409	1.524246
H	4.283118	1.154603	1.848601
H	5.016623	2.503650	1.000067
H	6.376078	1.004339	-.394131
H	4.110345	-1.027519	1.942207
H	1.243682	.784484	1.440260
H	.758606	2.429907	1.811506
H	7.063342	-1.142762	-1.227387
H	6.174689	-3.156208	-2.150874
H	5.677617	-3.763657	-.577468
H	3.527556	-2.823559	-.806411
H	3.935783	-2.355363	-2.455196
H	4.869414	-.257494	-1.772636
H	5.757163	-1.602102	2.212600
H	4.603677	-2.582997	1.282735
H	2.331258	1.846956	2.376027
H	3.382269	3.887268	1.266954
H	6.624421	.608111	1.306840
H	7.215221	-2.906846	.991801
H	-4.974469	.333411	.238344
H	-2.679704	-1.633618	-4.252338
H	-2.830460	3.745950	-.797073
H	-1.727237	.345874	4.499028
H	-1.609277	-5.032488	1.049428
H	-3.078411	.905566	-4.820522
H	-3.170669	3.181695	-3.354789
H	-2.605125	4.338119	1.762040
H	-2.139794	2.890642	4.004820
H	-1.358733	-2.203608	5.081109
H	-1.311753	-4.484595	3.626360

H	-1.878507	-5.635727	-1.496234
H	-2.325881	-4.198591	-3.747391

## Frequencies:

-16.2995	9.8269	16.0295
32.1700	35.6711	41.5281
51.6107	55.4390	58.5804
69.9807	77.1724	89.6702
98.9432	105.7952	116.4044
120.7901	136.4224	154.7912
155.0058	163.2311	169.2704
185.1557	201.8842	209.1197
212.2445	217.0861	218.6363
227.1744	230.6917	240.4920
254.1764	268.7943	270.4185
276.1253	278.3496	282.4996
284.0791	290.9174	294.7887
297.8754	302.8115	314.5302
318.4484	333.4578	348.3373
362.3694	369.0476	370.1762
371.7684	380.6952	385.8017
397.6002	409.7986	415.3576
418.9298	432.1618	433.0040
436.0773	439.9785	440.8269
456.2139	469.3888	480.6820
486.7231	511.4346	520.9742
553.2252	561.1672	563.0049
577.0437	618.4834	627.1958
648.0517	659.9211	679.0305
679.7665	681.9775	689.7726
690.3393	691.2922	700.3231
721.8374	726.8402	728.9612
731.9096	736.4520	744.5510
761.7762	766.4628	767.5731
768.3594	805.5430	806.0385
813.9978	815.8449	818.2975
824.2892	826.8547	834.5641
835.4107	850.0958	852.8532
854.3326	865.8086	868.7120
898.1799	909.0423	915.4746
920.2170	922.9126	935.1251
938.4780	944.0512	951.6012
954.9404	955.5741	958.2518
960.8096	974.4064	976.7773
987.2507	998.1723	1012.1521
1017.3790	1021.2991	1022.2305
1024.8219	1033.7358	1038.4862
1046.7005	1050.6555	1056.9272
1058.5070	1060.6871	1063.3378
1077.1012	1078.0014	1086.8211
1099.6053	1118.5583	1119.2143
1121.3751	1124.8992	1126.7250
1139.8586	1152.9238	1156.7295
1169.2280	1175.9635	1178.0910
1190.8731	1192.6512	1201.6830
1209.8119	1217.2777	1224.1993
1244.2444	1246.0268	1253.1279
1262.3455	1270.1472	1277.0549
1296.0414	1297.1779	1301.1308
1308.5924	1311.2162	1317.6270
1322.6119	1333.6634	1341.7817
1346.3478	1348.4046	1350.1141
1358.8941	1362.2968	1376.4598
1380.1537	1387.4555	1388.7505
1389.8551	1395.5251	1399.5551
1402.1394	1410.3465	1413.1965
1417.9457	1421.0781	1423.6233
1428.4614	1434.8094	1437.4809
1439.3003	1455.4090	1466.7129
1498.3791	1499.7711	1502.2524
1507.7334	1512.9254	1517.9312



1530.4759	1533.7784	1535.0421
1537.5054	1541.8132	1546.7285
1551.3965	1558.1840	1558.8416
1562.8577	1565.6552	1590.8609
1592.4060	1606.9014	1615.4897
1617.4422	1643.5453	1645.7437
1714.3163	1857.0586	2506.2290
2948.8630	2951.5405	2961.9421
3015.7579	3027.3285	3038.3990
3040.1745	3044.0400	3048.3425
3053.6886	3056.8307	3060.0201
3070.1064	3073.1941	3081.2044
3090.2330	3091.2798	3093.7368
3099.7747	3108.3400	3114.0082
3123.6643	3134.9414	3138.4445
3144.4346	3201.6560	3202.0550
3202.9692	3205.7005	3213.3151
3252.1085	3252.3088	3253.4382
3254.6672	3275.5356	3275.7787
3276.4936	3277.7751	3649.9813

## III.C.9. Point P9

Absolute energy: -2476.5974443

Geometry:

C	.463786	3.335797	-1.228003
C	.495270	4.609215	-.526354
C	1.552498	4.785110	.549139
C	5.446816	-.856076	.192588
O	-.352929	5.507037	-.762834
C	2.723200	3.799428	.397249
C	2.276832	2.316600	.227681
C	3.523868	1.438111	-.181512
C	3.122427	-.017660	-.581795
C	2.141260	.015318	-1.768733
C	.969112	.962034	-1.549135
C	1.225815	2.246879	-.894291
C	4.667913	1.471957	.871580
C	5.882377	.587408	.497488
C	4.388619	-.810014	-.942955
C	4.944763	-1.558970	1.476306
C	1.618621	1.806474	1.544422
C	6.522036	-1.747856	-.491423
C	5.700742	-2.864155	-1.207825
C	4.265008	-2.282389	-1.412987
O	7.578501	-2.244361	.372086
S	-4.529108	-.892879	.694647
Fe	-2.127225	-.637376	.108168
C	-2.561498	-1.395527	-3.199737
C	-2.715948	2.690339	-.572931
C	-1.853687	.102469	3.448852
C	-1.749363	-3.978268	.832655
N	-2.543654	.430353	-1.542573
C	-2.666070	-.061010	-2.836100
C	-2.936530	1.023319	-3.755090
C	-2.984234	2.171887	-3.016312
C	-2.745242	1.798278	-1.639129
N	-2.319321	1.041898	1.212922
C	-2.522198	2.337461	.753119
C	-2.477506	3.269099	1.858808
C	-2.238349	2.538018	2.987676
C	-2.129866	1.151254	2.586791
N	-1.863057	-1.724895	1.803313
C	-1.739740	-1.233285	3.088645
C	-1.488606	-2.321487	4.014169
C	-1.465726	-3.471648	3.280886
C	-1.696976	-3.096848	1.899640
N	-2.163701	-2.341890	-.963474
C	-1.962722	-3.626540	-.495885
C	-2.004460	-4.566658	-1.595602
C	-2.230252	-3.841605	-2.731357
C	-2.328569	-2.454201	-2.331805
O	-.378907	-.520370	.013732
H	3.316525	4.084054	-.483698
H	3.927533	1.901512	-1.100363
H	2.617857	-.505356	.263058
H	2.690819	.336476	-2.671499
H	1.760344	-.991779	-1.975242
H(iso=2)	.215602	.295374	-.740254
H	.313553	1.049294	-2.420527
H	-.267314	3.257690	-2.026154
H	1.901776	5.823701	.521978
H	1.059424	4.656595	1.523687
H	4.283452	1.154810	1.848375
H	5.016547	2.503293	1.000215
H	6.375729	1.004016	-.393907
H	4.110974	-1.027421	1.941766
H	1.244909	.784573	1.440886

H	.759662	2.430214	1.811502
H	7.063590	-1.143083	-1.226505
H	6.174572	-3.156198	-2.150278
H	5.678120	-3.763252	-.577553
H	3.527853	-2.823422	-.806771
H	3.935620	-2.354811	-2.454410
H	4.868972	-.257644	-1.772038
H	5.757036	-1.602142	2.212276
H	4.603869	-2.582582	1.282636
H	2.331672	1.845887	2.374840
H	3.382536	3.888074	1.267179
H	6.624177	.608271	1.306516
H	7.214676	-2.907437	.992951
H	-4.973708	.334401	.238374
H	-2.679212	-1.633349	-4.252079
H	-2.828061	3.745736	-.797228
H	-1.727242	.345901	4.498777
H	-1.609450	-5.032363	1.049314
H	-3.077538	.905283	-4.819661
H	-3.169381	3.181113	-3.353984
H	-2.604351	4.337273	1.761294
H	-2.139698	2.890213	4.004213
H	-1.358927	-2.202986	5.080069
H	-1.311888	-4.483888	3.625387
H	-1.878462	-5.634917	-1.495971
H	-2.325709	-4.197786	-3.746747

## Frequencies:

-1167.9694	10.1270	15.6548
19.2982	35.6696	37.5943
42.5581	53.5123	58.1898
59.6325	73.4946	81.3731
92.8052	100.8103	115.7578
130.7021	140.3422	142.1286
154.6567	156.9126	164.2812
174.2811	188.7201	202.9961
207.5512	211.1326	219.4224
224.0602	231.9480	233.4085
246.1424	266.0058	269.8884
272.9415	279.8131	281.6727
282.9219	287.1347	297.4911
298.7986	304.3395	315.0979
319.5250	329.0537	340.1049
360.7408	368.8850	370.1397
373.0513	379.7266	383.9217
399.0337	411.3496	415.6088
421.8787	433.6110	436.0585
438.0534	439.5779	443.0151
460.0964	472.0927	486.0568
505.5327	518.7684	525.9037
553.4636	556.9943	561.4270
576.4497	598.0195	621.7312
644.1590	654.8352	678.2105
678.9615	687.9324	689.7034
690.0429	693.6250	700.4678
725.3742	725.9395	728.9990
735.4857	740.2981	760.8395
762.2518	766.4705	766.8570
792.4362	802.5720	811.2099
812.7647	813.9805	818.1177
821.4015	834.3542	835.2309
847.8650	850.4173	852.2742
854.1476	859.5042	879.3823
906.1715	910.6203	917.9311
920.4017	926.3384	934.6872
936.6936	941.3073	952.1890
952.7701	953.0368	958.7459
962.8443	974.6050	983.4932
989.8335	998.9130	1016.3616
1016.7936	1019.7766	1021.7013
1023.5698	1032.4646	1038.2366

1048.0790	1050.0268	1056.9592
1057.7426	1060.5729	1062.6509
1076.7244	1077.9624	1086.2100
1101.3764	1116.9214	1117.4570
1119.4775	1123.0977	1125.3656
1137.3612	1150.2083	1155.4084
1159.4576	1172.2288	1176.4185
1189.6531	1191.1871	1199.3161
1205.6763	1215.5484	1215.7917
1238.3348	1242.3184	1244.6533
1256.0695	1262.9988	1273.5406
1280.2396	1294.7955	1296.3775
1299.6331	1306.9100	1310.8758
1315.3395	1322.1798	1331.7847
1336.4743	1345.4323	1347.8658
1349.5180	1357.6423	1362.8579
1376.2893	1378.6703	1385.6945
1387.8158	1389.3118	1394.8508
1398.8456	1400.6799	1409.3719
1411.3421	1415.9756	1420.2116
1422.8857	1427.2245	1429.3764
1436.2081	1437.7461	1453.7645
1463.2501	1498.0260	1499.3221
1501.5605	1510.0919	1523.9687
1529.8675	1533.3731	1534.2750
1536.7562	1540.7775	1545.6864
1550.6912	1557.1579	1558.0565
1562.2387	1565.0919	1589.9869
1591.5825	1604.0908	1606.5844
1614.3603	1643.0989	1645.2566
1645.9473	1714.5105	2502.3057
2953.7167	2964.4913	2978.9803
3019.6841	3032.5787	3041.2983
3043.7525	3047.7285	3052.6671
3055.7002	3060.7876	3061.6159
3074.5158	3078.6636	3082.1727
3093.8842	3097.3248	3098.2826
3103.2314	3109.9699	3112.4341
3119.3086	3129.8372	3143.3100
3151.2225	3209.1151	3210.0328
3210.4636	3211.4389	3221.8937
3263.0313	3263.1675	3264.4776
3265.5451	3286.1591	3286.4209
3287.3685	3288.5454	3631.8113

### III.C.10. Point P10

Absolute energy: -2476.6059498

Geometry:

C	.475413	3.344510	-1.231087
C	.494043	4.610869	-.526494
C	1.552695	4.786576	.550259
C	5.447520	-.856526	.193190
O	-.353936	5.507926	-.760211
C	2.725289	3.802016	.401311
C	2.278686	2.321171	.226583
C	3.524391	1.438702	-.181193
C	3.123277	-.016217	-.585446
C	2.163553	.025155	-1.788562
C	.978431	.965630	-1.572478
C	1.242203	2.269214	-.905344
C	4.667976	1.472002	.871731
C	5.882334	.587376	.497802
C	4.389804	-.810049	-.940881
C	4.945153	-1.558985	1.476501

C	1.617727	1.806752	1.540943
C	6.522739	-1.747765	-.491050
C	5.701038	-2.864197	-1.207542
C	4.265526	-2.281846	-1.412308
O	7.578369	-2.244697	.372034
S	-4.533280	-.891914	.694816
Fe	-2.114587	-.641814	.111220
C	-2.561648	-1.395346	-3.198647
C	-2.716208	2.688315	-.572009
C	-1.854101	.102869	3.448792
C	-1.749918	-3.977405	.832008
N	-2.548358	.428561	-1.541796
C	-2.666663	-.061754	-2.834279
C	-2.935663	1.021447	-3.751858
C	-2.983190	2.169528	-3.012742
C	-2.745133	1.796023	-1.637363
N	-2.322005	1.040585	1.215485
C	-2.522358	2.335383	.752851
C	-2.477304	3.266455	1.857169
C	-2.238351	2.536603	2.986219
C	-2.130485	1.151149	2.586883
N	-1.877875	-1.727058	1.807520
C	-1.743472	-1.232653	3.089275
C	-1.488266	-2.319370	4.011360
C	-1.465510	-3.469566	3.277771
C	-1.700978	-3.096785	1.899306
N	-2.166964	-2.343509	-.964050
C	-1.963483	-3.625748	-.496010
C	-2.004499	-4.564528	-1.594741
C	-2.230128	-3.839461	-2.730009
C	-2.329045	-2.453589	-2.330841
O	-.457825	-.564088	.056975
H	3.319015	4.086961	-.479890
H	3.929387	1.901948	-1.099934
H	2.610804	-.504955	.255444
H	2.734927	.338347	-2.678278
H	1.778465	-.981577	-1.996131
H(iso=2)	.295623	.425792	-.889438
H	.408128	1.110486	-2.498076
H	-.250575	3.264286	-2.035067
H	1.902503	5.825813	.523090
H	1.059632	4.658413	1.525607
H	4.283796	1.154804	1.849462
H	5.017391	2.503768	1.001095
H	6.375538	1.004360	-.394159
H	4.110448	-1.026663	1.941078
H	1.247227	.783148	1.435269
H	.758554	2.430081	1.810422
H	7.061855	-1.142354	-1.228430
H	6.174858	-3.155949	-2.151042
H	5.678072	-3.764202	-.577362
H	3.527764	-2.823754	-.806219
H	3.935718	-2.352620	-2.454378
H	4.870306	-.258378	-1.770695
H	5.756485	-1.602770	2.214515
H	4.603965	-2.583242	1.282846
H	2.330575	1.842277	2.372718
H	3.384365	3.892806	1.272484
H	6.625146	.608478	1.306933
H	7.213850	-2.906197	.992260
H	-4.980513	.336294	.248625
H	-2.676707	-1.632838	-4.251976
H	-2.822005	3.744877	-.797298
H	-1.723213	.346720	4.498685
H	-1.605878	-5.031617	1.048531
H	-3.074442	.905107	-4.817857
H	-3.165034	3.179917	-3.351684
H	-2.601627	4.335882	1.759493
H	-2.138182	2.891106	4.002783
H	-1.354588	-2.201958	5.077827
H	-1.307749	-4.481860	3.623289

H	-1.877645	-5.633769	-1.496379
H	-2.324670	-4.196752	-3.746082

## Frequencies:

-29.4585	-14.9556	-6.2608
8.7498	30.5202	34.1551
50.1698	51.8021	55.4077
57.5710	63.3728	89.5233
92.0305	107.0745	119.3301
127.3070	130.1906	143.4318
150.6523	156.2921	166.5384
183.5414	190.2168	200.2081
208.3271	213.6492	218.6952
220.3887	232.3168	242.7819
253.9152	267.0817	272.1155
279.7242	280.0926	280.5095
281.8633	291.0837	295.5816
301.7345	307.2672	312.8123
316.8145	334.2057	344.6504
359.0712	371.6982	373.9302
378.2436	381.5336	384.0499
400.6697	412.2803	415.3131
416.6311	434.8580	437.0184
438.7836	439.7390	441.0199
468.5615	475.4381	485.7916
506.1684	516.9582	528.8972
538.2161	560.7577	574.2495
576.0049	622.5009	643.5340
657.0893	678.7347	679.5241
687.7944	689.6590	690.4667
694.1326	725.6317	726.6025
729.7071	735.1678	742.0117
760.0963	761.6786	767.6858
767.8256	787.4733	797.1324
806.3938	811.4488	816.2467
817.6453	819.8465	826.2813
835.5611	836.1759	850.3370
851.2905	852.9393	855.5429
873.6278	895.8266	910.4396
917.8265	922.4367	925.1590
935.7637	940.8251	947.1477
951.5395	957.6230	958.3192
963.8215	965.0903	968.4250
979.9313	988.9027	994.2511
1006.6871	1021.5421	1022.6360
1024.6454	1026.3200	1028.2823
1037.0683	1038.9643	1049.3699
1051.7985	1061.0623	1062.2497
1063.8528	1064.4926	1080.8586
1083.6269	1088.4745	1102.3852
1120.4806	1121.0184	1122.8125
1126.5775	1128.4955	1140.4691
1149.4328	1161.3904	1172.4723
1176.3769	1195.5629	1196.6789
1197.2977	1200.8139	1214.9976
1220.2336	1237.8369	1242.9537
1248.9727	1256.3851	1264.3141
1275.9077	1283.0820	1295.0289
1301.5127	1303.1776	1306.3732
1307.9383	1313.7583	1315.7025
1323.9588	1334.4694	1337.6285
1346.3505	1353.0226	1354.1574
1358.1239	1364.7063	1376.7161
1379.2753	1389.9830	1390.7101
1393.3108	1396.6907	1400.4127
1405.0831	1409.9332	1415.1996
1416.2420	1420.3116	1426.8442
1428.9696	1431.2698	1438.0521
1440.7354	1454.4974	1460.5362
1501.4895	1502.9769	1504.2151
1510.6993	1530.3461	1534.8436

1536.5774	1537.4787	1538.1639
1541.2761	1546.0359	1551.0584
1556.6593	1560.4684	1562.7130
1565.5344	1593.1995	1594.5711
1609.2547	1617.1320	1645.4448
1646.9170	1648.5776	1670.3333
1718.1836	2019.6199	2514.0597
2951.2311	2961.8385	2995.4929
3014.4352	3027.2140	3034.2711
3036.7926	3041.1162	3044.1243
3045.8529	3054.2554	3054.5493
3067.1982	3069.1800	3071.8474
3072.4552	3085.2492	3090.5782
3090.7145	3094.4659	3105.3307
3112.3439	3123.8098	3136.4538
3143.6325	3195.8143	3205.0976
3205.5100	3206.1386	3216.1384
3254.6650	3254.8602	3256.3737
3257.3029	3277.6709	3277.9846
3279.1909	3280.1925	3647.1636

## III.C.11. Point P11

```
Absolute energy: -2476.5977507
Geometry:
C      0.464192   3.335760  -1.227940
C      0.495168   4.609196  -0.526426
C      1.552509   4.785119   0.549137
C      5.446827  -0.856089   0.192584
O     -0.352903   5.507015  -0.762788
C      2.723217   3.799441   0.397322
C      2.276786   2.316706   0.227645
C      3.523848   1.438092  -0.181517
C      3.122396  -0.017648  -0.581862
C      2.141793   0.015556  -1.769300
C      0.967542   0.960358  -1.548039
C      1.225988   2.247946  -0.894399
C      4.667909   1.471962   0.871572
C      5.882366   0.587405   0.497488
C      4.388625  -0.810010  -0.942909
C      4.944775  -1.558974   1.476295
C      1.618621   1.806469   1.544399
C      6.522046  -1.747850  -0.491408
C      5.700742  -2.864152  -1.207822
C      4.265020  -2.282372  -1.412975
O      7.578496  -2.244366   0.372102
S     -4.529143  -0.892872   0.694628
Fe    -2.126743  -0.637407   0.108189
C     -2.561500  -1.395509  -3.199697
C     -2.715959   2.690284  -0.572919
C     -1.853703   0.102474   3.448824
C     -1.749375  -3.978248   0.832636
N     -2.543829   0.430339  -1.542598
C     -2.666070  -0.061008  -2.836056
C     -2.936518   1.023282  -3.754997
C     -2.984222   2.171815  -3.016227
C     -2.745230   1.798232  -1.639106
N     -2.319367   1.041901   1.212994
C     -2.522185   2.337422   0.753112
C     -2.477508   3.269016   1.858770
C     -2.238354   2.537962   2.987620
C     -2.129874   1.151267   2.586763
N     -1.863216  -1.724922   1.803370
C     -1.739761  -1.233262   3.088669
C     -1.488622  -2.321413   4.014070
C     -1.465745  -3.471581   3.280780
C     -1.696998  -3.096863   1.899635
N     -2.163763  -2.341926  -0.963490
C     -1.962722  -3.626540  -0.495885
C     -2.004467  -4.566582  -1.595559
C     -2.230254  -3.841526  -2.731295
C     -2.328560  -2.454191  -2.331778
O     -0.381681  -0.521768   0.015075
H      3.316506   4.084021  -0.483720
H      3.927515   1.901479  -1.100407
H      2.617863  -0.505365   0.263147
H      2.692047   0.336352  -2.671505
H      1.760734  -0.991698  -1.975419
H(iso=2) 0.228280   0.308634  -0.753580
H      0.317296   1.051578  -2.423421
H     -0.266856   3.257644  -2.026300
H      1.901832   5.823781   0.522011
H      1.059416   4.656587   1.523751
H      4.283462   1.154790   1.848449
H      5.016594   2.503352   1.000262
H      6.375729   1.004041  -0.393952
H      4.110940  -1.027368   1.941773
H      1.245070   0.784450   1.440917
```



H	0.759685	2.430299	1.811561
H	7.063521	-1.143033	-1.226617
H	6.174599	-3.156178	-2.150369
H	5.678125	-3.763334	-0.577545
H	3.527815	-2.823462	-0.806729
H	3.935588	-2.354732	-2.454457
H	4.868916	-0.257647	-1.772054
H	5.757062	-1.602210	2.212351
H	4.603849	-2.582648	1.282598
H	2.331741	1.845751	2.374861
H	3.382648	3.888193	1.267303
H	6.624246	0.608266	1.306552
H	7.214686	-2.907405	0.992788
H	-4.973716	0.334324	0.238563
H	-2.679172	-1.633341	-4.252114
H	-2.827811	3.745781	-0.797254
H	-1.727185	0.345922	4.498809
H	-1.609422	-5.032404	1.049325
H	-3.077472	0.905292	-4.819690
H	-3.169256	3.181153	-3.353961
H	-2.604237	4.337312	1.761251
H	-2.139628	2.890246	4.004233
H	-1.358885	-2.202945	5.080077
H	-1.311850	-4.483906	3.625352
H	-1.878455	-5.634955	-1.495974
H	-2.325710	-4.197777	-3.746777

## Frequencies:

-1043.5505	9.8699	15.5134
18.7985	35.4755	36.3674
41.1083	53.4747	58.2347
59.4094	73.7358	80.9021
92.7679	100.5529	116.2093
130.9056	139.6112	143.4681
154.4072	156.6709	164.2991
174.3038	188.6307	202.9528
207.2659	211.2232	219.5400
223.6347	232.0882	233.3024
246.4867	266.5074	269.9487
272.8716	279.8168	281.6072
282.8897	286.9097	297.6633
299.4598	304.2959	315.0106
318.8988	328.2932	338.6090
360.4931	369.0657	370.2677
373.2613	379.8003	383.8658
399.1509	411.6039	415.5554
421.6831	433.7691	436.1148
438.0144	439.5626	443.3155
457.5677	471.3314	486.0080
504.6955	518.0583	520.7387
552.1980	556.0508	561.1201
576.1039	592.8484	621.6327
644.5569	655.3967	678.3210
679.0491	688.0186	689.6721
690.0018	700.3063	716.9787
725.5460	728.5917	730.1542
736.1856	740.9654	760.8812
762.1348	766.5095	766.8801
793.0794	803.0334	811.7431
813.3501	814.7049	817.9452
821.9365	834.4052	835.3040
848.5129	850.8774	852.2858
854.4980	865.5938	884.0989
906.7186	912.3117	918.5113
920.9810	931.5697	935.1788
937.2229	941.9910	952.5589
953.4038	953.5891	959.3963
963.6401	974.8867	984.2948
990.3107	999.5740	1016.8240
1017.6770	1019.8943	1021.8933
1023.7224	1032.6191	1038.3445

1048.4865	1050.1721	1057.2490
1057.9461	1060.9420	1062.7775
1076.9266	1078.6482	1086.4353
1101.5320	1117.3135	1117.8337
1119.8404	1123.4745	1126.4773
1138.5332	1150.6025	1155.3464
1168.9320	1172.7742	1177.2873
1189.9905	1191.5104	1199.6914
1209.5523	1215.8278	1216.0572
1239.4245	1242.4105	1244.9462
1256.4199	1263.3455	1274.3898
1280.8696	1294.8189	1296.6398
1299.8540	1306.8849	1310.4164
1315.4821	1322.3258	1331.9040
1336.4390	1345.5035	1348.0382
1349.7117	1357.6581	1363.0401
1376.4991	1378.7220	1385.8814
1388.0578	1389.4045	1394.9437
1399.0047	1400.8043	1409.4482
1411.6181	1415.9613	1420.1885
1423.0576	1427.4660	1429.3134
1436.4005	1437.6870	1453.8039
1463.0686	1498.1469	1499.4156
1501.6553	1510.1631	1525.7083
1529.9203	1533.4948	1534.4048
1536.8198	1540.8685	1545.7518
1550.7271	1557.2094	1558.2151
1562.2826	1565.1429	1590.0724
1591.6627	1606.2124	1610.9368
1614.3929	1643.2022	1645.9357
1648.0126	1714.6457	2503.3809
2953.6274	2964.3689	2981.0170
3019.1642	3032.0950	3040.5627
3043.0173	3047.0557	3051.9897
3054.4752	3060.1017	3060.8433
3073.7590	3077.9681	3081.0043
3092.9949	3096.6157	3097.4934
3102.3115	3105.2862	3111.6960
3118.5664	3129.2051	3142.6227
3150.6534	3207.6386	3209.4753
3209.9003	3210.8620	3221.2925
3262.0815	3262.2137	3263.5685
3264.6218	3285.1881	3285.4550
3286.4526	3287.6166	3633.6319

## III.C.12. Point P12

```

Absolute energy: -2476.5987934

Geometry:
C      0.464921   3.335771  -1.227795
C      0.494991   4.609089  -0.526567
C      1.552515   4.785131   0.549129
C      5.446853  -0.856123   0.192573
O     -0.352839   5.506957  -0.762704
C      2.723258   3.799467   0.397467
C      2.276705   2.316902   0.227569
C      3.523807   1.438066  -0.181540
C      3.122336  -0.017629  -0.581975
C      2.142852   0.016012  -1.770407
C      0.965066   0.957674  -1.546498
C      1.226396   2.250018  -0.894647
C      4.667895   1.471976   0.871564
C      5.882355   0.587402   0.497493
C      4.388648  -0.809999  -0.942830
C      4.944787  -1.558972   1.476298
C      1.618609   1.806466   1.544354
C      6.522104  -1.747829  -0.491392
C      5.700768  -2.864171  -1.207803
C      4.265044  -2.282341  -1.412953
O      7.578459  -2.244357   0.372079
S     -4.529224  -0.892858   0.694606
Fe    -2.125659  -0.637471   0.108235
C     -2.561495  -1.395454  -3.199533
C     -2.715983   2.690086  -0.572859
C     -1.853752   0.102461   3.448681
C     -1.749406  -3.978119   0.832581
N     -2.544292   0.430343  -1.542697
C     -2.666078  -0.061015  -2.835929
C     -2.936476   1.023157  -3.754768
C     -2.984184   2.171655  -3.015998
C     -2.745211   1.798119  -1.639037
N     -2.319534   1.041936   1.213192
C     -2.522162   2.337322   0.753072
C     -2.477512   3.268799   1.858644
C     -2.238364   2.537791   2.987486
C     -2.129883   1.151258   2.586696
N     -1.863668  -1.725018   1.803552
C     -1.739824  -1.233201   3.088687
C     -1.488665  -2.321223   4.013824
C     -1.465788  -3.471427   3.280506
C     -1.697065  -3.096866   1.899588
N     -2.163988  -2.342061  -0.963549
C     -1.962742  -3.626499  -0.495876
C     -2.004477  -4.566382  -1.595433
C     -2.230258  -3.841312  -2.731154
C     -2.328561  -2.454139  -2.331705
O     -0.387318  -0.524718   0.017880
H      3.316367   4.083917  -0.483619
H      3.927438   1.901374  -1.100405
H      2.617939  -0.505307   0.263192
H      2.694438   0.335962  -2.671433
H      1.761468  -0.991298  -1.975673
H(iso=2) 0.250796   0.333225  -0.777850
H      0.324729   1.056024  -2.428900
H     -0.265836   3.257609  -2.026351
H      1.901865   5.823701   0.522011
H      1.059468   4.656621   1.523731
H      4.283531   1.154820   1.848436
H      5.016624   2.503266   1.000328
H      6.375670   1.004040  -0.393895
H      4.111006  -1.027362   1.941661
H      1.245468   0.784404   1.440969

```

H	0.759845	2.430323	1.811568
H	7.063225	-1.143041	-1.226748
H	6.174557	-3.156120	-2.150305
H	5.678114	-3.763356	-0.577618
H	3.527884	-2.823431	-0.806752
H	3.935595	-2.354587	-2.454303
H	4.868768	-0.257700	-1.772013
H	5.756925	-1.602264	2.212433
H	4.603880	-2.582600	1.282618
H	2.331700	1.845551	2.374783
H	3.382736	3.888422	1.267359
H	6.624225	0.608246	1.306489
H	7.214453	-2.907550	0.992843
H	-4.973936	0.334430	0.238716
H	-2.678998	-1.633235	-4.251838
H	-2.827314	3.745497	-0.797218
H	-1.727111	0.345884	4.498513
H	-1.609363	-5.032121	1.049265
H	-3.077241	0.905346	-4.819311
H	-3.168911	3.180817	-3.353797
H	-2.603982	4.336936	1.761189
H	-2.139534	2.890170	4.003855
H	-1.358860	-2.202906	5.079649
H	-1.311827	-4.483524	3.625134
H	-1.878441	-5.634584	-1.496023
H	-2.325615	-4.197618	-3.746424

## Frequencies:

-701.2162	6.8409	14.1977
16.4281	30.6202	35.1264
38.7181	52.9314	57.3026
58.7767	74.1306	80.6869
92.7910	99.6710	116.8037
130.2683	139.8291	146.3263
154.0634	157.9836	163.8736
174.7149	187.3428	202.6785
205.6527	210.7799	219.5100
222.3785	231.5011	233.3638
246.0634	266.6603	269.8895
272.1347	279.7517	281.4158
282.7135	286.3152	297.6427
300.3152	304.3840	314.5802
318.6285	329.1436	340.7628
359.9495	369.4667	370.4324
373.4960	379.6590	383.6808
398.9357	411.9741	415.3891
421.1243	433.7888	436.0871
437.5797	439.3939	443.5054
449.8515	470.1558	485.7803
499.9369	511.1140	518.6342
549.1229	554.8463	560.5039
575.5901	584.8702	621.3512
644.4669	656.2059	678.0517
678.8010	687.5630	689.2948
689.7537	699.4617	724.0746
725.1558	728.5170	735.0598
740.1071	760.7014	761.7027
766.5247	766.8128	793.0878
802.6372	807.0147	811.4388
813.1132	817.6228	821.5031
834.5212	835.1261	840.7004
849.0210	851.3383	852.2815
854.8138	873.4570	901.0547
906.4864	915.7581	918.3974
920.8612	934.4311	937.2797
941.7267	950.2116	953.2649
953.3752	956.1578	959.3547
964.4623	975.2638	985.3805
990.9774	1000.9447	1017.2233
1019.4457	1020.1417	1022.3791
1024.0716	1033.0427	1038.4703

1048.9719	1050.3935	1057.7386
1058.2921	1061.4721	1062.8412
1077.3688	1079.5765	1086.7747
1101.5748	1117.1935	1117.6883
1119.6415	1123.3223	1127.2857
1139.3924	1150.6550	1155.0431
1172.0313	1175.6431	1187.1225
1190.4433	1191.9562	1200.2192
1216.1988	1216.3307	1221.9713
1241.5517	1243.6657	1245.1828
1256.9833	1263.9392	1275.9824
1282.2091	1294.6025	1297.1200
1300.2708	1306.6122	1309.3640
1315.5896	1322.3449	1332.1031
1336.2010	1345.3502	1348.1533
1349.8839	1357.4090	1363.1085
1376.5972	1378.5720	1386.1484
1388.6445	1389.3245	1394.8834
1399.0839	1400.9001	1409.2719
1411.6060	1415.6400	1420.0230
1423.2322	1427.7441	1428.8666
1436.6941	1437.4322	1453.5323
1462.3253	1498.3123	1499.5295
1501.7359	1510.1077	1528.4937
1529.8425	1533.7560	1534.4671
1536.7539	1540.8567	1545.6819
1550.5989	1557.1117	1558.2505
1562.1945	1565.0610	1590.1876
1591.7219	1605.5212	1614.2727
1622.4089	1643.5227	1646.2634
1652.5457	1715.0694	2503.1186
2954.4383	2965.1618	2986.0603
3019.6964	3032.7979	3040.7746
3043.3971	3047.4842	3052.4356
3053.7566	3060.6242	3061.2882
3074.2358	3078.7421	3080.8228
3093.2506	3097.4867	3098.0085
3098.7095	3102.5442	3112.1256
3119.3378	3129.8768	3143.3380
3151.4580	3207.4180	3210.9362
3211.3462	3212.2976	3222.7378
3264.0111	3264.1376	3265.5873
3266.5997	3287.0461	3287.3267
3288.4255	3289.5619	3630.6389

## III.C.13. Point P13

```
Absolute energy: -2476.6009048

Geometry:
C      0.466389   3.336151  -1.227741
C      0.494710   4.609013  -0.526733
C      1.552540   4.785186   0.549127
C      5.446917  -0.856172   0.192565
O     -0.352837   5.506957  -0.762493
C      2.723396   3.799584   0.397850
C      2.276607   2.317442   0.227437
C      3.523723   1.438012  -0.181563
C      3.122262  -0.017566  -0.582303
C      2.145349   0.017037  -1.772877
C      0.962667   0.954624  -1.546083
C      1.227817   2.253959  -0.895421
C      4.667863   1.472012   0.871543
C      5.882334   0.587389   0.497514
C      4.388694  -0.809986  -0.942612
C      4.944830  -1.558975   1.476302
C      1.618563   1.806459   1.544214
C      6.522125  -1.747797  -0.491373
C      5.700789  -2.864190  -1.207776
C      4.265102  -2.282284  -1.412905
O      7.578448  -2.244384   0.372077
S     -4.529472  -0.892786   0.694578
Fe    -2.123326  -0.637715   0.108396
C     -2.561513  -1.395383  -3.199362
C     -2.716070   2.689848  -0.572750
C     -1.853802   0.102493   3.448576
C     -1.749449  -3.978023   0.832507
N     -2.545051   0.430204  -1.542685
C     -2.666102  -0.061045  -2.835737
C     -2.936418   1.022993  -3.754447
C     -2.984132   2.171421  -3.015672
C     -2.745181   1.797916  -1.638906
N     -2.319811   1.041738   1.213455
C     -2.522154   2.337211   0.752956
C     -2.477519   3.268513   1.858490
C     -2.238386   2.537620   2.987305
C     -2.129905   1.151256   2.586676
N     -1.864759  -1.725120   1.803788
C     -1.739993  -1.233062   3.088768
C     -1.488704  -2.320952   4.013472
C     -1.465828  -3.471193   3.280117
C     -1.697249  -3.096930   1.899494
N     -2.164348  -2.342143  -0.963555
C     -1.962786  -3.626434  -0.495868
C     -2.004493  -4.566136  -1.595304
C     -2.230254  -3.841049  -2.730970
C     -2.328571  -2.454040  -2.331604
O     -0.400020  -0.530987   0.023912
H      3.316237   4.083765  -0.483500
H      3.927298   1.901227  -1.100485
H      2.617688  -0.505238   0.263004
H      2.699828   0.335465  -2.671792
H      1.763378  -0.990551  -1.976797
H(iso=2) 0.281050   0.369340  -0.812704
H      0.340120   1.065389  -2.440443
H     -0.263805   3.257553  -2.026879
H      1.901897   5.823813   0.522012
H      1.059478   4.656718   1.523813
H      4.283609   1.154831   1.848536
H      5.016708   2.503299   1.000440
H      6.375596   1.004044  -0.393928
H      4.111005  -1.027216   1.941494
H      1.246062   0.784150   1.440727
```

H	0.759956	2.430444	1.811627
H	7.063040	-1.142984	-1.226907
H	6.174599	-3.156100	-2.150346
H	5.678199	-3.763455	-0.577595
H	3.527897	-2.823454	-0.806710
H	3.935520	-2.354289	-2.454227
H	4.868607	-0.257725	-1.771909
H	5.756872	-1.602342	2.212622
H	4.603887	-2.582644	1.282587
H	2.331785	1.845099	2.374629
H	3.383073	3.888980	1.267693
H	6.624310	0.608250	1.306502
H	7.214242	-2.907449	0.992741
H	-4.974606	0.334396	0.239310
H	-2.678671	-1.633108	-4.251709
H	-2.826177	3.745367	-0.797253
H	-1.726852	0.345934	4.498355
H	-1.609152	-5.031984	1.049200
H	-3.076792	0.905310	-4.819068
H	-3.168258	3.180676	-3.353537
H	-2.603514	4.336710	1.760925
H	-2.139318	2.890140	4.003617
H	-1.358684	-2.202702	5.079293
H	-1.311655	-4.483260	3.624794
H	-1.878335	-5.634351	-1.496003
H	-2.325467	-4.197395	-3.746254

## Frequencies:

-171.3743	-16.5888	8.9791
12.1177	21.2516	34.1842
36.4251	52.5821	55.5984
58.6107	75.5094	80.8240
93.2892	98.2367	118.7751
129.0370	138.2123	148.6036
153.7031	158.3373	169.9494
183.1041	198.2750	201.8607
206.5417	211.4934	219.7198
220.9854	230.5907	237.6666
247.4973	267.4574	271.2179
274.9585	279.8057	281.5849
282.6073	288.1012	296.9176
301.0391	307.1262	313.5252
328.4027	335.2427	339.8572
359.7859	370.7662	373.0193
374.0481	379.8596	383.7557
398.4749	412.5842	414.3013
421.2364	434.0091	436.0396
436.4649	439.0966	439.7079
449.8174	468.9107	485.5826
495.0480	507.1368	517.9706
544.5787	550.6904	560.1018
575.2902	577.1525	621.3069
643.8406	656.8158	677.9155
678.6944	687.3853	689.0528
689.5692	696.7013	724.4995
725.0648	728.3428	735.0659
740.4177	760.2343	761.2647
766.5742	766.8157	792.0881
802.9328	810.2061	811.7648
813.5248	817.1930	821.8899
834.6751	835.5474	848.7732
849.9225	852.2740	853.7614
870.7933	887.7803	906.9403
915.3879	918.9453	921.3961
934.2901	937.8048	942.3300
945.7336	953.1964	953.8988
954.0638	960.1455	965.2003
975.8962	986.4598	991.7427
1001.6434	1017.6531	1020.2454
1021.5776	1022.6604	1024.5277
1033.4652	1038.4158	1049.2807

1050.8490	1058.2801	1058.7368
1062.0571	1062.8269	1077.8312
1080.5520	1086.8471	1101.6056
1117.5816	1118.0380	1119.9507
1123.6697	1127.0896	1139.5674
1149.5868	1154.6125	1171.0502
1174.9986	1190.9763	1191.8901
1192.7188	1197.4050	1213.6806
1216.8345	1234.9055	1240.7134
1244.3336	1245.6329	1258.1571
1264.0121	1278.7243	1281.6820
1294.4145	1297.6914	1300.7058
1306.0626	1308.1949	1313.5192
1322.4008	1331.7705	1334.9607
1345.3616	1348.5352	1350.1132
1357.2725	1363.1481	1376.5152
1378.1233	1386.4037	1388.9371
1389.2751	1395.0218	1398.8320
1400.7737	1405.1305	1411.7018
1412.1255	1415.4025	1419.9418
1423.5664	1427.7208	1429.9990
1437.2099	1437.3284	1453.4007
1461.2320	1498.7026	1499.8446
1501.9513	1510.1733	1529.7888
1532.6045	1534.1494	1534.5905
1536.7844	1540.8980	1545.6471
1550.5542	1556.9860	1558.4840
1562.1918	1565.0628	1590.4884
1591.9039	1604.8001	1614.4004
1639.4893	1644.1594	1646.7302
1660.8233	1715.6762	2504.4884
2954.7412	2965.4372	2992.6238
3019.3609	3032.5452	3039.9082
3042.7018	3046.8640	3051.4869
3051.8318	3060.1280	3060.6357
3073.5685	3078.2539	3078.9852
3089.1276	3092.2667	3097.2151
3097.3293	3101.5401	3111.4855
3118.8989	3129.5496	3142.9318
3150.9700	3205.6941	3211.2296
3211.6178	3212.5144	3222.8924
3264.0423	3264.1710	3265.7204
3266.6652	3287.0247	3287.3061
3288.5296	3289.6024	3631.5332



## III.C.14. Point P14

```
Absolute energy: -2476.6026921
Geometry:
C      0.468110    3.337453   -1.227874
C      0.494363    4.609009   -0.526920
C      1.552557    4.785292    0.549167
C      5.446996   -0.856250    0.192598
O     -0.352884    5.506978   -0.762169
C      2.723629    3.799840    0.398426
C      2.276664    2.318188    0.227329
C      3.523630    1.438015   -0.181554
C      3.122276   -0.017421   -0.582807
C      2.148818    0.018466   -1.776032
C      0.964580    0.955423   -1.550163
C      1.230378    2.258036   -0.896955
C      4.667822    1.472021    0.871494
C      5.882276    0.587375    0.497538
C      4.388800   -0.809985   -0.942282
C      4.944905   -1.558960    1.476277
C      1.618493    1.806498    1.543853
C      6.522226   -1.747775   -0.491308
C      5.700821   -2.864182   -1.207726
C      4.265196   -2.282189   -1.412806
O      7.578395   -2.244457    0.372093
S     -4.529905   -0.892636    0.694555
Fe    -2.120204   -0.638196    0.108716
C     -2.561534   -1.395305   -3.199117
C     -2.716169    2.689508   -0.572608
C     -1.853856    0.102547    3.448466
C     -1.749513   -3.977866    0.832389
N     -2.546021    0.430034   -1.542723
C     -2.666166   -0.061047   -2.835440
C     -2.936292    1.022689   -3.753888
C     -2.983997    2.171017   -3.015095
C     -2.745151    1.797549   -1.638721
N     -2.320244    1.041586    1.213907
C     -2.522149    2.336926    0.752909
C     -2.477502    3.268018    1.858213
C     -2.238411    2.537316    2.986989
C     -2.129969    1.151288    2.586587
N     -1.866656   -1.725427    1.804404
C     -1.740333   -1.232977    3.088770
C     -1.488737   -2.320560    4.012901
C     -1.465870   -3.470787    3.279523
C     -1.697625   -3.096859    1.899410
N     -2.164872   -2.342439   -0.963683
C     -1.962880   -3.626235   -0.495934
C     -2.004518   -4.565693   -1.595118
C     -2.230237   -3.840625   -2.730657
C     -2.328590   -2.453943   -2.331366
O     -0.417212   -0.539493    0.032163
H      3.316453    4.083944   -0.483360
H      3.927385    1.901209   -1.100648
H      2.616706   -0.505305    0.262308
H      2.707055    0.335190   -2.673061
H      1.766044   -0.989507   -1.979437
H(iso=2) 0.294971    0.394774   -0.836071
H      0.357275    1.076221   -2.454412
H     -0.261490    3.257864   -2.028099
H      1.902131    5.824289    0.522042
H      1.059450    4.656887    1.524203
H      4.283602    1.154787    1.848879
H      5.016900    2.503624    1.000570
H      6.375633    1.004198   -0.394135
H      4.110748   -1.026926    1.941481
H      1.246519    0.783572    1.440178
```

H	0.759691	2.430576	1.811898
H	7.062706	-1.142691	-1.227535
H	6.174768	-3.156121	-2.150739
H	5.678167	-3.763790	-0.577417
H	3.527739	-2.823644	-0.806466
H	3.935414	-2.353929	-2.454523
H	4.868623	-0.257725	-1.771882
H	5.756935	-1.602492	2.213131
H	4.603816	-2.582965	1.282580
H	2.331921	1.844457	2.374615
H	3.383673	3.889821	1.268496
H	6.624617	0.608253	1.306726
H	7.214252	-2.906867	0.992257
H	-4.975566	0.334009	0.240614
H	-2.678288	-1.633057	-4.251958
H	-2.824952	3.745592	-0.797380
H	-1.726356	0.346112	4.498605
H	-1.608733	-5.032209	1.049167
H	-3.076290	0.905292	-4.819230
H	-3.167544	3.180906	-3.353405
H	-2.603017	4.336920	1.760667
H	-2.139017	2.890406	4.003738
H	-1.358230	-2.202506	5.079325
H	-1.311208	-4.483317	3.624618
H	-1.878152	-5.634547	-1.496040
H	-2.325311	-4.197374	-3.746487

## Frequencies:

-30.1847	-13.9026	9.0778
16.6123	29.3440	35.1122
38.0368	53.4406	55.0292
59.1566	70.6602	87.2177
94.2266	100.1632	121.1897
128.4287	131.6225	146.4342
152.8849	157.5202	170.2258
184.9306	196.7475	201.6824
210.4313	216.0809	219.2467
220.7580	231.7528	243.1210
253.4344	268.1012	271.9396
279.0090	280.1486	281.5723
281.9583	292.2730	296.0518
301.5645	308.5177	313.2072
321.8155	334.7423	351.5993
359.6791	371.2223	374.5789
378.4424	379.7756	384.3623
399.6623	412.9018	414.6073
420.0839	434.4794	436.5872
438.6149	439.1595	440.5658
468.2205	473.5479	485.7154
506.1888	517.1767	535.2726
543.2253	558.8352	564.3190
574.7027	575.7693	621.8339
643.6695	657.1770	678.3767
679.1741	688.1760	689.4759
689.7943	694.7961	725.7925
726.0273	728.8879	735.7914
741.6330	760.0445	761.5257
766.9881	767.1539	791.6381
805.0841	809.8410	814.1353
815.9308	817.6694	824.4241
834.9369	835.7322	848.8908
850.4829	852.4812	854.5651
872.4842	890.1772	909.1995
916.1575	921.1694	923.7113
934.9691	939.7241	945.1552
950.5584	956.0071	956.4867
957.2978	962.7252	966.1156
977.3036	987.4142	992.8077
1003.1507	1018.9832	1020.8792
1023.3468	1023.8394	1025.4979
1034.4333	1038.5866	1049.5078

1051.2288	1059.2553	1059.8820
1062.9812	1063.3509	1078.7514
1081.5956	1087.2312	1101.9978
1119.2553	1119.6847	1121.5926
1125.3094	1127.9714	1139.7230
1149.6824	1156.3243	1172.0078
1175.7257	1192.7487	1193.9647
1196.8006	1198.3489	1214.6361
1218.0635	1236.8996	1242.3199
1246.9807	1254.2908	1262.2463
1269.1939	1280.9683	1290.3228
1294.8135	1298.9392	1301.7112
1306.5192	1309.1740	1314.6404
1323.0208	1333.1210	1336.0045
1345.8956	1349.9797	1351.5013
1357.7344	1363.9099	1376.8081
1378.9467	1387.7996	1389.6263
1390.4597	1395.6318	1399.8316
1402.6579	1409.5601	1413.3940
1415.7427	1420.0849	1424.7255
1427.9972	1429.4259	1437.5019
1438.3820	1453.9723	1461.0488
1499.5519	1500.7241	1502.6763
1510.5169	1530.1166	1533.3260
1534.8411	1535.2494	1537.1078
1541.1889	1545.9084	1550.8620
1556.9991	1559.2920	1562.4769
1565.3705	1591.3103	1592.6442
1605.5150	1615.1424	1627.3720
1644.9338	1647.2378	1659.4728
1716.2792	1751.1737	2509.5800
2953.0193	2963.6614	2993.7159
3016.5574	3029.4911	3036.6680
3039.2889	3043.5979	3047.3913
3048.4688	3056.7500	3057.0659
3069.9243	3073.9251	3074.7819
3081.3682	3088.3711	3093.3018
3093.5093	3097.6395	3107.9926
3115.0341	3126.0982	3139.2761
3146.9047	3200.5860	3207.2170
3207.5872	3208.4024	3218.6179
3258.0992	3258.2374	3259.8492
3260.7708	3281.1035	3281.3872
3282.6764	3283.7138	3641.6001

## III.C.15. Point P15

```
Absolute energy: -2476.5962701
Geometry:
C      0.476118    3.347941   -1.235885
C      0.497283    4.613361   -0.525481
C      1.553260    4.788008    0.552085
C      5.447840   -0.856402    0.193993
O     -0.355124    5.509023   -0.758166
C      2.725992    3.803329    0.401967
C      2.280720    2.320913    0.224748
C      3.527003    1.440242   -0.181275
C      3.125069   -0.014199   -0.587405
C      2.163391    0.027796   -1.788572
C      0.996192    0.984684   -1.590805
C      1.241784    2.258015   -0.908075
C      4.668989    1.471889    0.873037
C      5.883199    0.587256    0.498660
C      4.390872   -0.809786   -0.941272
C      4.945066   -1.559160    1.477123
C      1.616432    1.806711    1.537133
C      6.522803   -1.748039   -0.490627
C      5.701157   -2.864119   -1.207391
C      4.265690   -2.281769   -1.412060
O      7.579109   -2.245055    0.372290
S     -4.536684   -0.891431    0.695549
Fe    -2.126073   -0.644245    0.113014
C     -2.561882   -1.396257   -3.199486
C     -2.715742    2.688398   -0.571664
C     -1.854726    0.102525    3.450580
C     -1.750782   -3.978375    0.832820
N     -2.545238    0.427461   -1.540547
C     -2.666434   -0.062376   -2.834463
C     -2.935656    1.021842   -3.752831
C     -2.982848    2.170053   -3.013470
C     -2.744563    1.795650   -1.637092
N     -2.322451    1.039280    1.215445
C     -2.522770    2.335368    0.753582
C     -2.476981    3.267710    1.858122
C     -2.237880    2.537930    2.987589
C     -2.131050    1.150918    2.588348
N     -1.882750   -1.727548    1.807998
C     -1.747040   -1.233575    3.090725
C     -1.487167   -2.320984    4.013680
C     -1.464560   -3.471035    3.280129
C     -1.704785   -3.097746    1.900646
N     -2.167401   -2.343487   -0.963121
C     -1.964107   -3.626856   -0.495826
C     -2.003984   -4.566548   -1.595730
C     -2.229910   -3.841409   -2.731190
C     -2.329694   -2.454498   -2.331410
O     -0.411174   -0.548832    0.043335
H      3.322300    4.090955   -0.476305
H      3.933804    1.904328   -1.098647
H      2.608597   -0.502934    0.249854
H      2.731454    0.348393   -2.679601
H      1.781962   -0.977289   -2.005479
H(iso=2) 0.183989    0.305890   -0.790725
H      0.374161    1.091414   -2.474840
H     -0.249227    3.271634   -2.040137
H      1.902537    5.827038    0.526347
H      1.059136    4.658712    1.526231
H      4.283635    1.154023    1.849582
H      5.018159    2.503233    1.003060
H      6.376020    1.003961   -0.393282
H      4.110154   -1.027425    1.941141
H      1.242555    0.784988    1.428169
```

H	0.757211	2.430377	1.804730
H	7.063622	-1.142796	-1.226315
H	6.174949	-3.155890	-2.150355
H	5.678471	-3.763677	-0.577326
H	3.528001	-2.822870	-0.806019
H	3.936146	-2.353147	-2.453835
H	4.873782	-0.259023	-1.770211
H	5.756342	-1.602157	2.214632
H	4.604477	-2.583124	1.283218
H	2.327422	1.841762	2.369987
H	3.382207	3.890620	1.274846
H	6.625780	0.608288	1.307366
H	7.214932	-2.906531	0.993552
H	-4.981473	0.340339	0.253276
H	-2.677672	-1.633467	-4.252499
H	-2.824628	3.744325	-0.796752
H	-1.721666	0.346588	4.499850
H	-1.604202	-5.032042	1.048870
H	-3.075557	0.904558	-4.818143
H	-3.166238	3.180182	-3.350998
H	-2.602259	4.336479	1.759351
H	-2.137965	2.891656	4.003992
H	-1.350389	-2.202424	5.079171
H	-1.303907	-4.482893	3.624158
H	-1.876893	-5.635234	-1.496601
H	-2.324446	-4.197605	-3.747187

## Frequencies:

-1270.7095	11.1638	14.9810
19.6409	36.4342	37.8748
42.3084	53.2896	58.7222
59.3658	72.4304	76.9003
92.8446	100.3445	115.7464
131.5962	139.0818	143.4716
153.8139	155.9073	164.1581
178.2345	189.6197	201.4342
207.4756	211.8545	219.3646
224.1952	231.2481	232.2849
246.1433	267.0727	270.9358
274.1907	279.9219	281.5615
282.4515	287.5471	297.1260
302.0578	303.9788	314.8185
318.1187	323.4624	335.5017
359.8445	369.4044	370.8592
374.1518	379.8159	383.9817
400.0052	411.6384	414.4205
421.1699	434.2017	436.3761
437.3231	439.9437	441.9398
460.3706	471.7013	486.1076
500.2577	517.3728	519.2888
548.0650	554.6561	561.0750
576.5956	602.6624	622.4696
647.2754	656.6062	678.7793
679.4929	688.1957	690.0407
690.6346	703.1971	710.0004
726.2454	727.9970	730.1224
736.8248	742.8135	761.1741
763.7458	766.9609	767.0645
795.2806	804.2607	813.3186
815.1328	819.0654	819.2289
823.6412	834.8124	835.4695
849.3210	852.4945	853.1044
858.0667	867.1338	898.0990
907.9087	918.4256	919.6928
922.3085	933.0380	936.2893
938.1138	943.8045	953.5605
954.8668	955.0466	961.0938
964.8661	975.3816	984.8841
990.3584	1000.1906	1017.3348
1018.2769	1019.7408	1023.1098
1025.0529	1033.7627	1038.7951

1048.5948	1049.5777	1058.3211
1058.7865	1061.3593	1063.8117
1077.9920	1080.7666	1087.2701
1102.4398	1118.3569	1118.9291
1120.9176	1124.5374	1126.3592
1139.6411	1149.8460	1155.5621
1158.0834	1172.7071	1177.3570
1191.4270	1192.9286	1199.4855
1203.5727	1216.3686	1216.9192
1237.0375	1242.8247	1246.0339
1256.5144	1263.4900	1274.2952
1280.6751	1295.1402	1297.7543
1300.5880	1307.4241	1313.5616
1316.9634	1323.3377	1333.1115
1337.9876	1345.9352	1349.9997
1351.2824	1358.0019	1363.5869
1376.5206	1378.7912	1387.3683
1388.9295	1389.7107	1396.1771
1399.6915	1401.8685	1409.6746
1412.7256	1415.6874	1420.5648
1424.0558	1426.3944	1428.5079
1437.6806	1438.5942	1454.1688
1463.0425	1499.4678	1500.6511
1502.3921	1510.3607	1527.1330
1530.1272	1534.2651	1535.1875
1536.9537	1540.9274	1545.9034
1550.9045	1557.3430	1558.9182
1562.5567	1565.1809	1591.3003
1592.6887	1603.5609	1608.6933
1615.4075	1644.6724	1645.4746
1646.7668	1715.6947	2505.6411
2951.4794	2962.4527	2980.9584
3017.4227	3030.2865	3038.9188
3041.2007	3045.1163	3049.7768
3053.6593	3058.1675	3058.9923
3071.6513	3075.7871	3078.9498
3090.5636	3094.4004	3094.8713
3099.8425	3109.6256	3116.3615
3126.9485	3140.1211	3147.6824
3180.8831	3203.5123	3207.3260
3207.8249	3208.3468	3218.8561
3258.4862	3258.6800	3259.8709
3260.9422	3281.5779	3281.9558
3282.7731	3283.9054	3640.7629

## III.C.16. Point P16

```
Absolute energy: -2476.603168
Geometry:
C      0.490924   3.357810  -1.245254
C      0.500399   4.618096  -0.525337
C      1.554528   4.790661   0.555295
C      5.449044  -0.856643   0.195567
O     -0.356266   5.510246  -0.752268
C      2.728614   3.806724   0.406632
C      2.283893   2.325211   0.220327
C      3.531057   1.443107  -0.181944
C      3.128563  -0.009442  -0.595013
C      2.186302   0.042903  -1.810951
C      1.002435   0.986303  -1.611576
C      1.254471   2.272866  -0.920862
C      4.670258   1.471818   0.875127
C      5.884414   0.586992   0.500622
C      4.393919  -0.809016  -0.940435
C      4.945077  -1.559342   1.478080
C      1.613290   1.806412   1.527938
C      6.523774  -1.748297  -0.489428
C      5.701771  -2.864110  -1.206598
C      4.266716  -2.280854  -1.411060
O      7.579959  -2.245956   0.372780
S     -4.545697  -0.889955   0.696625
Fe    -2.124409  -0.650399   0.117643
C     -2.562360  -1.397252  -3.198756
C     -2.715139   2.685733  -0.570196
C     -1.857136   0.101983   3.452708
C     -1.753486  -3.979036   0.833460
N     -2.547093   0.424125  -1.538127
C     -2.666770  -0.064281  -2.832460
C     -2.934525   1.020156  -3.750294
C     -2.981051   2.167861  -3.010461
C     -2.743623   1.792663  -1.634632
N     -2.326146   1.036413   1.218325
C     -2.523402   2.332605   0.754514
C     -2.476088   3.265922   1.857759
C     -2.237110   2.537427   2.987862
C     -2.132988   1.150029   2.590335
N     -1.900529  -1.730253   1.812346
C     -1.755168  -1.234333   3.093457
C     -1.486132  -2.320782   4.013573
C     -1.463835  -3.470884   3.279694
C     -1.713392  -3.099362   1.902201
N     -2.171837  -2.345368  -0.962252
C     -1.966312  -3.628125  -0.495140
C     -2.003255  -4.566882  -1.595503
C     -2.229336  -3.841498  -2.730722
C     -2.331310  -2.455249  -2.330700
O     -0.438955  -0.566018   0.061757
H      3.328200   4.097683  -0.468185
H      3.941769   1.908623  -1.096804
H      2.601092  -0.499027   0.235079
H      2.770055   0.370922  -2.687524
H      1.809616  -0.961286  -2.040674
H(iso=2) 0.239451   0.367577  -0.890408
H      0.432069   1.130311  -2.528392
H     -0.229905   3.285060  -2.054112
H      1.903640   5.829841   0.532280
H      1.058264   4.659752   1.528154
H      4.283184   1.152455   1.850561
H      5.020078   2.502630   1.007772
H      6.376969   1.003929  -0.391347
H      4.108770  -1.027867   1.939920
H      1.238914   0.785559   1.413796
```

H	0.754682	2.430805	1.795320
H	7.063942	-1.142851	-1.225364
H	6.175465	-3.155517	-2.149722
H	5.678890	-3.763953	-0.576919
H	3.528583	-2.821207	-0.804821
H	3.936936	-2.351768	-2.452675
H	4.880241	-0.260714	-1.768941
H	5.754856	-1.601502	2.217331
H	4.605660	-2.583687	1.284013
H	2.321702	1.836219	2.363233
H	3.381200	3.891160	1.282629
H	6.627243	0.607840	1.309130
H	7.215099	-2.906409	0.994947
H	-4.986152	0.347722	0.267240
H	-2.676037	-1.633749	-4.252005
H	-2.820732	3.741753	-0.795865
H	-1.717635	0.346525	4.500877
H	-1.600326	-5.031745	1.048991
H	-3.073208	0.903543	-4.815699
H	-3.162316	3.178388	-3.347484
H	-2.599072	4.334688	1.757476
H	-2.135509	2.892438	4.003504
H	-1.341586	-2.202010	5.077869
H	-1.295650	-4.481693	3.622796
H	-1.874523	-5.635306	-1.497089
H	-2.322190	-4.197353	-3.746843

## Frequencies:

-157.3858	6.3350	10.8156
14.4036	25.5850	35.3390
36.7400	53.1944	55.8327
58.3616	70.6237	79.5395
92.8518	99.2938	119.5416
131.1870	140.2527	149.7857
152.7734	160.4707	174.6879
182.9953	192.4701	200.3176
202.7358	211.1329	219.5110
221.3676	232.1515	238.6098
250.7928	267.4641	274.0318
277.9712	280.3989	281.3415
281.5200	288.5849	297.0674
303.3868	308.4080	314.4122
323.7583	326.4190	335.9755
358.9140	371.7454	372.8135
376.9005	379.6972	384.1903
400.1791	413.0058	417.6249
419.9912	434.6505	436.8656
439.0264	440.0889	445.1022
466.8152	470.2271	485.5999
509.4708	517.7277	538.7719
547.3535	559.8774	575.1216
580.4862	614.0503	621.8554
645.6435	656.4501	678.4633
679.1979	687.8601	689.7070
690.2041	702.6092	725.5319
725.8494	729.5901	735.5732
741.4188	761.0221	763.3077
766.7973	767.1089	795.3433
804.3384	813.4970	815.4665
817.6322	818.8084	823.9196
835.2043	835.6422	849.8302
852.4615	853.5265	858.0390
871.9849	902.8733	908.2788
920.3134	922.6183	923.2282
934.8597	939.0108	944.5196
950.8801	955.4339	955.8662
962.0661	965.8562	969.2936
978.5382	989.2974	992.8050
1008.3663	1019.0246	1019.7803
1021.2991	1023.4019	1026.6158
1034.8817	1039.0805	1048.3217



1051.0016	1058.9946	1060.0606
1062.7478	1064.3107	1079.0372
1083.2610	1089.1789	1102.2848
1118.3616	1119.3365	1121.0047
1122.0836	1124.9433	1130.3021
1143.0858	1152.3684	1157.7218
1172.8772	1177.6962	1192.4011
1194.2122	1197.4235	1203.3250
1217.6205	1218.5047	1234.9468
1242.2917	1246.8739	1252.5625
1259.9673	1265.5742	1278.4108
1284.4750	1294.8014	1299.0010
1301.2291	1306.7308	1312.0261
1316.8257	1323.7301	1333.2165
1336.8500	1345.8514	1351.0898
1352.1648	1357.6530	1364.1941
1375.6592	1378.0892	1388.0682
1389.2745	1390.4615	1396.7240
1399.9316	1402.3368	1408.8651
1413.1881	1415.1396	1420.4597
1424.6682	1426.3814	1429.1791
1438.4803	1438.5622	1453.5472
1460.9388	1500.5970	1501.5325
1502.7574	1510.0466	1529.9642
1534.0538	1536.1006	1536.4175
1537.0214	1540.6889	1545.6777
1550.6665	1557.2970	1559.3948
1562.6529	1564.9132	1591.9497
1593.3852	1608.0171	1615.8431
1631.7482	1646.3070	1647.8390
1658.6541	1717.4078	2507.1888
2951.7896	2962.8781	2992.4646
3017.3182	3030.8518	3038.3474
3040.7154	3044.6512	3049.4051
3051.2177	3057.9820	3058.5745
3071.2447	3075.9670	3077.4510
3089.6244	3094.2228	3094.9386
3098.7753	3109.1021	3116.5168
3127.2568	3139.7182	3144.2085
3148.0163	3199.2536	3209.2140
3209.6302	3209.8507	3220.5170
3260.1726	3260.4266	3261.6557
3262.6512	3283.1429	3283.5354
3284.4890	3285.5228	3638.7687

## III.C.17. Point P17

```
Absolute energy: -2476.5982413
Geometry:
C      0.469667   3.344691  -1.233419
C      0.497499   4.611439  -0.525998
C      1.553052   4.786733   0.551182
C      5.447509  -0.856258   0.193595
O     -0.354170   5.508145  -0.759756
C      2.724819   3.801659   0.399868
C      2.279596   2.318622   0.225370
C      3.526374   1.439946  -0.181541
C      3.124700  -0.014977  -0.585704
C      2.152710   0.023172  -1.778964
C      0.996581   0.987194  -1.582039
C      1.234619   2.247401  -0.903138
C      4.668740   1.471760   0.872738
C      5.883027   0.587267   0.498495
C      4.390389  -0.809692  -0.942362
C      4.944806  -1.559058   1.476834
C      1.617012   1.806585   1.538903
C      6.522731  -1.748046  -0.490734
C      5.701099  -2.864106  -1.207383
C      4.265574  -2.281881  -1.412314
O      7.578779  -2.244849   0.372305
S     -4.534511  -0.891827   0.695341
Fe    -2.128570  -0.641782   0.1111382
C     -2.561742  -1.396167  -3.199051
C     -2.715634   2.688536  -0.571869
C     -1.854799   0.102098   3.449739
C     -1.750711  -3.978010   0.832973
N     -2.544344   0.428766  -1.541693
C     -2.666275  -0.061754  -2.834785
C     -2.935814   1.022144  -3.753363
C     -2.983082   2.170524  -3.014233
C     -2.744707   1.796220  -1.637925
N     -2.321815   1.040454   1.214805
C     -2.522701   2.335872   0.753806
C     -2.476981   3.267859   1.858320
C     -2.237903   2.537545   2.987549
C     -2.130937   1.150900   2.587686
N     -1.875549  -1.726918   1.806652
C     -1.744894  -1.234024   3.089773
C     -1.487798  -2.321373   4.013898
C     -1.465100  -3.471297   3.280543
C     -1.702484  -3.097104   1.900632
N     -2.166538  -2.343526  -0.963200
C     -1.964004  -3.626645  -0.495919
C     -2.004052  -4.566505  -1.595494
C     -2.229938  -3.841460  -2.731023
C     -2.329477  -2.454699  -2.331181
O     -0.384474  -0.530647   0.024516
H      3.320869   4.089188  -0.478859
H      3.932652   1.904298  -1.099124
H      2.612032  -0.503558   0.253848
H      2.710400   0.346586  -2.677098
H      1.772485  -0.982457  -1.994941
H(iso=2) 0.134598   0.242645  -0.706930
H      0.326953   1.060220  -2.435163
H     -0.258647   3.267823  -2.035022
H      1.902675   5.825780   0.525143
H      1.059193   4.657525   1.525543
H      4.283141   1.153887   1.849249
H      5.017772   2.503300   1.002635
H      6.376372   1.004202  -0.393199
H      4.109821  -1.027638   1.941435
H      1.242105   0.784846   1.431443
```

H	0.757301	2.430199	1.806105
H	7.063535	-1.142796	-1.226714
H	6.174945	-3.155974	-2.150482
H	5.678041	-3.763753	-0.577290
H	3.527905	-2.822769	-0.805882
H	3.936173	-2.354163	-2.454345
H	4.873022	-0.258570	-1.771402
H	5.756384	-1.601898	2.214178
H	4.604341	-2.583221	1.283163
H	2.328069	1.843385	2.371756
H	3.381906	3.888565	1.272174
H	6.625355	0.608020	1.307599
H	7.215162	-2.906714	0.992849
H	-4.978364	0.338191	0.247972
H	-2.678469	-1.633653	-4.252198
H	-2.827214	3.744519	-0.796663
H	-1.724035	0.346085	4.499613
H	-1.606286	-5.032209	1.049275
H	-3.076666	0.904891	-4.818883
H	-3.167873	3.180564	-3.352339
H	-2.603101	4.336943	1.760514
H	-2.138361	2.891226	4.004352
H	-1.353019	-2.203072	5.079995
H	-1.306386	-4.483598	3.625153
H	-1.877179	-5.635555	-1.496518
H	-2.324645	-4.198162	-3.747180

## Frequencies:

-1292.3041	8.7622	13.9447
19.4138	36.9736	39.0116
46.6071	53.0087	58.4735
59.7976	71.8964	76.5848
92.3976	100.2647	114.7947
130.8375	137.3193	138.6410
154.3492	154.9879	164.5400
175.1456	191.8062	201.0728
210.0170	212.6928	218.8451
223.7995	230.3169	233.1118
246.6411	268.1896	270.6569
274.4825	279.5112	281.7732
282.6432	287.5800	296.6755
297.7724	303.8509	315.5008
319.8910	322.3093	334.5127
361.5927	368.8521	369.9437
372.6704	380.2748	384.2672
399.5884	410.4447	416.4178
422.2594	433.4097	436.2482
437.6007	440.2663	441.4750
463.9772	476.0295	486.5945
505.8152	519.7601	531.2059
550.0312	559.2157	561.8441
578.0803	618.3238	627.9439
648.1020	658.5645	679.1567
679.7605	689.3119	689.9875
690.3390	691.1655	702.8028
726.7683	727.0244	731.1920
736.5127	742.0225	761.6505
765.1237	767.3281	767.8027
788.0532	804.7393	813.3869
814.7939	815.2317	819.6966
823.8438	829.5974	834.7897
835.4954	850.1916	852.6978
853.7508	855.9862	876.3276
904.2486	908.1706	913.3274
919.5602	922.2822	935.2288
937.8466	943.6369	952.2126
954.5583	954.9606	958.9884
960.5830	974.5145	979.7574
988.5988	997.4658	1012.0934
1018.3211	1020.7636	1023.5071
1025.0599	1034.1343	1038.1737

1045.3184	1049.9442	1057.9449
1058.7611	1058.9552	1063.3342
1074.5151	1077.7910	1084.2645
1094.0068	1102.6804	1118.3621
1119.0185	1121.0601	1124.6317
1129.3444	1141.3511	1152.1126
1159.0925	1172.4699	1176.7957
1191.5204	1193.1893	1195.3735
1201.2273	1214.6091	1217.4810
1234.4426	1243.4461	1246.2044
1255.3460	1263.1370	1271.8887
1278.9402	1295.6946	1297.7622
1301.3048	1308.1189	1314.5955
1316.7534	1322.9424	1333.2661
1339.1515	1346.2446	1349.7903
1351.3972	1358.6416	1363.1094
1376.4592	1379.5257	1388.0589
1389.1425	1389.8940	1395.9690
1399.5502	1401.8603	1410.1584
1413.1590	1416.6912	1420.8974
1424.3451	1427.6780	1429.1587
1437.9337	1439.0776	1454.9597
1465.5131	1499.4117	1500.6365
1502.7821	1510.5088	1517.9816
1530.3456	1534.4944	1535.1701
1537.1419	1541.0011	1546.0007
1551.2056	1557.1402	1558.7778
1562.1623	1563.1119	1565.4530
1591.5829	1593.0646	1609.6654
1616.0721	1630.2721	1644.6358
1646.6604	1715.2984	2506.7910
2950.0954	2960.9045	2969.2995
3016.4029	3028.7372	3038.7783
3040.5863	3044.4107	3048.9966
3054.2816	3057.4242	3059.4624
3070.7401	3074.2020	3080.6666
3090.3651	3092.5971	3094.2165
3099.7788	3108.8122	3114.9334
3125.2609	3138.9888	3145.9647
3180.7604	3204.0518	3204.6158
3204.7778	3205.2968	3215.5913
3254.8730	3255.0769	3256.0969
3257.2775	3278.1121	3278.5514
3279.1292	3280.3489	3646.1222

### III.D. Geometries, QM energy, and QM frequencies of the supplementary Shepard points in the MCOMM calculations for H-abstraction of testosterone by Cpd I of the $^4A$ state

#### III.D.1. Point P1

Absolute energy: -2476.5998587

Geometry:

C	.482874	3.381668	-1.224522
C	.520301	4.646327	-.512375
C	1.570635	4.801656	.574423
C	5.415166	-.872677	.211815
O	-.312341	5.556864	-.750400
C	2.734803	3.808849	.419314
C	2.277526	2.331666	.230998
C	3.521040	1.444536	-.168528
C	3.110199	-.003257	-.587350
C	2.148415	.051216	-1.789342
C	.981461	1.009522	-1.579465
C	1.239309	2.284909	-.904269
C	4.651047	1.457375	.900170
C	5.861162	.563729	.534681

C	4.373147	-.806242	-.937391
C	4.888601	-1.580533	1.482628
C	1.597263	1.818712	1.535456
C	6.490962	-1.769912	-.464489
C	5.667912	-2.871091	-1.202468
C	4.240738	-2.273251	-1.420903
O	7.528478	-2.285629	.409528
S	-4.547575	-.730270	.303034
Fe	-2.125896	-.667750	.163133
C	-1.747491	-3.985579	.904180
C	-2.419466	-1.440851	-3.183693
C	-2.714314	2.652027	-.588830
C	-1.955533	.117484	3.488104
N	-2.133796	-2.369044	-.912673
C	-1.934341	-3.649425	-.429900
C	-1.919807	-4.591847	-1.524625
C	-2.096095	-3.874135	-2.673470
C	-2.225317	-2.486606	-2.291955
N	-2.510146	.393016	-1.546267
C	-2.563403	-.105066	-2.837695
C	-2.809720	.973365	-3.769621
C	-2.903820	2.122453	-3.036807
C	-2.715253	1.758206	-1.649812
N	-2.341984	1.029250	1.235644
C	-2.545968	2.309164	.744667
C	-2.541067	3.258654	1.834704
C	-2.335298	2.548305	2.983256
C	-2.204034	1.158942	2.605244
N	-1.872325	-1.714551	1.844275
C	-1.802852	-1.213446	3.132019
C	-1.578437	-2.293500	4.068983
C	-1.524774	-3.447532	3.344144
C	-1.713550	-3.085451	1.955906
O	-.416934	-.461662	-.018101
H	3.336871	4.098771	-.455133
H	3.942622	1.911870	-1.077981
H	2.588892	-.493756	.247128
H	2.717910	.368261	-2.681126
H	1.757119	-.951023	-2.007253
H	.243899	.390896	-.827347
H	.353187	1.121858	-2.470175
H	-.244330	3.317733	-2.029534
H	1.929116	5.838630	.562448
H	1.069675	4.664748	1.544840
H	4.249881	1.135823	1.869898
H	5.009065	2.484841	1.042789
H	6.370982	.983516	-.346959
H	4.052782	-1.043964	1.941288
H	1.225980	.795427	1.425022
H	.732863	2.441633	1.790890
H	7.047879	-1.163850	-1.188723
H	6.151490	-3.158686	-2.142856
H	5.627408	-3.777026	-.581162
H	3.490265	-2.812569	-.827547
H	3.923467	-2.333916	-2.468157
H	4.870140	-.252387	-1.756336
H	5.689978	-1.637944	2.231010
H	4.540235	-2.600357	1.276447
H	2.296649	1.855854	2.378956
H	3.389724	3.883041	1.295484
H	6.593257	.569830	1.354259
H	7.149185	-2.948942	1.017195
H	-4.791399	-1.510480	-.808377
H	-1.608518	-5.036881	1.139689
H	-2.476119	-1.691977	-4.239216
H	-2.832447	3.706756	-.819388
H	-1.877811	.364846	4.543007
H	-1.785717	-5.660048	-1.415509
H	-2.136634	-4.238462	-3.691671
H	-2.903404	.852516	-4.840935
H	-3.087673	3.129445	-3.387451

H	-2.673873	4.325814	1.716133
H	-2.273257	2.918402	3.998214
H	-1.486242	-2.168783	5.139925
H	-1.378455	-4.458348	3.701534

## Frequencies:

-840.6932	-3.9746	9.4350
13.8538	25.9292	34.5936
37.5992	53.4497	56.6286
58.2656	71.6911	86.7873
94.7030	101.5491	117.8664
119.3439	134.6944	148.8732
154.2707	156.5490	168.0066
187.3356	193.2785	207.5031
214.2301	219.8597	224.1735
227.0494	234.1153	238.8771
246.9676	267.2107	273.6508
277.9105	280.5512	282.8022
287.0661	287.9024	298.5932
302.0377	306.6309	316.2461
321.5660	332.2171	335.0042
362.5190	370.3859	372.4665
375.0467	380.7265	384.8466
400.3766	419.4286	423.2946
424.7434	436.1327	437.3386
440.2944	442.2727	450.4964
460.7621	472.5837	486.7139
508.2929	519.6384	527.1150
559.3421	561.8356	572.7895
576.9885	606.4229	622.8800
650.8416	661.0339	680.0873
680.9468	687.2156	690.6727
693.6854	705.1413	726.1646
727.6356	731.5102	737.3748
741.4937	762.8294	765.8243
767.2198	767.6204	801.0626
807.6443	817.6211	819.0359
824.7813	825.7509	827.8409
834.6625	835.2102	850.9003
852.9964	855.9957	860.5316
879.8314	907.5055	909.3484
921.5462	923.2472	926.5047
935.4375	938.0644	949.3251
952.9038	958.3737	958.8483
963.1282	965.2610	972.8199
980.0526	987.2275	996.9285
1009.5205	1021.6735	1026.7409
1027.4669	1030.7236	1036.8296
1038.8426	1040.7034	1050.3162
1055.0567	1062.3362	1063.5980
1064.0981	1069.2764	1078.1292
1080.9690	1087.4671	1102.7748
1121.6477	1121.9261	1124.3515
1127.9784	1129.8837	1138.0693
1151.0529	1171.4950	1173.4814
1176.8024	1182.8606	1193.6426
1196.6628	1203.0577	1217.0822
1221.7148	1237.3650	1244.1280
1249.2232	1251.2856	1258.4196
1268.9842	1281.4175	1294.5694
1297.4767	1301.0016	1302.7463
1308.3930	1322.1589	1327.1221
1329.3878	1334.5472	1344.4292
1347.1613	1354.2286	1355.1932
1359.0747	1364.3310	1374.9908
1380.1296	1389.3572	1391.5908
1392.4327	1396.2742	1399.8122
1401.8801	1410.6106	1415.6186
1416.5406	1419.4759	1422.1673
1426.5983	1432.4897	1437.6073
1438.8120	1440.6399	1454.5969

1464.3067	1501.5314	1503.4133
1506.9331	1511.2349	1530.5472
1531.3501	1535.3028	1537.3593
1540.4074	1541.4626	1546.3979
1551.4546	1557.5676	1560.9660
1563.3265	1565.5752	1593.5066
1595.4940	1617.0312	1619.6066
1620.3930	1643.1672	1644.8750
1652.8747	1715.7242	2521.2992
2948.3439	2959.5869	2979.0695
3011.1744	3023.9486	3032.4026
3033.6640	3038.1689	3043.2929
3044.2994	3050.8561	3051.4587
3064.0886	3067.6273	3069.2552
3083.1389	3085.7547	3087.9187
3088.3321	3092.4431	3101.7775
3107.9921	3119.8494	3132.5639
3139.8106	3194.1536	3198.8558
3200.8560	3200.9677	3209.1422
3245.4174	3245.7669	3247.1749
3248.7197	3268.5383	3269.1749
3270.2378	3271.7541	3661.0385

### III.D.2. Point P2

Absolute energy: -2476.5997139

Geometry:

C	.480950	3.382371	-1.225260
C	.521043	4.646523	-.511873
C	1.570602	4.801670	.574497
C	5.415140	-.872569	.211849
O	-.312691	5.557155	-.750626
C	2.734803	3.808871	.419066
C	2.277807	2.331344	.231153
C	3.521137	1.444602	-.168462
C	3.110389	-.003307	-.587207
C	2.146108	.050173	-1.786928
C	.989194	1.017687	-1.584098
C	1.238711	2.278590	-.903974
C	4.651074	1.457382	.900236
C	5.861236	.563745	.534685
C	4.373117	-.806271	-.937530
C	4.888555	-1.580580	1.482675
C	1.597250	1.818761	1.535577
C	6.490777	-1.769941	-.464592
C	5.667864	-2.871090	-1.202544
C	4.240652	-2.273341	-1.420974
O	7.528621	-2.285597	.409542
S	-4.546743	-.730211	.303046
Fe	-2.128203	-.668210	.163568
C	-1.747298	-3.986278	.904459
C	-2.419475	-1.441361	-3.184374
C	-2.714519	2.652763	-.588818
C	-1.955330	.117320	3.488920
N	-2.133509	-2.368553	-.912110
C	-1.934300	-3.649553	-.429255
C	-1.919765	-4.592314	-1.524905
C	-2.096065	-3.874600	-2.673842
C	-2.225459	-2.486092	-2.292744
N	-2.508592	.393077	-1.546461
C	-2.563175	-.105341	-2.837742
C	-2.809788	.973530	-3.770196
C	-2.903881	2.122931	-3.037220
C	-2.715167	1.758528	-1.649543
N	-2.341437	1.028790	1.235656
C	-2.546126	2.309589	.744004
C	-2.541070	3.259218	1.834877

C	-2.335278	2.548689	2.983602
C	-2.203938	1.158527	2.605459
N	-1.871754	-1.713948	1.843153
C	-1.802917	-1.212528	3.132471
C	-1.578382	-2.293789	4.069486
C	-1.524715	-3.447833	3.344625
C	-1.713590	-3.086058	1.955326
O	-.408210	-.455461	-.024007
H	3.337010	4.098843	-.454939
H	3.942565	1.911964	-1.077751
H	2.588942	-.493737	.246509
H	2.712214	.369867	-2.681398
H	1.756856	-.951684	-2.007465
H	.149374	.294618	-.730800
H	.334478	1.110511	-2.455693
H	-.246626	3.317880	-2.028834
H	1.928645	5.838286	.562353
H	1.069687	4.664843	1.544480
H	4.249909	1.135910	1.869511
H	5.008764	2.484542	1.042549
H	6.370908	.983268	-.346781
H	4.053088	-1.044234	1.941277
H	1.225608	.796027	1.425117
H	.732830	2.441131	1.790810
H	7.048678	-1.164202	-1.187707
H	6.151352	-3.158738	-2.142382
H	5.627604	-3.776556	-.581301
H	3.490448	-2.812395	-.827876
H	3.923545	-2.334238	-2.467859
H	4.870453	-.252338	-1.756061
H	5.690000	-1.637715	2.230378
H	4.540288	-2.599963	1.276432
H	2.296504	1.856417	2.378548
H	3.389208	3.882487	1.294864
H	6.592914	.569942	1.354001
H	7.149312	-2.949485	1.017807
H	-4.790005	-1.511315	-.808995
H	-1.608494	-5.037044	1.139723
H	-2.476512	-1.692220	-4.239363
H	-2.833624	3.706815	-.819280
H	-1.877956	.364776	4.543223
H	-1.785808	-5.659873	-1.414991
H	-2.136776	-4.238051	-3.691754
H	-2.903725	.851957	-4.840838
H	-3.088337	3.129528	-3.387024
H	-2.674354	4.325702	1.715797
H	-2.273415	2.917795	3.998333
H	-1.486371	-2.168393	5.139799
H	-1.378594	-4.458403	3.701085

## Frequencies:

-1535.5630	9.3627	13.5802
19.0626	34.3505	36.9025
42.4765	54.3119	57.9126
58.8322	71.0733	95.6295
102.6298	104.7148	116.1042
134.1215	138.2798	147.1092
154.4898	157.2669	167.8692
187.0022	199.6462	209.1456
213.0226	214.5652	221.3482
225.0581	231.7107	234.3636
246.2739	267.9872	272.3025
272.8101	279.1006	284.6211
288.2997	289.6139	298.3697
301.9573	313.1382	318.1296
325.1560	331.7317	334.8415
364.4633	366.6779	372.8851
373.8614	380.0333	384.5012
399.4076	418.7792	424.1622
426.0537	437.0081	437.3117
439.5174	442.7076	443.2661



462.7372	476.5051	487.0759
507.1566	519.8329	536.7419
560.6966	561.7337	578.0208
585.9535	620.2112	632.9110
659.1338	669.7370	680.4551
681.8565	683.7832	691.6768
697.9843	704.1576	722.1841
726.3926	729.8839	731.4777
736.5893	738.4961	762.0711
765.7274	766.9100	767.1873
802.1147	803.2909	814.2408
815.6407	824.6077	828.1207
831.1008	833.2094	834.2452
850.3407	852.2285	855.2424
863.0771	885.8179	901.7819
902.4736	914.4883	916.7601
930.6136	934.0636	936.4208
945.3865	952.6426	954.0840
954.4352	959.1275	968.4290
974.8588	985.1301	993.7624
1002.5598	1020.5155	1022.3013
1024.6832	1026.0244	1032.8305
1035.1351	1038.6421	1049.0890
1049.9633	1061.7536	1062.2242
1063.0464	1063.6636	1075.2350
1080.8117	1085.9032	1099.3324
1106.5366	1119.5318	1119.9011
1122.1523	1125.1031	1128.8208
1142.4052	1151.2497	1172.0748
1175.7334	1179.5650	1192.7769
1193.8962	1195.4934	1199.6609
1211.1303	1219.2625	1226.4195
1243.8861	1246.7951	1252.6780
1261.8037	1269.6249	1277.4701
1291.2366	1295.8849	1296.9056
1299.5472	1308.1256	1315.9931
1322.6413	1332.8533	1338.4081
1346.6099	1352.4758	1357.2743
1357.4701	1359.0066	1363.6992
1377.5203	1379.8778	1389.1980
1390.3949	1391.2352	1395.9358
1399.0752	1401.4969	1410.3044
1414.9667	1417.5353	1420.9756
1427.9345	1432.4405	1432.9598
1438.1089	1439.8591	1454.3284
1464.6657	1501.9526	1503.8988
1507.1769	1510.6311	1520.9213
1530.3394	1534.4595	1536.9461
1540.5191	1542.2056	1545.7877
1551.2645	1555.2894	1558.9614
1560.5757	1563.1298	1565.3100
1594.3705	1596.1871	1619.0259
1632.1466	1637.7165	1643.3510
1644.7701	1714.7361	2515.1782
2949.0157	2960.3569	2967.9586
3014.2693	3026.7642	3036.8645
3038.0670	3042.1334	3047.4571
3050.3922	3054.9870	3055.8166
3068.5553	3071.7885	3074.2134
3088.5311	3089.9013	3092.6488
3097.9494	3106.2292	3112.3070
3113.5113	3124.1063	3136.5039
3144.2329	3202.9405	3203.7609
3205.1492	3205.2944	3213.1712
3250.3326	3250.6705	3251.8048
3253.4518	3273.5635	3274.1941
3274.9227	3276.5346	3651.3361

## III.D.3. Point P3

Absolute energy: -2476.6018907

Geometry:

C	.484035	3.381179	-1.224606
C	.520183	4.646479	-.512187
C	1.570710	4.801743	.574411
C	5.415214	-.872650	.211793
O	-.312483	5.557065	-.750267
C	2.734955	3.808941	.419614
C	2.277406	2.332135	.230925
C	3.521003	1.444460	-.168548
C	3.110097	-.003236	-.587562
C	2.150338	.051965	-1.791297
C	.979330	1.006939	-1.579757
C	1.240501	2.288941	-.904786
C	4.651033	1.457460	.900202
C	5.861204	.563725	.534715
C	4.373117	-.806229	-.937246
C	4.888610	-1.580584	1.482693
C	1.597179	1.818598	1.535496
C	6.490798	-1.769874	-.464567
C	5.667896	-2.871135	-1.202510
C	4.240735	-2.273264	-1.420928
O	7.528631	-2.285628	.409527
S	-4.548172	-.730299	.303079
Fe	-2.124527	-.667429	.162830
C	-1.747582	-3.985567	.904079
C	-2.419457	-1.440594	-3.183700
C	-2.714235	2.651999	-.588946
C	-1.955653	.117719	3.488007
N	-2.133679	-2.368514	-.912559
C	-1.934312	-3.649690	-.429943
C	-1.919770	-4.592330	-1.524857
C	-2.096069	-3.874532	-2.673744
C	-2.225264	-2.486761	-2.291874
N	-2.510648	.392430	-1.545257
C	-2.563574	-.105308	-2.838055
C	-2.809813	.973648	-3.769988
C	-2.903918	2.122627	-3.037208
C	-2.715445	1.758508	-1.649737
N	-2.341910	1.028698	1.235073
C	-2.545977	2.309203	.744691
C	-2.541114	3.259051	1.835007
C	-2.335340	2.548774	2.983557
C	-2.204059	1.159019	2.605606
N	-1.872465	-1.714425	1.844211
C	-1.802811	-1.213697	3.132039
C	-1.578338	-2.293700	4.069428
C	-1.524671	-3.447858	3.344524
C	-1.713485	-3.085493	1.956110
O	-.424637	-.467023	-.012946
H	3.336458	4.098272	-.454836
H	3.942226	1.911655	-1.077881
H	2.588776	-.493391	.246754
H	2.722444	.366961	-2.680982
H	1.757859	-.949805	-2.007273
H	.274536	.427040	-.862044
H	.368002	1.130948	-2.480774
H	-.241981	3.317663	-2.030012
H	1.928669	5.838360	.562433
H	1.069674	4.664846	1.544421
H	4.250061	1.135948	1.869606
H	5.008893	2.484478	1.042814
H	6.370733	.983213	-.346770
H	4.053178	-1.044025	1.940866
H	1.226200	.795803	1.424389
H	.733457	2.441721	1.790526

H	7.048271	-1.164175	-1.187875
H	6.151384	-3.158700	-2.142323
H	5.627811	-3.776681	-.581309
H	3.490499	-2.812338	-.827866
H	3.923401	-2.333726	-2.467548
H	4.869964	-.252430	-1.755912
H	5.689862	-1.637854	2.230609
H	4.540342	-2.599962	1.276349
H	2.296656	1.855484	2.378388
H	3.389719	3.883292	1.295344
H	6.593025	.569914	1.353947
H	7.148777	-2.949507	1.017847
H	-4.792851	-1.510819	-.809159
H	-1.608689	-5.036286	1.139536
H	-2.475717	-1.691702	-4.238635
H	-2.831126	3.706274	-.819343
H	-1.877766	.364802	4.542355
H	-1.785774	-5.659662	-1.415430
H	-2.136606	-4.238110	-3.691319
H	-2.903034	.852510	-4.840458
H	-3.087121	3.129077	-3.387118
H	-2.673486	4.325341	1.715880
H	-2.273218	2.918208	3.997855
H	-1.486181	-2.168586	5.139475
H	-1.378395	-4.458033	3.701199

## Frequencies:

-139.0975	-18.9883	-6.2699
10.1124	17.7458	33.4221
34.7360	53.5223	55.5452
56.8665	78.5872	87.1644
93.2046	100.0699	119.7875
129.9281	131.4877	151.9533
153.2336	159.3383	180.9221
183.4727	192.7350	206.1915
212.6272	219.6204	221.4082
227.2674	234.5551	242.0818
260.4100	268.4813	275.6551
276.9288	282.2112	284.5673
286.8956	289.8919	297.7130
309.6539	312.9918	318.0874
321.8446	331.5408	334.5016
361.7560	372.1923	373.9645
375.8276	380.2425	385.1594
399.5233	420.1507	422.0869
424.5825	435.5024	437.0552
440.0221	441.4929	448.2537
470.1563	471.5676	486.1320
509.6892	518.9704	548.7942
557.6330	562.3575	573.8067
576.6477	591.7555	621.7403
647.6402	660.6826	679.1799
679.9272	686.9835	690.1611
691.7196	702.6487	725.1455
726.5393	730.6488	736.5262
740.7738	762.3121	764.9755
766.6009	767.0705	799.5891
805.4251	815.1652	816.4249
823.1716	824.3010	825.1521
834.6139	835.1532	850.0610
852.7144	854.5311	858.4189
882.3791	906.2503	908.0102
920.3917	922.2613	930.9338
934.9666	937.6093	946.4831
953.3578	956.2541	956.7616
962.2454	968.2666	975.1728
985.9173	993.4271	1003.5081
1019.7016	1026.1016	1026.3325
1027.9448	1029.0632	1036.1581
1039.0187	1049.4482	1051.4042
1060.8216	1062.1904	1063.2809

1065.2715	1077.4123	1079.7969
1087.3237	1101.9399	1119.9130
1120.2401	1122.6835	1126.3154
1129.3992	1137.8794	1150.4043
1165.5551	1170.3844	1176.0587
1183.2063	1191.4915	1194.5090
1201.0567	1214.5468	1220.3776
1235.6054	1241.5881	1244.7609
1247.9695	1257.9278	1266.3939
1280.7744	1291.4212	1295.9156
1300.0805	1301.7748	1307.4149
1320.8920	1321.0270	1326.9867
1332.4312	1337.0808	1346.3407
1351.2929	1352.6513	1358.1951
1364.0274	1377.0818	1379.1112
1389.3334	1389.5919	1391.3499
1395.2836	1399.0550	1401.3885
1409.8541	1414.8452	1416.2980
1419.4694	1424.1489	1427.4417
1430.7110	1433.7225	1437.1117
1438.2320	1453.4651	1462.5201
1500.4341	1502.1711	1505.6891
1510.6798	1530.1045	1532.4753
1534.6603	1536.9000	1538.5701
1540.8979	1545.8184	1550.9410
1557.1023	1560.1864	1562.8784
1565.1104	1591.6711	1593.7424
1600.6481	1614.1026	1616.6359
1642.5819	1644.6138	1655.5368
1715.7749	1891.1296	2514.5729
2951.1594	2962.4048	2987.7780
3014.5655	3027.8251	3035.4304
3037.3099	3041.7173	3046.3542
3047.0412	3054.8852	3055.2232
3068.1176	3072.2038	3072.8974
3084.1145	3086.9203	3090.8426
3092.0707	3096.2255	3105.7197
3112.6823	3124.1677	3137.1066
3144.1311	3198.1717	3204.6859
3206.6737	3206.7696	3215.1400
3253.5411	3253.9246	3255.4272
3256.9170	3276.5505	3277.2163
3278.4132	3279.8862	3647.9035

### III.D.4. Point P4

Absolute energy: -2476.6019326

Geometry:

C	.480233	3.382528	-1.225646
C	.521432	4.646625	-.511553
C	1.570600	4.801702	.574536
C	5.415140	-.872505	.211857
O	-.312920	5.557361	-.750726
C	2.734857	3.808904	.419005
C	2.277922	2.331274	.231204
C	3.521190	1.444621	-.168437
C	3.110459	-.003339	-.587170
C	2.145344	.049807	-1.786159
C	.992468	1.021092	-1.586337
C	1.238609	2.276360	-.903934
C	4.651085	1.457418	.900296
C	5.861305	.563756	.534697
C	4.373099	-.806276	-.937577
C	4.888520	-1.580629	1.482739
C	1.597219	1.818752	1.535680

C	6.490634	-1.769933	-.464688
C	5.667848	-2.871123	-1.202599
C	4.240592	-2.273399	-1.421028
O	7.528742	-2.285550	.409526
S	-4.546425	-.730186	.303080
Fe	-2.129048	-.668361	.163713
C	-1.747217	-3.986637	.904571
C	-2.419483	-1.441551	-3.184724
C	-2.714622	2.653122	-.588841
C	-1.955253	.117302	3.489313
N	-2.133361	-2.368147	-.911780
C	-1.934268	-3.649696	-.428890
C	-1.919730	-4.592689	-1.525093
C	-2.096046	-3.874932	-2.674121
C	-2.225530	-2.485840	-2.293153
N	-2.507902	.392946	-1.546294
C	-2.563093	-.105590	-2.837869
C	-2.809846	.973673	-3.770595
C	-2.903940	2.123239	-3.037528
C	-2.715167	1.758806	-1.649351
N	-2.341153	1.028387	1.235512
C	-2.546223	2.309835	.743627
C	-2.541087	3.259623	1.835028
C	-2.335274	2.548995	2.983871
C	-2.203887	1.158299	2.605690
N	-1.871532	-1.713602	1.842545
C	-1.802952	-1.212083	3.132718
C	-1.578331	-2.293965	4.069870
C	-1.524659	-3.448088	3.344955
C	-1.713604	-3.086402	1.955050
O	-.406047	-.454151	-.025258
H	3.336830	4.098663	-.454605
H	3.942345	1.911900	-1.077499
H	2.589072	-.493557	.246027
H	2.710305	.370157	-2.681205
H	1.756827	-.951471	-2.007402
H	.118919	.266491	-.701800
H	.328368	1.106728	-2.450380
H	-.247078	3.318060	-2.028366
H	1.928180	5.837788	.562279
H	1.069765	4.664943	1.544022
H	4.250043	1.136043	1.869058
H	5.008483	2.484061	1.042402
H	6.370712	.982977	-.346498
H	4.053536	-1.044512	1.941034
H	1.225631	.796669	1.424983
H	.733163	2.440767	1.790554
H	7.049154	-1.164631	-1.186731
H	6.151130	-3.158704	-2.141750
H	5.627842	-3.776067	-.581544
H	3.490753	-2.812127	-.828264
H	3.923643	-2.334344	-2.467259
H	4.870502	-.252382	-1.755701
H	5.689835	-1.637548	2.229782
H	4.540409	-2.599455	1.276418
H	2.296297	1.856631	2.378035
H	3.388793	3.882231	1.294320
H	6.592522	.570019	1.353619
H	7.149036	-2.950291	1.018587
H	-4.789629	-1.512069	-.809798
H	-1.608558	-5.036635	1.139621
H	-2.476602	-1.692192	-4.238943
H	-2.833860	3.706365	-.819130
H	-1.878029	.364647	4.542826
H	-1.785922	-5.659207	-1.414700
H	-2.136831	-4.237542	-3.691280
H	-2.903754	.851661	-4.840191
H	-3.088454	3.129050	-3.386497
H	-2.674435	4.325044	1.715560
H	-2.273493	2.917213	3.997870
H	-1.486462	-2.168147	5.139145

H	-1.378713	-4.457921	3.700559
Frequencies:			
-975.3675	8.0674	13.2353	
18.4498	33.1477	35.8263	
41.6434	53.3638	57.3128	
58.4957	70.3788	94.8609	
102.6938	105.7101	114.9305	
131.6786	140.0773	153.8135	
156.9129	159.6010	165.4616	
183.3921	198.4536	208.3006	
210.7771	211.9109	221.3524	
222.7432	229.6378	234.1827	
244.8477	265.6961	270.3429	
271.4271	279.4024	284.9345	
288.4285	289.9356	297.8612	
301.8231	315.3603	325.1514	
327.9658	330.9828	337.9902	
364.4639	365.3263	372.8480	
373.6038	379.2404	384.3448	
398.3011	418.5344	424.8549	
426.7456	436.9377	437.1170	
440.9623	442.2626	443.1215	
462.5249	477.3232	486.7762	
508.8141	519.3743	554.9712	
559.8276	569.8086	585.7622	
594.3385	620.4359	635.6409	
664.8032	670.2694	679.3863	
681.2914	681.7075	691.7395	
698.6628	704.1572	722.0703	
724.8976	728.1092	730.7269	
735.6167	737.2298	761.2541	
765.1194	766.2817	766.9528	
798.8741	801.9540	810.2569	
811.6583	820.6711	826.5330	
832.0183	832.5248	833.8372	
849.3975	851.6511	853.7930	
861.0909	885.5624	897.2801	
899.1875	909.7193	912.1204	
926.1497	932.4377	936.1993	
941.0220	949.7982	950.0350	
951.1977	954.9503	966.3070	
974.3419	984.0904	993.7022	
999.6491	1011.6072	1018.0984	
1022.1195	1024.1920	1031.9727	
1034.1767	1035.4650	1039.1380	
1049.3766	1053.5722	1061.4562	
1062.0567	1062.6434	1064.6758	
1077.7016	1080.3902	1086.8545	
1100.7914	1117.1056	1117.2243	
1119.6193	1122.1479	1127.2770	
1139.7512	1151.1480	1169.9070	
1175.0285	1178.9547	1179.9278	
1191.1982	1193.4743	1197.7778	
1206.7325	1217.4644	1220.9706	
1243.2529	1244.7874	1251.6045	
1260.7020	1269.2146	1276.5300	
1294.6079	1295.2633	1296.8574	
1307.4914	1314.5158	1321.2299	
1328.0185	1335.9921	1345.4325	
1352.1216	1355.5788	1357.3177	
1358.3650	1359.5144	1365.3070	
1378.9246	1382.0482	1388.6841	
1389.6091	1392.3494	1395.2200	
1398.5420	1401.1380	1409.9789	
1413.0491	1416.8341	1420.7488	
1427.6470	1431.3148	1433.0516	
1437.9161	1439.3556	1453.3284	
1463.7305	1501.8027	1503.2957	
1506.4865	1509.9343	1518.0893	
1529.8158	1533.8039	1536.2684	

1539.3304	1542.1242	1544.5888
1550.4503	1550.9941	1556.7661
1559.1773	1562.5959	1564.7973
1593.8862	1595.7137	1618.7502
1624.9463	1641.7290	1642.9958
1646.3187	1714.3706	2507.6358
2951.5933	2962.4498	2967.8369
3018.5654	3031.3402	3041.5997
3043.2905	3047.0799	3052.5642
3055.5666	3060.3414	3061.0842
3074.1496	3077.6710	3079.9881
3094.3120	3096.0525	3098.3927
3103.9564	3111.6739	3118.3113
3124.2557	3129.6083	3142.1489
3150.1103	3210.0351	3211.9099
3212.3188	3212.5006	3220.3504
3259.6869	3260.0423	3261.1049
3262.8023	3282.8729	3283.5199
3284.1780	3285.8381	3635.5205

### III.D.5. Point P5

Absolute energy: -2476.6046678

Geometry:

C	.487295	3.384318	-1.224015
C	.519040	4.645961	-.513041
C	1.570605	4.801778	.574341
C	5.415367	-.872951	.211826
O	-.312014	5.556430	-.749743
C	2.735334	3.809278	.420713
C	2.277437	2.333476	.230811
C	3.520691	1.444607	-.168659
C	3.109981	-.002895	-.588158
C	2.156569	.054563	-1.796682
C	.982134	1.008559	-1.588190
C	1.245493	2.298206	-.907395
C	4.650908	1.457375	.900042
C	5.860998	.563684	.534692
C	4.373323	-.806185	-.936682
C	4.888715	-1.580469	1.482578
C	1.597142	1.818641	1.534650
C	6.491401	-1.769802	-.464342
C	5.668081	-2.871152	-1.202265
C	4.240964	-2.272978	-1.420617
O	7.528113	-2.285673	.409414
S	-4.550968	-.730516	.303113
Fe	-2.118585	-.666263	.161731
C	-1.748101	-3.983339	.903251
C	-2.419379	-1.439632	-3.181605
C	-2.713748	2.649879	-.588694
C	-1.956147	.117748	3.485607
N	-2.134736	-2.370355	-.914414
C	-1.934452	-3.648971	-.431108
C	-1.919907	-4.590835	-1.524010
C	-2.096122	-3.873039	-2.672529
C	-2.225051	-2.487379	-2.290024
N	-2.515074	.392162	-1.544960
C	-2.564542	-.104922	-2.837187
C	-2.809464	.972701	-3.767956
C	-2.903516	2.121151	-3.035400
C	-2.715967	1.757390	-1.649701
N	-2.343343	1.030258	1.235446
C	-2.545696	2.307891	.745722
C	-2.541013	3.257170	1.834235
C	-2.335393	2.547402	2.982483

C	-2.204388	1.159590	2.604675
N	-1.875482	-1.716614	1.847863
C	-1.803131	-1.215369	3.131027
C	-1.578418	-2.292690	4.067844
C	-1.524745	-3.446919	3.342934
C	-1.713787	-3.084029	1.957117
O	-.447020	-.485022	.004503
H	3.336933	4.098902	-.454558
H	3.942762	1.911712	-1.078244
H	2.586719	-.493458	.245741
H	2.735204	.366134	-2.683318
H	1.762371	-.947994	-2.011639
H	.285192	.468423	-.907989
H	.405460	1.153591	-2.510484
H	-.237433	3.318135	-2.031722
H	1.929764	5.839011	.562368
H	1.069867	4.665050	1.545361
H	4.249949	1.135785	1.870329
H	5.009470	2.485053	1.043137
H	6.370918	.983895	-.347096
H	4.052370	-1.043552	1.940858
H	1.226545	.794701	1.423414
H	.732989	2.442061	1.791309
H	7.046191	-1.163360	-1.190536
H	6.151580	-3.158421	-2.143374
H	5.627059	-3.777724	-.581175
H	3.490237	-2.812706	-.827126
H	3.923515	-2.332985	-2.468269
H	4.869743	-.252526	-1.756339
H	5.689444	-1.638311	2.232245
H	4.540219	-2.600742	1.276593
H	2.296491	1.853779	2.378878
H	3.390860	3.885207	1.297013
H	6.593617	.569664	1.354428
H	7.148343	-2.948330	1.016365
H	-4.797492	-1.508972	-.807619
H	-1.608706	-5.035059	1.139089
H	-2.474402	-1.690930	-4.237651
H	-2.828226	3.705452	-.819515
H	-1.877284	.364996	4.540980
H	-1.785595	-5.659651	-1.416468
H	-2.136334	-4.238591	-3.690793
H	-2.901878	.853631	-4.840051
H	-3.085204	3.128458	-3.387677
H	-2.672491	4.325063	1.716510
H	-2.272824	2.919333	3.997236
H	-1.485589	-2.169179	5.139333
H	-1.377751	-4.457617	3.701803

## Frequencies:

-31.0224	-18.5667	-10.8794
8.6175	28.9805	32.6437
47.1572	51.8911	53.1985
56.4791	62.9229	86.1705
96.2325	104.9488	109.8043
128.4372	129.4170	149.5618
151.1171	159.2108	178.3529
187.7385	196.9107	210.0867
215.0685	218.4259	221.7313
228.8843	233.7985	235.2970
262.0159	266.4050	275.6605
276.4427	280.7460	282.0066
286.3310	296.8046	297.6471
302.3115	306.3301	315.0543
327.5660	334.0876	346.7235
361.3135	372.2854	375.8454
379.7244	381.7032	386.0637
401.0596	419.8256	419.8998
423.6809	435.4158	437.1935
440.7196	441.4742	444.1039
469.7561	478.0576	486.2111



509.4582	518.8430	551.1252
557.4996	561.6991	576.7618
583.4335	622.8873	646.3048
660.9353	679.3893	680.1078
683.3489	689.5655	691.0132
697.8439	700.4968	727.1005
728.4725	731.9798	738.1605
743.7905	763.9839	765.9556
768.7881	769.3998	800.4937
810.7554	820.3270	821.3622
823.1514	823.3810	830.4660
835.9247	836.5857	851.7202
853.8644	856.7394	857.7767
882.6851	909.1342	914.0655
926.3008	928.3039	930.5111
936.4209	943.3119	952.5064
954.2550	961.6997	962.7686
968.2250	969.0353	976.6131
987.2969	994.7993	1004.2648
1022.4030	1030.7380	1031.3909
1031.4288	1032.8455	1039.3595
1041.6640	1049.9548	1052.4301
1064.5268	1064.9881	1066.3898
1067.4617	1078.0001	1083.9356
1087.5791	1102.9920	1123.6407
1123.9270	1126.3209	1130.0766
1130.5188	1138.2308	1149.8284
1169.6940	1171.7648	1176.9470
1184.2772	1197.9555	1200.4927
1200.9831	1214.6843	1225.9072
1239.2364	1243.5262	1247.8204
1252.6945	1259.2595	1268.7912
1283.9624	1295.8471	1301.9732
1306.3653	1307.6535	1308.4444
1318.0914	1322.8111	1334.9036
1335.2608	1340.6027	1347.7715
1354.4386	1356.0219	1359.3972
1365.6622	1378.7000	1380.3642
1390.6590	1395.5577	1396.5707
1398.0122	1400.3807	1403.4038
1411.4147	1417.3932	1419.2259
1420.7703	1428.1618	1432.7600
1434.8531	1437.7226	1442.2778
1455.0054	1458.6166	1470.2133
1502.5666	1505.0162	1507.8673
1511.6410	1530.8694	1535.3350
1536.2060	1537.6864	1541.3854
1541.6247	1546.5485	1551.6972
1557.5639	1562.6787	1563.6017
1565.8775	1594.6768	1596.5307
1611.9486	1618.6832	1639.6464
1644.2259	1646.3756	1670.4552
1717.5181	2528.5808	2577.7057
2946.7923	2957.9734	2988.0867
3007.9587	3020.5285	3028.1241
3029.4809	3034.3161	3038.5641
3039.3285	3046.7595	3047.3444
3059.6809	3062.6791	3063.7383
3067.5792	3078.0361	3081.6551
3083.4279	3087.4360	3097.4370
3103.7563	3115.6346	3128.5579
3134.8785	3187.2574	3195.0312
3196.6074	3196.7290	3205.1627
3241.2755	3241.6965	3243.2223
3244.6544	3264.3198	3264.9822
3266.2441	3267.6466	3670.0306

## III.D.6. Point P6

Absolute energy: -2476.6052307

Geometry:

C	.479269	3.383235	-1.225702
C	.521683	4.646414	-.511547
C	1.570553	4.801650	.574552
C	5.415129	-.872498	.211871
O	-.312993	5.557377	-.750853
C	2.734813	3.808864	.418868
C	2.278066	2.331041	.231258
C	3.521217	1.444685	-.168397
C	3.110565	-.003351	-.587061
C	2.144152	.049367	-1.784928
C	.998018	1.026726	-1.590006
C	1.238327	2.273231	-.903932
C	4.651097	1.457373	.900289
C	5.861300	.563757	.534685
C	4.373111	-.806288	-.937641
C	4.888504	-1.580620	1.482721
C	1.597280	1.818840	1.535663
C	6.490671	-1.769952	-.464679
C	5.667848	-2.871112	-1.202590
C	4.240587	-2.273402	-1.421021
O	7.528684	-2.285536	.409521
S	-4.545960	-.730202	.303107
Fe	-2.129972	-.668530	.163874
C	-1.747144	-3.986752	.904612
C	-2.419499	-1.441735	-3.184813
C	-2.714771	2.653197	-.588774
C	-1.955169	.117190	3.489471
N	-2.133454	-2.368324	-.911793
C	-1.934260	-3.649593	-.428643
C	-1.919742	-4.592509	-1.525006
C	-2.096053	-3.874785	-2.674029
C	-2.225595	-2.485594	-2.293316
N	-2.507370	.393135	-1.546708
C	-2.562981	-.105655	-2.837710
C	-2.809808	.973522	-3.770451
C	-2.903894	2.123199	-3.037333
C	-2.715078	1.758797	-1.649208
N	-2.341100	1.028521	1.235765
C	-2.546277	2.309881	.743379
C	-2.541065	3.259486	1.834890
C	-2.335254	2.548798	2.983763
C	-2.203840	1.158099	2.605609
N	-1.871613	-1.713651	1.842518
C	-1.803026	-1.211747	3.132781
C	-1.578373	-2.293836	4.069705
C	-1.524698	-3.447978	3.344767
C	-1.713679	-3.086477	1.954793
O	-.403117	-.452879	-.026499
H	3.337000	4.098855	-.454678
H	3.942437	1.912014	-1.077482
H	2.589122	-.493691	.246065
H	2.707688	.370385	-2.681360
H	1.756248	-.952003	-2.007362
H	.076949	.232310	-.665367
H	.318521	1.100593	-2.442691
H	-.248561	3.318274	-2.028029
H	1.928271	5.837799	.562220
H	1.069811	4.664948	1.544151
H	4.249984	1.136011	1.869103
H	5.008481	2.484131	1.042346
H	6.370786	.983041	-.346536
H	4.053433	-1.044535	1.941165
H	1.225635	.796635	1.425095
H	.732889	2.440615	1.790619

H	7.049133	-1.164575	-1.186885
H	6.151140	-3.158701	-2.141862
H	5.627726	-3.776134	-.581536
H	3.490706	-2.812183	-.828200
H	3.923691	-2.334468	-2.467422
H	4.870601	-.252343	-1.755800
H	5.689862	-1.637536	2.229832
H	4.540378	-2.599535	1.276447
H	2.296164	1.856818	2.378281
H	3.388736	3.882106	1.294270
H	6.592554	.569994	1.353679
H	7.149179	-2.950209	1.018392
H	-4.788612	-1.512265	-.809532
H	-1.608484	-5.036816	1.139648
H	-2.476818	-1.692307	-4.239113
H	-2.834524	3.706463	-.819120
H	-1.878045	.364655	4.543030
H	-1.785908	-5.659217	-1.414563
H	-2.136877	-4.237480	-3.691373
H	-2.903931	.851465	-4.840230
H	-3.088745	3.129146	-3.386393
H	-2.674641	4.325103	1.715514
H	-2.273495	2.917063	3.997963
H	-1.486480	-2.168049	5.139188
H	-1.378728	-4.457994	3.700463

## Frequencies:

-180.8015	5.3902	12.3854
16.8651	31.3782	33.9694
39.5297	52.3528	58.1871
58.9772	71.1188	100.3874
106.7943	113.8534	120.0501
129.0395	136.0998	154.7923
156.1502	162.6088	166.2081
181.9365	196.3550	209.8553
211.3312	217.9591	219.2978
227.1405	233.3861	241.7241
247.8350	266.3666	270.9883
273.7441	283.5531	285.2853
288.4234	294.6603	297.9403
300.9779	315.5843	320.4687
326.9537	334.6996	337.2707
363.6416	365.6630	372.9358
373.5142	379.6451	385.3690
398.1123	416.9332	420.2584
427.7619	437.2014	437.6017
442.0667	442.8495	449.7720
462.9359	478.7855	486.6696
511.0321	519.0629	555.0861
560.1817	575.0949	596.0555
617.5182	628.0807	647.7878
653.7296	678.2433	681.1632
681.5912	691.9463	697.8067
700.3276	716.0731	722.2035
724.8528	730.7164	732.9529
736.8674	749.3834	760.9861
765.0306	766.2071	771.0361
798.4610	806.3653	810.4896
811.9039	821.1494	829.4604
832.0411	833.0383	834.1909
849.0443	851.3938	853.9134
859.9047	884.9927	893.1764
895.9712	908.2619	910.6398
911.4964	924.3924	928.4920
936.2899	941.5826	949.8996
950.1367	951.0653	954.8871
961.0611	975.0191	980.9064
990.9199	998.7923	1011.3534
1017.7948	1021.8717	1023.2443
1032.2480	1035.4501	1038.1044
1046.5556	1049.6839	1060.1634

1062.3336	1062.6629	1062.9728
1076.9295	1081.0716	1086.3617
1098.7925	1117.3659	1117.4380
1119.7732	1121.8036	1126.2332
1139.0469	1151.4216	1165.4376
1175.0741	1176.4331	1183.0990
1192.1267	1194.0186	1197.4791
1206.4018	1217.3241	1222.1092
1243.6133	1244.8508	1252.3075
1261.1617	1269.7022	1276.2331
1293.8002	1295.5366	1296.0705
1307.8155	1315.1250	1321.7511
1332.0366	1338.0792	1345.9365
1356.9845	1358.4900	1358.5515
1361.9550	1367.2266	1375.1393
1379.4699	1385.1023	1389.6020
1390.1028	1395.3424	1398.5420
1401.3653	1409.2215	1413.6533
1417.1290	1420.9399	1429.2893
1431.6448	1431.9752	1438.1420
1440.1573	1453.6532	1464.0876
1500.6947	1503.8533	1506.0228
1507.0753	1515.5028	1516.3787
1529.9746	1534.3095	1536.7897
1541.0131	1543.3727	1546.1028
1550.8927	1556.4476	1559.1540
1562.6780	1564.9109	1594.3024
1596.0494	1618.0197	1619.2042
1642.3784	1643.0804	1652.6605
1714.1876	2107.6417	2508.6969
2950.6963	2958.8480	2964.9942
3017.8616	3030.3110	3041.1125
3042.6912	3046.4217	3051.8910
3055.4042	3059.5422	3060.4462
3073.4048	3076.6613	3079.0866
3093.7185	3094.8769	3097.5723
3103.4451	3110.9724	3117.3326
3128.5348	3129.2753	3141.1617
3149.3281	3209.0723	3211.3829
3211.5339	3211.6177	3219.1747
3257.7731	3258.1286	3259.1006
3260.8061	3280.9934	3281.6282
3282.1823	3283.8472	3638.6980

### III.D.7. Point P7

Absolute energy: -2476.6075111

Geometry:

C	.496253	3.392684	-1.227674
C	.519257	4.648201	-.512749
C	1.570710	4.803325	.575693
C	5.415917	-.873337	.212520
O	-.312916	5.556901	-.747542
C	2.737169	3.811821	.424222
C	2.279677	2.336646	.229968
C	3.521498	1.445737	-.168408
C	3.110667	-.001084	-.590746
C	2.171804	.062162	-1.809487
C	.994122	1.018528	-1.614327
C	1.256849	2.309292	-.915436
C	4.650996	1.457272	.900296
C	5.860940	.563664	.534928
C	4.374219	-.806120	-.935128
C	4.888851	-1.580434	1.482848
C	1.596186	1.818710	1.530877

C	6.492158	-1.769732	-.464087
C	5.668388	-2.871164	-1.201895
C	4.241358	-2.272442	-1.419859
O	7.527631	-2.285809	.409175
S	-4.560382	-.730733	.303060
Fe	-2.113994	-.665895	.161312
C	-1.749095	-3.980339	.902163
C	-2.419336	-1.438927	-3.179053
C	-2.712649	2.647567	-.588158
C	-1.957199	.117617	3.482643
N	-2.136592	-2.372153	-.916779
C	-1.934882	-3.648078	-.432157
C	-1.920027	-4.589681	-1.523340
C	-2.095945	-3.871926	-2.671604
C	-2.224915	-2.487968	-2.288740
N	-2.523026	.390213	-1.542387
C	-2.567775	-.105920	-2.834803
C	-2.808850	.970902	-3.764524
C	-2.902540	2.118970	-3.032151
C	-2.718161	1.755593	-1.647915
N	-2.344769	1.031650	1.235274
C	-2.545165	2.306613	.746244
C	-2.540716	3.255204	1.833335
C	-2.335674	2.545924	2.981397
C	-2.205164	1.159644	2.603424
N	-1.885395	-1.720048	1.853230
C	-1.805863	-1.217161	3.131139
C	-1.577628	-2.291940	4.067025
C	-1.523879	-3.446368	3.341924
C	-1.716289	-3.083264	1.958591
O	-.466545	-.519382	.038766
H	3.340380	4.102943	-.449791
H	3.945394	1.912928	-1.077342
H	2.579622	-.492400	.238081
H	2.763487	.373379	-2.687465
H	1.778061	-.939468	-2.031353
H	.271714	.490828	-.980243
H	.467192	1.194217	-2.561936
H	-.225191	3.326565	-2.038961
H	1.930467	5.840709	.563755
H	1.069974	4.666944	1.547017
H	4.249908	1.135626	1.870837
H	5.010136	2.485028	1.043924
H	6.370791	.984250	-.347042
H	4.051549	-1.043384	1.940005
H	1.225344	.794865	1.416353
H	.732356	2.442261	1.789558
H	7.044630	-1.162919	-1.192258
H	6.151506	-3.157985	-2.143755
H	5.626588	-3.778354	-.581261
H	3.490281	-2.812654	-.826698
H	3.924175	-2.331562	-2.467987
H	4.871450	-.253259	-1.755086
H	5.688333	-1.638374	2.234292
H	4.540515	-2.601108	1.277090
H	2.294458	1.849558	2.376611
H	3.391090	3.888363	1.302153
H	6.594030	.569821	1.354664
H	7.147306	-2.947676	1.015849
H	-4.811996	-1.506789	-.807397
H	-1.607508	-5.032210	1.137618
H	-2.470979	-1.689303	-4.235780
H	-2.823198	3.703667	-.819892
H	-1.875566	.365773	4.537931
H	-1.785662	-5.658990	-1.417199
H	-2.135929	-4.238730	-3.689783
H	-2.898331	.853970	-4.837458
H	-3.080449	3.126628	-3.386411
H	-2.671610	4.323656	1.716825
H	-2.272896	2.919580	3.995876
H	-1.482085	-2.169548	5.138746

H	-1.374086	-4.456608	3.701975
Frequencies:			
-28.6010	-22.0313	-19.1290	
-9.0962	16.3414	24.3407	
31.7769	42.1923	49.7416	
52.1966	63.4358	82.1359	
93.3472	100.6167	110.6158	
126.3605	129.6800	146.6568	
148.5136	158.3035	175.6744	
184.0097	192.8589	205.4491	
215.3012	217.3692	221.2618	
226.2382	228.5445	232.6885	
260.5050	264.4258	273.2420	
274.3970	279.2696	281.1978	
285.2973	296.7326	297.3526	
300.6393	302.5385	315.1991	
323.5936	334.5476	346.2281	
360.2559	372.0670	375.0378	
380.3361	382.4748	385.9718	
401.7194	417.3981	420.0628	
421.4179	434.9322	437.1809	
440.4761	441.0784	443.5746	
469.9844	476.7728	485.9502	
509.7044	518.5736	544.4070	
547.9223	562.1221	577.2717	
582.1566	623.6755	645.7543	
660.2803	679.0438	679.7918	
688.8665	689.3005	690.4636	
698.6553	727.6008	728.8382	
732.7987	738.6326	745.1222	
764.9713	765.9921	770.7968	
771.4374	800.2315	812.3779	
813.8492	821.7903	822.8765	
824.3132	825.0343	832.4378	
837.0472	838.9784	852.5029	
854.7495	857.8457	858.7055	
882.3696	911.0942	916.4024	
928.5600	930.7147	931.4460	
937.4390	945.8566	954.4388	
954.6900	963.5568	965.1292	
969.5018	970.9838	977.3630	
988.1739	995.3611	1004.4740	
1024.7934	1031.7065	1034.0027	
1036.3107	1037.1430	1039.7011	
1046.6300	1049.8572	1053.4260	
1065.5479	1068.3655	1068.6120	
1070.3510	1079.1869	1088.1206	
1088.3274	1103.4614	1125.1087	
1125.4185	1127.6896	1130.7815	
1131.5334	1139.2772	1148.6958	
1172.6660	1174.9761	1177.3997	
1185.4619	1199.6048	1203.5077	
1206.4545	1214.0727	1230.0550	
1238.1841	1244.6440	1251.1472	
1256.0576	1260.1178	1269.9702	
1285.4927	1296.2293	1305.1339	
1308.9941	1311.2557	1312.8047	
1319.6922	1323.8698	1335.8771	
1340.7842	1346.8390	1350.1868	
1358.1921	1359.9181	1359.9528	
1366.8646	1379.7685	1380.7107	
1391.1366	1398.1370	1401.0221	
1401.1493	1402.8330	1405.7195	
1411.8584	1417.8010	1421.1405	
1421.9303	1431.5630	1433.1891	
1438.1993	1438.8389	1448.0416	
1455.8385	1462.0573	1492.1674	
1505.3494	1508.0028	1509.8046	
1511.8718	1531.1213	1535.4135	
1537.6701	1539.0127	1541.8092	

1545.2070	1546.8110	1551.9461
1557.4553	1563.8931	1564.3736
1566.1078	1597.7627	1599.2273
1614.0937	1621.3253	1647.5781
1649.7457	1650.5222	1680.4847
1721.2174	2533.5905	2894.7505
2944.6975	2955.9317	2989.2494
3005.5513	3017.9687	3025.7791
3026.7840	3031.7670	3036.3287
3036.6229	3044.0053	3044.6926
3056.5550	3056.8272	3059.9978
3061.1580	3074.7395	3078.5757
3080.3836	3084.1042	3094.4592
3100.7332	3112.5969	3125.4578
3131.7194	3181.5040	3192.3066
3193.3179	3193.5830	3202.2851
3238.0490	3238.5142	3239.9991
3241.4074	3261.0889	3261.7333
3263.0115	3264.3911	3676.3449

### III.D.8. Point P8

Absolute energy: -2476.6088533

Geometry:

C	.476641	3.384509	-1.225409
C	.522187	4.645665	-.511512
C	1.570466	4.801486	.574592
C	5.415087	-.872472	.211885
O	-.313241	5.557557	-.751233
C	2.734678	3.808700	.418426
C	2.278510	2.330210	.231323
C	3.521375	1.444829	-.168229
C	3.110787	-.003435	-.586673
C	2.141122	.048395	-1.781947
C	1.013674	1.041999	-1.601124
C	1.237731	2.266590	-.904068
C	4.651158	1.457265	.900296
C	5.861326	.563764	.534672
C	4.373127	-.806307	-.937851
C	4.888446	-1.580616	1.482709
C	1.597463	1.819082	1.535708
C	6.490719	-1.769986	-.464690
C	5.667848	-2.871108	-1.202591
C	4.240551	-2.273436	-1.421042
O	7.528589	-2.285467	.409492
S	-4.544310	-.730356	.303334
Fe	-2.133025	-.668975	.164283
C	-1.746896	-3.987367	.904702
C	-2.419598	-1.442198	-3.185307
C	-2.715364	2.653566	-.588691
C	-1.954926	.117089	3.490155
N	-2.133755	-2.368686	-.911796
C	-1.934202	-3.649421	-.427858
C	-1.919763	-4.592083	-1.524770
C	-2.096065	-3.874429	-2.673844
C	-2.225787	-2.484942	-2.293765
N	-2.505241	.393547	-1.547655
C	-2.562554	-.106040	-2.837504
C	-2.809741	.973088	-3.770079
C	-2.903820	2.123122	-3.036793
C	-2.714776	1.759000	-1.648743
N	-2.340736	1.028764	1.236356
C	-2.546437	2.309999	.742697
C	-2.541027	3.259184	1.834544
C	-2.335202	2.548302	2.983518

C	-2.203625	1.157482	2.605606
N	-1.872004	-1.713780	1.842470
C	-1.803234	-1.210823	3.133007
C	-1.578492	-2.293375	4.069272
C	-1.524810	-3.447711	3.344163
C	-1.713893	-3.086752	1.954058
O	-.399347	-.454967	-.024751
H	3.337130	4.099130	-.454771
H	3.942504	1.912277	-1.077260
H	2.589763	-.493851	.246540
H	2.703171	.366909	-2.681069
H	1.751432	-.951914	-2.005021
H	.022191	.220172	-.639473
H	.296504	1.086949	-2.423638
H	-.251850	3.319668	-2.027135
H	1.928345	5.837508	.561986
H	1.070077	4.664985	1.544320
H	4.249948	1.135991	1.869029
H	5.008392	2.484021	1.042210
H	6.370855	.983070	-.346467
H	4.053431	-1.044709	1.941329
H	1.226265	.796708	1.425454
H	.732546	2.440262	1.790404
H	7.049096	-1.164636	-1.186901
H	6.151045	-3.158665	-2.141830
H	5.627551	-3.776098	-.581627
H	3.490756	-2.812182	-.828204
H	3.923840	-2.334769	-2.467458
H	4.870691	-.252329	-1.755924
H	5.689814	-1.637472	2.229721
H	4.540394	-2.599503	1.276524
H	2.295582	1.857510	2.378871
H	3.388435	3.881615	1.293863
H	6.592501	.569927	1.353631
H	7.149285	-2.950525	1.018370
H	-4.785015	-1.513717	-.808772
H	-1.608328	-5.037202	1.139680
H	-2.477507	-1.692602	-4.239394
H	-2.836353	3.706495	-.819037
H	-1.878111	.364649	4.543470
H	-1.785917	-5.658656	-1.414125
H	-2.136976	-4.237016	-3.691110
H	-2.904411	.850773	-4.839671
H	-3.089481	3.128877	-3.385670
H	-2.675104	4.324650	1.715293
H	-2.273535	2.916316	3.997694
H	-1.486555	-2.167648	5.138653
H	-1.378810	-4.457645	3.699765

## Frequencies:

-56.7356	-13.7559	12.4462
14.5838	26.4575	32.9932
37.4211	51.9943	58.7250
60.4952	72.1921	100.4081
106.2713	112.1842	123.4573
133.9983	140.6660	153.9967
156.0545	161.7452	178.9970
183.7553	193.4517	208.0172
211.2111	216.6121	223.1061
228.3176	234.9037	244.8820
251.1668	265.7417	270.8928
277.8221	285.5377	288.0581
288.7838	295.7027	297.8571
301.6146	311.1356	315.4289
326.5805	336.8146	344.5657
363.8713	370.5695	371.7933
373.0435	379.5340	385.7664
397.2370	406.4999	414.4246
427.0862	437.3126	438.1332
442.0328	442.4308	451.3629
460.1903	477.1165	485.9056



486.8324	512.1499	521.4128
559.6237	560.8251	576.0886
607.0419	618.7790	629.0845
651.2503	675.5064	680.6056
681.3165	682.0416	692.0332
699.0795	701.8255	704.3082
721.9099	724.4595	730.5730
731.9642	740.3979	760.1352
763.4980	765.5263	765.9164
795.2702	801.4279	809.5312
810.9129	812.3270	820.7549
830.5706	831.2621	833.6521
835.3334	849.0559	851.1099
853.4599	865.9780	871.4326
892.3511	893.3136	905.8603
908.5693	914.9796	922.1916
933.9606	941.1592	949.1411
949.2387	950.2582	954.0291
959.2162	973.8939	976.9443
987.1336	997.8707	1009.5061
1013.7076	1021.1106	1022.5181
1032.1894	1036.8031	1037.9837
1046.7124	1049.5652	1060.2428
1062.9852	1063.1483	1063.3423
1077.3182	1081.8465	1086.2998
1098.6320	1116.7560	1117.1487
1119.3109	1121.7421	1126.4329
1139.6640	1152.6042	1168.4376
1175.5751	1178.7444	1185.2472
1192.5151	1193.9519	1201.9923
1208.5527	1216.5590	1223.7240
1244.4234	1244.8708	1253.1798
1262.0303	1269.7845	1275.6801
1292.5975	1294.7019	1295.7904
1308.0900	1318.6236	1322.2414
1333.5972	1344.1083	1345.9830
1357.6517	1358.5206	1359.5083
1361.9502	1373.9868	1376.9250
1379.9026	1385.3925	1389.5283
1390.1836	1395.3246	1398.9972
1402.9323	1409.9992	1413.8931
1417.5447	1421.0296	1431.3386
1431.9359	1437.3081	1439.1819
1440.4016	1453.6664	1463.8000
1488.2304	1503.4749	1504.2355
1506.9727	1512.5950	1516.0663
1529.9112	1534.3606	1536.7436
1540.9860	1544.8909	1546.1226
1550.8792	1556.6336	1558.5751
1562.6428	1564.8875	1594.6727
1595.6475	1607.4427	1621.4341
1642.3012	1643.3138	1659.8100
1714.6071	2508.3773	2913.7086
2950.4587	2953.0387	2964.5427
3018.2734	3030.5757	3041.6849
3043.3580	3047.0245	3052.4701
3056.4664	3060.0618	3061.2319
3074.0839	3077.2604	3081.1998
3094.4174	3095.3165	3098.1329
3104.2547	3111.6102	3117.9221
3128.4999	3136.6551	3141.7051
3149.8946	3211.0081	3212.3604
3213.5246	3213.7958	3220.8222
3258.8700	3259.2660	3260.2212
3261.8999	3282.0770	3282.7141
3283.2318	3284.8841	3636.2751

## III.D.9. Point P9

Absolute energy: -2476.6029528

Geometry:

C	.484824	3.380985	-1.224854
C	.520171	4.646728	-.511913
C	1.570771	4.801845	.574417
C	5.415256	-.872612	.211779
O	-.312677	5.557298	-.750152
C	2.735131	3.809062	.419892
C	2.277370	2.332583	.230879
C	3.520981	1.444406	-.168557
C	3.110042	-.003210	-.587767
C	2.151888	.052537	-1.792808
C	.979211	1.006435	-1.581454
C	1.241718	2.291562	-.905313
C	4.651015	1.457545	.900243
C	5.861262	.563722	.534746
C	4.373090	-.806218	-.937114
C	4.888615	-1.580640	1.482765
C	1.597077	1.818499	1.535527
C	6.490587	-1.769838	-.464664
C	5.667869	-2.871170	-1.202562
C	4.240716	-2.273293	-1.420960
O	7.528811	-2.285639	.409545
S	-4.548646	-.730321	.303115
Fe	-2.123560	-.667181	.162599
C	-1.747642	-3.985682	.904025
C	-2.419447	-1.440438	-3.183841
C	-2.714191	2.652123	-.589062
C	-1.955740	.117926	3.488062
N	-2.133498	-2.367942	-.912402
C	-1.934280	-3.649958	-.429919
C	-1.919729	-4.592870	-1.525134
C	-2.096037	-3.874994	-2.674060
C	-2.225223	-2.486856	-2.291890
N	-2.510931	.391856	-1.544288
C	-2.563728	-.105555	-2.838403
C	-2.809907	.973938	-3.770415
C	-2.904014	2.122858	-3.037642
C	-2.715634	1.758827	-1.649643
N	-2.341729	1.028122	1.234519
C	-2.545999	2.309285	.744648
C	-2.541158	3.259512	1.835331
C	-2.335377	2.549293	2.983897
C	-2.204079	1.159057	2.605970
N	-1.872548	-1.714243	1.844032
C	-1.802783	-1.213833	3.132123
C	-1.578227	-2.293938	4.069939
C	-1.524555	-3.448219	3.344966
C	-1.713429	-3.085609	1.956246
O	-.431153	-.471777	-.008347
H	3.336142	4.097853	-.454531
H	3.941869	1.911488	-1.077773
H	2.588563	-.493069	.246217
H	2.725961	.365994	-2.680918
H	1.758536	-.948706	-2.007506
H	.286251	.446421	-.880449
H	.379161	1.137892	-2.488657
H	-.240109	3.317688	-2.030508
H	1.928194	5.838127	.562418
H	1.069658	4.664953	1.544019
H	4.250216	1.136049	1.869304
H	5.008708	2.484141	1.042781
H	6.370490	.982912	-.346602
H	4.053563	-1.044085	1.940482
H	1.226329	.796182	1.423864
H	.733971	2.441751	1.790234

H	7.048890	-1.164531	-1.186902
H	6.151278	-3.158717	-2.141812
H	5.628213	-3.776287	-.581405
H	3.490721	-2.812120	-.828170
H	3.923359	-2.333581	-2.466998
H	4.869870	-.252450	-1.755476
H	5.689809	-1.637734	2.230150
H	4.540445	-2.599571	1.276242
H	2.296685	1.855187	2.377763
H	3.389674	3.883527	1.295208
H	6.592771	.570012	1.353662
H	7.148465	-2.949977	1.018479
H	-4.794156	-1.511153	-.809850
H	-1.608854	-5.035845	1.139416
H	-2.475376	-1.691515	-4.238212
H	-2.830037	3.705943	-.819308
H	-1.877745	.364767	4.541873
H	-1.785847	-5.659381	-1.415263
H	-2.136609	-4.237741	-3.691100
H	-2.902720	.852405	-4.840088
H	-3.086703	3.128830	-3.386764
H	-2.673213	4.324974	1.715572
H	-2.273231	2.917969	3.997638
H	-1.486113	-2.168315	5.139137
H	-1.378323	-4.457846	3.700841

## Frequencies:

-27.8801	-16.5056	5.6878
13.8980	30.9604	33.4370
39.3579	54.0208	54.9755
57.1463	86.2667	92.4368
99.3306	99.9859	122.3613
128.0349	142.1164	150.2226
153.2551	157.6017	180.8097
182.1299	197.4977	208.1930
213.3141	218.9226	219.6010
228.3724	234.7876	241.1071
261.6461	268.4119	274.8985
276.8868	281.9557	282.2811
287.4238	295.1594	297.4155
309.5223	313.3102	326.3424
330.1804	336.2994	339.3526
361.4722	372.1621	375.0809
377.2812	380.3836	385.3482
398.8584	419.4680	421.7368
424.9455	435.0839	436.7988
439.8583	441.0018	445.1410
469.4976	475.3838	485.7178
508.2275	518.4733	550.9818
559.5979	572.5606	575.7740
584.7681	596.8703	621.0914
646.2597	660.5189	678.4928
679.1787	686.4125	689.8234
690.6492	700.5854	724.0438
725.4208	729.8959	735.5044
739.8616	761.7393	764.1971
766.0034	766.5137	798.1612
803.1168	812.6594	813.8698
821.6443	822.1479	822.5416
834.4044	834.9675	849.2021
852.3590	853.0659	855.9842
880.7565	904.7131	906.0101
918.5078	920.4007	928.7939
934.3891	936.3372	943.5463
952.1986	953.8486	954.4059
960.1149	967.2942	974.7614
985.4473	992.7806	1003.2291
1018.1044	1024.1657	1025.4570
1026.5495	1029.5934	1035.1132
1038.6838	1048.8772	1051.4872
1059.3912	1060.8188	1062.8938

1065.2304	1076.7370	1078.6832
1087.1029	1101.6228	1118.2193
1118.5159	1120.9652	1124.6512
1128.9096	1137.5471	1149.8990
1161.5498	1170.0265	1175.6373
1182.2078	1189.4891	1192.4340
1200.3851	1214.8080	1218.8845
1237.6723	1241.3737	1244.7415
1246.5106	1257.5988	1266.2483
1280.7208	1293.6232	1297.0399
1299.1179	1300.4627	1306.7734
1316.9385	1320.6220	1328.3751
1332.6754	1336.9403	1345.7648
1349.3072	1350.7887	1357.4420
1363.6115	1376.9055	1378.5719
1387.6052	1388.9415	1390.1691
1394.9560	1398.5899	1400.8405
1409.2925	1413.1260	1415.6671
1419.7011	1422.4296	1428.9275
1430.8374	1435.5799	1436.5885
1445.3360	1452.4808	1461.9887
1499.8762	1501.1420	1504.6616
1510.1889	1529.6812	1533.5771
1534.0326	1536.4562	1537.1245
1540.3410	1545.3026	1550.4714
1556.5605	1559.4299	1562.4495
1564.6640	1591.0871	1593.1495
1611.4071	1615.6216	1623.2507
1642.2812	1644.2799	1657.9427
1715.5755	2256.0257	2508.4539
2953.6340	2964.9191	2994.0815
3017.9000	3031.4983	3038.5791
3040.9874	3045.2629	3049.1686
3050.6495	3058.7493	3059.1502
3072.1555	3076.3000	3077.2212
3085.1194	3090.8667	3095.6923
3096.2197	3100.1856	3109.6693
3117.2792	3128.4812	3141.5199
3148.3899	3202.9395	3210.1143
3212.1007	3212.1908	3220.7171
3261.0287	3261.4537	3262.9676
3264.4283	3283.9625	3284.6636
3285.9023	3287.3518	3636.4566

### III.D.10. Point P10

Absolute energy: -2476.6068162

Geometry:

C	.491282	3.386517	-1.226928
C	.519489	4.648141	-.511660
C	1.570910	4.802803	.574993
C	5.415547	-.872806	.212096
O	-.313513	5.558086	-.748650
C	2.736535	3.810715	.422465
C	2.278526	2.335536	.230691
C	3.521020	1.444834	-.168388
C	3.110184	-.002283	-.589592
C	2.163897	.057708	-1.802980
C	.987647	1.013116	-1.601130
C	1.251801	2.303008	-.911316
C	4.650940	1.457623	.900220
C	5.861194	.563735	.534872
C	4.373445	-.806226	-.935840
C	4.888841	-1.580656	1.482842
C	1.596457	1.818423	1.533611

C	6.490856	-1.769783	-.464508
C	5.667975	-2.871168	-1.202478
C	4.240898	-2.273025	-1.420618
O	7.528875	-2.285869	.409535
S	-4.554530	-.730603	.303140
Fe	-2.117415	-.665916	.161403
C	-1.748324	-3.984250	.903230
C	-2.419274	-1.439674	-3.182839
C	-2.713393	2.651259	-.589094
C	-1.956474	.118379	3.486496
N	-2.133787	-2.368572	-.914218
C	-1.934233	-3.650039	-.430871
C	-1.919784	-4.593360	-1.525357
C	-2.095921	-3.875281	-2.674072
C	-2.224750	-2.487616	-2.290833
N	-2.516587	.389875	-1.541271
C	-2.565739	-.106164	-2.837988
C	-2.809761	.973573	-3.769452
C	-2.903736	2.122093	-3.036745
C	-2.717185	1.758456	-1.648858
N	-2.342090	1.028598	1.233576
C	-2.545580	2.308517	.745256
C	-2.541136	3.259246	1.835508
C	-2.335681	2.549623	2.984022
C	-2.204478	1.159609	2.605920
N	-1.877658	-1.716464	1.847866
C	-1.803594	-1.215497	3.132172
C	-1.577644	-2.293924	4.070423
C	-1.523938	-3.448647	3.345210
C	-1.714050	-3.085079	1.957671
O	-.463877	-.503351	.022712
H	3.337751	4.099439	-.452179
H	3.942665	1.911780	-1.077574
H	2.583362	-.492484	.241231
H	2.749838	.367038	-2.684424
H	1.769159	-.943147	-2.019550
H	.278616	.476555	-.942818
H	.439633	1.176974	-2.536832
H	-.229899	3.321561	-2.036406
H	1.928355	5.839455	.562974
H	1.069777	4.666089	1.544928
H	4.250292	1.136135	1.869709
H	5.008962	2.484432	1.043026
H	6.370347	.983025	-.346794
H	4.053343	-1.043668	1.940026
H	1.225847	.795938	1.419450
H	.733910	2.442122	1.790361
H	7.048239	-1.164157	-1.187689
H	6.151437	-3.158646	-2.142162
H	5.628239	-3.776609	-.581258
H	3.490616	-2.812336	-.828018
H	3.923389	-2.332422	-2.467006
H	4.870428	-.252708	-1.754502
H	5.689587	-1.638021	2.231145
H	4.540462	-2.599834	1.276299
H	2.296269	1.851807	2.376276
H	3.390824	3.886641	1.298349
H	6.593178	.570200	1.353817
H	7.148132	-2.949104	1.018508
H	-4.805474	-1.509476	-.809242
H	-1.608958	-5.034757	1.138749
H	-2.472733	-1.690625	-4.237739
H	-2.824320	3.705906	-.819759
H	-1.876956	.365395	4.540580
H	-1.785987	-5.660419	-1.415969
H	-2.136520	-4.238189	-3.691538
H	-2.900437	.853105	-4.839917
H	-3.083578	3.128780	-3.386769
H	-2.672122	4.325292	1.715480
H	-2.273277	2.919196	3.997929
H	-1.484290	-2.168367	5.139981

H	-1.376342	-4.458438	3.701474
Frequencies:			
-27.9988	-17.7226	-9.8022	
7.8155	30.9154	31.4083	
49.2735	51.3770	56.0968	
61.8840	79.7443	88.6804	
98.1699	110.6292	124.9642	
129.0011	133.6258	148.1862	
152.2780	156.5450	176.9488	
179.8192	193.4782	206.7841	
212.8564	218.8720	219.3971	
229.6786	234.2550	241.0705	
263.2322	267.3771	273.1890	
276.3289	279.8394	281.4792	
288.1664	295.7171	299.1951	
305.3377	312.9117	320.6326	
326.4030	334.4128	347.3504	
360.7500	372.1650	375.4079	
378.5525	382.1440	385.8270	
399.7012	419.2186	419.6449	
422.5877	435.0676	436.6858	
440.3048	440.9304	443.4101	
469.2973	476.8173	485.6600	
508.0670	518.1504	548.1831	
560.2460	560.6463	576.1729	
581.9433	621.8135	645.6242	
660.2460	678.6284	679.2797	
686.8025	689.4381	690.2141	
699.0046	725.1406	726.3835	
730.5834	735.6140	741.4219	
761.3659	763.7392	766.9191	
767.5767	777.9180	799.2516	
805.3032	814.7146	815.9656	
820.2668	822.4330	824.8701	
834.8493	835.9431	849.9529	
852.6663	854.2134	856.6862	
881.0395	906.7163	908.8216	
921.2695	923.4868	929.5241	
935.2662	939.4549	945.8273	
952.6202	955.9427	957.1170	
963.1478	968.1130	975.6292	
986.2963	993.0603	1003.4454	
1017.0772	1024.2085	1026.4234	
1028.8264	1030.4627	1036.8751	
1038.9248	1048.7453	1051.8696	
1060.1642	1061.8962	1063.7317	
1066.2633	1077.8100	1080.2356	
1087.6662	1102.2515	1119.5997	
1119.8773	1122.3024	1126.0269	
1129.2896	1138.5734	1148.9841	
1160.7155	1171.1537	1176.0316	
1184.5981	1191.6866	1194.5471	
1199.8918	1214.2030	1220.2240	
1237.6203	1242.7583	1247.8180	
1250.2798	1258.4795	1267.8852	
1282.4960	1294.5000	1300.5049	
1302.2167	1303.8442	1307.3785	
1313.3639	1321.9115	1333.8832	
1335.7622	1344.9335	1348.1664	
1349.7174	1351.6046	1357.8433	
1364.8095	1378.4372	1378.8715	
1389.0393	1389.4910	1391.7611	
1396.2784	1399.4418	1402.7089	
1409.8127	1414.3125	1416.0634	
1420.0555	1423.3141	1430.2155	
1431.5792	1437.1868	1438.7799	
1452.8758	1458.3500	1482.8636	
1500.5910	1501.8172	1504.3726	
1510.4455	1529.9477	1534.0118	
1536.2710	1537.0310	1537.1544	

1540.4574	1545.5051	1550.7140
1556.3597	1560.1119	1562.6925
1564.9107	1591.7890	1593.4971
1608.6395	1615.9262	1642.6477
1643.3402	1645.2740	1668.8406
1716.3279	2513.0919	2738.0622
2951.6323	2962.8942	2996.5453
3015.4230	3028.7971	3035.6804
3038.0386	3042.4587	3046.0579
3047.5936	3055.8442	3056.0847
3068.9305	3071.3144	3073.6862
3074.1745	3087.3447	3092.5023
3092.8763	3096.6087	3106.6122
3114.0779	3125.4637	3138.4017
3144.8728	3197.3408	3206.8501
3208.2657	3208.4467	3217.3141
3256.7306	3257.2764	3258.6388
3260.0996	3279.6650	3280.4233
3281.5725	3283.0385	3643.7782

### III.D.11. Point P11

Absolute energy: -2476.6037574

Geometry:

C	0.485699	3.381380	-1.225061
C	0.520051	4.646905	-0.511791
C	1.570810	4.801940	0.574431
C	5.415293	-0.872612	0.211781
O	-0.312805	5.557441	-0.749996
C	2.735321	3.809217	0.420240
C	2.277390	2.333096	0.230853
C	3.520930	1.444391	-0.168566
C	3.110009	-0.003140	-0.588010
C	2.153697	0.053224	-1.794434
C	0.979782	1.006634	-1.583885
C	1.243281	2.294092	-0.906011
C	4.650989	1.457595	0.900248
C	5.861273	0.563718	0.534766
C	4.373093	-0.806211	-0.936937
C	4.888639	-1.580669	1.482792
C	1.596990	1.818438	1.535424
C	6.490497	-1.769810	-0.464699
C	5.667864	-2.871185	-1.202581
C	4.240725	-2.273282	-1.420948
O	7.528901	-2.285664	0.409561
S	-4.549351	-0.730366	0.303138
Fe	-2.122345	-0.666889	0.162323
C	-1.747738	-3.985575	0.903909
C	-2.419427	-1.440258	-3.183781
C	-2.714107	2.652060	-0.589128
C	-1.955852	0.118081	3.487902
N	-2.133448	-2.367710	-0.912498
C	-1.934260	-3.650087	-0.430006
C	-1.919714	-4.593157	-1.525277
C	-2.096017	-3.875221	-2.674192
C	-2.225161	-2.486972	-2.291727
N	-2.511620	0.391383	-1.543509
C	-2.563955	-0.105702	-2.838562
C	-2.809943	0.974060	-3.770546
C	-2.904045	2.122897	-3.037788
C	-2.715841	1.758949	-1.649554
N	-2.341717	1.027868	1.234137
C	-2.545980	2.309206	0.744711
C	-2.541182	3.259693	1.835507
C	-2.335416	2.549571	2.984063
C	-2.204127	1.159139	2.606142
N	-1.872962	-1.714350	1.844307

C	-1.802799	-1.214079	3.132103
C	-1.578141	-2.294029	4.070198
C	-1.524466	-3.448420	3.345170
C	-1.713417	-3.085562	1.956442
O	-0.437557	-0.476694	-0.003558
H	3.336063	4.097687	-0.454295
H	3.941719	1.911399	-1.077763
H	2.588040	-0.492881	0.245608
H	2.729805	0.365441	-2.681297
H	1.759784	-0.947824	-2.008488
H	0.286863	0.453979	-0.889881
H	0.390521	1.144925	-2.497104
H	-0.238320	3.317774	-2.031237
H	1.927992	5.838137	0.562422
H	1.069650	4.665062	1.543897
H	4.250293	1.136095	1.869219
H	5.008650	2.484042	1.042793
H	6.370373	0.982792	-0.346568
H	4.053706	-1.044051	1.940268
H	1.226397	0.796267	1.423349
H	0.734210	2.441817	1.790207
H	7.049117	-1.164641	-1.186555
H	6.151262	-3.158724	-2.141639
H	5.628409	-3.776154	-0.581420
H	3.490799	-2.812050	-0.828277
H	3.923316	-2.333402	-2.466780
H	4.869822	-0.252452	-1.755223
H	5.689783	-1.637721	2.230034
H	4.540476	-2.599440	1.276180
H	2.296744	1.854760	2.377378
H	3.389827	3.883959	1.295375
H	6.592712	0.570067	1.353555
H	7.148296	-2.950119	1.018712
H	-4.795716	-1.511107	-0.810072
H	-1.608967	-5.035549	1.139317
H	-2.474977	-1.691348	-4.237968
H	-2.828916	3.705796	-0.819337
H	-1.877662	0.364800	4.541536
H	-1.785877	-5.659381	-1.415249
H	-2.136603	-4.237598	-3.691072
H	-2.902385	0.852444	-4.839972
H	-3.086228	3.128764	-3.386640
H	-2.672935	4.324877	1.715402
H	-2.273205	2.918003	3.997603
H	-1.485959	-2.168166	5.139083
H	-1.378151	-4.457855	3.700728

## Frequencies:

-28.4620	-15.6379	-3.0165
12.6103	31.0220	32.9952
46.2534	53.3822	56.1186
58.0179	85.6181	92.2132
99.2987	105.1202	123.6024
127.4526	145.6803	149.3229
153.3572	157.0942	179.1390
181.1403	196.6751	207.7109
213.6575	218.2408	219.5977
229.0677	234.8531	240.3949
261.3106	267.9325	273.9798
277.0089	281.4710	281.9162
287.7362	295.4827	297.8274
308.5449	313.0808	328.0621
329.9709	338.9955	343.6511
361.3220	372.1630	375.2624
377.6393	380.8281	385.4572
398.7269	419.2438	421.4679
424.8284	434.9321	436.6791
439.8269	440.8166	444.3107
469.2902	476.1964	485.5496
507.7657	518.2568	550.1353



559.5214	572.4500	575.7543
583.4041	620.9635	629.9300
645.9228	660.4253	678.2471
678.8968	686.5683	689.6353
690.2777	699.9684	723.6980
725.0549	729.6798	735.0752
739.6561	761.5359	764.0503
765.8592	766.3935	797.7928
802.4027	811.8551	813.0459
820.9420	821.6095	821.7979
834.3457	834.9400	848.9520
852.2194	852.6323	855.6431
880.3791	904.3498	905.4408
917.9594	919.9102	928.5222
934.2530	936.0870	942.5509
951.8671	953.0699	953.6976
959.5301	967.2051	974.6949
985.3726	992.4521	1003.0912
1017.2775	1023.2790	1025.0374
1026.3657	1029.6450	1034.8009
1038.6144	1048.6536	1051.4924
1058.8492	1060.3216	1062.7883
1065.2111	1076.7103	1078.3566
1087.1092	1101.5517	1117.6537
1117.9294	1120.3791	1124.0843
1128.7425	1137.6220	1149.5684
1159.9472	1170.0686	1175.4619
1182.5064	1188.8689	1191.7714
1199.9008	1214.4993	1218.3780
1237.3966	1241.5657	1245.5916
1246.0999	1257.4785	1266.2847
1280.7985	1293.7332	1297.8995
1299.5039	1300.0262	1306.5664
1315.2477	1320.6370	1329.8708
1332.9432	1337.2035	1345.6121
1348.5604	1350.1320	1357.1854
1363.5200	1376.8262	1378.3436
1386.8937	1388.7807	1389.7757
1394.9656	1398.5124	1400.8276
1409.0523	1412.5140	1415.4106
1419.6667	1421.8464	1428.4254
1430.5137	1435.4762	1436.5776
1450.4976	1452.3914	1462.9052
1499.6972	1500.7933	1504.2161
1510.0230	1529.5368	1533.8051
1533.9182	1536.3050	1536.5132
1540.1475	1545.1286	1550.3081
1556.3109	1559.2027	1562.3028
1564.5083	1590.7687	1592.7859
1610.2267	1615.2682	1630.4990
1642.2112	1644.2244	1659.9211
1715.5300	2384.6185	2506.5160
2954.3632	2965.6835	2996.7372
3018.9486	3032.6512	3039.5433
3042.1686	3046.4030	3050.0155
3051.7997	3059.9865	3060.4415
3073.4299	3077.3022	3078.7027
3084.7320	3092.1147	3097.3126
3097.5482	3101.4395	3110.9513
3118.8105	3129.9259	3142.9854
3149.7416	3204.5591	3211.9611
3213.8678	3213.9590	3222.6175
3263.6717	3264.1170	3265.5816
3267.0405	3286.5774	3287.2871
3288.5001	3289.9577	3632.3905

Absolute energy: -2476.6040876

Geometry:

C	0.486060	3.381692	-1.225098
C	0.519961	4.646933	-0.511812
C	1.570816	4.801972	0.574438
C	5.415309	-0.872627	0.211788
O	-0.312821	5.557457	-0.749922
C	2.735388	3.809282	0.420380
C	2.277413	2.333282	0.230848
C	3.520905	1.444400	-0.168567
C	3.110001	-0.003101	-0.588105
C	2.154419	0.053516	-1.795059
C	0.980324	1.007036	-1.585073
C	1.243917	2.294978	-0.906354
C	4.650978	1.457599	0.900236
C	5.861268	0.563716	0.534770
C	4.373105	-0.806209	-0.936863
C	4.888655	-1.580667	1.482787
C	1.596967	1.818432	1.535341
C	6.490512	-1.769804	-0.464687
C	5.667869	-2.871183	-1.202574
C	4.240739	-2.273265	-1.420929
O	7.528901	-2.285682	0.409566
S	-4.549644	-0.730387	0.303141
Fe	-2.121785	-0.666767	0.162209
C	-1.747784	-3.985465	0.903850
C	-2.419417	-1.440184	-3.183691
C	-2.714063	2.651972	-0.589133
C	-1.955900	0.118117	3.487774
N	-2.133468	-2.367765	-0.912627
C	-1.934259	-3.650083	-0.430093
C	-1.919718	-4.593159	-1.525277
C	-2.096013	-3.875211	-2.674167
C	-2.225128	-2.487037	-2.291606
N	-2.511981	0.391271	-1.543333
C	-2.564058	-0.105704	-2.838552
C	-2.809935	0.974042	-3.770479
C	-2.904033	2.122836	-3.037734
C	-2.715918	1.758915	-1.649541
N	-2.341761	1.027908	1.234079
C	-2.545955	2.309127	0.744784
C	-2.541182	3.259648	1.835514
C	-2.335431	2.549577	2.984054
C	-2.204154	1.159198	2.606130
N	-1.873200	-1.714495	1.844569
C	-1.802814	-1.214222	3.132059
C	-1.578121	-2.294008	4.070189
C	-1.524445	-3.448425	3.345150
C	-1.713425	-3.085482	1.956546
O	-0.440391	-0.478914	-0.001399
H	3.336120	4.097725	-0.454245
H	3.941741	1.911401	-1.077794
H	2.587758	-0.492868	0.245407
H	2.731310	0.365328	-2.681560
H	1.760331	-0.947580	-2.009039
H	0.287171	0.458090	-0.894782
H	0.394751	1.147576	-2.500462
H	-0.237727	3.317849	-2.031579
H	1.928034	5.838238	0.562438
H	1.069651	4.665098	1.543969
H	4.250288	1.136087	1.869278
H	5.008683	2.484103	1.042814
H	6.370379	0.982821	-0.346608
H	4.053660	-1.043995	1.940259
H	1.226397	0.796182	1.423171
H	0.734188	2.441871	1.790279
H	7.049059	-1.164586	-1.186670
H	6.151294	-3.158725	-2.141713
H	5.628398	-3.776209	-0.581383
H	3.490767	-2.812085	-0.828233

H	3.923300	-2.333329	-2.466836
H	4.869822	-0.252449	-1.755208
H	5.689793	-1.637752	2.230129
H	4.540463	-2.599498	1.276179
H	2.296765	1.854559	2.377356
H	3.389955	3.884169	1.295556
H	6.592771	0.570067	1.353595
H	7.148301	-2.950000	1.018644
H	-4.796318	-1.510948	-0.809953
H	-1.608992	-5.035523	1.139295
H	-2.474825	-1.691300	-4.237969
H	-2.828534	3.705830	-0.819375
H	-1.877624	0.364839	4.541495
H	-1.785869	-5.659508	-1.415304
H	-2.136593	-4.237648	-3.691146
H	-2.902264	0.852514	-4.840042
H	-3.086050	3.128819	-3.386695
H	-2.672847	4.324959	1.715402
H	-2.273188	2.918127	3.997671
H	-1.485878	-2.168166	5.139185
H	-1.378057	-4.457942	3.700791

## Frequencies:

-28.9434	-15.7729	-5.2698
12.0487	31.1171	32.7375
47.3657	53.2335	56.2811
58.8071	85.0052	91.7596
99.1401	106.6358	124.2713
127.5864	143.9918	148.9804
153.2232	157.0254	179.2606
180.8304	196.2928	207.7722
213.6618	218.3381	219.5627
229.3905	234.8290	240.5899
261.6221	267.9690	273.7130
277.0535	281.1843	281.8557
287.8157	295.5859	298.0627
307.9257	313.0651	327.3884
329.6576	337.8001	344.7838
361.2883	372.1840	375.3795
377.8251	381.0123	385.4725
398.8720	419.1914	421.2966
424.7135	434.9652	436.6879
439.9135	440.8338	444.0016
469.2153	476.4924	485.5653
507.7095	518.2471	549.8542
559.6395	571.2615	575.8043
582.8285	621.0600	645.2818
646.1675	660.4946	678.3110
678.9561	687.1741	689.6295
690.2619	699.7410	723.9096
725.2653	729.7854	735.2181
739.8890	761.6055	764.1356
765.9692	766.5190	797.8669
802.8471	812.2954	813.4880
820.8002	821.6018	822.1538
834.4002	835.0136	849.0813
852.2736	852.8179	855.5823
880.4033	904.6110	905.9331
918.4598	920.4284	928.4720
934.3673	936.5713	943.0551
951.9554	953.4987	954.2008
960.0443	967.2733	974.8183
985.4817	992.5346	1003.1370
1017.2395	1023.3579	1025.1647
1026.6548	1029.8195	1035.0112
1038.6366	1048.6770	1051.5168
1058.9786	1060.4599	1062.8910
1065.3717	1076.7693	1078.5107
1087.1302	1101.6480	1117.9491
1118.2201	1120.6717	1124.3803
1128.8327	1137.6641	1149.5240

1159.8969	1170.1670	1175.5367
1182.6372	1189.1580	1192.0480
1199.8795	1214.4966	1218.6048
1237.5778	1241.7136	1245.9024
1246.3771	1257.5990	1266.4762
1281.0279	1293.8969	1298.2763
1300.0764	1300.2575	1306.6461
1314.8042	1320.7904	1330.5694
1333.1993	1337.6021	1345.7364
1348.6307	1350.2419	1357.2748
1363.6582	1376.9843	1378.4348
1387.0964	1388.8886	1389.9757
1395.1161	1398.6360	1400.9956
1409.1614	1412.7576	1415.4901
1419.7299	1422.0012	1428.5943
1430.5979	1435.7833	1436.6562
1451.6830	1453.3001	1464.0576
1499.7687	1500.8914	1504.2416
1510.0935	1529.5970	1533.8402
1534.2418	1536.3622	1536.5254
1540.1917	1545.1807	1550.3664
1556.3303	1559.3357	1562.3569
1564.5663	1590.8497	1592.8448
1609.8562	1615.3054	1632.8197
1642.2397	1644.2664	1661.0818
1715.5510	2445.7757	2507.4897
2953.9978	2965.3193	2996.7171
3018.4514	3032.0888	3038.9574
3041.5525	3045.8170	3049.4039
3051.1880	3059.3718	3059.7891
3072.7842	3076.5056	3078.0093
3083.3740	3091.4217	3096.5942
3096.8539	3100.7417	3110.3197
3118.1027	3129.2679	3142.3167
3149.0150	3203.6252	3211.1678
3213.0396	3213.1316	3221.8001
3262.5836	3263.0588	3264.5064
3265.9713	3285.4939	3286.2303
3287.4310	3288.8908	3634.1975

### III.D.13. Point P13

Absolute energy: -2476.6032313

Geometry:

C	0.485121	3.381017	-1.224973
C	0.520171	4.646827	-0.511807
C	1.570790	4.801886	0.574423
C	5.415272	-0.872600	0.211776
O	-0.312753	5.557382	-0.750108
C	2.735213	3.809120	0.420017
C	2.277374	2.332779	0.230864
C	3.520970	1.444392	-0.168562
C	3.110027	-0.003193	-0.587853
C	2.152532	0.052767	-1.793402
C	0.979214	1.006308	-1.582197
C	1.242272	2.292536	-0.905521
C	4.651006	1.457576	0.900259
C	5.861284	0.563721	0.534755
C	4.373085	-0.806213	-0.937054
C	4.888616	-1.580664	1.482791
C	1.597034	1.818462	1.535522
C	6.490518	-1.769821	-0.464701
C	5.667864	-2.871185	-1.202582
C	4.240707	-2.273300	-1.420968
O	7.528875	-2.285636	0.409548

S	-4.548890	-0.730333	0.303129
Fe	-2.123182	-0.667083	0.162505
C	-1.747670	-3.985691	0.903994
C	-2.419442	-1.440376	-3.183866
C	-2.714169	2.652145	-0.589101
C	-1.955777	0.118000	3.488050
N	-2.133455	-2.367746	-0.912367
C	-1.934269	-3.650044	-0.429903
C	-1.919715	-4.593058	-1.525225
C	-2.096027	-3.875149	-2.674168
C	-2.225209	-2.486879	-2.291879
N	-2.511116	0.391626	-1.543906
C	-2.563804	-0.105658	-2.838511
C	-2.809935	0.974026	-3.770549
C	-2.904042	2.122931	-3.037772
C	-2.715716	1.758932	-1.649587
N	-2.341692	1.027922	1.234310
C	-2.546008	2.309292	0.744629
C	-2.541173	3.259666	1.835437
C	-2.335390	2.549468	2.984015
C	-2.204092	1.159060	2.606093
N	-1.872660	-1.714205	1.844015
C	-1.802790	-1.213881	3.132145
C	-1.578184	-2.294010	4.070118
C	-1.524510	-3.448350	3.345114
C	-1.713422	-3.085640	1.956291
O	-0.433246	-0.473386	-0.006777
H	3.336030	4.097708	-0.454373
H	3.941742	1.911422	-1.077719
H	2.588439	-0.492938	0.245930
H	2.727326	0.365720	-2.680926
H	1.758955	-0.948250	-2.007748
H	0.286818	0.448785	-0.883564
H	0.383397	1.140500	-2.491603
H	-0.239350	3.317729	-2.030687
H	1.928007	5.838005	0.562404
H	1.069666	4.665005	1.543853
H	4.250284	1.136094	1.869166
H	5.008630	2.483983	1.042764
H	6.370389	0.982795	-0.346522
H	4.053728	-1.044130	1.940322
H	1.226391	0.796351	1.423655
H	0.734183	2.441724	1.790144
H	7.049080	-1.164679	-1.186538
H	6.151220	-3.158704	-2.141595
H	5.628350	-3.776125	-0.581470
H	3.490826	-2.812024	-0.828300
H	3.923362	-2.333516	-2.466756
H	4.869834	-0.252464	-1.755297
H	5.689751	-1.637698	2.229968
H	4.540487	-2.599400	1.276205
H	2.296683	1.855060	2.377482
H	3.389642	3.883646	1.295148
H	6.592660	0.570050	1.353529
H	7.148306	-2.950240	1.018736
H	-4.794751	-1.511278	-0.810141
H	-1.608914	-5.035598	1.139350
H	-2.475223	-1.691426	-4.237981
H	-2.829587	3.705748	-0.819282
H	-1.877719	0.364745	4.541611
H	-1.785886	-5.659196	-1.415210
H	-2.136613	-4.237567	-3.690939
H	-2.902581	0.852376	-4.839861
H	-3.086508	3.128659	-3.386596
H	-2.673088	4.324751	1.715461
H	-2.273229	2.917854	3.997478
H	-1.486077	-2.168218	5.138929
H	-1.378288	-4.457700	3.700678

Frequencies:  
-28.0034      -15.9799      3.5277

13.2889	30.8267	33.2575
42.8497	53.5015	55.3623
57.1731	86.3227	92.6123
99.3985	102.0957	122.4343
127.4177	146.4237	149.7262
153.4596	157.1482	179.1275
181.6667	196.9534	207.5740
213.3612	218.2679	219.6084
228.5899	234.8417	240.2589
260.8882	267.8461	274.3429
276.8971	281.7968	282.0163
287.5405	295.2428	297.4543
309.1146	313.1387	328.4734
330.2870	339.2328	342.0426
361.3632	372.1322	375.0904
377.3078	380.5002	385.3137
398.5880	419.3041	421.6747
424.9206	434.9067	436.6875
439.7285	440.8239	444.7371
469.3667	475.6058	485.5622
507.8453	518.3041	550.4207
559.3776	573.5540	575.7025
584.0707	607.3382	620.8707
646.0313	660.3932	678.1991
678.8647	686.0202	689.6754
690.3464	700.2454	723.5012
724.8672	729.5968	734.9942
739.4461	761.5197	763.9703
765.7969	766.3163	797.7339
802.0004	811.4670	812.6648
821.1105	821.4350	821.7950
834.3222	834.8922	848.8434
852.2021	852.5007	855.6433
880.3391	904.0813	904.9762
917.4789	919.3900	928.4691
934.1397	935.5701	942.1387
951.7837	952.7186	953.2377
959.0339	967.0841	974.5652
985.2551	992.4314	1003.0589
1017.5708	1023.4685	1025.0667
1026.2179	1029.4543	1034.7443
1038.5858	1048.6652	1051.4705
1058.9002	1060.3490	1062.6950
1065.0495	1076.6059	1078.3397
1087.0657	1101.4567	1117.4155
1117.7038	1120.1432	1123.8452
1128.6708	1137.5235	1149.6889
1160.4436	1169.8907	1175.4198
1182.1417	1188.7773	1191.7024
1200.0377	1214.6157	1218.3124
1237.3582	1241.2896	1244.8908
1245.9126	1257.3743	1266.0328
1280.5226	1293.4906	1297.2742
1298.8623	1299.9693	1306.5099
1316.0908	1320.4341	1328.6945
1332.6017	1336.7259	1345.4994
1348.6892	1350.1906	1357.1304
1363.3830	1376.6698	1378.2926
1386.9237	1388.6924	1389.7458
1394.7853	1398.3750	1400.6459
1408.9710	1412.3927	1415.3601
1419.5894	1421.8687	1428.3965
1430.4501	1435.2389	1436.4656
1447.0847	1452.0916	1461.8632
1499.6795	1500.7912	1504.3061
1509.9758	1529.4913	1533.5391
1533.8025	1536.2669	1536.6923
1540.1300	1545.1007	1550.2700
1556.3321	1559.1065	1562.2664
1564.4717	1590.7846	1592.8311
1610.8754	1615.3149	1626.2155

1642.2010	1644.2025	1658.3491
1715.5361	2303.7430	2505.9672
2954.6404	2965.9643	2996.2411
3019.3607	3033.0962	3040.0364
3042.6483	3046.8729	3050.5760
3052.2916	3060.4646	3060.9447
3073.9399	3078.0764	3079.2459
3086.3410	3092.6830	3097.8515
3098.1190	3102.0101	3111.4391
3119.3458	3130.4027	3143.4751
3150.3175	3205.3240	3212.5668
3214.5429	3214.6313	3223.2486
3264.4828	3264.9289	3266.4089
3267.8783	3287.3860	3288.1045
3289.3218	3290.7899	3630.9718

### III.D.14. Point P14

Absolute energy: -2476.6015976

Geometry:

C	0.483611	3.380862	-1.224889
C	0.520456	4.646659	-0.511895
C	1.570722	4.801780	0.574439
C	5.415214	-0.872591	0.211793
O	-0.312646	5.557234	-0.750338
C	2.734990	3.808962	0.419539
C	2.277464	2.332056	0.230944
C	3.521062	1.444454	-0.168533
C	3.110124	-0.003273	-0.587523
C	2.149756	0.051680	-1.790773
C	0.979628	1.007437	-1.579555
C	1.240186	2.287727	-0.904613
C	4.651043	1.457504	0.900263
C	5.861273	0.563734	0.534725
C	4.373094	-0.806227	-0.937301
C	4.888576	-1.580633	1.482760
C	1.597133	1.818560	1.535627
C	6.490634	-1.769860	-0.464664
C	5.667875	-2.871165	-1.202566
C	4.240674	-2.273323	-1.420986
O	7.528763	-2.285589	0.409523
S	-4.547909	-0.730264	0.303092
Fe	-2.125263	-0.667571	0.162964
C	-1.747514	-3.985905	0.904196
C	-2.419464	-1.440731	-3.184031
C	-2.714292	2.652344	-0.588994
C	-1.955592	0.117735	3.488371
N	-2.133496	-2.368074	-0.912208
C	-1.934290	-3.649851	-0.429694
C	-1.919734	-4.592709	-1.525049
C	-2.096051	-3.874872	-2.674025
C	-2.225313	-2.486621	-2.292220
N	-2.510042	0.392304	-1.545051
C	-2.563498	-0.105488	-2.838229
C	-2.809878	0.973831	-3.770402
C	-2.903986	2.122928	-3.037557
C	-2.715444	1.758757	-1.649644
N	-2.341645	1.028291	1.234885
C	-2.546048	2.309431	0.744445
C	-2.541135	3.259464	1.835183
C	-2.335335	2.549102	2.983824
C	-2.204024	1.158878	2.605833
N	-1.872140	-1.714038	1.843572
C	-1.802812	-1.213385	3.132254
C	-1.578285	-2.293907	4.069816

C	-1.524616	-3.448107	3.344880
C	-1.713472	-3.085797	1.955929
O	-0.422676	-0.465720	-0.014199
H	3.336227	4.098051	-0.454542
H	3.942000	1.911576	-1.077650
H	2.588995	-0.493207	0.246443
H	2.721100	0.366995	-2.680484
H	1.757550	-0.949452	-2.006911
H	0.272481	0.423143	-0.858366
H	0.364232	1.128769	-2.477390
H	-0.242121	3.317854	-2.029634
H	1.928227	5.837905	0.562387
H	1.069718	4.664907	1.543973
H	4.250191	1.136057	1.869186
H	5.008649	2.484027	1.042688
H	6.370532	0.982931	-0.346510
H	4.053612	-1.044268	1.940616
H	1.226243	0.796382	1.424341
H	0.733858	2.441466	1.790244
H	7.048794	-1.164601	-1.186895
H	6.151178	-3.158661	-2.141734
H	5.628059	-3.776214	-0.581513
H	3.490781	-2.812081	-0.828222
H	3.923489	-2.333798	-2.466965
H	4.869976	-0.252489	-1.755571
H	5.689735	-1.637705	2.230030
H	4.540462	-2.599487	1.276310
H	2.296540	1.855702	2.377862
H	3.389319	3.883006	1.294855
H	6.592654	0.569990	1.353599
H	7.148513	-2.950247	1.018565
H	-4.792612	-1.511441	-0.809939
H	-1.608759	-5.035926	1.139460
H	-2.475801	-1.691684	-4.238256
H	-2.831306	3.705882	-0.819205
H	-1.877843	0.364676	4.542008
H	-1.785894	-5.659037	-1.415191
H	-2.136652	-4.237669	-3.690855
H	-2.903060	0.852273	-4.839856
H	-3.087216	3.128615	-3.386659
H	-2.673533	4.324725	1.715682
H	-2.273302	2.917692	3.997409
H	-1.486281	-2.168399	5.138858
H	-1.378526	-4.457564	3.700744

## Frequencies:

-192.2106	-17.2793	-6.1612
10.3663	18.1632	32.6632
34.8598	52.8879	55.0110
56.6881	76.3140	89.0137
94.7329	100.2826	118.0896
129.2530	144.2330	151.6984
153.3350	158.0374	176.5760
182.6968	189.2859	204.2007
210.8129	219.5796	220.4813
227.0978	234.6552	240.5438
256.3596	267.6103	274.7407
276.3445	282.2467	284.4728
286.2643	287.6933	297.3804
307.4242	313.4975	320.0021
328.2236	332.1076	338.9864
361.5748	372.0616	373.2983
375.2559	379.5269	384.5851
398.6956	420.1026	422.2362
424.4001	435.1149	436.8282
439.5830	441.1610	448.5775
468.7067	470.8506	485.8400
508.8933	518.7205	542.2133
555.9650	560.8037	575.9620
577.7465	592.2923	621.0799
647.5258	660.3725	678.5138



679.2509	685.4227	690.0283
691.2442	702.5058	723.6624
725.0479	729.8342	735.3665
739.3368	761.7104	764.3182
765.9422	766.4063	798.6376
802.0940	811.7512	812.9969
821.5453	823.0609	823.5651
834.3161	834.8520	849.0444
852.3403	852.9146	857.9216
881.2305	904.2364	904.8730
917.1333	918.9852	930.1208
934.1569	934.8659	942.5659
952.2698	952.9895	953.2421
958.8542	967.5847	974.4775
985.2477	992.5657	1002.9957
1018.8231	1024.7193	1025.1447
1026.7064	1028.0503	1034.9485
1038.7414	1048.9836	1051.1744
1059.6271	1061.0060	1062.6132
1064.4803	1076.9674	1078.8269
1087.1506	1101.4182	1117.6545
1117.9932	1120.4079	1124.0431
1128.6994	1137.6946	1150.2752
1163.8008	1169.5327	1175.5316
1182.4109	1189.4771	1192.4938
1200.7800	1214.2161	1218.6967
1233.7042	1240.7420	1243.8482
1246.2157	1257.3308	1265.2451
1279.5341	1289.1563	1295.1029
1298.4894	1300.2505	1306.7403
1319.9022	1320.8783	1325.5132
1331.5572	1336.1012	1345.5517
1350.0244	1351.3238	1357.3828
1363.2591	1376.4081	1378.3361
1387.8448	1388.5281	1389.9398
1394.4644	1398.2904	1400.7216
1408.7760	1412.8440	1415.3009
1417.8440	1422.7068	1423.2868
1429.2371	1432.4343	1435.9348
1437.3347	1452.3921	1461.3912
1499.8291	1501.2558	1504.8915
1510.1114	1529.5766	1531.4265
1534.0979	1536.3899	1537.7551
1540.3682	1545.3035	1550.4180
1556.6114	1559.1938	1562.3898
1564.6058	1585.6508	1591.8826
1594.2492	1614.2457	1615.9465
1642.2810	1644.3153	1652.8377
1715.5701	1818.8882	2507.7066
2953.9758	2965.2821	2990.3511
3018.6544	3032.3386	3039.7276
3042.0658	3046.2839	3050.7582
3051.7379	3059.7850	3060.2446
3073.2557	3077.8799	3078.4978
3090.3700	3092.1943	3096.7425
3097.4071	3101.5183	3110.7121
3118.3704	3129.4418	3142.4918
3149.6507	3205.0794	3211.3689
3213.4691	3213.5721	3222.0228
3262.6768	3263.0522	3264.5617
3266.0592	3285.6206	3286.2828
3287.4914	3288.9824	3633.2953

### III.D.15. Point P15

Absolute energy: -2476.59621

Geometry:

C	0.490294	3.390440	-1.230558
C	0.522304	4.649516	-0.510880
C	1.571123	4.803900	0.576373
C	5.415643	-0.872689	0.212693
O	-0.314775	5.558981	-0.747654
C	2.736856	3.811672	0.422780
C	2.280225	2.334649	0.229773
C	3.522572	1.445842	-0.168110
C	3.111301	-0.001161	-0.590523
C	2.162211	0.058638	-1.801297
C	1.009622	1.034909	-1.619308
C	1.250710	2.288636	-0.913215
C	4.651468	1.457511	0.900921
C	5.861580	0.563745	0.535241
C	4.373968	-0.806171	-0.935961
C	4.888734	-1.580752	1.483251
C	1.595801	1.818631	1.531349
C	6.490891	-1.769935	-0.464340
C	5.667981	-2.871075	-1.202429
C	4.240847	-2.273004	-1.420441
O	7.529115	-2.285940	0.409544
S	-4.556132	-0.730484	0.303094
Fe	-2.126687	-0.668293	0.163679
C	-1.748136	-3.986041	0.903930
C	-2.419506	-1.441250	-3.184457
C	-2.713863	2.652965	-0.588844
C	-1.956368	0.117870	3.488733
N	-2.134281	-2.368659	-0.913653
C	-1.934388	-3.650155	-0.429362
C	-1.919671	-4.593722	-1.525531
C	-2.095648	-3.875983	-2.674649
C	-2.225117	-2.486819	-2.292979
N	-2.513555	0.390003	-1.541994
C	-2.566037	-0.107355	-2.836929
C	-2.809748	0.972856	-3.768968
C	-2.903466	2.122227	-3.035975
C	-2.717312	1.758523	-1.647473
N	-2.341048	1.028488	1.234342
C	-2.545513	2.309689	0.743860
C	-2.540895	3.259841	1.835422
C	-2.335719	2.549435	2.984211
C	-2.204305	1.158385	2.606075
N	-1.881686	-1.716571	1.847293
C	-1.805928	-1.213762	3.134094
C	-1.577012	-2.294290	4.071294
C	-1.523249	-3.449028	3.345877
C	-1.716328	-3.086906	1.956864
O	-0.432420	-0.496484	0.016238
H	3.340249	4.102500	-0.449309
H	3.945167	1.913247	-1.076382
H	2.581937	-0.491593	0.237544
H	2.744538	0.373547	-2.685353
H	1.771074	-0.940659	-2.026928
H	0.140240	0.349863	-0.820758
H	0.395143	1.150791	-2.504286
H	-0.231658	3.327904	-2.038585
H	1.928412	5.840069	0.564807
H	1.069635	4.666935	1.545494
H	4.250265	1.135927	1.869574
H	5.009106	2.483936	1.043665
H	6.370437	0.982746	-0.346297
H	4.053308	-1.044415	1.940281
H	1.223491	0.797438	1.415642
H	0.733095	2.441795	1.787460
H	7.049114	-1.164516	-1.186327
H	6.151174	-3.158487	-2.141591
H	5.628268	-3.776086	-0.581500
H	3.490829	-2.811961	-0.828163
H	3.923827	-2.332841	-2.466524

H	4.872466	-0.253127	-1.753870
H	5.689331	-1.637585	2.231034
H	4.540802	-2.599549	1.276639
H	2.293985	1.851403	2.374710
H	3.388754	3.884858	1.299755
H	6.593210	0.570308	1.353752
H	7.148651	-2.949738	1.019548
H	-4.804431	-1.511053	-0.809886
H	-1.607393	-5.035716	1.138612
H	-2.473521	-1.690974	-4.238841
H	-2.827514	3.706465	-0.819821
H	-1.876434	0.365811	4.541752
H	-1.786088	-5.660019	-1.414954
H	-2.136438	-4.238207	-3.691677
H	-2.900796	0.851327	-4.838626
H	-3.084343	3.128389	-3.385027
H	-2.673321	4.325050	1.715274
H	-2.274104	2.917542	3.998008
H	-1.481940	-2.168127	5.139990
H	-1.373948	-4.458288	3.700994

## Frequencies:

-1870.1696	8.4644	10.9551
17.2347	33.9089	38.8238
41.4703	53.9110	57.3328
57.9941	69.8373	92.8498
100.0271	104.2228	114.8515
131.3225	142.0730	153.3119
155.7733	159.8173	162.9558
183.4682	197.5586	207.2883
210.9028	218.2449	221.1572
224.2074	231.7429	234.5929
243.9371	264.9604	271.4477
275.7289	278.3692	283.8237
287.8195	288.8077	297.2233
302.3589	314.7139	321.9973
328.8849	333.6129	340.1034
362.4211	368.4044	372.4228
373.9259	378.6479	383.8171
399.0079	413.8071	421.4161
424.7818	435.7036	436.9409
437.5011	442.1335	442.3735
462.6219	474.0129	486.3538
497.1689	516.4205	519.6889
560.0166	560.1344	575.5274
576.8944	618.0363	628.3365
656.2920	665.3223	679.2916
680.1504	683.9002	690.9223
694.1275	704.6867	723.5164
724.9938	730.5974	735.0794
738.1810	761.0931	764.7759
765.8161	766.1975	769.5142
800.4280	801.3800	811.0052
812.2615	821.0292	826.8531
828.9095	833.8084	834.5107
849.1949	852.0970	853.3211
864.2790	883.6044	901.4613
903.2387	913.9591	916.2066
931.2566	934.0241	936.4794
941.3577	950.9933	951.4707
952.3968	957.1395	969.2416
974.3444	984.5467	992.0391
1002.2447	1018.9086	1023.4206
1024.3668	1024.7324	1028.2394
1033.7663	1038.8054	1048.7346
1049.7373	1059.7213	1061.0916
1062.2572	1063.5455	1078.5396
1079.3924	1087.4555	1101.8128
1117.0778	1117.4872	1119.6378
1123.1672	1127.8520	1138.6665
1150.4458	1169.8327	1171.8150

1175.8963	1181.0081	1189.8117
1192.3895	1201.9960	1214.3307
1217.6338	1230.7942	1239.9364
1243.8075	1245.2246	1257.0925
1265.5467	1277.8290	1282.4630
1295.2302	1296.4070	1298.4650
1307.4140	1320.6933	1325.4239
1332.7024	1334.9584	1339.7963
1342.9133	1345.7683	1352.6748
1353.5637	1357.8075	1363.5082
1378.2472	1380.1651	1387.8737
1388.5281	1389.8501	1396.0015
1398.9548	1401.8865	1409.6935
1412.2700	1415.9896	1420.4822
1424.3575	1428.5091	1430.5951
1436.3912	1437.5565	1452.7285
1462.3938	1500.9171	1502.2220
1504.5326	1510.1374	1526.2983
1529.6746	1533.8213	1536.3346
1539.5251	1540.1595	1545.3683
1550.5364	1556.2797	1558.4467
1562.4473	1564.5927	1576.7826
1592.8737	1594.1475	1616.7878
1625.0673	1636.6389	1643.5124
1645.6713	1716.2450	2506.6403
2952.2760	2964.0366	2978.7974
3018.9956	3032.3117	3041.1192
3043.2506	3047.1139	3052.3783
3054.8996	3060.5687	3061.1975
3074.2266	3078.5445	3079.7829
3093.5269	3097.1390	3098.0773
3102.9530	3111.6557	3118.9923
3129.7791	3142.7298	3150.4212
3203.9688	3210.4011	3212.9545
3214.6861	3214.7694	3223.4233
3262.3068	3262.7471	3263.9635
3265.5720	3285.3654	3286.0110
3286.9364	3288.5389	3632.2098

### III.D.16. Point P16

Absolute energy: -2476.6026742

Geometry:

C	0.502054	3.397018	-1.236330
C	0.523734	4.652772	-0.511084
C	1.571807	4.805966	0.578383
C	5.416217	-0.872958	0.213695
O	-0.315579	5.559429	-0.743888
C	2.738455	3.814056	0.426532
C	2.281856	2.337883	0.227387
C	3.524413	1.447440	-0.168343
C	3.112707	0.001722	-0.595051
C	2.179626	0.068955	-1.817781
C	1.009194	1.031390	-1.633014
C	1.259991	2.302522	-0.921690
C	4.651948	1.457521	0.901896
C	5.861921	0.563656	0.536097
C	4.375350	-0.805832	-0.934761
C	4.888793	-1.580780	1.483848
C	1.593877	1.818282	1.525796
C	6.491466	-1.769957	-0.463695
C	5.668230	-2.870992	-1.201961
O	4.241318	-2.272385	-1.419630
O	7.529208	-2.286382	0.409584
S	-4.567478	-0.730312	0.302590

Fe	-2.122178	-0.668926	0.164331
C	-1.749622	-3.984419	0.903437
C	-2.419773	-1.440820	-3.182798
C	-2.712556	2.651565	-0.588466
C	-1.958053	0.117852	3.487188
N	-2.136151	-2.369802	-0.915224
C	-1.935180	-3.650175	-0.430443
C	-1.919483	-4.593762	-1.525339
C	-2.095137	-3.876211	-2.674466
C	-2.225083	-2.488253	-2.292102
N	-2.520518	0.387631	-1.538471
C	-2.569122	-0.108426	-2.834954
C	-2.809607	0.971596	-3.766334
C	-2.902761	2.120477	-3.033683
C	-2.719113	1.756932	-1.645938
N	-2.342236	1.028947	1.233759
C	-2.544668	2.309049	0.744868
C	-2.540412	3.259102	1.835427
C	-2.335980	2.548872	2.983925
C	-2.205205	1.158679	2.605662
N	-1.892311	-1.719596	1.852003
C	-1.809953	-1.216195	3.135098
C	-1.575791	-2.294530	4.071877
C	-1.521922	-3.449340	3.346302
C	-1.720169	-3.087029	1.959164
O	-0.447617	-0.522191	0.041567
H	3.344233	4.106881	-0.443698
H	3.949569	1.915546	-1.075394
H	2.575087	-0.489314	0.228011
H	2.775019	0.388458	-2.690140
H	1.791568	-0.930408	-2.051553
H	0.205297	0.411890	-0.920054
H	0.451837	1.187043	-2.553865
H	-0.216234	3.336760	-2.048929
H	1.929549	5.842614	0.568312
H	1.068817	4.668360	1.547123
H	4.249994	1.135211	1.870549
H	5.010299	2.484075	1.046093
H	6.370627	0.982952	-0.345873
H	4.052039	-1.044335	1.939591
H	1.219626	0.797778	1.405831
H	0.732360	2.443243	1.783330
H	7.048277	-1.163961	-1.187081
H	6.151421	-3.158110	-2.141914
H	5.628240	-3.776715	-0.581230
H	3.490719	-2.811508	-0.827265
H	3.924107	-2.331470	-2.466212
H	4.875598	-0.254158	-1.752837
H	5.688413	-1.637373	2.233433
H	4.541350	-2.600267	1.277216
H	2.291238	1.845666	2.370735
H	3.388275	3.886151	1.305986
H	6.594307	0.570290	1.354655
H	7.148426	-2.948552	1.019470
H	-4.819453	-1.507634	-0.810865
H	-1.605492	-5.034528	1.137683
H	-2.470750	-1.689637	-4.238254
H	-2.821992	3.706007	-0.820455
H	-1.874673	0.366776	4.540477
H	-1.785588	-5.660884	-1.415569
H	-2.135362	-4.239547	-3.691912
H	-2.898006	0.851407	-4.837125
H	-3.079998	3.127588	-3.384147
H	-2.671916	4.325250	1.715818
H	-2.274445	2.918167	3.998105
H	-1.476417	-2.168820	5.140989
H	-1.368164	-4.458493	3.702125

## Frequencies:

-406.5347	-6.5620	6.9797
12.2187	23.8141	33.2339

36.9300	52.7541	55.6507
56.7342	71.2660	84.8860
93.8158	100.8276	117.3090
131.8040	136.3229	147.0602
152.7797	155.7111	164.0524
185.4436	189.5240	203.7725
211.5014	219.0056	220.0700
222.5016	233.6635	238.2387
248.8492	266.5675	273.0607
277.4366	280.9770	282.0317
285.8720	287.7391	297.0135
303.9371	313.6785	318.8310
320.4897	329.3214	335.2401
360.2592	371.8650	372.4264
376.8856	379.5054	384.4169
400.0723	418.7427	421.0400
423.4492	435.2450	436.9379
439.5315	441.1468	449.1124
469.7680	471.5022	485.8327
510.1264	518.5725	554.3168
560.1758	560.2799	575.3471
579.1934	620.6266	631.9313
655.0344	660.0178	678.9836
679.6023	687.5313	689.9353
691.1393	705.4299	725.0388
726.2875	731.0178	735.8504
741.1103	761.9303	765.7487
767.0501	767.4588	799.8040
805.0502	814.6850	816.0911
822.1401	824.8728	825.9677
834.8700	835.5213	850.0357
852.7314	854.6161	862.5704
879.2427	907.3871	908.1459
920.4895	922.7591	931.6830
935.0299	938.3997	945.8900
953.3646	955.7460	956.8401
962.8033	968.4464	974.8098
985.0967	991.2565	1000.5166
1018.2416	1020.9822	1025.7256
1026.6569	1028.4144	1036.5740
1039.2475	1048.2275	1049.2975
1060.5935	1062.5510	1062.7497
1064.4044	1079.3737	1080.8392
1088.1060	1102.7648	1119.5657
1120.0196	1122.3004	1125.9680
1128.3612	1138.1073	1149.2756
1163.8000	1169.8633	1176.1203
1183.3223	1192.0218	1194.9426
1200.6279	1203.5678	1219.7794
1220.3451	1243.0858	1248.0285
1255.4344	1256.8112	1261.3601
1272.2943	1286.2693	1294.9659
1300.3026	1302.1119	1305.1558
1309.4356	1318.6783	1322.6029
1333.4652	1335.5893	1346.2030
1351.5044	1353.0752	1358.1021
1363.2736	1370.7438	1378.3272
1389.1113	1389.8237	1391.4361
1397.0590	1397.8943	1399.7471
1406.1527	1412.3433	1414.5084
1418.7417	1420.4666	1423.9687
1431.1186	1436.4591	1438.4636
1448.2962	1453.1397	1458.6084
1468.9150	1501.7670	1502.6372
1504.4517	1510.4744	1530.0087
1534.1513	1536.1087	1536.8693
1538.9191	1540.4742	1545.6051
1550.7970	1557.1851	1559.8176
1562.9066	1564.8291	1592.7974
1594.2996	1613.0063	1616.6185
1632.0543	1644.2924	1646.8963

1658.4866	1717.8093	2512.2963
2950.0526	2961.7355	2988.6962
3015.1533	3028.6539	3036.4774
3038.3368	3042.5081	3047.5585
3048.8681	3055.8831	3056.2800
3068.9926	3073.3141	3074.0371
3087.6438	3092.1718	3092.5460
3096.8391	3106.5554	3113.8861
3124.9295	3137.6394	3145.2748
3161.2833	3196.6827	3207.3210
3208.3022	3208.5943	3217.8536
3255.5479	3256.0769	3257.4357
3258.9061	3278.5247	3279.2296
3280.3893	3281.8518	3645.5984

### III.D.17. Point P17

Absolute energy: -2476.6012371

Geometry:

C	0.484466	3.389006	-1.228689
C	0.522682	4.647688	-0.511460
C	1.570892	4.802880	0.575835
C	5.415443	-0.872642	0.212484
O	-0.314048	5.558220	-0.748888
C	2.735848	3.810392	0.420977
C	2.279761	2.332495	0.230000
C	3.522436	1.445722	-0.168191
C	3.111465	-0.001732	-0.589332
C	2.153252	0.055084	-1.793193
C	1.016704	1.042757	-1.615187
C	1.244992	2.277266	-0.910059
C	4.651449	1.457286	0.900795
C	5.861493	0.563719	0.535139
C	4.373863	-0.806157	-0.936872
C	4.888567	-1.580646	1.483043
C	1.596360	1.818907	1.532380
C	6.490993	-1.770004	-0.464315
C	5.667969	-2.871032	-1.202358
C	4.240836	-2.273072	-1.420555
O	7.528721	-2.285809	0.409563
S	-4.551523	-0.730451	0.303193
Fe	-2.130437	-0.669033	0.164350
C	-1.747741	-3.986522	0.904255
C	-2.419699	-1.441809	-3.184564
C	-2.714635	2.652922	-0.588603
C	-1.955914	0.117377	3.489301
N	-2.134695	-2.369277	-0.913054
C	-1.934521	-3.649599	-0.428604
C	-1.919691	-4.592355	-1.524845
C	-2.095760	-3.874814	-2.673862
C	-2.225591	-2.485962	-2.293189
N	-2.509634	0.391720	-1.544876
C	-2.564601	-0.106901	-2.836627
C	-2.809665	0.972415	-3.768534
C	-2.903430	2.122066	-3.035471
C	-2.716113	1.758342	-1.647739
N	-2.341124	1.029017	1.235678
C	-2.545871	2.309629	0.743375
C	-2.540805	3.258896	1.834710
C	-2.335451	2.548241	2.983453
C	-2.204084	1.157778	2.605602
N	-1.878976	-1.715889	1.845869
C	-1.805531	-1.212524	3.133679
C	-1.577650	-2.293557	4.069834
C	-1.523907	-3.448039	3.344556

C	-1.716056	-3.086790	1.955649
O	-0.414338	-0.478502	-0.001668
H	3.339690	4.101900	-0.451461
H	3.945008	1.913539	-1.076755
H	2.584978	-0.492503	0.240966
H	2.726977	0.371805	-2.684223
H	1.762272	-0.944816	-2.019183
H	0.070829	0.285413	-0.728247
H	0.343770	1.117921	-2.463352
H	-0.241118	3.325822	-2.034596
H	1.929024	5.839577	0.564003
H	1.069650	4.666041	1.545670
H	4.249823	1.135597	1.869885
H	5.009192	2.484442	1.043554
H	6.370955	0.983208	-0.346520
H	4.052589	-1.044382	1.941006
H	1.224177	0.796593	1.419000
H	0.732052	2.441483	1.788065
H	7.048841	-1.164116	-1.187460
H	6.151368	-3.158570	-2.142356
H	5.627661	-3.776647	-0.581274
H	3.490475	-2.812185	-0.827595
H	3.923831	-2.333736	-2.467585
H	4.872379	-0.252846	-1.755170
H	5.689601	-1.637493	2.231273
H	4.540595	-2.600168	1.276712
H	2.294201	1.853816	2.376761
H	3.388623	3.883026	1.298188
H	6.593420	0.569993	1.354296
H	7.149472	-2.949070	1.017907
H	-4.795175	-1.511921	-0.808601
H	-1.607246	-5.037073	1.139161
H	-2.475515	-1.691838	-4.239725
H	-2.832153	3.706978	-0.819616
H	-1.876928	0.365530	4.543246
H	-1.785691	-5.660048	-1.414504
H	-2.136468	-4.238090	-3.692024
H	-2.902492	0.850778	-4.839448
H	-3.086646	3.129079	-3.385284
H	-2.674209	4.325533	1.715393
H	-2.273800	2.917099	3.998477
H	-1.483106	-2.167905	5.140070
H	-1.375153	-4.458538	3.700680

## Frequencies:

-1348.3685	9.1622	12.3053
18.4388	34.8485	38.0085
43.7607	53.5273	57.4163
59.5309	70.2106	90.6655
101.2531	105.8027	115.0157
132.0518	137.4330	150.0760
154.6191	156.9867	165.9275
186.0730	198.4003	202.9621
212.3902	213.3176	218.7164
221.1571	230.7838	233.5141
244.5868	267.2793	267.4574
271.5778	279.1500	285.2385
288.3295	289.8843	297.5980
302.0359	309.7155	317.1997
323.6972	329.1188	333.5246
364.2176	365.1802	372.8274
373.3887	379.8089	384.3913
399.2894	417.3140	424.4289
425.2489	437.3142	437.4033
437.6725	442.2289	443.3861
462.8773	477.6922	487.1014
505.5416	519.9362	529.0268
560.5909	561.2784	577.7661
584.1044	620.1207	633.0299
657.5240	676.5303	680.4546
682.1787	683.2095	691.9826



699.3159	703.3637	724.2727
726.5948	731.8530	734.0890
737.1153	747.4841	761.8660
765.7701	766.8948	767.3798
802.9934	803.7999	814.3592
815.8402	824.9835	827.3409
832.3515	833.1150	834.2706
850.6681	852.2060	855.6996
862.4540	884.2372	900.1550
900.9618	913.0029	915.5582
928.9548	933.5450	935.3297
945.6102	951.4041	953.9465
954.2381	958.9676	967.7752
974.7644	984.7674	994.4616
1001.9603	1019.1302	1022.0312
1024.7217	1026.2622	1033.7476
1035.8047	1038.5361	1048.8239
1049.8055	1061.9885	1062.9120
1063.5433	1063.7861	1077.2843
1081.4573	1086.2420	1096.2698
1106.5599	1119.6754	1120.2759
1122.1485	1124.8409	1128.7311
1141.5639	1151.9504	1171.8502
1176.6040	1182.0736	1192.6252
1193.5336	1195.7080	1201.7027
1210.2019	1219.2044	1225.2750
1244.6329	1246.9920	1254.4828
1262.9170	1270.6406	1277.5939
1296.1337	1296.2524	1297.8485
1303.2301	1308.9640	1318.6553
1323.3498	1334.2453	1343.5263
1346.8142	1357.6433	1358.9123
1359.3055	1360.8254	1363.8929
1378.9455	1380.4237	1388.6039
1390.4001	1391.7795	1396.4868
1399.6446	1402.9695	1411.0629
1415.3210	1417.6039	1421.1984
1428.9729	1431.3542	1433.3146
1438.4671	1440.2978	1454.6231
1465.2217	1502.2285	1505.0561
1507.0386	1509.2434	1517.2335
1526.9675	1530.5350	1534.8004
1537.3802	1541.6996	1544.1720
1546.7276	1551.3895	1556.9955
1559.7605	1563.1892	1565.3455
1595.6087	1596.7925	1617.8561
1619.2749	1643.1426	1645.5300
1647.2034	1716.2187	2514.7607
2948.2134	2959.0997	2964.6210
3013.8823	3026.2397	3036.6879
3037.8220	3041.7430	3046.9190
3051.1765	3054.5144	3055.8411
3068.1098	3071.2061	3075.3220
3087.9564	3089.2022	3091.9215
3097.4280	3105.8355	3111.7434
3123.0683	3135.8189	3143.9241
3196.2629	3203.1074	3203.4466
3205.5093	3205.5996	3213.2580
3248.4900	3248.9045	3249.9495
3251.5590	3271.7877	3272.4135
3273.0901	3274.6623	3656.5793

### III.E. Geometries, QM energy, and QM frequencies of the supplementary Shepard points in the MCMC calculations for D-abstraction of 6 $\beta$ -d<sub>1</sub>-testosterone by Cpd I of the <sup>4</sup>A state

#### III.E.1. Point P1

Absolute energy: -2476.5997599

Geometry:

C	.482953	3.381366	-1.223328
C	.519942	4.645739	-.511430
C	1.570335	4.801151	.575518
C	5.414912	-.873201	.212924
O	-.312515	5.556234	-.749254
C	2.734546	3.808370	.420509
C	2.277203	2.331293	.232072
C	3.520714	1.444064	-.167452
C	3.109904	-.003718	-.586281
C	2.148466	.050932	-1.788549
C	.979470	1.007475	-1.576941
C	1.239062	2.285004	-.903187
C	4.650753	1.456880	.901268
C	5.860860	.563240	.535782
C	4.372899	-.806714	-.936241
C	4.888325	-1.581009	1.483726
C	1.597006	1.818230	1.536500
C	6.490782	-1.770383	-.463354
C	5.667663	-2.871591	-1.201322
C	4.240485	-2.273698	-1.419752
O	7.528107	-2.286089	.410607
S	-4.548153	-.730770	.304139
Fe	-2.125474	-.668113	.164127
C	-1.747835	-3.985705	.905186
C	-2.419735	-1.441203	-3.182239
C	-2.714512	2.651202	-.587673
C	-1.955868	.116971	3.488837
N	-2.134287	-2.369800	-.911795
C	-1.934643	-3.649793	-.428913
C	-1.920105	-4.592078	-1.523358
C	-2.096389	-3.874362	-2.672175
C	-2.225585	-2.487138	-2.290611
N	-2.511053	.392548	-1.545194
C	-2.563788	-.105498	-2.836441
C	-2.809944	.972729	-3.768212
C	-2.904040	2.121762	-3.035423
C	-2.715573	1.757555	-1.648693
N	-2.342549	1.029002	1.236832
C	-2.546215	2.308504	.745892
C	-2.541331	3.257883	1.835669
C	-2.335574	2.547573	2.984195
C	-2.204355	1.158499	2.606211
N	-1.872992	-1.715314	1.845842
C	-1.803178	-1.214107	3.132978
C	-1.578742	-2.293829	4.069840
C	-1.525079	-3.447862	3.345003
C	-1.713874	-3.085748	1.957106
O	-.419326	-.464123	-.015089
H	3.336575	4.098325	-.453949
H	3.942383	1.911355	-1.076881
H	2.588560	-.494236	.248161
H	2.718036	.368589	-2.680039
H	1.757844	-.951535	-2.006734
H(iso=2)	.236651	.382941	-.819605
H	.355070	1.122096	-2.470192
H	-.244228	3.317161	-2.028271
H	1.928942	5.838063	.563532
H	1.069447	4.664280	1.545969
H	4.249623	1.135344	1.871008
H	5.008826	2.484308	1.043935
H	6.370691	.983088	-.345818

H	4.052481	-1.044468	1.942347
H	1.225867	.794894	1.426173
H	.732623	2.441095	1.792077
H	7.047223	-1.164296	-1.187916
H	6.151172	-3.159084	-2.141764
H	5.627022	-3.777595	-.580140
H	3.490026	-2.813034	-.826415
H	3.923253	-2.334315	-2.467001
H	4.869803	-.252913	-1.755275
H	5.689544	-1.638492	2.232265
H	4.539966	-2.600841	1.277601
H	2.296306	1.855231	2.380073
H	3.389483	3.882726	1.296641
H	6.592972	.569306	1.355337
H	7.148719	-2.949538	1.018197
H	-4.792214	-1.510797	-.807291
H	-1.608787	-5.036971	1.140698
H	-2.476239	-1.692312	-4.237743
H	-2.832406	3.705922	-.818241
H	-1.878011	.364323	4.543706
H	-1.785996	-5.660239	-1.414555
H	-2.136872	-4.238910	-3.690228
H	-2.903544	.852202	-4.839503
H	-3.087677	3.128631	-3.386323
H	-2.673977	4.325022	1.717364
H	-2.273458	2.917947	3.998975
H	-1.486490	-2.169395	5.140741
H	-1.378716	-4.458513	3.702642

## Frequencies:

-775.1503	-4.6476	9.1479
13.6138	26.1437	34.1751
37.5555	52.8925	56.0424
58.0854	71.3903	86.6644
94.5055	101.3006	117.5818
119.2094	134.5916	147.8825
153.8612	155.9690	167.7258
186.9921	193.1682	207.1389
214.1502	219.6482	223.7681
226.3780	233.9073	237.4192
245.9573	267.4228	273.2573
277.4053	280.1102	282.6097
286.8821	287.2838	298.2811
301.4760	307.1767	316.0436
319.4574	331.8951	334.7876
362.4555	370.1012	372.4327
374.7688	380.2788	384.2862
400.1624	418.3726	421.4007
423.2337	436.0264	437.3061
440.1418	442.2414	447.2940
455.0805	470.6157	486.6916
508.2301	518.8631	524.0786
551.2585	561.5576	572.0754
576.0234	588.0956	622.0152
644.9101	656.9789	680.0105
680.8649	687.0136	690.6021
693.6937	701.0691	726.0149
727.5212	730.1834	737.5165
741.4359	762.2935	763.0621
767.3419	767.8817	794.4342
807.3817	810.2519	817.4473
818.7926	826.1678	827.5850
834.8099	835.3115	840.2545
850.2708	853.1228	853.8579
857.4121	872.0340	897.1661
909.1535	915.9430	921.3922
923.3095	935.4492	937.8692
946.0128	949.1415	954.8917
958.3478	958.7041	963.9489
965.2928	975.8127	985.7104
992.4825	1001.3939	1020.0123

1022.1429	1027.3341	1028.2322
1031.5587	1037.7123	1038.7618
1049.1468	1051.0812	1062.2494
1062.9592	1063.9485	1064.2076
1079.9536	1081.6195	1086.7043
1102.0328	1121.5663	1121.8795
1124.2700	1127.8393	1128.5602
1139.4266	1150.7390	1172.6544
1173.1080	1176.3287	1186.2363
1194.4507	1197.4574	1200.9016
1216.2277	1219.9317	1222.5652
1243.0076	1243.9456	1249.6262
1257.8002	1265.1895	1276.3991
1282.5525	1295.9830	1301.4832
1303.4629	1308.1524	1317.1484
1323.3225	1330.4795	1333.2282
1337.9811	1346.9715	1354.7597
1355.7352	1359.0658	1364.5443
1377.8704	1379.9797	1390.6522
1392.4186	1393.4305	1396.5982
1399.8757	1402.2145	1410.8587
1416.7932	1417.4975	1420.7812
1427.0251	1432.3838	1433.1682
1437.6253	1439.3678	1454.6316
1463.7652	1501.7481	1503.8105
1507.2873	1511.1726	1530.3862
1530.7915	1535.1704	1537.3376
1540.9941	1541.4024	1546.3628
1551.4389	1557.3540	1561.1709
1563.3073	1565.5744	1593.8954
1595.8419	1607.9600	1618.4024
1620.4071	1643.3762	1645.1889
1653.0804	1716.0487	2521.6529
2948.3303	2959.6242	2979.2365
3011.2139	3023.9763	3032.4896
3033.7489	3038.2476	3043.3789
3044.3194	3050.9565	3051.5381
3064.1469	3067.6777	3069.0049
3083.2301	3085.8748	3087.5189
3088.0784	3092.5255	3101.8172
3108.1003	3119.9155	3132.6468
3139.8901	3194.5397	3199.0898
3201.0515	3201.1581	3209.3943
3246.0466	3246.3876	3247.7900
3249.3533	3269.1584	3269.7838
3270.8501	3272.3814	3659.9776

## III.E.2. Point P2

Absolute energy: -2476.5997129

Geometry:

C	.480342	3.382187	-1.223892
C	.520696	4.645809	-.510925
C	1.570280	4.801112	.575591
C	5.414854	-.873093	.212962
O	-.312829	5.556488	-.749586
C	2.734459	3.808321	.420084
C	2.277558	2.330687	.232267
C	3.520858	1.444153	-.167354
C	3.110130	-.003792	-.585989
C	2.145477	.049568	-1.785413
C	.990906	1.019198	-1.584323
C	1.238274	2.277443	-.902875
C	4.650800	1.456848	.901325
C	5.860924	.563258	.535774
C	4.372869	-.806755	-.936460
C	4.888270	-1.581038	1.483747
C	1.597027	1.818331	1.536640
C	6.490650	-1.770433	-.463430
C	5.667615	-2.871572	-1.201391
C	4.240393	-2.273793	-1.419828
O	7.528197	-2.286050	.410625
S	-4.546862	-.730705	.304152
Fe	-2.128469	-.668715	.164696
C	-1.747577	-3.986522	.905520
C	-2.419762	-1.441843	-3.183011
C	-2.714824	2.652014	-.587623
C	-1.955594	.116738	3.489802
N	-2.134014	-2.369450	-.911210
C	-1.934606	-3.649831	-.428191
C	-1.920074	-4.592380	-1.523563
C	-2.096368	-3.874703	-2.672465
C	-2.225760	-2.486536	-2.291475
N	-2.509036	.392847	-1.545814
C	-2.563420	-.105719	-2.836390
C	-2.809984	.972803	-3.768691
C	-2.904072	2.122208	-3.035720
C	-2.715364	1.757816	-1.648437
N	-2.341957	1.028691	1.237073
C	-2.546390	2.308951	.745173
C	-2.541318	3.258334	1.835744
C	-2.335531	2.547798	2.984441
C	-2.204222	1.158014	2.606326
N	-1.872288	-1.714686	1.844622
C	-1.803257	-1.213036	3.133440
C	-1.578734	-2.294033	4.070186
C	-1.525069	-3.448045	3.345336
C	-1.713943	-3.086360	1.956398
O	-.406300	-.454071	-.024706
H	3.336841	4.098542	-.453916
H	3.942459	1.911539	-1.076670
H	2.588743	-.494335	.247849
H	2.711282	.368991	-2.680417
H	1.755856	-.952275	-2.006043
H(iso=2)	.152971	.298041	-.733116
H	.331346	1.108331	-2.452722
H	-.247533	3.317460	-2.027437
H	1.928633	5.837809	.563429
H	1.069470	4.664313	1.545769
H	4.249583	1.135377	1.870734
H	5.008586	2.484145	1.043692
H	6.370717	.982940	-.345713
H	4.052641	-1.044728	1.942515
H	1.225333	.795397	1.426460

H	.732353	2.440586	1.792062
H	7.047905	-1.164532	-1.187183
H	6.151072	-3.159148	-2.141486
H	5.627080	-3.777253	-.580224
H	3.490113	-2.812953	-.826630
H	3.923335	-2.334741	-2.466934
H	4.870149	-.252835	-1.755162
H	5.689640	-1.638291	2.231751
H	4.539977	-2.600598	1.277609
H	2.296142	1.856016	2.379932
H	3.388946	3.881979	1.296029
H	6.592728	.569384	1.355196
H	7.149036	-2.949916	1.018566
H	-4.789801	-1.511648	-.807579
H	-1.608681	-5.037466	1.140812
H	-2.476895	-1.692703	-4.238192
H	-2.834318	3.706214	-.818144
H	-1.878184	.364279	4.544281
H	-1.786067	-5.660217	-1.414024
H	-2.137048	-4.238623	-3.690472
H	-2.904088	.851584	-4.839607
H	-3.088673	3.128886	-3.385985
H	-2.674674	4.325111	1.717115
H	-2.273635	2.917364	3.999263
H	-1.486656	-2.169046	5.140790
H	-1.378895	-4.458704	3.702273

## Frequencies:

-1179.2255	8.8579	13.3300
18.9987	34.4069	36.3496
42.5460	53.9287	57.3326
59.0985	71.0771	95.4067
102.2135	104.3995	116.1852
131.9555	136.1534	145.4661
154.1561	156.9260	168.0379
187.3018	199.7543	209.1594
213.4730	214.9602	221.2711
224.0838	231.0797	234.1424
246.1554	268.2133	272.2571
272.4787	279.1954	284.4448
287.9652	289.2642	298.2549
301.5398	311.0581	317.3359
323.4072	331.3874	334.6147
364.3543	366.4944	372.8165
373.5759	380.1018	384.3896
399.6234	417.9135	423.6525
425.0667	437.0331	437.3839
439.1585	442.4949	443.2539
462.2481	475.1470	487.1382
507.0082	519.6444	533.4724
557.4525	561.7568	577.2935
584.2708	614.6403	623.9340
644.9547	658.3286	680.5502
681.9613	683.8933	691.6382
698.0878	700.7070	712.4412
725.9566	727.0980	730.7356
736.8200	738.6852	761.9175
762.5181	766.7172	767.4315
784.6798	803.9952	810.6670
814.7855	816.2711	818.0438
825.5709	831.4195	833.7265
834.4684	844.1590	851.0232
852.4735	855.9787	871.5945
903.0114	903.9584	910.3938
915.2700	917.5438	931.2903
935.2275	946.4335	952.0122
955.0156	955.2891	958.4704
960.0404	974.1963	979.7955
989.1275	997.7365	1012.8014
1021.3183	1024.2271	1026.1958
1033.8626	1036.1184	1037.9125

1045.6499	1050.3063	1059.4878
1063.0226	1063.2426	1063.9153
1074.4086	1081.6585	1084.8981
1100.0197	1105.9214	1120.1506
1120.3471	1122.7818	1125.7868
1130.6589	1141.9855	1151.5464
1172.0200	1176.0921	1180.9782
1194.0005	1196.4067	1196.9507
1200.9778	1213.2347	1220.4604
1233.8943	1244.1631	1247.6754
1255.8444	1263.1535	1272.3638
1278.7917	1296.1199	1297.8853
1300.1627	1308.3447	1316.2146
1322.7472	1332.7827	1338.5923
1346.7980	1353.4480	1358.1381
1358.3816	1359.2620	1363.5825
1376.7983	1380.0913	1389.6567
1390.6094	1392.4525	1396.1514
1399.3637	1401.8667	1410.5309
1415.7826	1417.8060	1421.0386
1428.7283	1433.2673	1433.5120
1438.1920	1440.6359	1454.7227
1465.0000	1502.2641	1504.4666
1507.7146	1510.7392	1521.0549
1530.4825	1534.5434	1537.0408
1540.4269	1543.0222	1545.6255
1551.2121	1551.5129	1557.5815
1560.6437	1563.2203	1565.4662
1594.9512	1596.7290	1619.5303
1632.5979	1638.2232	1643.6797
1645.1331	1715.1137	2517.8432
2948.1657	2959.3135	2966.2302
3013.0436	3025.3989	3035.6860
3036.6939	3040.8022	3046.0999
3049.2782	3053.5137	3054.4868
3067.0210	3070.1360	3073.0557
3087.0424	3088.1591	3091.1303
3096.4374	3104.7113	3110.6674
3112.8513	3122.4731	3134.8793
3142.5531	3201.1652	3202.0003
3203.3563	3203.5230	3211.3211
3248.0037	3248.3182	3249.4476
3251.1091	3271.2499	3271.8524
3272.5700	3274.1946	3654.8670

## III.E.3. Point P3

Absolute energy: -2476.6020827

Geometry:

C	.484428	3.381116	-1.223582
C	.519846	4.645951	-.511279
C	1.570421	4.801264	.575517
C	5.414970	-.873176	.212909
O	-.312702	5.556462	-.749053
C	2.734748	3.808520	.420926
C	2.277090	2.331932	.232000
C	3.520646	1.443995	-.167471
C	3.109813	-.003661	-.586610
C	2.150748	.051898	-1.790833
C	.976415	1.003939	-1.576502
C	1.240480	2.289165	-.903780
C	4.650725	1.456968	.901285
C	5.860892	.563234	.535823
C	4.372877	-.806699	-.936033
C	4.888351	-1.581056	1.483779
C	1.596916	1.818109	1.536468
C	6.490608	-1.770346	-.463423
C	5.667647	-2.871625	-1.201364
C	4.240502	-2.273696	-1.419760
O	7.528266	-2.286116	.410624
S	-4.549063	-.730817	.304179
Fe	-2.123785	-.667730	.163762
C	-1.747962	-3.985641	.905052
C	-2.419716	-1.440906	-3.182214
C	-2.714384	2.651158	-.587802
C	-1.956024	.117230	3.488678
N	-2.134180	-2.369238	-.911725
C	-1.934620	-3.650059	-.429003
C	-1.920066	-4.592624	-1.523628
C	-2.096355	-3.874809	-2.672466
C	-2.225516	-2.487320	-2.290465
N	-2.511818	.391826	-1.543959
C	-2.564066	-.105761	-2.836783
C	-2.810042	.973028	-3.768580
C	-2.904135	2.121922	-3.035831
C	-2.715852	1.757836	-1.648581
N	-2.342490	1.028400	1.236167
C	-2.546218	2.308492	.745941
C	-2.541378	3.258302	1.836011
C	-2.335630	2.548103	2.984526
C	-2.204414	1.158603	2.606564
N	-1.873323	-1.715252	1.845896
C	-1.803163	-1.214435	3.132986
C	-1.578612	-2.294057	4.070342
C	-1.524944	-3.448232	3.345438
C	-1.713825	-3.085761	1.957375
O	-.429132	-.471564	-.007904
H	3.336263	4.097889	-.453661
H	3.942010	1.911164	-1.076846
H	2.588180	-.493917	.247606
H	2.722967	.368387	-2.680049
H	1.759779	-.950484	-2.007700
H(iso=2)	.267382	.417248	-.854296
H	.371129	1.131616	-2.481370
H	-.241674	3.317040	-2.029034
H	1.928524	5.837984	.563536
H	1.069394	4.664406	1.545654
H	4.249765	1.135444	1.870820
H	5.008690	2.484082	1.043976
H	6.370469	.982818	-.345721
H	4.052778	-1.044433	1.941946
H	1.226080	.795114	1.425368



H	.733123	2.441249	1.791806
H	7.047662	-1.164527	-1.187173
H	6.151140	-3.159142	-2.141367
H	5.627451	-3.777330	-.580190
H	3.490179	-2.812868	-.826655
H	3.923142	-2.334080	-2.466533
H	4.869687	-.252928	-1.754848
H	5.689513	-1.638414	2.231968
H	4.540038	-2.600561	1.277477
H	2.296399	1.854706	2.379538
H	3.389637	3.883130	1.296716
H	6.592839	.569408	1.355119
H	7.148412	-2.949873	1.018692
H	-4.794222	-1.510904	-.807883
H	-1.608946	-5.036500	1.140556
H	-2.475682	-1.692027	-4.237316
H	-2.830707	3.705637	-.818273
H	-1.877910	.364355	4.543163
H	-1.786013	-5.660170	-1.414468
H	-2.136837	-4.238644	-3.690154
H	-2.903064	.852206	-4.839297
H	-3.086995	3.128522	-3.386085
H	-2.673533	4.324833	1.717048
H	-2.273386	2.917902	3.998888
H	-1.486335	-2.169144	5.140594
H	-1.378537	-4.458489	3.702410

## Frequencies:

-167.6063	-19.0267	-7.3061
9.6276	18.2497	33.2062
34.7294	53.1624	55.3469
56.7877	76.8604	85.9438
92.5782	99.8973	119.5716
126.6801	131.5527	151.5600
153.1884	159.6728	178.2479
183.0335	191.5665	205.5537
212.9674	219.4813	221.4104
226.6093	234.4570	241.8959
256.7931	268.2627	275.3174
276.8707	282.0730	284.0863
286.3997	288.0101	297.3672
305.0797	311.7982	316.5069
320.0395	330.8683	334.2524
361.6401	372.1857	373.6123
375.7868	379.4421	384.4413
399.4487	416.1168	420.9640
423.5822	435.5403	437.0824
440.0202	441.5394	442.7995
465.8093	469.6730	486.1740
509.0596	518.0662	539.4478
558.5715	565.0691	572.4845
576.4398	579.6507	621.5037
644.0746	657.1103	679.2973
680.0337	687.2778	690.1506
691.8329	698.4003	725.4559
726.8396	729.4819	736.8184
741.1900	761.3406	762.6239
766.8581	767.4209	793.6016
806.1110	812.6584	815.9010
817.1475	823.4510	825.8695
834.7871	835.3278	849.6324
851.4776	852.8786	855.6192
871.6681	890.7594	908.7216
916.2715	921.1124	923.0216
934.9235	938.2572	947.2940
947.6538	955.2537	956.9921
957.5700	963.0809	965.8243
976.1796	986.8402	992.7978
1002.2720	1020.0405	1021.8915
1026.9732	1027.0933	1028.7320
1036.8727	1038.5468	1049.3777

1051.1420	1061.4673	1062.3408
1062.8310	1063.5847	1080.4606
1080.8813	1086.7066	1101.8244
1120.4052	1120.7573	1123.1805
1126.7546	1127.7531	1139.7027
1149.3233	1166.7482	1170.2184
1174.7665	1189.4180	1192.5750
1195.4924	1196.5223	1211.5621
1221.1489	1232.2640	1238.0050
1243.5638	1248.5942	1258.2609
1264.2263	1278.4713	1279.4715
1295.3511	1300.8391	1302.5776
1306.7580	1311.6023	1321.6957
1322.8188	1329.1034	1334.3090
1345.7390	1346.8699	1352.9447
1353.6423	1358.4320	1364.7063
1377.5518	1379.5078	1390.1722
1390.5109	1393.0281	1396.2854
1399.7473	1402.1875	1410.4251
1415.4525	1416.6861	1420.4193
1425.0454	1430.7167	1431.4580
1437.1661	1437.8878	1453.7181
1461.8242	1501.1042	1502.6393
1506.1022	1510.7971	1530.2412
1533.7727	1534.7283	1537.0079
1539.1224	1540.9746	1545.9242
1551.0509	1557.0406	1560.5661
1562.9861	1565.2304	1592.6820
1594.7139	1614.5382	1617.0338
1631.7442	1643.1759	1645.0002
1659.4354	1716.1376	2516.6754
2950.4077	2961.6811	2986.7773
3013.5746	3026.6945	3034.4131
3036.1786	3040.6269	3045.1868
3045.9231	3053.7109	3054.0335
3066.8884	3070.5414	3071.3540
3081.7034	3085.6797	3089.4706
3090.8119	3094.9869	3104.5078
3111.3577	3122.8843	3135.8391
3142.8308	3196.8456	3203.2601
3205.1625	3205.2546	3213.6888
3251.7349	3252.1168	3253.6100
3255.1015	3274.7539	3275.4133
3276.6055	3278.0775	3650.9997

## III.E.4. Point P4

Absolute energy: -2476.6019663

Geometry:

C	.479297	3.382199	-1.224411
C	.521250	4.645992	-.510397
C	1.570298	4.801152	.575644
C	5.414854	-.872985	.212970
O	-.313197	5.556853	-.749743
C	2.734519	3.808358	.419974
C	2.277732	2.330557	.232337
C	3.520954	1.444163	-.167297
C	3.110228	-.003843	-.585932
C	2.144453	.049072	-1.784387
C	.995786	1.024107	-1.587873
C	1.238196	2.274610	-.902825
C	4.650822	1.456900	.901407
C	5.861024	.563269	.535794
C	4.372829	-.806767	-.936529
C	4.888221	-1.581111	1.483837
C	1.596978	1.818312	1.536812
C	6.490385	-1.770430	-.463577
C	5.667573	-2.871606	-1.201481
C	4.240311	-2.273885	-1.419914
O	7.528398	-2.286002	.410628
S	-4.546320	-.730676	.304204
Fe	-2.129767	-.668938	.164907
C	-1.747444	-3.987151	.905704
C	-2.419779	-1.442128	-3.183619
C	-2.715002	2.652626	-.587684
C	-1.955475	.116751	3.490478
N	-2.133737	-2.368705	-.910629
C	-1.934557	-3.650088	-.427634
C	-1.920016	-4.593007	-1.523897
C	-2.096334	-3.875279	-2.672925
C	-2.225867	-2.486179	-2.292114
N	-2.507872	.392591	-1.545455
C	-2.563277	-.106118	-2.836648
C	-2.810090	.973083	-3.769361
C	-2.904178	2.122706	-3.036272
C	-2.715362	1.758283	-1.648160
N	-2.341459	1.027964	1.236777
C	-2.546543	2.309348	.744612
C	-2.541348	3.259015	1.836034
C	-2.335526	2.548342	2.984879
C	-2.204140	1.157674	2.606729
N	-1.871872	-1.714065	1.843564
C	-1.803298	-1.212373	3.133836
C	-1.578648	-2.294347	4.070825
C	-1.524978	-3.448459	3.345901
C	-1.713956	-3.086909	1.955990
O	-.403085	-.451856	-.026834
H	3.336603	4.098250	-.453546
H	3.942122	1.911473	-1.076354
H	2.588939	-.494091	.247310
H	2.709076	.368634	-2.680065
H	1.755072	-.951848	-2.005538
H(iso=2)	.126258	.273172	-.707170
H	.323380	1.103740	-2.445860
H	-.248235	3.317816	-2.027011
H	1.927942	5.837238	.563318
H	1.069513	4.664432	1.545172
H	4.249736	1.135531	1.870170
H	5.008205	2.483574	1.043496
H	6.370463	.982517	-.345391
H	4.053208	-1.045046	1.942202
H	1.225309	.796220	1.426203

H	.732773	2.440196	1.791644
H	7.048821	-1.165105	-1.185707
H	6.150834	-3.159168	-2.140677
H	5.627493	-3.776599	-.580473
H	3.490463	-2.812622	-.827135
H	3.923403	-2.334909	-2.466191
H	4.870244	-.252855	-1.754647
H	5.689544	-1.638032	2.230900
H	4.540117	-2.599964	1.277531
H	2.295965	1.856375	2.379259
H	3.388426	3.881559	1.295344
H	6.592241	.569515	1.354740
H	7.148798	-2.950876	1.019536
H	-4.789090	-1.512722	-.808621
H	-1.608744	-5.037162	1.140732
H	-2.477059	-1.692740	-4.237857
H	-2.834701	3.705840	-.817980
H	-1.878280	.364152	4.543995
H	-1.786202	-5.659567	-1.413516
H	-2.137148	-4.237957	-3.690107
H	-2.904170	.851057	-4.838985
H	-3.088932	3.128513	-3.385274
H	-2.674844	4.324477	1.716679
H	-2.273748	2.916576	3.998920
H	-1.486764	-2.168596	5.140153
H	-1.379027	-4.458323	3.701561

## Frequencies:

-844.3844	7.7772	13.6294
18.6491	33.4121	35.9783
41.9059	53.4941	57.5549
58.2950	70.4240	95.0358
102.8047	105.9389	114.9386
131.6687	139.8734	153.6721
156.7994	158.9938	165.1873
183.0999	198.6923	208.8223
210.9155	212.6175	221.2263
221.6562	229.4536	234.1643
244.9443	265.7868	270.3675
271.4565	279.2094	284.9158
288.2983	289.4945	297.7322
301.5347	315.2529	323.7177
327.3055	330.4314	337.5412
364.3823	365.1028	372.7544
373.2549	379.1311	384.2268
398.3255	417.9989	423.6819
426.0549	436.9578	437.1676
440.0659	441.9322	442.9612
462.2143	476.2670	486.7558
508.2585	519.1465	548.2671
558.4778	564.5908	580.1801
592.0849	615.3963	623.5284
642.9926	661.4567	679.2734
681.2577	681.5825	691.7259
698.6165	699.0058	710.9620
723.4943	725.0405	729.7772
735.0591	736.1014	759.5549
761.2949	765.0299	766.3451
770.0668	792.7061	799.1513
808.4713	810.4051	811.8211
820.9017	832.1108	832.7515
833.8687	838.2044	849.5213
851.7019	853.9704	868.8365
894.9981	897.4385	905.4450
909.7783	912.1604	926.1905
934.1688	941.1934	949.9212
950.1408	950.9850	953.9210
955.1595	972.9846	976.9768
987.2948	996.6740	1010.1056
1018.5110	1022.0425	1023.7489
1032.1334	1034.3279	1037.7286

1044.3467	1049.6321	1058.7344
1061.6139	1062.2351	1062.5686
1074.6993	1080.4307	1085.0943
1097.5906	1110.0328	1117.2063
1117.2951	1119.7405	1122.4867
1131.3761	1142.0258	1151.5070
1171.1267	1175.3906	1180.1134
1191.3429	1193.5459	1198.7547
1200.2316	1214.0564	1217.5581
1238.2106	1243.4554	1244.9384
1256.1412	1263.0656	1271.9647
1277.0851	1294.6651	1295.3802
1296.9932	1307.6606	1315.6420
1321.8393	1332.5030	1338.4618
1345.8524	1355.6999	1357.0588
1358.3179	1359.8576	1362.5173
1376.3850	1379.2919	1386.7084
1389.5853	1389.7759	1395.2784
1398.5789	1401.2946	1409.5049
1413.1809	1416.9552	1420.7339
1427.5742	1431.3357	1433.2650
1437.8741	1439.3079	1453.3978
1463.7543	1501.6821	1503.4375
1506.5989	1509.5653	1517.9708
1529.7020	1531.6155	1534.3138
1536.9963	1541.4517	1542.4880
1546.1925	1550.7880	1556.5224
1559.1437	1562.5899	1564.8203
1594.0764	1595.8572	1618.9079
1623.7892	1642.0746	1643.2959
1646.7433	1714.7219	2507.7528
2951.5195	2961.8943	2967.0893
3018.4162	3031.1656	3041.4955
3043.1314	3046.9138	3052.3938
3055.5698	3060.1506	3060.9632
3073.9698	3077.4446	3080.4536
3094.1435	3095.7792	3098.2108
3103.7875	3111.4826	3118.0763
3125.5763	3129.3379	3141.9117
3149.8349	3209.8563	3211.5911
3212.1835	3212.3772	3220.1288
3259.2648	3259.5954	3260.6645
3262.3615	3282.4572	3283.0744
3283.7307	3285.3963	3636.1041

## III.E.5. Point P5

Absolute energy: -2476.6047673

Geometry:

C	.487602	3.383940	-1.223334
C	.519013	4.645569	-.512131
C	1.570336	4.801353	.575496
C	5.415124	-.873443	.212963
O	-.312342	5.555880	-.748516
C	2.735127	3.808904	.421970
C	2.277167	2.333151	.231899
C	3.520391	1.444174	-.167560
C	3.109769	-.003311	-.587262
C	2.156509	.054456	-1.795846
C	.979091	1.004921	-1.583409
C	1.244712	2.296971	-.905996
C	4.650606	1.456895	.901144
C	5.860712	.563206	.535808
C	4.373102	-.806652	-.935519
C	4.888445	-1.580956	1.483688
C	1.596884	1.818151	1.535654
C	6.491163	-1.770277	-.463226
C	5.667822	-2.871638	-1.201140
C	4.240713	-2.273432	-1.419466
O	7.527806	-2.286162	.410515
S	-4.551940	-.731010	.304204
Fe	-2.118620	-.666750	.162833
C	-1.748447	-3.983626	.904294
C	-2.419646	-1.440056	-3.180336
C	-2.713911	2.649280	-.587575
C	-1.956489	.117257	3.486511
N	-2.135187	-2.370901	-.913429
C	-1.934767	-3.649403	-.430038
C	-1.920188	-4.591297	-1.522878
C	-2.096391	-3.873483	-2.671388
C	-2.225333	-2.487870	-2.288831
N	-2.515976	.391493	-1.543561
C	-2.565069	-.105489	-2.835920
C	-2.809714	.972129	-3.766679
C	-2.903740	2.120561	-3.034125
C	-2.716425	1.756800	-1.648450
N	-2.343779	1.029801	1.236473
C	-2.545964	2.307313	.746836
C	-2.541275	3.256606	1.835299
C	-2.335689	2.546862	2.983555
C	-2.204745	1.159085	2.605706
N	-1.876422	-1.717310	1.849295
C	-1.803561	-1.215946	3.132136
C	-1.578641	-2.293156	4.068960
C	-1.524963	-3.447414	3.344038
C	-1.714197	-3.084479	1.958306
O	-.449368	-.489296	.009343
H	3.336780	4.098589	-.453235
H	3.942513	1.911277	-1.077110
H	2.586241	-.494001	.246415
H	2.734221	.369307	-2.681933
H	1.764834	-.948675	-2.012870
H(iso=2)	.287624	.456042	-.895427
H	.400783	1.149156	-2.504762
H	-.237585	3.317659	-2.030598
H	1.929487	5.838577	.563554
H	1.069514	4.664637	1.546461
H	4.249663	1.135321	1.871430
H	5.009179	2.484554	1.044246
H	6.370611	.983415	-.345979
H	4.052079	-1.044040	1.941902
H	1.226422	.794188	1.424334

H	.732704	2.441452	1.792473
H	7.045831	-1.163830	-1.189483
H	6.151289	-3.158881	-2.142253
H	5.626784	-3.778219	-.580085
H	3.489981	-2.813172	-.826012
H	3.923294	-2.333394	-2.467111
H	4.869581	-.253058	-1.755177
H	5.689095	-1.638806	2.233425
H	4.539951	-2.601222	1.277710
H	2.296197	1.853112	2.379910
H	3.390585	3.884846	1.298301
H	6.593332	.569211	1.355525
H	7.147983	-2.948859	1.017457
H	-4.798979	-1.509238	-.806608
H	-1.608910	-5.035313	1.140098
H	-2.474363	-1.691290	-4.236387
H	-2.827909	3.704869	-.818431
H	-1.877416	.364559	4.541833
H	-1.785864	-5.660085	-1.415378
H	-2.136577	-4.239021	-3.689622
H	-2.901887	.853154	-4.838775
H	-3.085122	3.127869	-3.386462
H	-2.672609	4.324481	1.717558
H	-2.273061	2.918837	3.998256
H	-1.485674	-2.169652	5.140404
H	-1.377823	-4.458054	3.702909

## Frequencies:

-30.5783	-18.4169	-9.3723
8.6496	28.9148	32.6522
46.9248	51.9133	53.2834
57.1337	63.0373	86.1764
96.2191	104.8858	109.4540
128.0564	129.6086	149.5318
150.9121	159.4601	177.7345
187.8198	195.7431	210.1951
214.9988	218.3956	221.4860
228.4622	233.7690	235.8208
260.5784	264.9796	275.4433
276.3288	280.6970	281.5576
286.3333	296.6172	297.0854
302.3969	302.8323	314.7358
327.2088	333.8782	342.8703
361.0029	372.2568	375.6657
378.7405	379.8807	384.5665
400.9535	415.1128	419.6550
422.9889	435.3885	437.1832
439.8246	440.9923	441.4695
468.6665	475.2639	486.1904
507.8945	517.7946	539.5858
556.9188	561.2202	575.3543
576.0022	622.5596	643.5722
657.4981	679.3744	680.0943
685.1484	689.5567	691.0094
694.6825	702.6666	727.0867
728.4499	730.6140	738.2073
743.7762	761.4720	764.1316
768.8451	769.4903	793.3450
810.5576	811.7187	820.2392
821.3127	823.2395	830.3784
835.9713	836.6429	850.8535
851.7288	853.9014	857.4986
874.1026	893.2489	913.9778
917.1698	926.2267	928.2673
936.3035	943.2694	952.2400
952.3999	961.5754	961.9458
962.7639	967.4628	968.3348
979.2690	988.6210	994.6630
1005.1191	1022.4132	1024.7660
1030.9386	1031.6269	1032.9324
1038.9457	1041.8332	1049.9551

1052.0651	1064.1670	1064.5944
1065.1227	1066.5553	1082.6624
1084.1524	1087.3897	1102.6324
1123.5966	1123.8817	1126.2616
1129.2995	1130.0218	1139.9998
1149.4045	1170.0800	1173.2566
1176.4494	1197.6123	1198.3072
1199.6214	1201.1896	1214.5221
1226.0274	1237.7208	1244.0850
1252.7445	1256.2288	1264.6652
1273.2932	1283.2335	1295.7515
1297.2552	1306.4461	1307.9021
1308.1491	1316.1793	1318.4957
1324.0678	1334.8448	1338.0912
1347.4896	1354.6556	1356.2325
1359.3506	1365.5020	1377.7944
1380.2877	1390.8557	1395.7724
1397.1623	1398.1137	1400.5888
1404.6804	1411.1416	1417.3679
1419.2502	1420.7721	1428.3073
1430.5044	1435.1074	1437.5109
1442.5925	1455.1288	1462.4785
1502.6565	1505.1204	1507.9221
1511.5341	1530.8589	1535.3028
1536.1591	1537.6659	1541.4926
1541.6440	1546.5064	1551.6719
1557.4106	1562.6971	1563.5868
1565.8707	1594.7908	1596.6226
1612.2684	1618.7755	1634.0173
1644.4390	1646.6147	1668.4711
1717.7722	1852.7006	2528.4531
2946.8547	2958.0601	2987.8291
3008.0619	3020.6110	3028.2357
3029.5890	3034.3850	3038.3610
3039.4184	3046.8559	3047.4143
3059.7948	3062.3772	3063.8098
3067.6460	3078.1570	3081.8073
3083.5282	3087.5575	3097.5276
3103.8949	3115.6979	3128.6571
3134.9644	3187.3896	3195.2436
3196.7801	3196.9081	3205.3998
3241.5807	3242.0152	3243.5124
3244.9558	3264.6219	3265.2948
3266.5319	3267.9505	3669.4800

### III.E.6. Point P6

Absolute energy: -2476.605368

Geometry:

C	.478032	3.382918	-1.224347
C	.521503	4.645696	-.510366
C	1.570246	4.801072	.575658
C	5.414833	-.872975	.212980
O	-.313279	5.556885	-.749925
C	2.734451	3.808284	.419770
C	2.277923	2.330208	.232389
C	3.521012	1.444231	-.167234
C	3.110344	-.003871	-.585758
C	2.143086	.048563	-1.782966
C	1.003055	1.031325	-1.592962
C	1.237946	2.271211	-.902873
C	4.650845	1.456843	.901405
C	5.861024	.563270	.535781
C	4.372839	-.806780	-.936623
C	4.888197	-1.581103	1.483818



C	1.597053	1.818421	1.536816
C	6.490412	-1.770451	-.463574
C	5.667573	-2.871594	-1.201474
C	4.240300	-2.273896	-1.419914
O	7.528335	-2.285979	.410624
S	-4.545626	-.730706	.304254
Fe	-2.130922	-.669129	.165089
C	-1.747340	-3.987351	.905759
C	-2.419812	-1.442352	-3.183775
C	-2.715224	2.652748	-.587615
C	-1.955364	.116645	3.490726
N	-2.133850	-2.368876	-.910607
C	-1.934552	-3.649963	-.427330
C	-1.920028	-4.592781	-1.523787
C	-2.096343	-3.875098	-2.672816
C	-2.225954	-2.485891	-2.292304
N	-2.507098	.392817	-1.545950
C	-2.563108	-.106207	-2.836476
C	-2.810045	.972899	-3.769188
C	-2.904126	2.122661	-3.036039
C	-2.715228	1.758281	-1.647990
N	-2.341366	1.028087	1.237076
C	-2.546617	2.309395	.744327
C	-2.541323	3.258852	1.835868
C	-2.335496	2.548100	2.984745
C	-2.204073	1.157424	2.606644
N	-1.871957	-1.714080	1.843469
C	-1.803394	-1.211970	3.133909
C	-1.578707	-2.294171	4.070610
C	-1.525033	-3.448315	3.345648
C	-1.714057	-3.086999	1.955671
O	-.399060	-.449568	-.029069
H	3.336761	4.098444	-.453660
H	3.942219	1.911608	-1.076314
H	2.589103	-.494225	.247485
H	2.706567	.367724	-2.680221
H	1.753375	-.952153	-2.004832
H(iso=2)	.090988	.242960	-.674999
H	.312455	1.097129	-2.437105
H	-.249984	3.318208	-2.026605
H	1.928040	5.837217	.563230
H	1.069588	4.664419	1.545317
H	4.249674	1.135487	1.870210
H	5.008201	2.483633	1.043435
H	6.370543	.982582	-.345426
H	4.053101	-1.045082	1.942346
H	1.225330	.796211	1.426352
H	.732474	2.440038	1.791650
H	7.048826	-1.165058	-1.185842
H	6.150839	-3.159164	-2.140789
H	5.627371	-3.776658	-.580460
H	3.490420	-2.812678	-.827062
H	3.923455	-2.335064	-2.466359
H	4.870333	-.252811	-1.754764
H	5.689576	-1.638012	2.230931
H	4.540090	-2.600047	1.277561
H	2.295792	1.856678	2.379563
H	3.388330	3.881349	1.295241
H	6.592273	.569482	1.354800
H	7.148957	-2.950834	1.019327
H	-4.787575	-1.513069	-.808251
H	-1.608637	-5.037414	1.140772
H	-2.477367	-1.692895	-4.238080
H	-2.835610	3.705957	-.817960
H	-1.878296	.364166	4.544277
H	-1.786184	-5.659524	-1.413331
H	-2.137203	-4.237854	-3.690173
H	-2.904407	.850785	-4.838972
H	-3.089318	3.128583	-3.385098
H	-2.675106	4.324492	1.716611
H	-2.273756	2.916345	3.998987

H	-1.486795	-2.168456	5.140135
H	-1.379058	-4.458353	3.701385

## Frequencies:

-235.1523	6.0177	12.9868
17.8170	32.0357	34.6305
40.3119	52.5386	58.1428
59.0369	70.9366	100.0748
107.1810	111.1993	114.5293
129.3572	136.2325	154.4568
156.2239	159.8652	165.1410
182.0649	197.4583	210.5366
211.4496	217.4396	217.5854
227.3825	233.4688	237.7909
246.4599	266.4646	271.0204
273.2216	282.2002	285.2737
288.3402	292.2746	297.8367
300.5650	315.0448	319.9903
326.6160	329.8108	336.0842
363.9058	365.4429	372.7511
373.0508	379.5448	385.1250
398.1416	416.5089	419.2245
427.2985	437.2624	437.6127
441.8869	442.6556	447.6299
462.4060	478.0965	486.6461
510.6029	518.1851	543.0288
559.9455	571.1066	580.2448
603.2600	616.8767	624.8973
647.5415	676.6084	680.0831
681.0864	681.5686	691.9208
696.5973	700.2641	702.6211
721.8446	725.0911	728.8784
732.2873	734.1042	740.0185
760.8392	765.3151	765.9616
767.3281	798.6161	805.1479
810.3395	811.9752	818.6986
821.5536	831.7818	833.1077
834.2346	837.9537	850.3032
851.4593	855.0655	866.4667
891.0297	895.8860	906.0959
908.2941	910.8420	924.5168
934.2280	941.6856	949.9610
950.0440	951.0537	953.3479
954.9699	972.5267	975.9117
986.6729	997.1400	1010.1260
1015.4530	1021.8638	1023.2177
1032.3877	1035.6031	1038.0932
1045.7450	1049.7285	1059.6401
1062.4660	1062.7582	1063.0273
1076.8683	1081.1560	1086.2553
1098.2261	1117.4136	1117.5288
1119.8655	1121.8803	1125.4419
1138.8758	1151.9273	1162.0662
1173.7289	1175.6076	1183.1890
1192.2414	1194.0857	1199.9230
1206.4318	1217.2845	1221.0346
1243.9639	1244.9975	1252.2165
1261.2126	1269.5046	1276.1200
1293.8592	1295.6771	1296.1292
1307.9787	1316.5641	1321.8666
1332.3002	1339.1142	1345.9534
1357.1565	1358.5037	1358.6708
1361.6671	1367.4740	1374.2233
1379.6124	1384.9542	1389.5786
1390.2374	1395.3791	1398.6884
1401.6158	1408.9276	1413.7623
1417.3050	1420.9513	1428.0549
1431.0773	1431.8616	1437.9899
1440.2255	1453.7191	1459.6632
1465.9359	1502.9170	1504.0004
1506.9556	1509.8904	1515.2161

1529.9413	1533.2959	1535.9967
1538.1988	1542.7183	1543.9975
1547.3323	1550.9267	1556.6110
1559.1121	1562.7079	1564.9327
1594.5111	1596.1586	1616.4864
1620.2407	1642.8075	1643.5837
1653.1072	1714.5644	2509.0104
2950.6977	2957.8567	2964.7407
3017.7359	3030.1715	3041.0167
3042.5504	3046.2807	3051.7518
3055.4517	3059.3722	3060.4021
3073.2507	3076.4672	3079.8664
3093.5746	3094.6377	3097.3981
3103.3013	3110.8098	3117.1312
3128.2989	3130.9792	3140.9538
3149.0694	3209.0024	3211.2448
3211.4153	3211.6238	3219.0557
3257.4232	3257.7972	3258.7763
3260.4764	3280.6472	3281.2960
3281.8494	3283.5125	3639.0782

### III.E.7. Point P7

Absolute energy: -2476.6074669

Geometry:

C	.496503	3.392226	-1.227140
C	.519413	4.647572	-.512125
C	1.570444	4.802815	.576735
C	5.415711	-.873840	.213658
O	-.313135	5.556017	-.746370
C	2.736929	3.811373	.425449
C	2.279459	2.336279	.231105
C	3.521309	1.445359	-.167325
C	3.110763	-.001491	-.590079
C	2.172033	.062548	-1.808878
C	.992355	1.015122	-1.607266
C	1.256348	2.308502	-.914036
C	4.650709	1.456771	.901438
C	5.860654	.563185	.536061
C	4.374193	-.806569	-.934106
C	4.888543	-1.580905	1.483961
C	1.596030	1.818267	1.531967
C	6.491973	-1.770205	-.462956
C	5.668160	-2.871656	-1.200722
C	4.241163	-2.272878	-1.418690
O	7.527261	-2.286290	.410258
S	-4.561727	-.731186	.304126
Fe	-2.114403	-.666654	.162640
C	-1.749503	-3.980480	.903197
C	-2.419657	-1.439358	-3.177581
C	-2.712824	2.646782	-.586965
C	-1.957603	.117043	3.483409
N	-2.137420	-2.372849	-.915795
C	-1.935343	-3.648382	-.431076
C	-1.920293	-4.589850	-1.522052
C	-2.096188	-3.872140	-2.670308
C	-2.225317	-2.488450	-2.287489
N	-2.524015	.389574	-1.541055
C	-2.568381	-.106513	-2.833252
C	-2.809047	.970122	-3.762873
C	-2.902675	2.118164	-3.030536
C	-2.718644	1.754785	-1.646542
N	-2.345434	1.031251	1.236411
C	-2.545467	2.305955	.747369
C	-2.540920	3.254394	1.834228

C	-2.335943	2.545081	2.982251
C	-2.205601	1.159048	2.604304
N	-1.887146	-1.720911	1.854838
C	-1.806664	-1.217784	3.132246
C	-1.577822	-2.292296	4.067922
C	-1.524064	-3.446698	3.342827
C	-1.717082	-3.083698	1.959797
O	-.466788	-.524114	.044077
H	3.340278	4.102628	-.448433
H	3.945308	1.912690	-1.076137
H	2.579370	-.493039	.238441
H	2.762231	.377853	-2.686400
H	1.780320	-.939339	-2.033332
H(iso=2)	.283467	.482927	-.957343
H	.454139	1.184164	-2.549533
H	-.225567	3.325735	-2.037786
H	1.930254	5.840185	.564903
H	1.069447	4.666427	1.547926
H	4.249585	1.135098	1.871954
H	5.009883	2.484508	1.045138
H	6.370511	.983830	-.345880
H	4.051143	-1.043925	1.941037
H	1.225440	.794308	1.417675
H	.732021	2.441571	1.790683
H	7.044212	-1.163380	-1.191291
H	6.151225	-3.158408	-2.142633
H	5.626265	-3.778909	-.580185
H	3.490058	-2.813019	-.825487
H	3.924018	-2.332020	-2.466826
H	4.871582	-.253884	-1.754086
H	5.687878	-1.638823	2.235568
H	4.540273	-2.601619	1.278240
H	2.294192	1.849243	2.377790
H	3.390706	3.887898	1.303485
H	6.593739	.569346	1.355803
H	7.146856	-2.948203	1.016842
H	-4.813518	-1.506884	-.806519
H	-1.607399	-5.032298	1.138538
H	-2.470946	-1.689570	-4.234351
H	-2.822813	3.702908	-.818781
H	-1.875506	.365354	4.538615
H	-1.785819	-5.659138	-1.416067
H	-2.136033	-4.239096	-3.688413
H	-2.898281	.853372	-4.835827
H	-3.080266	3.125793	-3.384972
H	-2.671576	4.322861	1.717831
H	-2.273109	2.918873	3.996655
H	-1.481829	-2.170043	5.139596
H	-1.373817	-4.456805	3.702992

## Frequencies:

-29.2230	-22.2811	-19.7211
-9.7796	14.9851	23.2814
31.3744	41.4421	49.1253
52.4145	63.4062	81.9683
92.9009	100.2518	110.2489
126.4899	129.3467	146.2912
148.0361	158.3277	175.1701
184.1639	191.6724	205.6938
215.2791	217.2288	221.0654
225.7358	228.6952	232.6121
257.2582	262.2027	272.8534
274.4024	279.0511	280.8325
285.0598	295.7928	296.9570
299.5673	300.6630	314.7188
323.3422	334.3050	342.1565
359.8567	372.0364	374.7871
378.7497	381.1809	384.4992
401.7038	415.4511	417.3744
420.4554	434.8312	437.1932
439.0986	440.9051	441.0824

468.9966	474.0817	485.8878
507.6516	517.4584	536.7280
543.9723	561.6708	574.7727
576.5139	623.3294	643.1719
657.2373	678.9487	679.6995
688.7673	689.1922	690.3714
693.3161	727.5359	728.7579
731.4705	738.7188	745.1479
760.7129	765.1499	771.0029
771.6603	791.7424	809.5727
812.3237	818.8959	821.8809
822.9446	824.5416	832.3894
837.1990	839.1241	851.8980
852.5687	854.8771	858.7073
874.8019	896.8387	916.4080
918.0280	928.5768	930.8898
937.3948	945.8964	953.0913
954.4662	963.5551	965.0704
965.7058	968.8410	971.0759
981.9834	989.9820	995.5879
1008.2631	1025.1164	1025.8641
1034.5878	1036.9744	1037.7087
1039.4226	1047.2968	1050.1933
1052.9802	1065.3394	1065.6313
1069.1248	1070.8834	1084.3318
1088.5158	1088.6864	1103.0128
1125.1662	1125.4678	1127.7224
1129.7685	1131.5795	1140.5396
1148.6935	1173.9262	1175.8808
1177.1364	1196.7101	1201.7342
1204.1430	1207.1239	1214.6698
1230.6328	1237.8285	1244.8959
1256.4460	1257.7483	1266.1946
1278.1326	1285.3053	1296.4195
1308.1310	1311.8036	1313.3152
1315.7629	1317.6110	1320.3227
1324.9986	1336.0523	1340.9955
1348.0151	1358.7804	1359.9165
1360.4833	1366.4833	1377.2847
1380.7145	1391.2700	1398.6069
1401.2484	1401.9007	1403.6942
1407.4050	1411.6026	1417.7691
1421.0376	1422.2291	1430.7521
1432.0581	1437.8884	1439.3938
1448.6120	1455.9158	1463.3111
1505.6687	1508.4072	1510.1879
1511.7654	1531.1258	1535.4187
1537.7013	1539.1346	1541.7577
1545.8500	1546.7894	1551.9381
1557.4892	1563.9061	1564.5830
1566.1109	1598.1835	1599.6554
1614.7317	1621.7298	1648.0487
1649.4624	1650.7177	1679.9535
1721.8004	2099.1176	2533.7474
2944.7329	2955.9538	2988.7786
3005.5355	3017.9223	3025.7634
3026.7660	3031.7138	3036.0009
3036.5064	3043.9520	3044.6507
3056.5337	3056.5984	3060.0002
3061.0618	3074.7212	3078.5665
3080.3586	3084.0865	3094.3974
3100.7119	3112.5200	3125.3772
3131.6052	3181.9461	3192.4024
3193.3660	3193.6430	3202.4008
3238.2560	3238.7180	3240.1842
3241.6122	3261.2914	3261.9329
3263.1959	3264.6028	3676.2514

## III.E.8. Point P8

Absolute energy: -2476.6088406

Geometry:

C	.475664	3.383930	-1.223899
C	.521815	4.645007	-.510300
C	1.570175	4.800902	.575677
C	5.414790	-.872953	.212982
O	-.313476	5.557060	-.750281
C	2.734328	3.808103	.419363
C	2.278320	2.329477	.232433
C	3.521171	1.444333	-.167074
C	3.110519	-.003959	-.585375
C	2.140797	.047775	-1.780643
C	1.016852	1.044607	-1.603191
C	1.237706	2.266207	-.903071
C	4.650911	1.456746	.901415
C	5.861051	.563271	.535770
C	4.372840	-.806803	-.936804
C	4.888145	-1.581099	1.483802
C	1.597210	1.818633	1.536870
C	6.490438	-1.770480	-.463584
C	5.667568	-2.871588	-1.201480
C	4.240268	-2.273932	-1.419940
O	7.528255	-2.285922	.410608
S	-4.544032	-.730875	.304489
Fe	-2.133436	-.669403	.165336
C	-1.747111	-3.987945	.905835
C	-2.419914	-1.442742	-3.184247
C	-2.715787	2.653082	-.587554
C	-1.955150	.116607	3.491372
N	-2.134103	-2.369149	-.910585
C	-1.934506	-3.649827	-.426660
C	-1.920044	-4.592400	-1.523578
C	-2.096355	-3.874786	-2.672646
C	-2.226129	-2.485349	-2.292657
N	-2.505153	.393160	-1.546741
C	-2.562687	-.106550	-2.836330
C	-2.809992	.972536	-3.768863
C	-2.904070	2.122578	-3.035581
C	-2.714926	1.758452	-1.647592
N	-2.341022	1.028259	1.237575
C	-2.546761	2.309457	.743774
C	-2.541296	3.258584	1.835585
C	-2.335443	2.547677	2.984527
C	-2.203875	1.156897	2.606673
N	-1.872270	-1.714151	1.843400
C	-1.803578	-1.211197	3.134087
C	-1.578820	-2.293742	4.070201
C	-1.525143	-3.448063	3.345080
C	-1.714252	-3.087225	1.955039
O	-.395152	-.450007	-.028892
H	3.336835	4.098626	-.453832
H	3.942288	1.911809	-1.076133
H	2.589732	-.494344	.248068
H	2.703867	.362974	-2.680285
H	1.748159	-.951812	-2.001983
H(iso=2)	.049442	.220494	-.645848
H	.295828	1.087052	-2.422325
H	-.252708	3.319385	-2.025868
H	1.928119	5.836973	.562997
H	1.069843	4.664416	1.545491
H	4.249650	1.135455	1.870180
H	5.008146	2.483567	1.043343
H	6.370617	.982613	-.345388
H	4.053078	-1.045208	1.942506
H	1.225813	.796268	1.426719
H	.732154	2.439796	1.791390

H	7.048810	-1.165086	-1.185870
H	6.150775	-3.159152	-2.140795
H	5.627239	-3.776642	-.580511
H	3.490449	-2.812700	-.827037
H	3.923539	-2.335322	-2.466430
H	4.870362	-.252774	-1.754897
H	5.689560	-1.637963	2.230844
H	4.540097	-2.600055	1.277617
H	2.295321	1.857348	2.380103
H	3.388114	3.880922	1.294872
H	6.592263	.569411	1.354779
H	7.149095	-2.951054	1.019242
H	-4.784027	-1.514485	-.807457
H	-1.608488	-5.037857	1.140822
H	-2.478018	-1.693179	-4.238408
H	-2.837292	3.706052	-.817886
H	-1.878344	.364192	4.544769
H	-1.786171	-5.659090	-1.412937
H	-2.137287	-4.237471	-3.690003
H	-2.904852	.850164	-4.838552
H	-3.089999	3.128407	-3.384479
H	-2.675510	4.324163	1.716401
H	-2.273787	2.915721	3.998819
H	-1.486858	-2.168073	5.139709
H	-1.379121	-4.458095	3.700760

## Frequencies:

-28.4500	-9.2428	13.7234
17.9622	28.9976	34.2754
39.0594	52.1347	58.6454
63.0614	74.7152	100.8672
107.3256	112.6232	124.3020
134.1009	140.1234	154.2890
156.0969	161.7774	179.3721
186.2378	195.0487	208.6063
211.3364	216.5420	223.1159
228.4354	235.6178	245.0530
251.1033	266.0138	270.9508
278.1504	285.5752	288.0664
288.8580	293.8597	297.8292
300.3617	309.8872	315.3672
325.4234	334.5748	340.0180
363.3883	370.4610	370.7983
372.5678	379.2647	385.2844
388.1464	399.4822	410.0543
420.0572	428.5886	437.6368
438.1757	441.8889	442.9613
453.1635	466.2584	479.3865
486.2730	511.4392	520.0671
558.3935	560.1752	575.5250
595.1720	608.9373	620.0359
635.3966	653.2979	676.2897
680.6390	681.3948	690.0727
690.8668	692.0644	701.8102
702.3238	722.5957	724.4769
730.8726	733.7140	740.2206
760.1936	764.6853	765.5670
766.3595	797.7590	804.4963
810.0007	811.4625	821.0944
824.8234	830.9895	832.2809
835.3492	849.0698	851.1052
853.3198	860.0374	870.0035
890.9766	893.5415	906.1300
908.7850	913.0271	922.3808
934.0487	941.5636	949.3909
949.4971	950.5566	954.3346
958.1285	973.3354	976.5811
986.8509	997.7823	1009.8399
1013.3829	1021.2388	1022.5929
1032.3016	1036.9469	1038.0272
1046.6286	1049.6866	1060.2159

1063.0513	1063.2554	1063.4382
1077.3729	1081.8625	1086.3215
1098.6206	1117.0231	1117.4169
1119.6178	1122.0710	1126.4337
1139.6923	1152.6950	1168.6651
1175.7117	1178.3356	1185.3773
1192.6387	1194.0707	1202.5538
1209.2185	1216.6403	1223.6916
1244.6427	1245.1169	1253.3996
1262.1863	1269.8448	1275.8221
1292.6669	1294.7940	1295.9086
1308.2107	1319.0552	1322.4737
1333.7195	1345.0366	1346.1821
1357.8111	1358.6238	1359.6857
1362.0372	1374.1263	1377.2875
1380.0584	1385.5416	1389.6604
1390.3363	1395.4170	1399.1158
1403.2499	1410.2598	1414.1140
1417.7245	1421.0797	1431.4230
1431.9688	1437.6826	1439.9034
1440.9397	1453.8030	1463.9106
1487.1811	1503.6790	1504.3896
1507.2356	1512.5955	1515.9934
1529.9725	1534.3217	1536.7936
1540.9773	1545.0579	1546.1146
1550.9295	1556.6111	1558.6870
1562.6921	1564.9434	1594.7951
1595.7372	1607.0708	1621.7256
1642.4121	1643.4425	1659.9635
1714.7047	2042.2724	2509.0567
2950.2029	2952.4996	2964.2915
3017.8454	3030.0990	3041.2354
3042.8354	3046.5143	3051.9672
3056.0350	3059.5021	3060.7660
3073.5157	3076.6293	3080.7699
3093.8622	3094.6354	3097.5667
3103.6668	3111.0505	3117.2880
3128.0364	3137.5306	3141.0885
3149.2838	3210.1756	3211.7020
3212.7399	3213.0226	3219.9389
3257.7232	3258.1088	3259.0488
3260.7365	3280.9439	3281.5673
3282.0708	3283.7319	3638.3053

### III.E.9. Point P9

Absolute energy: -2476.5985081

Geometry:

C	.481582	3.380848	-1.224372
C	.520759	4.646386	-.510455
C	1.570418	4.801305	.575623
C	5.414886	-.872990	.212941
O	-.313161	5.556949	-.749409
C	2.734658	3.808479	.420351
C	2.277428	2.331166	.232204
C	3.520879	1.444031	-.167360
C	3.110016	-.003806	-.586257
C	2.147032	.050131	-1.787158
C	.984168	1.012319	-1.580170
C	1.238857	2.281115	-.902997
C	4.650795	1.457006	.901411
C	5.861045	.563266	.535832
C	4.372792	-.806742	-.936347
C	4.888271	-1.581137	1.483882
C	1.596858	1.818137	1.536829



C	6.490237	-1.770387	-.463601
C	5.667552	-2.871622	-1.201514
C	4.240324	-2.273885	-1.419937
O	7.528594	-2.286074	.410666
S	-4.547354	-.730684	.304183
Fe	-2.127957	-.668554	.164543
C	-1.747600	-3.987069	.905607
C	-2.419747	-1.441732	-3.183584
C	-2.714735	2.652593	-.587871
C	-1.955664	.117067	3.490283
N	-2.133465	-2.368258	-.910625
C	-1.934536	-3.650411	-.428109
C	-1.919983	-4.593528	-1.524155
C	-2.096307	-3.875713	-2.673198
C	-2.225696	-2.486712	-2.291808
N	-2.508822	.392060	-1.544388
C	-2.563530	-.106064	-2.837102
C	-2.810207	.973464	-3.769756
C	-2.904312	2.122842	-3.036773
C	-2.715595	1.758451	-1.648420
N	-2.341412	1.027569	1.236146
C	-2.546432	2.309320	.745078
C	-2.541410	3.259419	1.836405
C	-2.335593	2.548889	2.985189
C	-2.204216	1.158104	2.607031
N	-1.871714	-1.713995	1.843683
C	-1.803104	-1.213089	3.133765
C	-1.578534	-2.294647	4.071301
C	-1.524864	-3.448796	3.346383
C	-1.713754	-3.086801	1.956562
O	-.413623	-.459646	-.019358
H	3.336231	4.097803	-.453429
H	3.941828	1.911242	-1.076427
H	2.588769	-.493837	.247242
H	2.714878	.368424	-2.679579
H	1.756957	-.950968	-2.006042
H(iso=2)	.202899	.347562	-.783544
H	.344557	1.116489	-2.461670
H	-.244904	3.317474	-2.028018
H	1.927744	5.837375	.563492
H	1.069408	4.664447	1.544993
H	4.249853	1.135587	1.870154
H	5.008213	2.483519	1.043612
H	6.370310	.982363	-.345376
H	4.053410	-1.044898	1.941920
H	1.225561	.796150	1.425763
H	.733333	2.440647	1.791450
H	7.049101	-1.165211	-1.185261
H	6.150876	-3.159227	-2.140506
H	5.627827	-3.776467	-.580382
H	3.490504	-2.812554	-.827228
H	3.923249	-2.334604	-2.465919
H	4.870030	-.252915	-1.754399
H	5.689619	-1.638052	2.230792
H	4.540171	-2.599865	1.277421
H	2.296237	1.855766	2.378874
H	3.388701	3.881980	1.295614
H	6.592252	.569577	1.354675
H	7.148592	-2.950826	1.019945
H	-4.791355	-1.512353	-.808938
H	-1.608979	-5.036991	1.140720
H	-2.476541	-1.692518	-4.237702
H	-2.832923	3.705872	-.818074
H	-1.878279	.364187	4.543765
H	-1.786218	-5.659784	-1.413709
H	-2.137056	-4.238078	-3.690165
H	-2.903746	.851369	-4.839106
H	-3.088261	3.128548	-3.385455
H	-2.674344	4.324573	1.716613
H	-2.273747	2.916921	3.998973
H	-1.486673	-2.168657	5.140288

H                    -1.378917            -4.458434            3.701747

Frequencies:

-1208.3256	7.2291	13.0228
17.6229	33.6012	35.6288
39.9474	54.0766	57.3838
58.3983	70.8759	94.1780
100.2716	103.8391	115.5675
131.2544	144.6823	154.0758
155.1630	158.4681	164.6315
183.4071	196.2088	206.9481
210.6346	219.0448	223.5760
225.0017	232.7865	235.1409
244.5555	265.1251	271.2950
276.1006	278.7824	283.7818
287.8023	288.0636	297.8822
301.9740	314.5049	321.9745
328.7308	334.6918	340.4095
363.0804	368.2915	372.4778
373.8108	378.7736	383.8173
398.5815	417.6404	423.2142
423.8853	435.9018	436.9341
439.5204	442.1436	443.8817
458.8988	471.7834	486.4351
504.6474	518.8299	523.5166
552.8604	560.1631	575.7380
583.9168	599.3637	621.0635
644.6818	656.4710	679.2232
680.2393	683.5049	690.9587
694.5193	701.0173	721.9278
724.8488	728.8286	733.5687
735.5284	738.7218	761.1638
761.5434	765.4912	766.0907
791.2846	800.3398	810.7282
811.9739	814.2888	820.7186
827.3819	833.4649	834.1697
846.9997	850.1068	851.9682
854.1941	859.4008	880.7025
901.0935	910.0469	913.5994
915.5723	922.2744	930.6834
934.2938	941.2154	950.9463
951.0695	952.0197	956.4645
962.1751	973.6226	982.6665
989.7598	998.6830	1015.9505
1019.2859	1022.7711	1024.0734
1028.4965	1033.3145	1038.0100
1047.7152	1049.7956	1059.5900
1060.1388	1060.7336	1062.6322
1077.2999	1078.6416	1085.8112
1100.7835	1116.9734	1117.2772
1119.6565	1123.0223	1125.0448
1136.5329	1149.5974	1155.5071
1170.5859	1171.9254	1175.9027
1189.1298	1191.9447	1198.5920
1204.2775	1214.9698	1217.3851
1236.5336	1242.6350	1244.8598
1255.8015	1262.5887	1272.7752
1278.8868	1294.8197	1295.8853
1298.0658	1306.9922	1315.5981
1321.8144	1331.6966	1336.6261
1337.0435	1345.5127	1352.5362
1353.1796	1357.6478	1362.8703
1376.4160	1378.6335	1387.3384
1388.2113	1389.4348	1395.1426
1398.4643	1400.7307	1409.2252
1412.2087	1416.1834	1420.2728
1424.0004	1429.5750	1431.4939
1436.3136	1437.1364	1452.5998
1462.2772	1500.4261	1501.7035
1505.3251	1509.9993	1525.7648
1529.6348	1533.8388	1536.3293

1539.0494	1540.1891	1545.3227
1550.4838	1556.1334	1558.8236
1562.3540	1564.5954	1581.5310
1592.2756	1594.1979	1616.9559
1626.1064	1640.3545	1642.6699
1644.1412	1714.8045	2506.2434
2953.3425	2964.8478	2978.6005
3019.3548	3032.7559	3041.4162
3043.4942	3047.4884	3052.9282
3054.0824	3060.9161	3061.4919
3074.6482	3078.8327	3080.5076
3094.1944	3097.4246	3098.8128
3103.6275	3108.1374	3112.0936
3119.3105	3130.5362	3143.2800
3150.8395	3209.7146	3211.7356
3213.9553	3214.1165	3222.3704
3262.4888	3262.8364	3264.1550
3265.7613	3285.5474	3286.1913
3287.1504	3288.7437	3632.0036

### III.E.10. Point P10

Absolute energy: -2476.6068297

Geometry:

C	.491427	3.385940	-1.226241
C	.519520	4.647607	-.510876
C	1.570642	4.802338	.576090
C	5.415304	-.873302	.213230
O	-.313764	5.557382	-.747461
C	2.736252	3.810256	.423638
C	2.278205	2.335089	.231798
C	3.520744	1.444404	-.167298
C	3.110070	-.002733	-.588737
C	2.163835	.057664	-1.802143
C	.985628	1.009872	-1.595513
C	1.251005	2.301978	-.909873
C	4.650642	1.457138	.901330
C	5.860908	.563258	.535989
C	4.373276	-.806690	-.934751
C	4.888558	-1.581139	1.483959
C	1.596252	1.817945	1.534714
C	6.490624	-1.770259	-.463389
C	5.667726	-2.871657	-1.201339
C	4.240659	-2.273479	-1.419474
O	7.528552	-2.286352	.410629
S	-4.555523	-.731076	.304218
Fe	-2.117827	-.666554	.162645
C	-1.748666	-3.984545	.904283
C	-2.419551	-1.440116	-3.181559
C	-2.713578	2.650644	-.587959
C	-1.956811	.117866	3.487409
N	-2.134343	-2.369197	-.913238
C	-1.934579	-3.650453	-.429808
C	-1.920061	-4.593737	-1.524184
C	-2.096180	-3.875669	-2.672896
C	-2.225052	-2.488127	-2.289653
N	-2.517357	.389266	-1.539976
C	-2.566231	-.106713	-2.836669
C	-2.809999	.972949	-3.768084
C	-2.903941	2.121457	-3.035390
C	-2.717595	1.757824	-1.647612
N	-2.342555	1.028194	1.234673
C	-2.545839	2.307965	.746382
C	-2.541382	3.258625	1.836528
C	-2.335969	2.548996	2.985032

C	-2.204836	1.159100	2.606922
N	-1.878817	-1.717226	1.849357
C	-1.804104	-1.216090	3.133302
C	-1.577854	-2.294365	4.071479
C	-1.524144	-3.449090	3.346263
C	-1.714550	-3.085540	1.958874
O	-.465451	-.508069	.027944
H	3.337537	4.099050	-.450916
H	3.942409	1.911407	-1.076425
H	2.583064	-.493087	.241906
H	2.748604	.370305	-2.683161
H	1.770995	-.943501	-2.020700
H(iso=2)	.287038	.471068	-.925978
H	.430181	1.169244	-2.527416
H	-.230280	3.320844	-2.035181
H	1.928115	5.838963	.564158
H	1.069345	4.665620	1.545925
H	4.250000	1.135655	1.870804
H	5.008678	2.483916	1.044146
H	6.370051	.982560	-.345658
H	4.053041	-1.044178	1.941092
H	1.225847	.795396	1.420727
H	.733648	2.441508	1.791526
H	7.047890	-1.164643	-1.186633
H	6.151140	-3.159087	-2.141033
H	5.627943	-3.777113	-.580176
H	3.490373	-2.812762	-.826884
H	3.923196	-2.332868	-2.465847
H	4.870343	-.253269	-1.753411
H	5.689216	-1.638504	2.232326
H	4.540206	-2.600310	1.277430
H	2.295980	1.851299	2.377421
H	3.390459	3.886124	1.299558
H	6.592871	.569742	1.354923
H	7.147756	-2.949649	1.019580
H	-4.806806	-1.509731	-.808247
H	-1.609069	-5.035000	1.139742
H	-2.472765	-1.690975	-4.236455
H	-2.824164	3.705277	-.818673
H	-1.877055	.364958	4.541424
H	-1.786239	-5.660747	-1.414881
H	-2.136726	-4.238627	-3.690290
H	-2.900501	.852595	-4.838526
H	-3.083556	3.128101	-3.385497
H	-2.672260	4.324638	1.716563
H	-2.273545	2.918630	3.998861
H	-1.484295	-2.168879	5.140975
H	-1.376342	-4.458779	3.702572

## Frequencies:

-28.3044	-17.9414	-9.9290
6.8734	30.6164	31.1767
49.1739	51.0125	55.8478
61.8325	79.5224	88.3054
97.8682	110.4309	124.6086
128.7762	133.4755	148.0021
152.0145	156.3902	176.4340
180.1020	190.7414	206.6971
212.7002	218.4907	219.2148
229.3949	234.1907	241.2032
259.3431	266.1813	272.4993
276.0975	279.2194	281.3666
288.0683	295.1583	298.2788
301.9668	312.5923	321.0863
326.0646	334.3132	343.3137
360.3034	372.1322	375.1817
377.1154	380.7986	383.9179
399.6405	414.5062	419.1233
422.0500	434.9914	436.6711
438.9405	440.7045	440.9302
468.1159	474.0802	485.6242

506.1264	517.0581	536.5944
559.7209	560.1896	573.7142
575.2985	621.4082	642.9825
657.0622	678.5563	679.2062
686.7432	689.3695	690.1413
693.4600	725.0654	726.2934
729.1547	735.6381	741.3976
758.4968	761.7683	767.0055
767.7012	780.9215	794.0179
805.1262	810.6636	814.5832
815.8139	820.4042	824.7074
834.9244	836.0784	849.6122
850.0346	852.7349	854.6932
872.9011	892.6983	908.6621
916.6111	921.1564	923.3840
935.0224	939.3780	945.6611
950.9470	955.7913	956.9883
962.8042	963.7795	967.5865
978.5687	988.4355	993.6246
1005.9854	1017.2777	1023.8819
1024.5288	1026.7554	1029.2595
1037.2256	1038.5142	1049.1295
1051.3539	1060.4030	1062.1591
1063.0417	1063.7405	1080.5271
1082.7785	1087.6707	1101.8334
1119.5394	1119.8123	1122.2257
1125.9573	1128.0423	1139.9784
1148.7590	1161.1449	1172.2224
1175.7479	1192.0074	1194.8767
1197.1447	1199.7051	1214.3766
1220.4866	1236.9278	1242.8910
1248.0046	1255.9607	1263.9149
1275.0148	1282.0740	1294.7216
1300.9193	1302.3673	1305.3655
1307.3331	1313.5870	1315.1647
1323.0932	1333.7967	1336.5307
1346.0917	1349.9337	1351.8013
1357.7761	1364.4086	1376.4612
1378.8196	1389.3718	1389.6426
1392.1398	1396.6149	1399.7185
1404.0126	1409.5141	1414.3838
1415.8671	1420.0454	1423.5060
1428.7373	1430.4994	1436.8924
1439.1159	1452.9017	1459.7621
1500.7037	1501.9740	1504.4988
1510.3303	1529.9272	1533.9784
1536.3083	1537.0594	1537.3975
1540.3871	1545.4550	1550.6781
1556.2486	1560.1674	1562.6723
1564.8937	1591.9589	1593.6629
1608.8848	1616.0826	1641.7630
1643.3564	1645.4758	1667.8847
1716.5716	1999.7405	2513.1023
2951.7728	2963.0592	2996.6383
3015.5720	3028.9459	3035.8173
3038.2053	3042.5972	3045.8465
3047.7716	3056.0218	3056.2493
3069.1228	3071.4202	3074.1277
3074.7402	3087.5249	3092.7322
3093.0344	3096.8006	3106.7895
3114.2988	3125.6233	3138.5752
3145.0088	3197.7609	3207.1853
3208.5642	3208.7353	3217.6611
3257.2346	3257.7670	3259.1171
3260.5896	3280.1630	3280.9071
3282.0464	3283.5259	3643.1390

## III.E.11. Point P11

Absolute energy: -2476.6000796

Geometry:

C	0.482849	3.380511	-1.224153
C	0.520441	4.646348	-0.510655
C	1.570451	4.801335	0.575596
C	5.414923	-0.873032	0.212922
O	-0.313063	5.556874	-0.749257
C	2.734727	3.808515	0.420586
C	2.277268	2.331503	0.232108
C	3.520810	1.443988	-0.167400
C	3.109909	-0.003769	-0.586416
C	2.148579	0.050838	-1.788775
C	0.979334	1.007314	-1.577335
C	1.239400	2.284798	-0.903239
C	4.650776	1.457031	0.901395
C	5.861024	0.563259	0.535837
C	4.372801	-0.806722	-0.936226
C	4.888295	-1.581141	1.483878
C	1.596847	1.818079	1.536770
C	6.490285	-1.770359	-0.463577
C	5.667568	-2.871641	-1.201496
C	4.240359	-2.273841	-1.419907
O	7.528568	-2.286075	0.410663
S	-4.547998	-0.730724	0.304186
Fe	-2.126450	-0.668241	0.164245
C	-1.747728	-3.986700	0.905439
C	-2.419737	-1.441413	-3.183237
C	-2.714598	2.652217	-0.587907
C	-1.955802	0.117206	3.489836
N	-2.133588	-2.368358	-0.910888
C	-1.934538	-3.650429	-0.428402
C	-1.919994	-4.593461	-1.524089
C	-2.096315	-3.875610	-2.673107
C	-2.225608	-2.486975	-2.291416
N	-2.509786	0.391835	-1.543970
C	-2.563712	-0.106031	-2.837175
C	-2.810203	0.973461	-3.769587
C	-2.904309	2.122667	-3.036677
C	-2.715710	1.758392	-1.648490
N	-2.341681	1.027639	1.235963
C	-2.546362	2.309128	0.745368
C	-2.541421	3.259272	1.836408
C	-2.335616	2.548845	2.985122
C	-2.204275	1.158302	2.607039
N	-1.872104	-1.714281	1.844256
C	-1.803074	-1.213575	3.133565
C	-1.578523	-2.294566	4.071210
C	-1.524854	-3.448762	3.346276
C	-1.713723	-3.086536	1.956885
O	-0.420519	-0.464975	-0.014251
H	3.336048	4.097633	-0.453358
H	3.941728	1.911125	-1.076478
H	2.588678	-0.493726	0.247280
H	2.718356	0.368118	-2.679367
H	1.757987	-0.950440	-2.006394
H(iso=2)	0.240744	0.386809	-0.823421
H	0.356638	1.123468	-2.470277
H	-0.243156	3.317362	-2.028387
H	1.927801	5.837391	0.563535
H	1.069424	4.664455	1.544994
H	4.249920	1.135601	1.870200
H	5.008278	2.483490	1.043723
H	6.370236	0.982367	-0.345376
H	4.053441	-1.044832	1.941775
H	1.225845	0.796042	1.425514
H	0.733580	2.440843	1.791419

H	7.048800	-1.165176	-1.185450
H	6.150871	-3.159169	-2.140515
H	5.627853	-3.776554	-0.580431
H	3.490524	-2.812536	-0.827220
H	3.923221	-2.334379	-2.465806
H	4.869839	-0.252964	-1.754367
H	5.689529	-1.638160	2.230921
H	4.540182	-2.599873	1.277388
H	2.296282	1.855337	2.378825
H	3.388909	3.882353	1.295820
H	6.592310	0.569556	1.354640
H	7.148364	-2.950912	1.019858
H	-4.792651	-1.512081	-0.809023
H	-1.609061	-5.036613	1.140632
H	-2.476203	-1.692292	-4.237346
H	-2.831879	3.705596	-0.818096
H	-1.878181	0.364192	4.543340
H	-1.786223	-5.659651	-1.413932
H	-2.136999	-4.238111	-3.689921
H	-2.903463	0.851644	-4.838894
H	-3.087732	3.128303	-3.385500
H	-2.673956	4.324379	1.716694
H	-2.273639	2.917107	3.998710
H	-1.486577	-2.168782	5.140112
H	-1.378827	-4.458220	3.701818

## Frequencies:

-711.5250	-4.9572	8.9926
13.6850	26.4456	32.9890
37.2925	53.1419	56.2951
57.4572	71.3415	91.3263
97.0084	101.8495	116.0924
130.1992	146.4181	152.5355
154.1292	157.0413	164.0433
182.8988	190.4337	204.4920
210.4366	219.5496	221.6108
226.7207	234.4492	237.2348
245.5674	265.7154	271.5646
276.7517	279.8488	282.8759
286.1660	287.5436	297.5128
302.0564	313.7838	319.4115
329.0094	333.1335	341.1801
361.9984	370.1444	372.2773
374.4296	378.6657	383.7469
398.4837	418.5777	420.6393
423.5209	435.3775	436.8370
439.4680	441.5296	446.7513
454.9122	470.0264	486.0621
507.0706	518.1177	523.4941
549.2903	560.0185	575.2500
579.8142	585.8679	620.6004
644.2632	656.5034	678.7572
679.5675	684.5504	690.4025
692.4089	700.1001	723.4013
724.8663	728.4442	735.1574
738.7357	760.9428	761.5559
765.6115	766.1449	792.4533
801.1064	810.0780	811.4631
812.2905	820.8778	824.6827
833.9854	834.5229	846.8989
849.6609	852.1587	852.8736
858.2507	873.1732	898.7070
902.9714	915.4702	915.5391
917.4326	933.0214	933.8870
941.6206	947.7869	951.8814
952.0572	954.6063	957.6438
964.0935	974.2713	984.9494
991.0292	1000.7238	1018.7476
1019.0954	1024.2049	1024.5028
1026.9568	1034.0611	1038.2642
1048.6420	1050.2078	1059.3561

1060.6663	1060.9374	1062.8555
1078.5402	1079.2760	1086.4678
1101.0789	1117.1750	1117.4733
1119.8588	1123.4531	1127.1622
1139.2915	1150.3589	1166.1337
1171.8992	1175.4108	1186.4855
1189.0285	1191.9626	1200.5407
1216.2458	1217.7894	1220.9499
1242.1425	1243.1993	1245.4118
1256.7503	1263.7228	1275.2541
1280.9877	1294.6082	1297.2020
1299.2021	1306.7434	1315.9279
1321.9813	1326.6293	1331.9456
1336.3846	1345.4235	1350.7931
1351.8252	1357.3767	1363.1443
1376.7691	1378.5021	1387.3982
1389.0409	1389.4569	1395.1939
1398.6580	1400.8418	1409.1496
1412.3067	1415.8428	1420.0609
1423.0240	1429.2064	1430.5784
1435.6463	1436.8075	1452.3242
1461.1934	1500.0734	1501.2295
1504.9207	1509.9990	1529.4832
1530.0916	1533.9673	1536.3097
1538.0078	1540.2614	1545.2728
1550.3738	1556.3377	1558.9305
1562.3190	1564.5436	1591.5303
1593.5492	1608.2650	1616.2871
1618.3281	1642.3540	1644.1448
1649.1805	1715.1907	2506.1688
2954.0202	2965.4417	2985.9192
3019.3981	3033.0281	3040.8825
3043.1739	3047.2743	3052.3533
3052.8536	3060.7847	3061.3038
3074.3735	3078.9209	3079.6272
3093.5711	3096.9475	3097.7711
3098.5816	3102.9308	3111.8126
3119.3999	3130.4683	3143.4325
3150.8089	3207.5665	3212.2431
3214.3764	3214.4934	3222.9438
3263.6299	3263.9986	3265.4201
3266.9788	3286.6077	3287.2685
3288.3686	3289.9199	3630.8051

### III.E.12. Point P12

Absolute energy: -2476.5987756

Geometry:

C	0.481942	3.380721	-1.224325
C	0.520673	4.646401	-0.510500
C	1.570432	4.801317	0.575617
C	5.414891	-0.872997	0.212937
O	-0.313143	5.556943	-0.749367
C	2.734676	3.808490	0.420415
C	2.277382	2.331262	0.232179
C	3.520862	1.444016	-0.167367
C	3.109986	-0.003796	-0.586305
C	2.147450	0.050324	-1.787601
C	0.982657	1.010770	-1.579219
C	1.238989	2.282127	-0.903053
C	4.650792	1.457013	0.901406
C	5.861040	0.563264	0.535832
C	4.372790	-0.806737	-0.936311
C	4.888280	-1.581143	1.483877
C	1.596857	1.818117	1.536817



C	6.490237	-1.770382	-0.463594
C	5.667552	-2.871622	-1.201515
C	4.240332	-2.273873	-1.419931
O	7.528599	-2.286077	0.410681
S	-4.547526	-0.730697	0.304178
Fe	-2.127586	-0.668476	0.164466
C	-1.747632	-3.986998	0.905574
C	-2.419744	-1.441653	-3.183519
C	-2.714697	2.652523	-0.587888
C	-1.955699	0.117111	3.490193
N	-2.133467	-2.368254	-0.910672
C	-1.934533	-3.650431	-0.428191
C	-1.919985	-4.593539	-1.524156
C	-2.096308	-3.875714	-2.673189
C	-2.225667	-2.486792	-2.291715
N	-2.509044	0.391989	-1.544256
C	-2.563576	-0.106052	-2.837139
C	-2.810214	0.973486	-3.769741
C	-2.904318	2.122811	-3.036777
C	-2.715627	1.758445	-1.648449
N	-2.341460	1.027560	1.236078
C	-2.546415	2.309283	0.745159
C	-2.541414	3.259409	1.836427
C	-2.335599	2.548908	2.985188
C	-2.204234	1.158166	2.607045
N	-1.871776	-1.714042	1.843796
C	-1.803089	-1.213219	3.133725
C	-1.578526	-2.294646	4.071305
C	-1.524857	-3.448802	3.346387
C	-1.713738	-3.086743	1.956657
O	-0.415459	-0.461045	-0.018018
H	3.336200	4.097758	-0.453435
H	3.941803	1.911217	-1.076457
H	2.588729	-0.493818	0.247271
H	2.715832	0.368371	-2.679529
H	1.757240	-0.950865	-2.006148
H(iso=2)	0.214026	0.358822	-0.795049
H	0.347846	1.118418	-2.464065
H	-0.244442	3.317437	-2.028175
H	1.927765	5.837428	0.563519
H	1.069398	4.664439	1.545016
H	4.249865	1.135577	1.870193
H	5.008241	2.483548	1.043647
H	6.370294	0.982365	-0.345408
H	4.053400	-1.044864	1.941903
H	1.225615	0.796089	1.425682
H	0.733389	2.440733	1.791461
H	7.049075	-1.165189	-1.185304
H	6.150892	-3.159214	-2.140551
H	5.627842	-3.776513	-0.580381
H	3.490479	-2.812568	-0.827215
H	3.923227	-2.334538	-2.465932
H	4.869989	-0.252918	-1.754396
H	5.689640	-1.638101	2.230823
H	4.540160	-2.599896	1.277381
H	2.296295	1.855635	2.378872
H	3.388780	3.882073	1.295704
H	6.592300	0.569576	1.354685
H	7.148592	-2.950835	1.019839
H	-4.791713	-1.512232	-0.808931
H	-1.609006	-5.036969	1.140719
H	-2.476466	-1.692480	-4.237682
H	-2.832636	3.705880	-0.818096
H	-1.878247	0.364205	4.543729
H	-1.786228	-5.659847	-1.413754
H	-2.137064	-4.238113	-3.690189
H	-2.903691	0.851435	-4.839145
H	-3.088145	3.128574	-3.385488
H	-2.674240	4.324619	1.716623
H	-2.273706	2.916997	3.998995
H	-1.486632	-2.168676	5.140335

H            -1.378880    -4.458467    3.701793

Frequencies:

-1111.1915	6.5422	12.4633
16.9732	33.5976	33.7483
39.3202	53.9357	57.2542
58.2850	70.9251	93.4605
99.3271	103.3813	115.7468
131.1950	145.0016	153.9103
154.2101	157.8436	164.6236
183.6150	194.9012	206.4454
210.6916	219.3670	223.1873
225.7808	233.4625	235.4398
244.8615	265.4483	271.4276
276.5525	278.9759	283.5619
287.5354	287.9165	297.8714
301.9614	314.3601	321.4290
328.5581	334.3574	339.6061
362.7884	368.7714	372.4260
373.9934	378.7990	383.7890
398.6410	417.9116	422.7145
423.7385	435.7972	436.9267
439.5839	442.0078	444.8522
457.4042	471.1879	486.3600
505.0736	518.7020	522.7984
551.8312	560.1609	575.5926
582.4940	595.1778	620.9146
644.6458	656.4399	679.1675
680.1146	683.9415	690.8315
693.9415	700.9741	723.0321
725.0030	728.7575	735.2153
738.0337	750.8002	761.2077
761.6579	765.5133	766.1520
792.0577	800.8292	811.1063
812.3259	815.1332	821.0343
826.5704	833.6266	834.2645
847.5400	850.5850	852.0274
854.5088	863.7236	884.5316
901.9022	911.8145	914.4116
916.3625	927.3188	931.6032
934.5933	941.6185	951.4010
951.6052	952.3368	957.0408
962.9138	973.8282	983.3990
990.1517	999.2111	1016.8571
1019.1595	1023.1371	1024.1772
1027.9786	1033.4470	1038.1016
1048.0733	1049.9153	1059.4657
1060.4000	1060.6680	1062.7277
1077.9809	1078.5351	1086.0276
1100.9243	1117.1821	1117.4880
1119.8722	1123.3136	1126.1751
1138.0157	1150.2675	1164.4133
1169.2484	1172.2693	1176.3048
1189.0607	1191.9230	1199.3194
1206.9142	1215.4025	1217.5364
1237.9401	1242.5926	1245.0489
1256.0705	1262.8856	1273.4150
1279.4021	1294.8017	1296.2235
1298.3621	1306.9611	1315.7162
1321.9029	1331.7464	1333.7470
1336.6755	1345.5376	1351.9983
1352.7869	1357.6182	1362.9977
1376.5899	1378.6356	1387.3493
1388.3454	1389.4770	1395.1966
1398.5507	1400.7754	1409.2639
1412.3027	1416.1402	1420.2350
1423.6807	1429.4438	1431.3224
1436.0547	1437.0678	1452.5742
1462.0656	1500.3077	1501.5598
1505.2003	1510.0392	1527.0689
1529.6545	1533.9254	1536.3588

1538.6842	1540.2575	1545.3529
1550.4853	1556.2437	1558.8929
1562.3765	1564.6107	1589.0547
1592.2153	1594.1268	1616.7313
1623.6489	1642.1534	1643.2327
1644.2144	1714.8798	2506.5987
2953.3582	2964.8368	2980.4343
3019.1132	3032.5514	3040.9767
3043.0900	3047.1373	3052.5387
3053.3825	3060.5613	3061.1064
3074.2414	3078.5155	3079.9111
3093.6789	3097.1105	3098.3780
3103.0788	3104.6190	3111.7055
3118.9584	3130.1937	3142.9822
3150.4989	3208.6484	3211.4189
3213.6251	3213.7604	3222.0732
3262.1322	3262.4856	3263.8369
3265.4270	3285.1735	3285.8280
3286.8218	3288.4007	3632.8649

### III.E.13. Point P13

Absolute energy: -2476.6024074

Geometry:

C	0.484444	3.380487	-1.224112
C	0.520140	4.646391	-0.510790
C	1.570498	4.801408	0.575571
C	5.414976	-0.873071	0.212907
O	-0.313057	5.556885	-0.749026
C	2.734883	3.808627	0.420988
C	2.277128	2.332090	0.232006
C	3.520713	1.443941	-0.167442
C	3.109806	-0.003695	-0.586707
C	2.150908	0.051848	-1.791080
C	0.976070	1.003531	-1.576649
C	1.240706	2.289241	-0.903796
C	4.650740	1.457076	0.901374
C	5.861008	0.563249	0.535858
C	4.372813	-0.806702	-0.936020
C	4.888335	-1.581150	1.483888
C	1.596799	1.818005	1.536654
C	6.490274	-1.770324	-0.463571
C	5.667584	-2.871659	-1.201482
C	4.240409	-2.273794	-1.419869
O	7.528594	-2.286111	0.410667
S	-4.548978	-0.730788	0.304208
Fe	-2.124424	-0.667797	0.163826
C	-1.747895	-3.986324	0.905215
C	-2.419716	-1.441026	-3.182901
C	-2.714440	2.651849	-0.587974
C	-1.955987	0.117416	3.489356
N	-2.133681	-2.368323	-0.911184
C	-1.934534	-3.650517	-0.428707
C	-1.919995	-4.593553	-1.524118
C	-2.096307	-3.875648	-2.673090
C	-2.225500	-2.487273	-2.290974
N	-2.511004	0.391363	-1.543154
C	-2.564008	-0.106087	-2.837326
C	-2.810220	0.973525	-3.769497
C	-2.904322	2.122521	-3.036674
C	-2.715933	1.758417	-1.648495
N	-2.341898	1.027550	1.235591
C	-2.546291	2.308920	0.745647
C	-2.541441	3.259230	1.836512
C	-2.335662	2.548962	2.985145

C	-2.204352	1.158524	2.607144
N	-1.872698	-1.714612	1.844935
C	-1.803055	-1.214150	3.133375
C	-1.578465	-2.294544	4.071263
C	-1.524794	-3.448840	3.346286
C	-1.713689	-3.086266	1.957285
O	-0.430347	-0.472492	-0.006992
H	3.335880	4.097414	-0.453247
H	3.941559	1.910998	-1.076567
H	2.588291	-0.493562	0.247027
H	2.723342	0.367942	-2.679458
H	1.759793	-0.949686	-2.007404
H(iso=2)	0.272432	0.422601	-0.859754
H	0.372761	1.132825	-2.481723
H	-0.240815	3.317198	-2.029115
H	1.927772	5.837518	0.563569
H	1.069391	4.664520	1.544992
H	4.249985	1.135618	1.870266
H	5.008332	2.483508	1.043828
H	6.370146	0.982336	-0.345408
H	4.053460	-1.044684	1.941558
H	1.226088	0.795902	1.424967
H	0.733819	2.441095	1.791373
H	7.048731	-1.165149	-1.185484
H	6.150918	-3.159168	-2.140515
H	5.627991	-3.776610	-0.580398
H	3.490531	-2.812526	-0.827204
H	3.923139	-2.334096	-2.465704
H	4.869676	-0.252978	-1.754242
H	5.689492	-1.638217	2.231045
H	4.540192	-2.599889	1.277332
H	2.296373	1.854717	2.378672
H	3.389241	3.882942	1.296163
H	6.592379	0.569567	1.354635
H	7.148153	-2.950805	1.019833
H	-4.794609	-1.511754	-0.809050
H	-1.609179	-5.036249	1.140520
H	-2.475665	-1.692017	-4.237030
H	-2.830325	3.705404	-0.818170
H	-1.878055	0.364248	4.542908
H	-1.786195	-5.659725	-1.414095
H	-2.136923	-4.238121	-3.689876
H	-2.903015	0.851873	-4.838829
H	-3.087021	3.128229	-3.385539
H	-2.673499	4.324342	1.716637
H	-2.273538	2.917354	3.998642
H	-1.486398	-2.168775	5.140116
H	-1.378624	-4.458223	3.701875

## Frequencies:

-106.4003	-20.4437	-6.0625
9.3109	17.0172	32.2934
34.4807	52.9556	54.6908
56.9353	80.7438	88.4362
94.2589	100.1272	118.8329
128.4478	146.9616	151.4094
153.7085	157.9535	179.1975
182.0182	192.2588	204.1926
210.6641	219.1238	219.7768
226.8106	234.7960	240.4160
256.4376	267.4114	275.2326
275.8013	282.1628	282.7343
287.3515	290.2947	296.6333
305.5544	313.0349	322.9787
328.6150	331.6449	340.7657
361.3302	372.0960	373.9741
375.8739	378.4160	384.0822
398.2687	415.0391	421.3045
423.8601	435.0384	436.7270
439.5869	441.0225	441.6386
466.8837	469.5440	485.7206

507.6173	517.5588	538.4870
558.3813	569.7060	574.9247
577.3025	580.2346	620.4972
643.4765	656.7721	678.3816
679.0728	685.5507	689.9229
690.8757	697.1179	723.5291
724.8970	728.2246	735.0918
739.2989	760.1844	761.5861
765.7032	766.2685	791.7796
801.8153	810.9469	811.5374
812.6514	821.1755	822.2910
834.2488	834.7961	848.2056
849.6685	852.2329	853.5879
870.5196	888.7071	904.4240
915.3662	917.0286	918.9278
933.7284	934.9336	942.0668
947.3405	952.4290	952.9627
954.7597	958.7754	964.9711
975.0156	986.3131	991.7994
1001.7879	1017.9199	1021.1936
1024.0377	1025.0019	1026.1424
1034.5434	1038.1609	1048.9005
1050.6397	1059.0526	1060.4727
1061.4786	1062.7913	1078.4151
1080.3636	1086.5447	1101.1186
1117.3536	1117.6765	1120.0959
1123.7396	1126.9713	1139.4545
1149.2540	1162.1036	1170.6889
1174.6013	1188.8350	1191.8254
1192.5760	1196.7381	1212.9651
1218.2269	1234.0554	1241.4564
1244.9509	1245.7777	1258.2663
1263.9984	1278.3308	1280.6187
1294.3630	1298.0746	1299.8277
1306.1791	1313.4642	1318.8578
1321.9689	1331.3128	1334.7902
1345.3822	1349.1030	1350.6457
1357.1751	1363.0874	1376.3814
1378.1868	1386.9735	1387.5010
1389.2518	1395.2993	1398.4156
1401.0647	1404.7494	1412.2480
1412.3905	1415.6074	1419.9376
1422.8326	1428.7715	1429.9363
1435.4326	1436.6018	1452.1144
1459.9781	1500.0116	1500.8742
1504.5058	1509.9885	1529.5193
1533.6796	1533.8600	1536.2810
1537.0416	1540.1705	1545.1527
1550.2977	1556.3065	1559.0481
1562.2907	1564.5060	1591.0460
1593.1236	1612.7357	1615.5372
1634.9168	1642.4295	1644.1487
1658.4010	1715.3998	2506.2450
2954.4234	2965.7936	2992.9444
3019.2954	3033.0062	3040.2046
3042.7130	3046.8995	3050.8334
3052.3447	3060.4678	3060.9392
3073.9651	3077.9895	3079.1357
3088.0520	3092.8376	3097.7217
3098.1245	3102.1719	3111.4467
3119.2697	3130.2862	3143.3643
3150.4403	3205.7256	3212.3864
3214.4004	3214.4892	3223.0838
3264.1200	3264.5420	3266.0127
3267.5073	3287.0415	3287.7444
3288.9352	3290.4242	3631.0255

## III.E.14. Point P14

Absolute energy: -2476.6035999

Geometry:

C	0.485565	3.381089	-1.224043
C	0.519847	4.646337	-0.511028
C	1.570505	4.801450	0.575555
C	5.415013	-0.873133	0.212914
O	-0.312992	5.556795	-0.748830
C	2.734991	3.808734	0.421320
C	2.277086	2.332527	0.231964
C	3.520620	1.443952	-0.167465
C	3.109764	-0.003601	-0.586942
C	2.152762	0.052677	-1.792782
C	0.976372	1.003226	-1.578487
C	1.241998	2.292040	-0.904458
C	4.650708	1.457069	0.901323
C	5.860956	0.563238	0.535862
C	4.372848	-0.806693	-0.935844
C	4.888381	-1.581126	1.483852
C	1.596787	1.817999	1.536446
C	6.490370	-1.770312	-0.463509
C	5.667610	-2.871647	-1.201436
C	4.240475	-2.273725	-1.419799
O	7.528520	-2.286163	0.410676
S	-4.549799	-0.730853	0.304210
Fe	-2.122732	-0.667451	0.163501
C	-1.748038	-3.985881	0.905007
C	-2.419692	-1.440754	-3.182497
C	-2.714306	2.651434	-0.587964
C	-1.956134	0.117505	3.488847
N	-2.133846	-2.368639	-0.911630
C	-1.934548	-3.650437	-0.429038
C	-1.920021	-4.593360	-1.524016
C	-2.096308	-3.875448	-2.672886
C	-2.225406	-2.487507	-2.290507
N	-2.512135	0.391152	-1.542818
C	-2.564278	-0.106014	-2.837241
C	-2.810172	0.973406	-3.769138
C	-2.904263	2.122226	-3.036389
C	-2.716104	1.758236	-1.648514
N	-2.342160	1.027806	1.235528
C	-2.546205	2.308634	0.745941
C	-2.541430	3.258918	1.836445
C	-2.335696	2.548808	2.984982
C	-2.204434	1.158731	2.607019
N	-1.873397	-1.715121	1.845828
C	-1.803084	-1.214660	3.133152
C	-1.578449	-2.294389	4.071040
C	-1.524777	-3.448721	3.346055
C	-1.713711	-3.085921	1.957629
O	-0.438336	-0.478825	-0.000858
H	3.336034	4.097534	-0.453293
H	3.941658	1.911020	-1.076746
H	2.587706	-0.493609	0.246833
H	2.727205	0.368069	-2.680074
H	1.761295	-0.949328	-2.008772
H(iso=2)	0.284275	0.440780	-0.877737
H	0.383619	1.139256	-2.490192
H	-0.239429	3.317144	-2.029879
H	1.928050	5.837915	0.563623
H	1.069346	4.664554	1.545307
H	4.249925	1.135552	1.870572
H	5.008514	2.483821	1.043939
H	6.370230	0.982514	-0.345604
H	4.053178	-1.044445	1.941608
H	1.226131	0.795459	1.424605
H	0.733642	2.441349	1.791603

H	7.048403	-1.164859	-1.186135
H	6.151077	-3.159178	-2.140917
H	5.627885	-3.776941	-0.580237
H	3.490353	-2.812698	-0.826954
H	3.923066	-2.333881	-2.466051
H	4.869641	-0.252953	-1.754364
H	5.689560	-1.638349	2.231499
H	4.540117	-2.600211	1.277332
H	2.296476	1.854161	2.378879
H	3.389692	3.883507	1.296749
H	6.592654	0.569531	1.354865
H	7.148227	-2.950240	1.019341
H	-4.796088	-1.511119	-0.808489
H	-1.609210	-5.036268	1.140486
H	-2.475269	-1.691876	-4.237111
H	-2.829302	3.705567	-0.818308
H	-1.877928	0.364381	4.542879
H	-1.786120	-5.660191	-1.414325
H	-2.136868	-4.238394	-3.690174
H	-2.902703	0.852138	-4.839172
H	-3.086528	3.128490	-3.385830
H	-2.673231	4.324723	1.716717
H	-2.273443	2.917825	3.998915
H	-1.486181	-2.168856	5.140538
H	-1.378369	-4.458556	3.702181

## Frequencies:

-27.6970	-15.8245	5.9895
13.6131	31.8005	33.1156
44.0627	53.8927	55.6928
57.8129	84.9430	91.5408
99.2723	102.4057	123.4814
128.2616	137.1663	150.4795
153.0085	157.9236	180.5287
182.4398	196.4841	208.8320
213.6446	218.8180	219.5024
228.3931	234.7185	241.7659
260.6926	268.2488	274.3652
276.9145	281.0570	281.9522
287.5872	295.5543	296.9467
304.7575	313.0111	322.9320
329.5289	334.7888	338.3443
361.2237	372.1971	375.1010
377.6227	378.7090	384.2310
399.0232	414.1540	421.2094
424.1991	435.1862	436.8229
439.9053	440.2179	441.1098
468.1183	473.0381	485.7984
506.9232	517.4966	538.8582
559.4817	570.1432	574.7350
575.2030	620.9649	625.3298
643.2900	657.0509	678.6970
679.3675	687.2341	689.8386
690.7192	695.3414	724.5898
725.9508	728.7424	735.8742
740.4586	760.0110	762.0024
766.2397	766.8365	791.4688
804.2229	810.3277	813.8097
815.0046	821.5311	823.6866
834.5429	835.1304	848.7964
849.6828	852.5105	854.2913
871.7462	889.1824	907.1639
915.6598	919.6893	921.6316
934.4146	937.4392	944.8238
949.8785	954.9133	955.6220
957.6792	961.4420	965.7338
976.1848	987.0975	992.7365
1002.9100	1018.1579	1022.6627
1024.7054	1025.9104	1027.2401
1035.6544	1038.3195	1049.1519
1050.9722	1059.8201	1061.2687

1062.2861	1063.2086	1079.1532
1081.0814	1086.8119	1101.4937
1118.9700	1119.2580	1121.7083
1125.3925	1127.7440	1139.5056
1149.3513	1161.9819	1171.8592
1175.2954	1190.3327	1193.2533
1196.6695	1197.6264	1214.2161
1219.5291	1236.2034	1242.5097
1247.0924	1253.5888	1261.7710
1268.1791	1280.1416	1287.8900
1294.7724	1299.5143	1301.1401
1306.6636	1314.5995	1316.5453
1322.5287	1332.5112	1335.7220
1345.9180	1349.6659	1351.2327
1357.6750	1363.8693	1376.8471
1378.7487	1388.2378	1389.5933
1390.6795	1395.8698	1399.3354
1402.1002	1409.3578	1413.7753
1415.8495	1420.0674	1422.9282
1428.9114	1429.6137	1436.5376
1436.7821	1452.7332	1460.1849
1499.9536	1501.4234	1504.7885
1510.2774	1529.8430	1533.4182
1534.1246	1536.6073	1537.2527
1540.4335	1545.4201	1550.6235
1556.4492	1559.7737	1562.5811
1564.8283	1590.7084	1592.8828
1601.7031	1610.9323	1615.9209
1642.2737	1644.3777	1655.7172
1709.0183	1715.6711	2511.2119
2952.6309	2963.9479	2993.2301
3016.4996	3029.9383	3037.0552
3039.3521	3043.6944	3047.3375
3049.0304	3057.0959	3057.4004
3070.3894	3073.7902	3075.3059
3081.5020	3089.0544	3093.7418
3094.3475	3098.3722	3107.9834
3115.3796	3126.6802	3139.7297
3146.5085	3200.6756	3208.0067
3209.9020	3209.9937	3218.5573
3258.2087	3258.6346	3260.1301
3261.5868	3281.1575	3281.8518
3283.0797	3284.5242	3641.1669

### III.E.15. Point P15

Absolute energy: -2476.5963757

Geometry:

C	0.487694	3.388762	-1.228241
C	0.521714	4.648156	-0.509902
C	1.570730	4.802890	0.576993
C	5.415299	-0.873129	0.213600
O	-0.314887	5.558322	-0.747343
C	2.736368	3.810715	0.423236
C	2.279879	2.333630	0.231371
C	3.522099	1.445099	-0.166909
C	3.111038	-0.002174	-0.588772
C	2.159456	0.056894	-1.797647
C	1.012503	1.036880	-1.616231
C	1.249754	2.286849	-0.910784
C	4.651134	1.456993	0.901871
C	5.861254	0.563271	0.536219
C	4.373610	-0.806704	-0.935168
C	4.888419	-1.581224	1.484224
C	1.595980	1.818303	1.533530



C	6.490528	-1.770418	-0.463338
C	5.667679	-2.871586	-1.201388
C	4.240537	-2.273586	-1.419483
O	7.528792	-2.286345	0.410669
S	-4.554430	-0.731083	0.304381
Fe	-2.127980	-0.668666	0.164642
C	-1.748190	-3.986858	0.905080
C	-2.419811	-1.441793	-3.183623
C	-2.714516	2.652659	-0.587789
C	-1.956402	0.117463	3.490137
N	-2.134568	-2.368966	-0.912282
C	-1.934632	-3.650597	-0.427986
C	-1.919957	-4.594055	-1.524365
C	-2.095994	-3.876300	-2.673463
C	-2.225516	-2.487028	-2.291875
N	-2.512422	0.389771	-1.541268
C	-2.565758	-0.107814	-2.836066
C	-2.810028	0.972442	-3.768061
C	-2.903822	2.121881	-3.035014
C	-2.717245	1.758247	-1.646451
N	-2.341174	1.027838	1.235519
C	-2.545988	2.309147	0.744792
C	-2.541233	3.259312	1.836460
C	-2.335925	2.548897	2.985264
C	-2.204459	1.157736	2.607271
N	-1.880934	-1.716702	1.847835
C	-1.805776	-1.213873	3.134997
C	-1.577488	-2.294585	4.072146
C	-1.523745	-3.449358	3.346709
C	-1.716211	-3.087331	1.957563
O	-0.430558	-0.494695	0.014998
H	3.339283	4.101161	-0.449263
H	3.944181	1.912510	-1.075375
H	2.583111	-0.492553	0.240223
H	2.740459	0.368673	-2.683789
H	1.765121	-0.941627	-2.020812
H(iso=2)	0.152634	0.347735	-0.806391
H	0.382177	1.142197	-2.490908
H	-0.234726	3.325746	-2.035726
H	1.927908	5.839035	0.565084
H	1.069469	4.666099	1.546219
H	4.250021	1.135497	1.870545
H	5.008649	2.483432	1.044436
H	6.370162	0.982253	-0.345257
H	4.053159	-1.044893	1.941449
H	1.224327	0.796804	1.418829
H	0.732903	2.441070	1.789192
H	7.048998	-1.165082	-1.185132
H	6.150897	-3.159070	-2.140452
H	5.628014	-3.776506	-0.580393
H	3.490575	-2.812447	-0.827128
H	3.923490	-2.333595	-2.465504
H	4.871840	-0.253476	-1.753068
H	5.689184	-1.638069	2.231759
H	4.540438	-2.599961	1.277619
H	2.294253	1.852360	2.376705
H	3.388680	3.884276	1.299809
H	6.592787	0.569802	1.354756
H	7.148423	-2.950477	1.020498
H	-4.801633	-1.512444	-0.808362
H	-1.607804	-5.036486	1.139845
H	-2.474318	-1.691706	-4.237873
H	-2.828823	3.706061	-0.818603
H	-1.876847	0.365243	4.543151
H	-1.786320	-5.660268	-1.413657
H	-2.136812	-4.238334	-3.690492
H	-2.901556	0.850645	-4.837584
H	-3.085332	3.127958	-3.383805
H	-2.673752	4.324431	1.716172
H	-2.274243	2.916820	3.999058
H	-1.482921	-2.168341	5.140816

H        -1.374963    -4.458667    3.701715

Frequencies:

-1416.3274	7.9866	11.1816
17.1548	33.9864	39.2322
41.6037	54.0326	57.3643
58.3511	69.8890	93.2113
100.5539	104.3512	114.7693
131.0904	142.0929	153.4228
156.1523	160.8527	162.8864
182.7266	197.8090	207.6388
210.8506	218.3342	221.7295
223.4609	230.7517	234.6567
243.7358	264.6807	271.2390
274.9178	278.3406	283.9893
287.7341	288.8321	297.0970
302.3500	314.6403	320.4988
328.9229	333.8595	341.0678
362.5857	368.1055	372.4491
373.5714	378.3100	383.6553
398.8703	413.1086	421.6161
423.6236	435.7626	436.9707
437.3468	441.9692	442.2353
461.4541	471.9894	486.3866
496.3131	515.7288	519.2026
555.6211	559.8828	575.8810
577.9972	608.9402	621.9344
647.1937	656.4082	679.2586
680.1774	683.5109	690.9821
694.3986	702.5448	723.2025
724.8063	729.5389	734.9269
737.7699	752.6207	761.4173
762.4194	765.6366	766.0820
792.1638	800.2179	810.6148
811.9096	816.9548	820.7132
827.2116	833.6547	834.4069
846.7726	850.7993	852.0638
855.1746	864.1975	891.8214
900.8420	913.0893	913.3148
915.5284	920.3759	930.5633
934.4716	940.9483	950.5952
950.9718	952.0455	956.5921
962.4641	973.9267	982.4212
989.6798	998.8402	1015.1902
1018.9317	1023.9072	1024.4901
1028.3220	1033.5562	1038.3526
1047.5852	1049.2334	1059.6014
1060.1412	1060.9145	1063.2246
1078.8488	1079.1876	1086.0632
1101.4459	1113.5681	1117.0453
1117.3088	1119.4100	1122.9418
1129.2420	1141.7411	1151.1857
1170.1159	1171.9841	1176.5637
1189.4888	1191.9759	1195.6018
1202.7589	1215.6153	1217.4483
1233.3835	1243.1139	1244.9647
1256.3449	1262.6693	1272.5977
1278.5300	1295.0123	1295.9650
1298.2174	1307.5340	1318.0356
1322.8010	1333.0541	1336.2563
1339.6336	1345.6022	1352.7534
1353.5092	1357.7495	1363.0675
1376.8431	1378.7707	1387.4352
1388.0015	1389.4508	1395.9503
1398.9596	1401.8232	1409.6287
1412.0789	1415.7735	1420.3873
1424.1999	1427.8633	1430.3418
1436.1132	1437.4017	1452.6710
1462.1909	1500.7877	1502.2532
1504.5303	1510.1300	1525.7125
1529.6383	1533.7334	1536.2956

1539.6420	1540.0942	1545.2944
1550.4955	1556.0731	1558.2234
1562.3841	1564.5600	1569.1808
1592.8847	1594.0981	1616.7968
1626.2459	1634.1737	1643.5074
1645.6003	1716.1835	2506.0733
2952.6413	2964.3163	2977.7629
3019.3193	3032.6370	3041.4814
3043.6586	3047.5128	3052.8003
3055.0966	3060.9452	3061.5962
3074.6840	3079.0100	3080.3389
3093.9936	3097.5666	3098.5865
3103.4388	3112.1142	3119.4398
3130.2468	3143.1891	3150.7907
3206.1501	3213.0660	3213.4903
3215.3210	3215.3989	3223.9268
3262.8496	3263.2862	3264.4900
3266.1022	3285.9192	3286.5556
3287.4562	3289.0772	3631.1914

### III.E.16. Point P16

Absolute energy: -2476.6025143

Geometry:

C	0.501392	3.396052	-1.235187
C	0.523597	4.652050	-0.510374
C	1.571546	4.805361	0.579228
C	5.416002	-0.873420	0.214724
O	-0.315860	5.558781	-0.743078
C	2.738326	3.813623	0.427575
C	2.281898	2.337442	0.228857
C	3.524345	1.446980	-0.167125
C	3.112828	0.001167	-0.594008
C	2.178476	0.068721	-1.815668
C	1.009256	1.030552	-1.627491
C	1.259578	2.301388	-0.919678
C	4.651804	1.457015	0.903048
C	5.861729	0.563167	0.537210
C	4.375305	-0.806291	-0.933944
C	4.888502	-1.581245	1.484866
C	1.593997	1.818048	1.527408
C	6.491226	-1.770489	-0.462571
C	5.667988	-2.871508	-1.200865
C	4.241122	-2.272875	-1.418620
O	7.528993	-2.286896	0.410750
S	-4.567611	-0.730787	0.303718
Fe	-2.123331	-0.669707	0.165691
C	-1.749921	-3.985210	0.904626
C	-2.420097	-1.441399	-3.181907
C	-2.712943	2.651288	-0.587387
C	-1.958340	0.117394	3.488586
N	-2.136700	-2.370318	-0.914041
C	-1.935563	-3.650778	-0.429217
C	-1.919712	-4.594346	-1.524274
C	-2.095375	-3.876806	-2.673416
C	-2.225481	-2.488751	-2.291089
N	-2.520246	0.387133	-1.537328
C	-2.569252	-0.108983	-2.833872
C	-2.809922	0.971120	-3.765267
C	-2.903072	2.120030	-3.032608
C	-2.719271	1.756510	-1.644781
N	-2.342492	1.028390	1.234882
C	-2.544981	2.308642	0.745926
C	-2.540675	3.258706	1.836595
C	-2.336239	2.548443	2.985092

C	-2.205493	1.158131	2.606877
N	-1.893162	-1.720184	1.853194
C	-1.810473	-1.216651	3.136386
C	-1.575999	-2.295076	4.073111
C	-1.522134	-3.449906	3.347518
C	-1.720705	-3.087709	1.960302
O	-0.446674	-0.523497	0.043448
H	3.344079	4.106358	-0.442785
H	3.949371	1.915249	-1.074195
H	2.575585	-0.490036	0.229310
H	2.772378	0.389261	-2.688715
H	1.790065	-0.930448	-2.049924
H(iso=2)	0.214433	0.407076	-0.904778
H	0.440216	1.179074	-2.541901
H	-0.217461	3.335229	-2.047410
H	1.929162	5.842140	0.569178
H	1.068396	4.667740	1.547945
H	4.249796	1.134653	1.871736
H	5.010146	2.483646	1.047295
H	6.370465	0.982506	-0.344793
H	4.051711	-1.044758	1.940678
H	1.220180	0.797250	1.407943
H	0.732144	2.442806	1.784655
H	7.048171	-1.164475	-1.185969
H	6.151264	-3.158705	-2.140854
H	5.627984	-3.777249	-0.580046
H	3.490436	-2.811876	-0.826122
H	3.923856	-2.332104	-2.465276
H	4.875652	-0.254659	-1.752034
H	5.688211	-1.637821	2.234457
H	4.541053	-2.600799	1.278232
H	2.291289	1.846045	2.372469
H	3.388219	3.885999	1.307060
H	6.594173	0.569754	1.355818
H	7.148360	-2.948985	1.020462
H	-4.819150	-1.508156	-0.809683
H	-1.605554	-5.035406	1.138852
H	-2.471176	-1.690224	-4.237469
H	-2.822647	3.705810	-0.819421
H	-1.874821	0.366388	4.541961
H	-1.785688	-5.661608	-1.414426
H	-2.135515	-4.240129	-3.691042
H	-2.898500	0.850782	-4.836189
H	-3.080529	3.127299	-3.383013
H	-2.672263	4.325005	1.716937
H	-2.274690	2.917706	3.999455
H	-1.476399	-2.169278	5.142354
H	-1.368143	-4.459204	3.703326

## Frequencies:

-400.9874	-5.6692	7.7743
12.9216	24.4440	33.6104
37.0574	53.0394	56.1260
57.0672	71.2232	84.9952
93.8675	101.0188	117.3573
132.0099	135.1419	147.0216
153.1861	155.8463	164.4947
185.9820	190.1874	203.9357
211.8131	219.0813	220.1623
222.4038	233.6031	236.9978
247.0943	266.7252	273.1107
277.2120	279.9270	282.2136
285.7572	287.8512	296.8449
303.1314	312.9491	317.1919
318.7917	329.6375	334.8832
360.3398	371.7915	372.4016
376.5296	378.9644	384.0095
400.0364	418.5795	419.7191
421.2090	435.3715	437.0039
439.5921	441.2756	445.3519
465.2869	469.8497	485.9271

509.5041	518.0817	547.0366
558.9623	560.5569	569.4559
576.4001	610.3068	621.6835
646.0785	656.8645	679.1351
679.7783	687.4247	690.0322
691.3420	703.0770	725.2557
726.5155	730.0213	735.9260
741.2093	761.8616	763.3810
766.8707	767.3623	795.6603
805.5402	815.1276	816.6085
817.6982	822.1549	825.4549
834.8057	835.3942	849.5143
852.6987	853.7964	857.6190
871.5662	902.0609	908.4432
918.6314	920.8441	923.1374
935.0731	938.5674	946.4296
947.8203	956.1350	957.2704
961.8699	963.8969	965.2557
976.3953	981.0350	990.2276
997.7933	1009.7842	1018.4763
1020.8993	1025.6221	1026.4467
1028.2561	1036.3974	1039.0444
1048.6270	1051.1406	1060.4348
1062.3902	1062.5688	1064.3744
1080.6204	1083.9216	1088.7069
1102.9462	1119.9217	1120.3161
1122.6054	1126.3522	1128.1129
1142.2503	1150.2225	1163.7038
1172.7604	1177.0740	1191.9563
1194.8266	1195.2385	1202.0835
1216.8171	1219.9920	1229.2570
1242.8842	1244.8238	1248.0215
1258.1475	1264.9288	1277.6982
1282.6405	1295.2632	1300.0970
1301.8966	1307.5357	1317.6972
1318.8382	1323.8109	1333.6337
1338.0560	1346.3411	1351.3727
1353.0169	1358.2205	1364.6067
1376.7235	1378.7662	1389.5773
1389.8162	1391.1030	1397.2139
1399.7905	1402.6054	1409.6819
1414.6036	1415.8148	1420.4758
1423.8442	1427.2890	1431.0466
1437.5858	1438.3205	1453.2777
1461.2668	1501.4295	1502.5862
1504.3555	1510.4805	1530.0762
1534.1810	1535.6560	1536.8229
1538.7841	1540.5188	1545.6554
1550.8508	1557.1637	1559.7860
1562.9668	1564.8968	1592.6478
1594.1529	1613.0416	1616.4851
1620.3218	1643.9655	1646.7169
1655.4510	1717.5915	2512.9058
2949.7870	2961.4279	2988.1660
3014.6183	3028.0614	3035.9451
3037.7318	3041.9101	3046.9434
3048.0723	3055.2329	3055.6229
3068.3189	3072.6134	3073.4225
3086.9328	3091.3521	3091.8442
3096.1275	3105.9356	3113.1096
3124.2507	3136.9397	3144.5683
3165.1914	3195.7537	3206.3044
3207.2662	3207.5697	3216.7891
3253.9989	3254.5255	3255.8810
3257.3496	3276.9939	3277.6934
3278.8451	3280.3066	3648.4702

## III.E.17. Point P17

Absolute energy: -2476.6017205

Geometry:

C	0.482950	3.388531	-1.226840
C	0.522242	4.646732	-0.510465
C	1.570585	4.802180	0.576813
C	5.415155	-0.873135	0.213546
O	-0.314271	5.557672	-0.748091
C	2.735511	3.809746	0.421818
C	2.279771	2.331649	0.231212
C	3.522330	1.445243	-0.166960
C	3.111351	-0.002292	-0.587964
C	2.152318	0.054454	-1.791207
C	1.022641	1.047722	-1.617849
C	1.244963	2.276101	-0.908871
C	4.651267	1.456718	0.901909
C	5.861224	0.563215	0.536234
C	4.373652	-0.806652	-0.935937
C	4.888267	-1.581104	1.484074
C	1.596308	1.818613	1.533671
C	6.490772	-1.770527	-0.463170
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C	4.240598	-2.273559	-1.419474
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S	-4.550852	-0.731076	0.304459
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C	-2.420064	-1.442416	-3.183612
C	-2.715250	2.652479	-0.587456
C	-1.956115	0.116935	3.490668
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C	-1.919969	-4.592475	-1.523550
C	-2.096042	-3.875015	-2.672531
C	-2.225996	-2.486337	-2.292045
N	-2.508952	0.391436	-1.544157
C	-2.564575	-0.107464	-2.835427
C	-2.809902	0.971707	-3.767076
C	-2.903668	2.121375	-3.034014
C	-2.716130	1.757799	-1.646528
N	-2.341372	1.028681	1.237047
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H	2.585295	-0.493177	0.242930
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H	-0.242874	3.325446	-2.033255
H	1.928958	5.839221	0.564847
H	1.069422	4.665400	1.547018
H	4.249490	1.134959	1.871274
H	5.009106	2.484225	1.044760
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H	4.052003	-1.044743	1.942325
H	1.224226	0.795813	1.420782
H	0.731415	2.441145	1.789096

H	7.048492	-1.164390	-1.186826
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H	5.627241	-3.777417	-0.580014
H	3.490019	-2.812795	-0.826238
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H	4.540233	-2.600970	1.277782
H	2.294017	1.854080	2.378586
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H	6.593422	0.569407	1.355641
H	7.149577	-2.949148	1.018299
H	-4.793079	-1.513003	-0.806573
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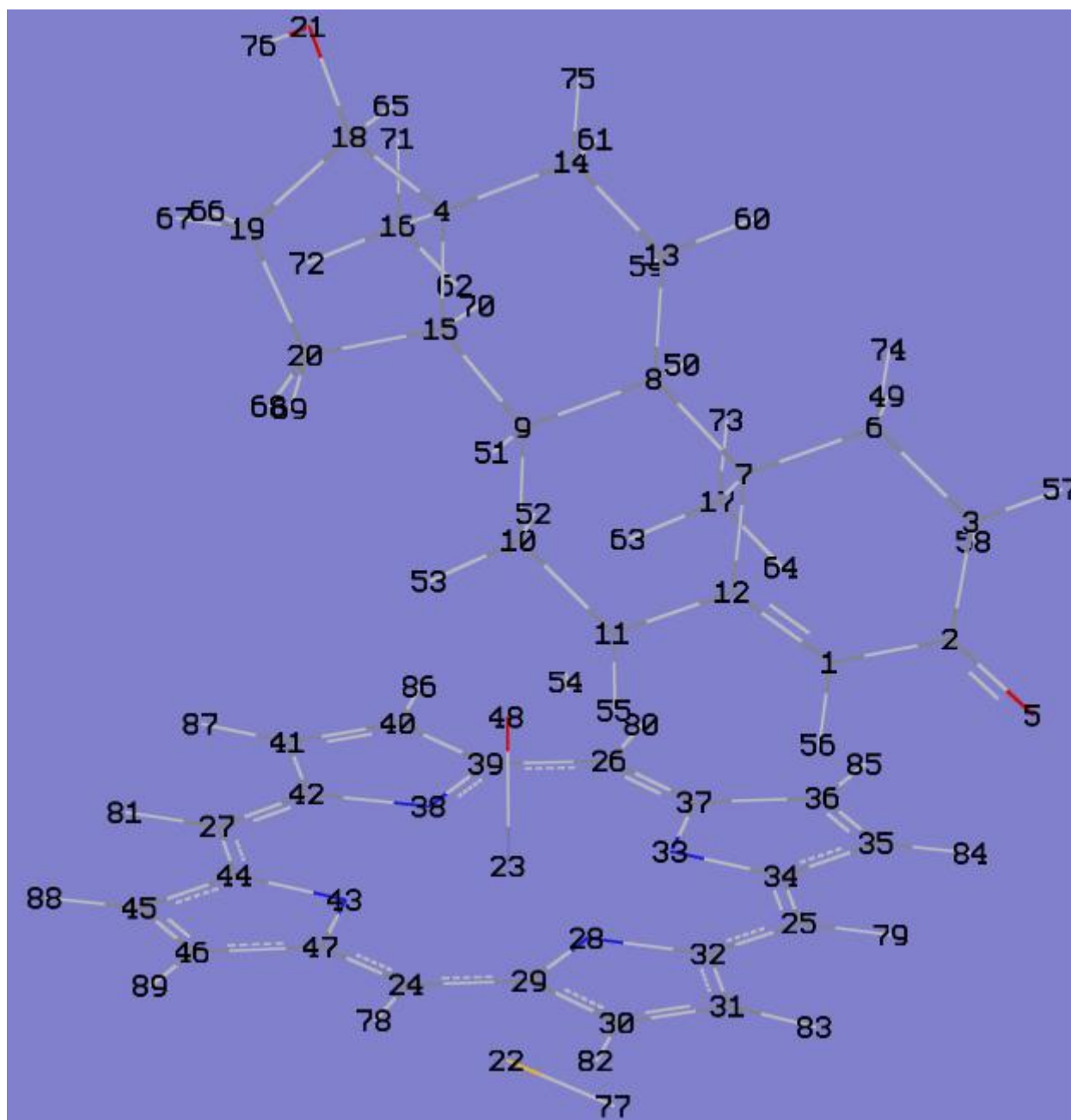
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505.6649	520.1444	527.8651
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IV. Atomic index and the internal coordinates used for generalized normal mode analysis in the MCMM reaction dynamics calculations.



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89-46-47-24	89-46-47-43	23-48-54-11		

Figure S1.  $V_{\text{MEP}}$  (kcal/mol) as a function of mass-scaled reactant coordinate  $s$  (bohr) by the MCMM-8, MCMM-9 and MCMM-10 reaction dynamics calculations for the  $6\beta$  H-abstraction of testosterone in the (A) doublet and (B) quartet spin states and for the  $6\beta$  D-abstraction of  $6\beta$ - $d_1$ - testosterone in the (C) doublet and (D) quartet spin states.

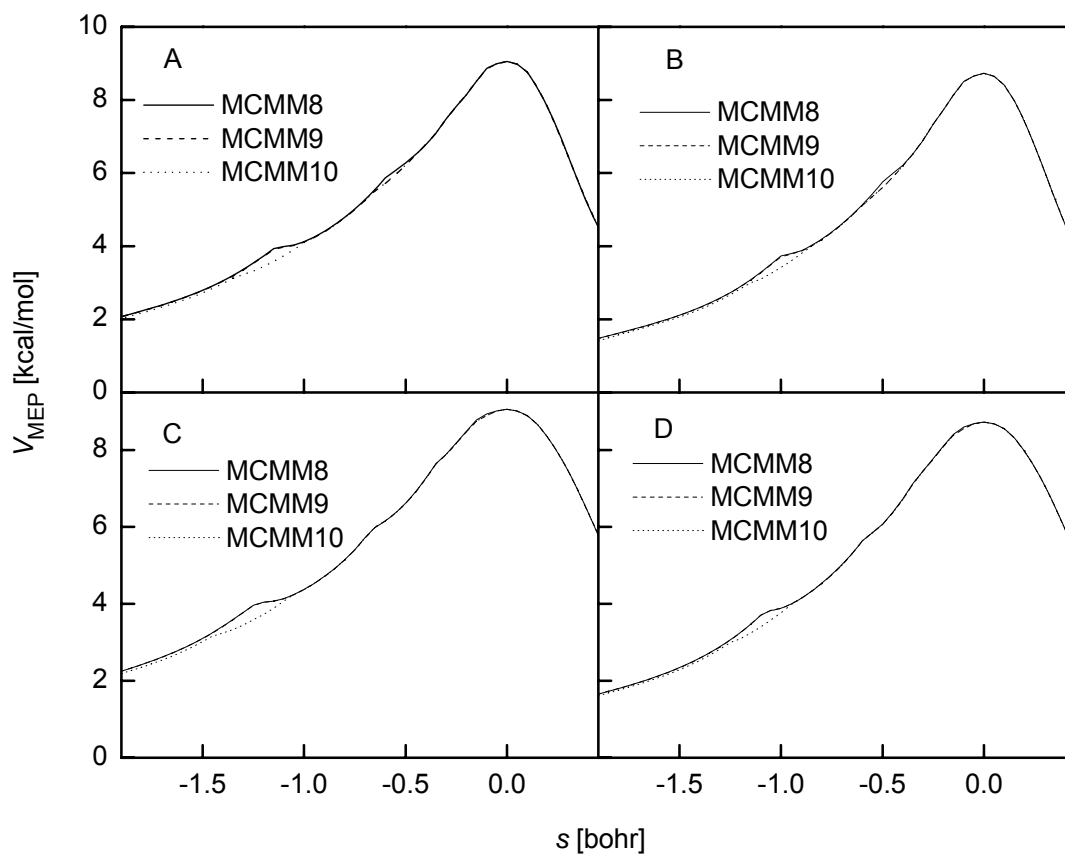


Figure S2.  $V_a^G$  (kcal/mol) at  $T = 300$  K as a function of mass-scaled reactant coordinate  $s$  (bohr) by the MCMM-8, MCMM-9 and MCMM-10 reaction dynamics calculations for the  $6\beta$  H-abstraction of testosterone in the (A) doublet and (B) quartet spin states and for the  $6\beta$  D-abstraction of  $6\beta$ - $d_1$ - testosterone in the (C) doublet and (D) quartet spin states.

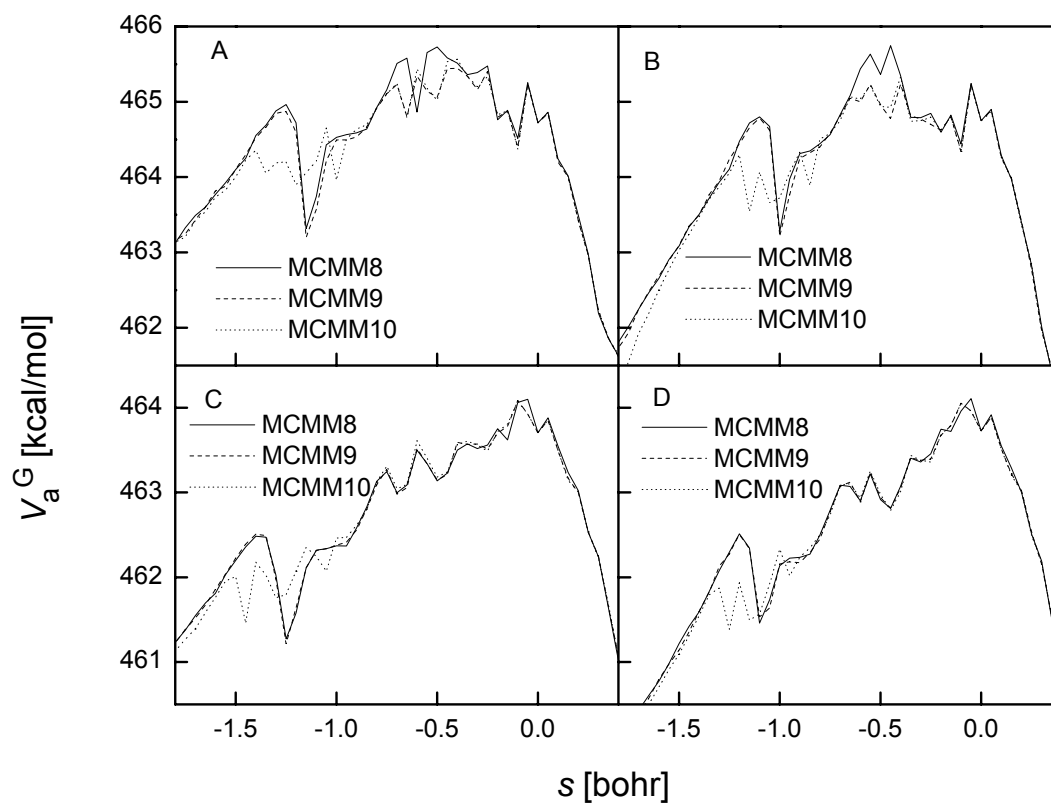


Table S1. Rate constants and transmission coefficients by MCMM-10 reaction dynamics calculations using different step sizes when following the MEP <sup>a</sup>

Rate Constants (cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> )				
Step Size (bohr)	TST	CVT	CVT/ZCT	CVT/SCT
0.0005	3.84E-20	8.47E-23	1.51E-22	2.59E-22
0.001	3.84E-20	8.65E-23	1.52E-22	2.65E-22
0.002	3.84E-20	9.00E-23	1.55E-22	3.62E-22
0.003	3.84E-20	9.16E-23	1.55E-22	4.29E-22
0.004	3.84E-20	8.51E-23	1.02E-22	3.45E-22
0.005	3.84E-20	1.09E-22	1.58E-22	6.08E-22

Transmission Coefficient			
Step Size (bohr)	TST/W	ZCT	SCT
0.0005	3.66	1.78	3.05
0.001	3.66	1.75	3.06
0.002	3.66	1.72	4.03
0.003	3.66	1.70	4.69
0.004	3.66	1.71	5.77
0.005	3.66	1.76	6.76

<sup>a</sup> Testosterone H-abstraction in the <sup>4</sup>A state at *T* = 300K.