

Supplementary Material

Computational investigation of cyclic substituted iodine(III) halogen bond donors

Raphaël Robidas,^a Stefan M. Huber,^{b*} and Claude Y. Legault^{a*}

^a*Department of Chemistry, Université de Sherbrooke, Sherbrooke, Canada*

^b*Department of Chemistry and Biochemistry, Ruhr-Universität Bochum, Bochum, Germany*

Email: claudel.legault@usherbrooke.ca, stefan.m.huber@rub.de

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Comparison with Experimental Data

We compared calculated bromide complexation free energies with experimental values obtained from isothermal calorimetry (ITC) for a few compounds (Figure S1). For unfunctionalized iodolium cation **1_H** as triflate salt, the approximate experimental complexation free energy of bromide (as tetrabutylammonium bromide in an acetonitrile solution) is -37 kJ/mol.¹ ITC measurements performed at a different temperature in another work lead to the similar value of -33 kJ/mol.² These values are respectively 7 kJ/mol and 11 kJ/mol lower than the calculated value, which could be attributed to the influence of the counter-ion. It has been shown previously that the triflate counter-ion can influence the measured Lewis acidity by competitive binding.² Computationally, a “naked” cation is used, and thus this influence is not taken into consideration.

Iodolium cation **9**, as triflate salt, was shown to have a bromide complexation free energy of -42 kJ/mol,¹ which deviates significantly from the calculated value. This could be explained by competitive binding of the triflate counter-ion, and possibly of the solvent (acetonitrile) as well. Due to the large number of combinations that could be modeled as well as the complexity of the system, we did not seek to exactly reproduce the experimental values. Nevertheless, iodolium cation **9** is indeed more Lewis acidic than **1_H**, as could be expected. These preliminary results suggest that the calculated bromide complexation free energies are indeed representative of the experimental values, although not in a direct fashion due to the complexity of the experimental system. The calculated values can be considered as maximal Lewis acidity values (*i.e.* when the counter-ion binds so weakly that it can be neglected).

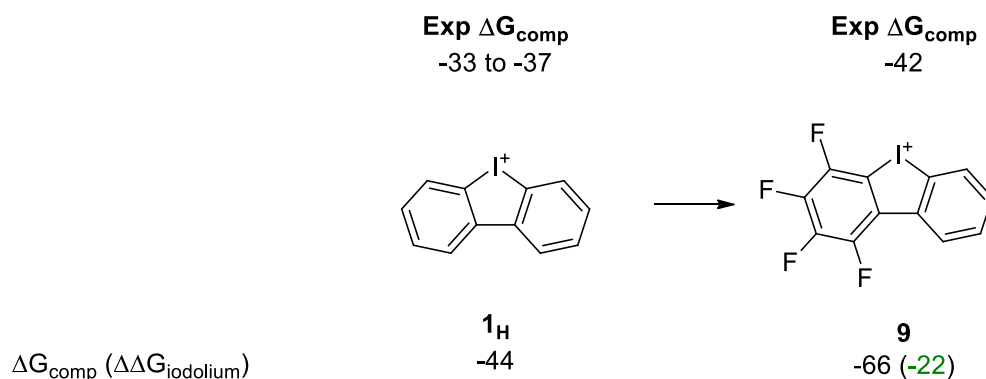


Figure S1. Comparison between the experimental and computational bromide complexation free energies of iodolium **1_H** and **9** (values in kJ/mol)

In the recent work on iodonium salts, the approximate bromide complexation constant of iodonium **10_{CH2}** was also determined. The calculations reproduce very closely the difference in bromide complexation free energy between **1_H** and **10_{CH2}**, namely 10 kJ/mol (Figure S2).

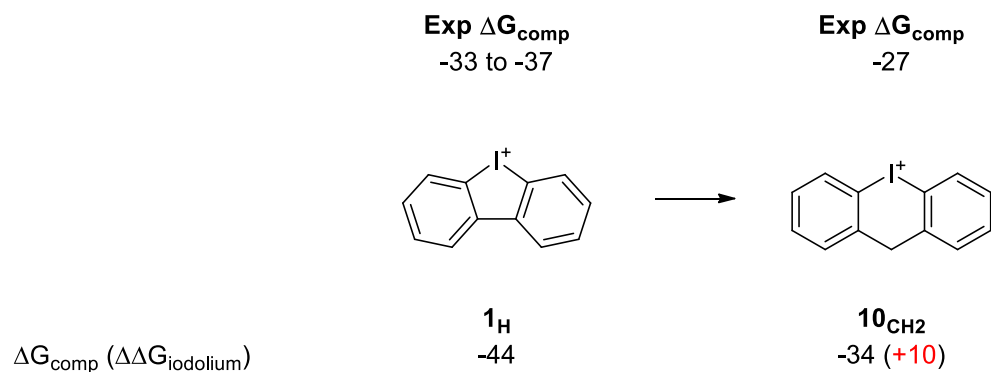


Figure S2. Comparison between the experimental and computational bromide complexation free energies of iodolium **1_H** and **10_{CH2}** (values in kJ/mol)

References of the Supporting Material

1. Reinhard, D. L.; Heinen, F.; Stoesser, J.; Engelage, E.; Huber, S. M. *Helv. Chim. Acta* **2021**, *104* (2), e2000221. <https://doi.org/10.1002/hlca.202000221>.
2. Mayer, R. J.; Ofial, A. R.; Mayr, H.; Legault, C. Y. *J. Am. Chem. Soc.* **2020**, *142* (11), 5221–5233. <https://doi.org/10.1021/jacs.9b12998>.

Structures

1_CF3_cation_conf1

H -3.468923 -0.059263 2.235840
C -2.391669 -0.032811 2.329229
C 0.413025 0.037710 2.545176
C -1.555116 -0.039104 1.235290
C -1.776502 0.011513 3.573336
C -0.389130 0.046182 3.674004
C -0.163960 -0.006842 1.275054
H -2.389608 0.019192 4.464593
H 0.074114 0.080985 4.651015
H 1.489459 0.067504 2.648423
C 0.558018 -0.011080 0.000820
C 1.735693 0.010557 -2.550116
C -0.190647 -0.043586 -1.171114
C 1.947995 0.022130 -0.145688
C 2.521460 0.027785 -1.402552
C 0.355329 -0.025260 -2.442228
H 2.578856 0.042426 0.732857
H 3.598277 0.051446 -1.498315
H 2.192494 0.027180 -3.530476
I -2.231419 -0.121637 -0.739106
C -0.502639 0.031691 -3.675405
F -1.598812 -0.742122 -3.549410
F -0.949575 1.273281 -3.900604
F 0.143180 -0.367876 -4.760721
SCF: -1096.561568
ZPE: 0.165836
H: -1096.381358
G: -1096.435229

1_CN_cation_conf1

H -3.665966 0.000000 -1.573809
C -2.600332 0.000000 -1.758044
C 0.178315 0.000000 -2.214745
C -1.673119 0.000000 -0.741237
C -2.091111 0.000000 -3.050778
C -0.717367 0.000000 -3.271078
C -0.289695 0.000000 -0.900841
H -2.778421 0.000000 -3.886291
H -0.339849 0.000000 -4.284860
H 1.243723 0.000000 -2.404321
C 0.538750 0.000000 0.304388

C 1.921281 0.000000 2.760642
C -0.112718 0.000000 1.528261
C 1.936405 0.000000 0.343111
C 2.608361 0.000000 1.552673
C 0.530287 0.000000 2.758139
H 2.495058 0.000000 -0.583395
H 3.689717 0.000000 1.560598
H 2.447788 0.000000 3.705083
I -2.179452 0.000000 1.294122
C -0.234555 0.000000 3.966332
N -0.907003 0.000000 4.895848
SCF: -851.719953
ZPE: 0.159685
H: -851.547711
G: -851.596182

1_F_cation_conf1

H -3.547054 0.000000 -1.704195
C -2.468358 0.000000 -1.782245
C 0.340776 0.000000 -1.961699
C -1.646442 0.000000 -0.678429
C -1.834594 0.000000 -3.018528
C -0.445656 0.000000 -3.101616
C -0.253586 0.000000 -0.699446
H -2.436103 0.000000 -3.917669
H 0.030360 0.000000 -4.073080
H 1.419910 0.000000 -2.042927
C 0.452479 0.000000 0.582369
C 1.536843 0.000000 3.186797
C -0.338164 0.000000 1.726842
C 1.833380 0.000000 0.776084
C 2.355140 0.000000 2.060583
C 0.171149 0.000000 3.004630
H 2.496136 0.000000 -0.078850
H 3.428251 0.000000 2.195989
H 1.939478 0.000000 4.190991
I -2.360467 0.000000 1.297108
F -0.673379 0.000000 4.037091
SCF: -858.723410
ZPE: 0.152820
H: -858.558961
G: -858.605315

1_H_cation_conf1

H 0.000000 0.051540 0.105931
C 0.000000 0.075444 1.186712
C 0.000000 0.109430 3.997489
C 0.000000 -1.072184 1.948142
C 0.000000 1.277843 1.880647
C 0.000000 1.288771 3.272071
C 0.000000 -1.121730 3.340220
H 0.000000 2.206252 1.325745
H 0.000000 2.233538 3.798923
H 0.000000 0.139202 5.079159
C 0.000000 -2.438047 3.980952
C 0.000000 -5.068188 4.966534
C 0.000000 -3.563575 3.160396
C 0.000000 -2.681185 5.355234
C 0.000000 -3.980273 5.834413
C 0.000000 -4.871388 3.592283
H 0.000000 -1.848677 6.046467
H 0.000000 -4.149825 6.902845
H 0.000000 -5.705862 2.904433
H 0.000000 -6.077787 5.354630
I 0.000000 -3.004099 1.145174
SCF: -759.477091
ZPE: 0.161048
H: -759.305304
G: -759.349589

1_NMe2_cation_conf1

H -1.601081 3.178720 -2.759835
C -1.035994 3.224628 -1.839230
C 0.434087 3.325458 0.554971
C -0.680520 2.092794 -1.139209
C -0.632074 4.441873 -1.305395
C 0.096729 4.486543 -0.121053
C 0.044969 2.083666 0.053100
H -0.889678 5.356245 -1.823251
H 0.406529 5.442626 0.279615
H 1.004225 3.374898 1.473691
C 0.329115 0.783817 0.664222
C 0.635245 -1.859113 1.586273
C -0.123240 -0.333188 -0.016914
C 0.967496 0.533223 1.880508
C 1.103358 -0.773218 2.324683

C 0.002863 -1.653717 0.362237
H 1.333875 1.355402 2.480945
H 1.590987 -0.957592 3.273104
H 0.766189 -2.866877 1.959076
I -1.172676 0.141034 -1.739526
N -0.507030 -2.650966 -0.503610
C 0.474893 -3.060680 -1.515960
C -1.064237 -3.814866 0.178985
H -0.028475 -3.673772 -2.262735
H 1.288686 -3.641169 -1.064678
H 0.905590 -2.188795 -2.008671
H -1.592880 -4.420453 -0.556514
H -0.287850 -4.435755 0.641452
H -1.768802 -3.490970 0.943615
SCF: -893.438729
ZPE: 0.234015
H: -893.189724
G: -893.243513

1_NMe2_cation_conf2

H 0.070597 3.775809 -2.100040
C 0.397560 3.913665 -1.078496
C 1.247961 4.254793 1.579936
C 0.667182 2.851281 -0.243947
C 0.565307 5.185181 -0.544432
C 0.987340 5.348886 0.771238
C 1.089650 2.961633 1.081945
H 0.364108 6.048573 -1.164605
H 1.114783 6.346263 1.170848
H 1.577330 4.397493 2.601209
C 1.324930 1.721673 1.824345
C 1.614858 -0.839328 2.959341
C 1.133390 0.539026 1.131176
C 1.680888 1.584053 3.167609
C 1.811779 0.316311 3.713958
C 1.271037 -0.746076 1.612820
H 1.833684 2.462466 3.780525
H 2.078219 0.219423 4.758394
H 1.733823 -1.814183 3.414734
I 0.484798 0.837317 -0.813521
N 1.058212 -1.822881 0.718062
C 0.437908 -2.995948 1.326577
C 2.284262 -2.194935 0.000063
H 1.121433 -3.521578 2.003732

H 0.150556 -3.681773 0.530214
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1_OMe_cation_conf1

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C -1.101013 -0.288257 1.925866
C -0.663741 -0.337975 4.235813
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C 0.230656 -0.043122 1.593018
H -0.999937 -0.449570 5.258040
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C 1.962318 0.433410 -1.748035
C -0.384769 0.046822 -2.102402
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H 2.941046 0.624329 -2.168549
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H -0.796733 -0.807741 -4.608193
H -1.106519 0.952853 -4.522364
H -2.470305 -0.194305 -4.568778
SCF: -874.007441
ZPE: 0.193857
H: -873.800219
G: -873.850197

1_OMe_cation_conf2

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C 0.677078 0.000745 2.806024
C -1.429581 -0.001141 1.722058
C -1.382660 -0.000971 4.072972
C 0.007877 0.000238 4.018706
C -0.040079 0.000054 1.609592
H -1.892278 -0.001367 5.027218
H 0.577763 0.000781 4.938346
H 1.759160 0.001677 2.778152
C 0.537052 0.000459 0.264723
C 1.327598 0.000914 -2.440637
C -0.357905 -0.000393 -0.792490
C 1.891971 0.001607 -0.069816
C 2.260648 0.001799 -1.405277
C -0.030342 -0.000199 -2.137236
H 2.643107 0.002337 0.708377
H 3.312314 0.002679 -1.660402
H 1.655814 0.001104 -3.470608
I -2.332039 -0.002036 -0.172983
O -1.053446 -0.001089 -3.003714
C -0.740187 -0.000791 -4.397359
H -0.173116 -0.895089 -4.658968
H -0.174528 0.894421 -4.658901
H -1.694527 -0.001529 -4.915436
SCF: -874.007488
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2_CF3_cation_conf1

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C 2.577320 -0.059385 0.139302
C 1.395379 0.060787 -1.907252
C 3.742690 0.014165 -1.977871
C 3.755382 -0.052061 -0.588223
C 1.346813 -0.001695 -0.516838
H 4.670769 0.020034 -2.533635
H 4.700794 -0.098512 -0.064504
H 2.608583 -0.111060 1.219671
C 0.031436 -0.003770 0.123317
C -2.585473 0.000274 1.105136
C -1.091472 0.050680 -0.697207
C -0.208549 -0.056008 1.498416
C -1.502956 -0.053352 1.979685

C -2.399824 0.054355 -0.266295
H 0.621468 -0.098250 2.190602
H -1.677826 -0.094183 3.047566
I -0.537660 0.129076 -2.708268
H -3.236222 0.096500 -0.950197
C -3.974822 0.001363 1.681296
F -4.919105 0.025865 0.738951
F -4.195625 -1.084146 2.434782
F -4.178464 1.063189 2.472974
SCF: -1096.564659
ZPE: 0.165726
H: -1096.384517
G: -1096.438572

2_CN_cation_conf1

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C 1.255349 0.023493 -1.824095
C -1.108533 0.014770 -1.686501
C -0.117062 0.020554 -3.814659
C 1.132993 0.025504 -3.203325
C 0.114537 0.014925 -1.020728
H -0.197445 0.021349 -4.893491
H 2.025589 0.031296 -3.814461
H 2.234551 0.030413 -1.363249
C 0.099313 0.008792 0.440151
C -0.183577 0.009211 3.219808
C -1.140377 0.015005 1.078069
C 1.225190 -0.004301 1.263958
C 1.086426 -0.003211 2.637910
C -1.336916 0.016287 2.437575
H 2.212888 -0.016373 0.823509
H 1.962483 -0.011621 3.271907
I -2.692011 0.017757 -0.316621
H -2.318154 0.022345 2.891663
C -0.311758 0.013627 4.648628
N -0.410219 0.018012 5.791435
SCF: -851.724054
ZPE: 0.159302
H: -851.552101
G: -851.601212

2_F_cation_conf1

H -2.388206 0.000000 -3.153898

C -1.394734 0.000000 -2.727219
C 1.177906 0.000000 -1.589948
C -1.175961 0.000000 -1.367937
C -0.263003 0.000000 -3.532186
C 1.007448 0.000000 -2.964106
C 0.068476 0.000000 -0.744225
H -0.381413 0.000000 -4.607368
H 1.879001 0.000000 -3.605139
H 2.172554 0.000000 -1.164350
C 0.105238 0.000000 0.717503
C -0.078687 0.000000 3.485992
C -1.107516 0.000000 1.400352
C 1.257820 0.000000 1.506211
C 1.169500 0.000000 2.885475
C -1.259784 0.000000 2.768916
H 2.231452 0.000000 1.033925
H 2.056369 0.000000 3.504552
I -2.707981 0.000000 0.058806
H -2.215485 0.000000 3.274361
F -0.153096 0.000000 4.820384
SCF: -858.726437
ZPE: 0.152125
H: -858.562592
G: -858.609430

2_NMe2_cation_conf1

H -1.240891 3.482721 -3.750137
C -0.714882 3.481870 -2.808365
C 0.639592 3.381887 -0.355464
C -0.558894 2.333926 -2.076739
C -0.154002 4.667356 -2.275930
C 0.523111 4.573101 -1.032064
C 0.094650 2.193375 -0.858094
H 0.962580 5.456824 -0.594275
H 1.165997 3.364122 0.590715
C 0.151333 0.876039 -0.241228
C 0.123002 -1.763202 0.739522
C -0.457177 -0.187404 -0.906039
C 0.766009 0.558605 0.973446
C 0.748138 -0.741550 1.449295
C -0.500223 -1.493493 -0.471995
H 1.258007 1.338761 1.539906
H 1.230576 -0.965525 2.391773
I -1.317170 0.477860 -2.697134

H -0.990936 -2.274438 -1.036545
N -0.263773 5.842129 -2.935278
C -0.968587 5.900254 -4.201836
H -0.973807 6.926690 -4.555261
H -2.004577 5.568096 -4.092455
H -0.482992 5.274944 -4.956604
C 0.342284 7.042613 -2.388732
H 1.421235 6.919629 -2.263547
H -0.090853 7.300573 -1.418695
H 0.167361 7.865728 -3.074649
H 0.117093 -2.774288 1.123812
SCF: -893.442063
ZPE: 0.234322
H: -893.192540
G: -893.246957

2_OMe_cation_conf1

H -1.647076 0.000000 4.293971
C -0.710503 0.000000 3.753705
C 1.710066 0.000000 2.320869
C -0.653646 0.000000 2.377935
C 0.507727 0.000000 4.420436
C 1.702088 0.000000 3.705627
C 0.508306 0.000000 1.610252
H 0.517155 0.000000 5.502169
H 2.642927 0.000000 4.239849
H 2.648276 0.000000 1.781272
C 0.370093 0.000000 0.156884
C -0.154506 0.000000 -2.613545
C -0.906004 0.000000 -0.385671
C 1.417555 0.000000 -0.773726
C 1.160283 0.000000 -2.124250
C -1.230554 0.000000 -1.725770
H 2.441371 0.000000 -0.423020
H 1.972825 0.000000 -2.838882
I -2.341038 0.000000 1.138519
H -2.254714 0.000000 -2.066973
O -0.292437 0.000000 -3.946194
C -1.609214 0.000000 -4.485623
H -2.154700 0.893919 -4.176191
H -2.154700 -0.893919 -4.176191
H -1.489681 0.000000 -5.565349
SCF: -874.005124
ZPE: 0.193852

H: -873.797989

G: -873.847975

2_OMe_cation_conf2

H -2.167854 -0.000012 4.314777
C -1.218426 -0.000007 3.797513
C 1.237899 0.000005 2.427146
C -1.126286 -0.000004 2.423542
C -0.017576 -0.000004 4.495253
C 1.194650 0.000002 3.811220
C 0.054673 0.000002 1.685684
H -0.035935 -0.000006 5.576922
H 2.121536 0.000005 4.369409
H 2.189911 0.000009 1.911922
C -0.045253 0.000004 0.229013
C -0.497354 0.000007 -2.555708
C -1.314762 0.000001 -0.346174
C 1.016966 0.000009 -0.672701
C 0.802581 0.000011 -2.039848
C -1.594754 0.000002 -1.686906
H 2.032303 0.000012 -0.297799
H 1.655564 0.000014 -2.702543
I -2.785683 -0.000008 1.142372
H -2.598924 -0.000001 -2.087823
O -0.794613 0.000008 -3.862634
C 0.280394 0.000012 -4.796379
H 0.896090 -0.893624 -4.678241
H 0.896085 0.893651 -4.678240
H -0.181333 0.000012 -5.779777
SCF: -874.004824
ZPE: 0.193904
H: -873.797651
G: -873.847591

3_CF3_cation_conf1

H 2.168769 -0.020445 -4.028050
C 2.198041 -0.002079 -2.947586
C 2.249571 0.046048 -0.135146
C 1.056948 -0.009718 -2.177672
C 3.404107 0.031215 -2.259782
C 3.423794 0.055743 -0.868842
C 1.015318 0.011627 -0.785851
H 4.329279 0.038273 -2.820325
H 4.371905 0.082426 -0.348650

H 2.287744 0.065403 0.946130
C -0.297911 -0.004075 -0.140927
C -2.926606 -0.042357 0.854421
C -1.426388 -0.035572 -0.953794
C -0.529294 0.008308 1.235861
C -1.827145 -0.009515 1.708981
C -2.733551 -0.055881 -0.516241
H 0.304917 0.031185 1.923689
H -3.932846 -0.058066 1.253481
I -0.880576 -0.052228 -2.969888
H -3.572768 -0.080999 -1.197370
C -2.094939 -0.001000 3.190355
F -2.889309 1.019962 3.538915
F -2.718677 -1.120665 3.582686
F -0.980384 0.102206 3.915601
SCF: -1096.564946
ZPE: 0.165767
H: -1096.384770
G: -1096.439256

3_CN_cation_conf1

H -0.310797 0.000000 -4.196818
C 0.288679 0.000000 -3.296695
C 1.830273 0.000000 -0.941467
C -0.266851 0.000000 -2.037204
C 1.676438 0.000000 -3.355144
C 2.433625 0.000000 -2.187901
C 0.438875 0.000000 -0.836937
H 2.162252 0.000000 -4.321678
H 3.513506 0.000000 -2.252452
H 2.437760 0.000000 -0.046091
C -0.330157 0.000000 0.407724
C -2.033833 0.000000 2.651925
C -1.720919 0.000000 0.321131
C 0.206787 0.000000 1.692138
C -0.644484 0.000000 2.790094
C -2.595323 0.000000 1.386118
H 1.277918 0.000000 1.841265
H -2.669198 0.000000 3.526806
I -2.328469 0.000000 -1.676184
H -3.669093 0.000000 1.258902
C -0.074160 0.000000 4.109134
N 0.377474 0.000000 5.163234
SCF: -851.724247

ZPE: 0.159805
H: -851.551929
G: -851.600455

3_F_cation_conf1

H -0.658378 0.000000 3.899927
C 0.023966 0.000000 3.061044
C 1.774921 0.000000 0.860118
C -0.415829 0.000000 1.756215
C 1.399572 0.000000 3.248843
C 2.261551 0.000000 2.156361
C 0.399355 0.000000 0.627026
H 1.793578 0.000000 4.256157
H 3.330820 0.000000 2.320054
H 2.460815 0.000000 0.023111
C -0.250246 0.000000 -0.684570
C -1.730999 0.000000 -3.079481
C -1.643563 0.000000 -0.723354
C 0.408949 0.000000 -1.911869
C -0.345968 0.000000 -3.064714
C -2.407839 0.000000 -1.870881
H 1.488765 0.000000 -1.977153
H -2.264581 0.000000 -4.019812
I -2.433972 0.000000 1.207398
H -3.488506 0.000000 -1.845512
F 0.297489 0.000000 -4.238907
SCF: -858.727590
ZPE: 0.152740
H: -858.563272
G: -858.609552

3_NMe2_cation_conf1

H 0.180489 2.331645 -4.840929
C 0.248283 2.396229 -3.763516
C 0.420091 2.533042 -0.960974
C 0.090526 1.296549 -2.949256
C 0.501388 3.604497 -3.127495
C 0.585630 3.666241 -1.739660
C 0.163241 1.298452 -1.558947
H 0.632842 4.497660 -3.723627
H 0.784090 4.614922 -1.258615
H 0.489699 2.599583 0.116956
C -0.032468 0.026897 -0.856567
C -0.443958 -2.506413 0.261575

C -0.279582 -1.103402 -1.632645
C 0.008004 -0.134472 0.520273
C -0.192692 -1.400013 1.112221
C -0.487150 -2.363380 -1.110130
H 0.195213 0.732121 1.136389
H -0.605317 -3.490112 0.675942
I -0.296502 -0.632582 -3.662698
H -0.679117 -3.221902 -1.739610
N -0.146607 -1.554744 2.458111
C -0.396090 -2.854676 3.051646
C 0.109077 -0.411113 3.311825
H -1.391321 -3.227109 2.793185
H -0.334032 -2.764334 4.131928
H 0.342505 -3.591376 2.723939
H -0.674990 0.345859 3.214015
H 0.140422 -0.743376 4.345011
H 1.068326 0.055408 3.071554
SCF: -893.441102
ZPE: 0.234384
H: -893.191539
G: -893.245948

3_OMe_cation_conf1

H 0.256347 0.000000 -4.847887
C 0.776766 0.000000 -3.900145
C 2.110835 0.000000 -1.424351
C 0.113610 0.000000 -2.693203
C 2.164387 0.000000 -3.841462
C 2.819713 0.000000 -2.613858
C 0.715850 0.000000 -1.438007
H 2.730676 0.000000 -4.763159
H 3.901289 0.000000 -2.586087
H 2.635361 0.000000 -0.477924
C -0.151737 0.000000 -0.258839
C -2.015910 0.000000 1.843843
C -1.532095 0.000000 -0.468209
C 0.281408 0.000000 1.057307
C -0.642130 0.000000 2.103780
C -2.473326 0.000000 0.533487
H 1.337389 0.000000 1.294399
H -2.736836 0.000000 2.647925
I -1.972455 0.000000 -2.507689
H -3.534775 0.000000 0.326977
O -0.118406 0.000000 3.340117

C -1.009800 0.000000 4.448887
H -1.637271 -0.893589 4.444376
H -1.637271 0.893589 4.444376
H -0.381521 0.000000 5.335346
SCF: -874.005111
ZPE: 0.194128
H: -873.797770
G: -873.847551

3_OMe_cation_conf2

H -0.221819 -0.000142 -4.709067
C 0.314793 -0.000086 -3.770502
C 1.690410 0.000060 -1.317571
C -0.327756 -0.000087 -2.552479
C 1.703053 -0.000009 -3.735607
C 2.378723 0.000064 -2.519111
C 0.294977 -0.000017 -1.306849
H 2.253685 -0.000005 -4.666718
H 3.460624 0.000123 -2.509482
H 2.234190 0.000116 -0.382145
C -0.554525 -0.000030 -0.114485
C -2.375022 -0.000067 2.012073
C -1.931128 -0.000109 -0.300022
C -0.086425 0.000031 1.199820
C -0.993367 0.000012 2.254458
C -2.861626 -0.000129 0.722138
H 0.977756 0.000095 1.382817
H -3.054383 -0.000078 2.854146
I -2.408208 -0.000196 -2.330432
H -3.926451 -0.000191 0.533430
O -0.631789 0.000065 3.547187
C 0.756758 0.000132 3.854714
H 1.242652 0.893601 3.457280
H 1.242732 -0.893306 3.457306
H 0.822346 0.000150 4.939104
SCF: -874.005377
ZPE: 0.194310
H: -873.797889
G: -873.847548

4_CF3_cation_conf1

H 2.103189 0.081625 -3.707768
C 2.073082 0.048932 -2.627272
C 1.938575 -0.054418 0.166348

C 0.886470 0.042292 -1.930346
C 3.237399 0.006977 -1.875793
C 3.157836 -0.050120 -0.491698
C 0.730943 0.002847 -0.540361
H 4.196337 0.011504 -2.376029
H 4.064262 -0.094464 0.097032
H 1.957915 -0.110424 1.238838
C -0.653848 0.005783 -0.014427
C -3.439089 -0.038495 0.585595
C -1.677593 -0.000985 -0.966694
C -1.125880 0.017503 1.317652
C -2.485108 -0.010083 1.592351
C -3.035881 -0.023966 -0.734592
H -4.491503 -0.061234 0.831711
I -0.946601 0.055748 -2.912930
H -3.754897 -0.029238 -1.542845
H -2.815414 -0.003967 2.620237
C -0.207725 0.081374 2.516170
F -0.881552 0.188117 3.661009
F 0.555986 -1.015084 2.629970
F 0.613000 1.139777 2.463742
SCF: -1096.553122
ZPE: 0.166120
H: -1096.372835
G: -1096.425470

4_CN_cation_conf1

H -3.131536 0.000000 -2.594390
C -2.070018 0.000000 -2.387762
C 0.678681 0.000000 -1.815378
C -1.571798 0.000000 -1.105660
C -1.136127 0.000000 -3.415141
C 0.221831 0.000000 -3.123218
C -0.221953 0.000000 -0.746448
H -1.477914 0.000000 -4.441385
H 0.943083 0.000000 -3.929541
H 1.742089 0.000000 -1.636431
C 0.094217 0.000000 0.688059
C 0.373892 0.000000 3.514050
C -0.975938 0.000000 1.582518
C 1.360095 0.000000 1.303849
C 1.488177 0.000000 2.691624
C -0.895395 0.000000 2.957743
H 0.490174 0.000000 4.588772

I -2.801751 0.000000 0.579679
H -1.778034 0.000000 3.582869
H 2.480748 0.000000 3.121113
C 2.587159 0.000000 0.561459
N 3.600416 0.000000 0.023518
SCF: -851.718978
ZPE: 0.159651
H: -851.546825
G: -851.595179

4_F_cation_conf1

H 1.029793 0.000000 3.798765
C 1.306753 0.000000 2.753560
C 1.989594 0.000000 0.025539
C 0.368580 0.000000 1.747595
C 2.637831 0.000000 2.358060
C 2.966999 0.000000 1.007977
C 0.636620 0.000000 0.377809
H 3.413252 0.000000 3.112344
H 4.007534 0.000000 0.712147
H 2.277104 0.000000 -1.014133
C -0.513553 0.000000 -0.527384
C -2.887454 0.000000 -2.058281
C -1.796936 0.000000 0.022630
C -0.498844 0.000000 -1.921700
C -1.648552 0.000000 -2.682355
C -2.983632 0.000000 -0.672287
H -3.790250 0.000000 -2.653560
I -1.689209 0.000000 2.107216
H -3.944807 0.000000 -0.177914
H -1.558480 0.000000 -3.760370
F 0.677555 0.000000 -2.555561
SCF: -858.723590
ZPE: 0.152685
H: -858.559297
G: -858.605646

4_NMe2_cation_conf1

H 2.323657 0.715539 -4.108910
C 2.222868 0.472039 -3.060011
C 1.916854 -0.189784 -0.351979
C 0.995332 0.373169 -2.444972
C 3.336581 0.229244 -2.267994
C 3.172943 -0.115340 -0.932229

C 0.761738 0.073705 -1.099927
H 4.324152 0.296279 -2.704243
H 4.042468 -0.330378 -0.325077
H 1.823432 -0.472262 0.684851
C -0.635860 -0.006729 -0.647479
C -3.380380 -0.453795 -0.187011
C -1.624984 0.086517 -1.626850
C -1.106773 -0.243926 0.672621
C -2.469085 -0.507877 0.854539
C -2.975466 -0.114552 -1.470621
H -4.428072 -0.644082 0.006042
I -0.801121 0.564649 -3.488935
H -3.679123 -0.026237 -2.286008
H -2.831947 -0.728943 1.847704
N -0.219704 -0.225895 1.747434
C 0.408557 1.067464 2.018158
C -0.651029 -0.868265 2.977862
H 0.651496 1.587865 1.095143
H 1.327289 0.913678 2.585426
H -0.266128 1.702687 2.604700
H -1.029523 -1.867882 2.768891
H 0.215015 -0.953256 3.634017
H -1.423290 -0.293633 3.504861
SCF: -893.430569
ZPE: 0.234449
H: -893.181458
G: -893.233930

4_NMe2_cation_conf2

H 3.168245 1.710753 -3.556660
C 3.173261 1.442883 -2.509224
C 3.134623 0.719293 0.199596
C 2.017461 1.383272 -1.764414
C 4.354203 1.126971 -1.851958
C 4.321698 0.753148 -0.514436
C 1.918328 1.055167 -0.409597
H 5.289648 1.160851 -2.394037
H 5.241175 0.482885 -0.011922
H 3.141792 0.412812 1.233781
C 0.575776 1.022398 0.190982
C -2.120075 0.680758 0.938463
C -0.508065 1.188670 -0.671224
C 0.240495 0.765251 1.548056
C -1.104607 0.555231 1.872025

C -1.841412 1.041460 -0.372616
H -3.148384 0.530442 1.240280
I 0.130379 1.689375 -2.599657
H -2.624517 1.185769 -1.103065
H -1.367302 0.319484 2.893038
N 1.239882 0.711841 2.518027
C 0.918811 0.046244 3.769502
C 1.948656 1.969856 2.754040
H 0.468937 -0.926189 3.574510
H 0.240966 0.636671 4.398864
H 1.848133 -0.102983 4.319094
H 2.114448 2.508989 1.824594
H 1.368008 2.613056 3.426352
H 2.914837 1.761745 3.215307
SCF: -893.430568
ZPE: 0.234529
H: -893.181395
G: -893.233776

4_OMe_cation_conf1

H 2.087368 0.000000 -4.045643
C 2.071582 0.000000 -2.964496
C 1.985154 0.000000 -0.157760
C 0.896030 0.000000 -2.250325
C 3.247077 0.000000 -2.225667
C 3.193293 0.000000 -0.837929
C 0.772229 0.000000 -0.857938
H 4.197853 0.000000 -2.741334
H 4.112862 0.000000 -0.267777
H 1.978556 0.000000 0.919422
C -0.585440 0.000000 -0.302047
C -3.293395 0.000000 0.474114
C -1.656663 0.000000 -1.192842
C -0.944854 0.000000 1.064952
C -2.289432 0.000000 1.430720
C -2.995921 0.000000 -0.880600
H -4.328360 0.000000 0.789232
I -0.978508 0.000000 -3.168112
H -3.771346 0.000000 -1.633133
H -2.562257 0.000000 2.475279
O 0.059061 0.000000 1.951658
C -0.255416 0.000000 3.341748
H -0.820137 -0.894222 3.610276
H -0.820137 0.894222 3.610276

H 0.700405 0.000000 3.858031
SCF: -874.001939
ZPE: 0.194133
H: -873.794598
G: -873.844269

4_OMe_cation_conf2

H 1.552722 -0.157327 -4.278393
C 1.673605 -0.146340 -3.203824
C 1.945592 -0.118872 -0.408829
C 0.600667 -0.068177 -2.346416
C 2.931564 -0.212411 -2.619586
C 3.055172 -0.197718 -1.236430
C 0.655421 -0.050434 -0.949623
H 3.807426 -0.274194 -3.251386
H 4.038500 -0.248748 -0.787782
H 2.076162 -0.109598 0.660349
C -0.617718 0.036073 -0.225721
C -3.199240 0.208114 0.889010
C -1.792262 0.095701 -0.972705
C -0.798737 0.066134 1.175900
C -2.082987 0.153184 1.709925
C -3.078332 0.179414 -0.492569
H -4.183660 0.274195 1.333112
I -1.372780 0.041104 -3.018283
H -3.942879 0.220303 -1.139257
H -2.219537 0.178366 2.780684
O 0.307682 0.007393 1.928365
C 0.170766 0.028112 3.346792
H -0.296728 0.957260 3.676247
H 1.181808 -0.033757 3.739298
H -0.412231 -0.827580 3.691223
SCF: -874.001870
ZPE: 0.193799
H: -873.794742
G: -873.844968

5_CF3_cation_conf1

H 1.838353 1.358037 -3.505705
C 1.881989 1.078646 -2.461838
C 1.988640 0.152206 0.175078
C 0.792394 0.567792 -1.796203
C 3.054690 1.199883 -1.734456
C 3.109541 0.682085 -0.451613

C 0.727190 0.189738 -0.448798
H 3.937488 1.619170 -2.196498
H 4.060048 0.650686 0.066395
C -0.619903 -0.185443 0.053900
C -3.216586 -1.205451 0.607567
C -1.552492 -0.562568 -0.921115
C -1.162802 -0.152534 1.352301
C -2.417700 -0.688350 1.613342
C -2.810319 -1.077212 -0.710662
H -4.184206 -1.629215 0.837562
I -0.928866 0.005702 -2.824925
H -3.461674 -1.353495 -1.528797
H -2.795077 -0.662985 2.628118
C -0.584975 0.634450 2.508787
F -1.490630 1.534320 2.922036
F -0.295119 -0.116462 3.573918
F 0.507324 1.326931 2.185391
C 2.309205 -0.632095 1.429149
F 1.271956 -1.322246 1.903265
F 2.789276 0.122289 2.420832
F 3.262955 -1.533880 1.151168
SCF: -1433.618847
ZPE: 0.170316
H: -1433.430884
G: -1433.490847

5_CN_cation_conf1

H -3.238540 -0.225782 -2.358468
C -2.170091 -0.120138 -2.227131
C 0.571034 0.307052 -1.849833
C -1.584017 -0.082116 -0.982134
C -1.326018 0.000909 -3.321178
C 0.021402 0.256760 -3.129926
C -0.219657 0.041295 -0.714500
H -1.735022 -0.040368 -4.321056
H 0.661761 0.458087 -3.977891
C 0.194156 -0.036221 0.691506
C 0.671085 -0.004999 3.483921
C -0.808657 0.086775 1.654693
C 1.472718 -0.304312 1.219364
C 1.701300 -0.257479 2.593740
C -0.629708 0.118915 3.018924
H 0.867079 0.032277 4.546442
I -2.696959 0.005961 0.777564

H -1.459197 0.221887 3.705300
H 2.698489 -0.459664 2.960282
C 2.542897 -0.827216 0.420725
N 3.397607 -1.332217 -0.153649
C 1.903391 0.828370 -1.754000
N 2.933445 1.332224 -1.729294
SCF: -943.951304
ZPE: 0.158088
H: -943.778969
G: -943.831124

5_F_cation_conf1

H 0.987882 -0.049222 3.782045
C 1.295346 -0.024943 2.745889
C 2.037096 0.071980 0.067697
C 0.388630 -0.011694 1.713670
C 2.637397 -0.001300 2.391875
C 3.000272 0.054077 1.058189
C 0.665044 0.016978 0.339166
H 3.396299 -0.014307 3.162257
H 4.038516 0.093508 0.756621
C -0.486833 0.008613 -0.580379
C -2.924714 0.025289 -2.049566
C -1.766057 0.041934 -0.006377
C -0.525584 -0.051697 -1.978287
C -1.704545 -0.034245 -2.698556
C -2.973176 0.053814 -0.662531
H -3.843820 0.036692 -2.619087
I -1.660859 0.018282 2.072165
H -3.916492 0.078717 -0.135417
H -1.640450 -0.077115 -3.777685
F 0.598448 -0.147853 -2.683474
F 2.476704 0.162493 -1.184516
SCF: -957.965009
ZPE: 0.144398
H: -957.808129
G: -957.857026

5_NMe2_cation_conf1

H 1.857932 1.394327 -4.258255
C 1.759748 1.034404 -3.244445
C 1.486114 -0.164722 -0.671116
C 0.553736 0.725469 -2.672916
C 2.867715 0.840072 -2.418843

C 2.737010 0.239895 -1.183353
C 0.317465 0.258720 -1.375734
H 3.852742 1.097171 -2.786173
H 3.631740 0.011441 -0.622418
C -1.077658 0.228736 -0.920410
C -3.813965 -0.229330 -0.435273
C -2.069716 0.246864 -1.906012
C -1.569074 0.217974 0.421197
C -2.925965 -0.116687 0.614872
C -3.412629 0.028609 -1.746430
H -4.854440 -0.448687 -0.233703
I -1.241908 0.792072 -3.753016
H -4.116034 0.059145 -2.565817
H -3.301073 -0.221396 1.622769
N -0.760794 0.521863 1.478504
C 0.148222 1.653954 1.418019
C -1.165009 0.173388 2.824860
H 0.209025 2.053409 0.409745
H 1.149415 1.371804 1.749614
H -0.224218 2.448723 2.072815
H -1.567796 -0.838294 2.855655
H -0.282475 0.210029 3.464098
H -1.911776 0.868214 3.228099
N 1.401315 -0.933684 0.453361
C 0.490621 -2.064277 0.515965
H -0.095634 -2.044987 1.436672
H 1.070290 -2.992889 0.491955
H -0.185704 -2.071233 -0.334091
C 2.544075 -1.060959 1.334127
H 3.016441 -0.092512 1.493450
H 3.291415 -1.763757 0.946046
H 2.190846 -1.432768 2.296381
SCF: -1027.381379
ZPE: 0.307669
H: -1027.054887
G: -1027.115728

5_NMe2_cation_conf2

H 2.869670 2.156604 -3.209594
C 2.729953 1.886182 -2.173048
C 2.345100 0.919259 0.482290
C 1.499981 1.631629 -1.626025
C 3.802936 1.760002 -1.290525
C 3.618088 1.271210 -0.013507

C 1.207551 1.279426 -0.304266
H 4.803865 1.979188 -1.638989
H 4.487672 1.087600 0.600849
C -0.206559 1.289065 0.091892
C -2.965096 0.877722 0.492299
C -1.154815 1.223866 -0.934323
C -0.757095 1.391405 1.406822
C -2.123320 1.077891 1.567088
C -2.504643 1.021746 -0.816672
H -4.014649 0.678306 0.665529
I -0.247092 1.611438 -2.783589
H -3.171156 0.983533 -1.666010
H -2.543371 1.060735 2.562398
N 0.004590 1.777819 2.472082
C 0.918269 2.902564 2.363282
C -0.466368 1.543695 3.821604
H 1.048258 3.204068 1.328042
H 1.893713 2.655365 2.786229
H 0.506517 3.755694 2.912891
H -0.873178 0.537651 3.917241
H 0.383952 1.635200 4.497869
H -1.230112 2.268977 4.127838
N 2.212175 0.258167 1.669631
C 3.319769 0.213454 2.601891
H 4.083244 -0.516599 2.306537
H 2.929404 -0.075131 3.578244
H 3.783766 1.194625 2.694677
C 1.302486 -0.868014 1.795332
H 0.645156 -0.940200 0.933709
H 0.696015 -0.780780 2.698691
H 1.883017 -1.794862 1.853893
SCF: -1027.381391
ZPE: 0.307445
H: -1027.055055
G: -1027.116081

5_OMe_cation_conf1

H 3.079401 -0.583543 -3.107215
C 2.690669 -0.455799 -2.106533
C 1.648651 0.004518 0.465463
C 1.357752 -0.236756 -1.857770
C 3.522329 -0.494586 -0.995429
C 3.002867 -0.244396 0.261196
C 0.736356 -0.063323 -0.612993

H 4.580762 -0.677330 -1.123783
H 3.648643 -0.209229 1.128945
C -0.736356 0.063323 -0.612993
C -3.522329 0.494586 -0.995429
C -1.357752 0.236756 -1.857770
C -1.648651 -0.004518 0.465463
C -3.002867 0.244396 0.261196
C -2.690669 0.455799 -2.106533
H -4.580762 0.677330 -1.123783
I 0.000000 0.000000 -3.422792
H -3.079401 0.583543 -3.107215
H -3.648643 0.209230 1.128945
O -1.273544 -0.298061 1.730866
C -0.842348 -1.644833 1.932345
H -0.046791 -1.921691 1.239169
H -1.689233 -2.323577 1.805560
H -0.469503 -1.700778 2.951523
O 1.273544 0.298061 1.730866
C 0.842348 1.644833 1.932345
H 1.689233 2.323577 1.805560
H 0.469503 1.700778 2.951523
H 0.046791 1.921691 1.239169
SCF: -988.508492
ZPE: 0.225980
H: -988.266611
G: -988.321320

5_OMe_cation_conf2

H 2.998076 -0.081981 -3.167979
C 2.570405 -0.069647 -2.175653
C 1.442899 0.120312 0.403188
C 1.237467 0.174214 -1.946493
C 3.343691 -0.288594 -1.043973
C 2.794723 -0.177220 0.222090
C 0.579079 0.209297 -0.715083
H 4.398030 -0.505710 -1.153252
H 3.434981 -0.288512 1.084658
C -0.881959 0.415283 -0.724010
C -3.614215 1.110696 -1.105378
C -1.446156 0.826125 -1.941526
C -1.840486 0.219991 0.300613
C -3.163334 0.613248 0.102170
C -2.748348 1.181437 -2.189444
H -4.650907 1.394774 -1.226741

I -0.052722 0.711739 -3.492403
H -3.089284 1.490120 -3.167859
H -3.845735 0.478810 0.931229
O -1.571669 -0.339621 1.499651
C -1.088781 -1.681060 1.471797
H -0.224953 -1.797742 0.816802
H -1.885290 -2.350689 1.138183
H -0.804402 -1.927155 2.492157
O 0.910478 0.375521 1.598309
C 1.669683 0.095774 2.768281
H 2.004526 -0.943293 2.772590
H 0.995345 0.269428 3.602681
H 2.528956 0.764453 2.845396
SCF: -988.512066
ZPE: 0.226235
H: -988.269921
G: -988.325500

6_CF3_cation_conf1

H 2.191175 -0.094536 -4.000226
C 2.208005 -0.074804 -2.919759
C 2.230440 -0.024015 -0.103310
C 1.058510 -0.046026 -2.160127
C 3.406021 -0.078553 -2.225763
C 3.402839 -0.053570 -0.833385
C 1.004784 -0.018399 -0.770579
H 4.339470 -0.102120 -2.773764
H 2.259708 -0.005443 0.977584
C -0.312942 0.011826 -0.135816
C -2.952919 0.062015 0.833158
C -1.435567 0.007942 -0.962331
C -0.558990 0.043627 1.233167
C -1.865172 0.065963 1.695840
C -2.743563 0.032895 -0.539391
H 0.266662 0.050316 1.934162
H -3.964024 0.080627 1.215162
I -0.867322 -0.041916 -2.972301
H -3.576975 0.030274 -1.228347
C -2.076340 0.108563 3.186526
F -3.363551 0.018031 3.522978
F -1.434140 -0.891309 3.804726
F -1.609098 1.247699 3.716380
C 4.733477 -0.073707 -0.128479
F 4.615034 0.027649 1.196327

F 5.520375 0.931636 -0.533670
F 5.402505 -1.207464 -0.379064
SCF: -1433.652188
ZPE: 0.170686
H: -1433.463495
G: -1433.526695

6_CF3_cation_conf2

H 2.591790 0.934120 -3.038472
C 2.616349 0.953222 -1.958129
C 2.659807 1.005189 0.856548
C 1.473698 0.966606 -1.190579
C 3.821834 0.967677 -1.273914
C 3.828801 0.995980 0.116405
C 1.429685 0.992533 0.201060
H 4.749546 0.959042 -1.830147
H 2.699264 1.025265 1.937767
C 0.115679 1.006106 0.844455
C -2.515571 1.025081 1.827952
C -1.009556 0.992687 0.026767
C -0.119469 1.031017 2.220121
C -1.419607 1.039575 2.687233
C -2.318473 1.001938 0.457877
H 0.711659 1.043122 2.912070
H -3.523484 1.031424 2.223130
I -0.457727 0.954695 -1.987747
H -3.155466 0.992118 -0.226506
C -1.694976 1.061732 4.167401
F -2.382018 -0.021982 4.553554
F -0.580500 1.102640 4.898463
F -2.433805 2.124954 4.512082
C 5.150826 0.970016 0.837701
F 5.085097 1.562801 2.033170
F 6.111974 1.584934 0.142389
F 5.569648 -0.286491 1.049747
SCF: -1433.652186
ZPE: 0.170598
H: -1433.463530
G: -1433.527346

6_CF3_cation_conf3

H 1.598346 -0.006615 -4.030126
C 1.620756 -0.004923 -2.949580
C 1.657600 -0.000959 -0.132751

C 0.475144 0.001471 -2.183597
C 2.822327 -0.010243 -2.262124
C 2.826164 -0.008143 -0.869534
C 0.428026 0.004237 -0.793225
H 3.752897 -0.016901 -2.815391
H 1.693138 0.000114 0.948105
C -0.887120 0.009271 -0.152234
C -3.520376 0.012555 0.825930
C -2.010728 0.008429 -0.972478
C -1.125085 0.013469 1.223187
C -2.426172 0.014970 1.687597
C -3.320515 0.009799 -0.543876
H -0.295511 0.015548 1.917075
H -4.529035 0.012845 1.219244
I -1.453952 0.004468 -2.985579
H -4.156065 0.008587 -1.230089
C -2.705087 0.017312 3.167196
F -3.405010 -1.064600 3.534932
F -1.592245 0.034660 3.901604
F -3.432987 1.083395 3.526253
C 4.161019 -0.028093 -0.172636
F 4.937219 0.989600 -0.567456
F 4.837594 -1.152572 -0.444475
F 4.049660 0.052321 1.154028
SCF: -1433.652320
ZPE: 0.170471
H: -1433.463734
G: -1433.528164

6_CN_cation_conf1

H -0.287887 0.000000 -4.196067
C 0.307647 0.000000 -3.293504
C 1.841703 0.000000 -0.925242
C -0.249459 0.000000 -2.034029
C 1.690905 0.000000 -3.358332
C 2.439226 0.000000 -2.180000
C 0.453072 0.000000 -0.830916
H 2.187624 0.000000 -4.318637
H 2.456289 0.000000 -0.035230
C -0.318726 0.000000 0.412297
C -2.031423 0.000000 2.646178
C -1.708745 0.000000 0.318141
C 0.213750 0.000000 1.697958
C -0.643029 0.000000 2.791636

C -2.588327 0.000000 1.378143
H 1.284132 0.000000 1.852775
H -2.671182 0.000000 3.517908
I -2.307754 0.000000 -1.682374
H -3.661614 0.000000 1.246823
C -0.079915 0.000000 4.113816
N 0.366511 0.000000 5.169951
C 3.873613 0.000000 -2.268813
N 5.017889 0.000000 -2.342081
SCF: -943.970616
ZPE: 0.158431
H: -943.797832
G: -943.850831

6_F_cation_conf1

H -0.648349 0.000000 3.903118
C 0.029270 0.000000 3.060527
C 1.775461 0.000000 0.847285
C -0.416296 0.000000 1.756062
C 1.400928 0.000000 3.256298
C 2.232238 0.000000 2.147878
C 0.400121 0.000000 0.627050
H 1.823882 0.000000 4.251646
H 2.482849 0.000000 0.028418
C -0.248362 0.000000 -0.684558
C -1.728165 0.000000 -3.076690
C -1.641208 0.000000 -0.721817
C 0.412373 0.000000 -1.910764
C -0.342833 0.000000 -3.063837
C -2.406285 0.000000 -1.868506
H 1.492451 0.000000 -1.975572
H -2.262045 0.000000 -4.017152
I -2.430504 0.000000 1.210454
H -3.487005 0.000000 -1.844368
F 0.298862 0.000000 -4.237595
F 3.554415 0.000000 2.350823
SCF: -957.977896
ZPE: 0.144414
H: -957.821062
G: -957.869345

6_NMe2_cation_conf1

H -0.208690 2.497596 -4.633057
C -0.020257 2.483798 -3.568047

C 0.468938 2.442200 -0.808367
C -0.151508 1.333490 -2.817168
C 0.364439 3.638861 -2.918400
C 0.621512 3.648743 -1.524282
C 0.079980 1.272573 -1.444723
H 0.468417 4.541478 -3.501321
H 0.655851 2.414790 0.254325
C -0.106170 -0.026312 -0.784192
C -0.521229 -2.597194 0.249963
C -0.489219 -1.102456 -1.581736
C 0.067167 -0.263554 0.571610
C -0.133178 -1.548086 1.120901
C -0.700310 -2.378538 -1.100640
H 0.358065 0.558881 1.207701
H -0.685208 -3.593550 0.631615
I -0.709892 -0.526938 -3.573383
H -0.997417 -3.193208 -1.747312
N 0.040027 -1.774379 2.447073
C -0.207232 -3.092572 2.999414
C 0.408405 -0.683179 3.327515
H -1.243850 -3.404888 2.842758
H -0.013768 -3.067161 4.067627
H 0.448885 -3.841905 2.548794
H -0.348831 0.106786 3.325024
H 0.504187 -1.064757 4.339525
H 1.364928 -0.241990 3.034174
N 1.004496 4.788326 -0.896437
C 1.270313 4.778389 0.528631
H 2.073855 4.079766 0.778432
H 0.380562 4.496869 1.099641
H 1.574774 5.774192 0.836494
C 1.139247 6.022780 -1.645765
H 1.444518 6.813375 -0.967011
H 0.192559 6.313375 -2.109914
H 1.893539 5.932201 -2.432364
SCF: -1027.404753
ZPE: 0.307648
H: -1027.077327
G: -1027.142841

6_NMe2_cation_conf2

H 0.196041 2.453757 -3.544113
C 0.500034 2.451294 -2.506097
C 1.293381 2.437257 0.182729

C 0.335759 1.344574 -1.698496
C 1.074289 3.576194 -1.950538
C 1.483875 3.600270 -0.593645
C 0.717363 1.297402 -0.359257
H 1.208898 4.443852 -2.578455
H 1.595341 2.422142 1.219172
C 0.479430 0.042877 0.367606
C -0.063468 -2.445348 1.536768
C -0.110157 -1.004584 -0.337012
C 0.798540 -0.181112 1.698975
C 0.536755 -1.423588 2.314864
C -0.388440 -2.239829 0.211567
H 1.258401 0.616917 2.262106
H -0.280042 -3.409128 1.972100
I -0.505663 -0.461387 -2.309759
H -0.846613 -3.032589 -0.364544
N 0.851112 -1.636133 3.617071
C 0.589461 -2.925219 4.228261
C 1.443785 -0.572046 4.403343
H -0.478347 -3.161940 4.222594
H 0.929989 -2.900703 5.259009
H 1.121764 -3.727141 3.709438
H 0.791990 0.305594 4.439287
H 1.595944 -0.926344 5.418423
H 2.411156 -0.264429 3.995523
N 2.044841 4.712799 -0.057641
C 2.499881 4.705825 1.318802
H 3.255236 3.932098 1.484403
H 1.672421 4.531720 2.012667
H 2.942607 5.670581 1.547735
C 2.226119 5.900661 -0.869923
H 2.652243 6.685697 -0.252517
H 1.272946 6.257515 -1.268824
H 2.902132 5.714599 -1.709723
SCF: -1027.404748
ZPE: 0.307895
H: -1027.077189
G: -1027.141899

6_NMe2_cation_conf3

H 0.614856 2.316810 -3.637450
C 0.831163 2.302034 -2.577561
C 1.395460 2.255601 0.167740
C 0.633089 1.174547 -1.806948

C 1.322109 3.431551 -1.955084
C 1.614691 3.439727 -0.567904
C 0.902534 1.111249 -0.441629
H 1.479870 4.316376 -2.553118
H 1.610583 2.225411 1.225015
C 0.643282 -0.163325 0.241041
C 0.074810 -2.685408 1.320793
C 0.146352 -1.213408 -0.528050
C 0.855591 -0.402300 1.590894
C 0.578508 -1.662334 2.162928
C -0.142581 -2.465018 -0.023897
H 1.239954 0.399087 2.203789
H -0.150429 -3.662389 1.720812
I -0.102851 -0.641987 -2.517171
H -0.527956 -3.259649 -0.648423
N 0.787744 -1.889967 3.483503
C 0.489987 -3.189433 4.054888
C 1.282895 -0.825544 4.334016
H -0.569160 -3.440823 3.947957
H 0.733272 -3.171364 5.113012
H 1.079704 -3.977998 3.579732
H 0.600823 0.029807 4.340447
H 1.373354 -1.199597 5.349317
H 2.266322 -0.477315 4.005435
N 2.093018 4.556636 0.034833
C 2.306239 5.766395 -0.736088
H 1.375764 6.121108 -1.188093
H 3.037285 5.608784 -1.533922
H 2.682705 6.540890 -0.074700
C 2.388404 4.547015 1.454105
H 2.756216 5.526854 1.743270
H 3.154688 3.805216 1.696974
H 1.495805 4.324664 2.046135
SCF: -1027.404759
ZPE: 0.307782
H: -1027.077239
G: -1027.142481

6_NMe2_cation_conf4

H 0.830629 2.263306 -3.618444
C 1.033126 2.283276 -2.555969
C 1.548976 2.334156 0.199162
C 0.742002 1.212700 -1.735235
C 1.598203 3.402883 -1.980314

C 1.872278 3.458006 -0.590612
C 0.982431 1.199615 -0.362996
H 1.827900 4.243940 -2.616883
H 1.740858 2.344972 1.261570
C 0.616173 -0.015421 0.376681
C -0.158174 -2.429845 1.568680
C 0.058508 -1.065160 -0.349762
C 0.783587 -0.198654 1.741413
C 0.401439 -1.402925 2.370031
C -0.330925 -2.264922 0.209567
H 1.218501 0.601581 2.320930
H -0.464114 -3.365274 2.012155
I -0.104782 -0.583183 -2.370886
H -0.760539 -3.061229 -0.383189
N 0.564509 -1.574321 3.705538
C 0.178024 -2.824081 4.331943
C 1.109576 -0.501225 4.513787
H -0.894501 -3.011353 4.225785
H 0.414921 -2.774386 5.390470
H 0.718621 -3.669659 3.898429
H 0.497259 0.402106 4.440195
H 1.129155 -0.817311 5.552388
H 2.129843 -0.249573 4.209595
N 2.430552 4.562559 -0.035894
C 2.769538 5.702949 -0.865443
H 1.883875 6.121196 -1.351873
H 3.491459 5.431995 -1.640963
H 3.211854 6.472075 -0.239352
C 2.701208 4.602151 1.387647
H 3.140569 5.563657 1.635391
H 3.402062 3.815876 1.683223
H 1.784098 4.481218 1.971238
SCF: -1027.404703
ZPE: 0.307363
H: -1027.077500
G: -1027.143122

6_OMe_cation_conf1

H -0.052777 0.002893 -4.910674
C 0.499848 -0.011309 -3.981387
C 1.926516 -0.048204 -1.568884
C -0.123782 -0.014301 -2.756362
C 1.887732 -0.027485 -3.996223
C 2.598017 -0.046039 -2.792389

C 0.541715 -0.031975 -1.529303
H 2.398188 -0.024605 -4.947742
C -0.274678 -0.031682 -0.312213
C -2.044313 -0.027317 1.870235
C -1.662658 -0.014129 -0.461845
C 0.215319 -0.047254 0.983610
C -0.660808 -0.045158 2.069928
C -2.558690 -0.011424 0.581055
H 1.280626 -0.061285 1.174060
H -2.729193 -0.025388 2.705290
I -2.192714 0.007553 -2.481584
H -3.628807 0.002462 0.423833
O -0.083242 -0.061203 3.282154
C -0.925729 -0.058171 4.428313
H -1.563412 -0.944285 4.445579
H -1.541757 0.842803 4.456342
H -0.259951 -0.071389 5.286863
H 2.508623 -0.062271 -0.656707
O 3.938621 -0.062380 -2.718758
C 4.678470 -0.064674 -3.933601
H 5.725629 -0.080602 -3.644391
H 4.472908 0.835370 -4.516016
H 4.448896 -0.951551 -4.527185
SCF: -988.532995
ZPE: 0.227031
H: -988.290093
G: -988.346099

6_OMe_cation_conf2

H 0.351723 0.985729 -3.343248
C 0.914256 0.994025 -2.419827
C 2.366737 1.014650 -0.022451
C 0.303964 1.006687 -1.188172
C 2.301860 0.991527 -2.449541
C 3.024858 1.002271 -1.253246
C 0.981825 1.016488 0.032697
H 2.802101 0.981196 -3.406410
C 0.176153 1.026159 1.257019
C -1.565377 1.040326 3.448932
C -1.206227 1.025819 1.121375
C 0.691377 1.034204 2.553576
C -0.176086 1.041189 3.640895
C -2.098536 1.032573 2.177460
H 1.761373 1.034645 2.699365

H -2.213638 1.045535 4.315251
I -1.760476 1.013081 -0.890873
H -3.170031 1.031612 2.030000
O 0.232107 1.048768 4.919552
C 1.630765 1.049719 5.177924
H 2.102674 1.940980 4.759301
H 2.102382 0.154178 4.768211
H 1.734241 1.055106 6.259429
H 2.961740 1.022218 0.881487
O 4.366295 1.001148 -1.193901
C 5.093274 0.990589 -2.416682
H 6.143556 0.992381 -2.138431
H 4.869773 1.879445 -3.009658
H 4.868938 0.092255 -2.994838
SCF: -988.533267
ZPE: 0.227129
H: -988.290334
G: -988.345973

6_OMe_cation_conf3

H 0.338400 0.932768 -3.306841
C 0.894197 0.933870 -2.379399
C 2.330421 0.935398 0.042567
C 0.272055 0.985057 -1.146194
C 2.271572 0.881451 -2.384811
C 2.990987 0.883022 -1.180698
C 0.935831 0.986444 0.074245
H 2.814289 0.838894 -3.319723
C 0.120567 1.037079 1.291261
C -1.641283 1.127839 3.466332
C -1.260165 1.082307 1.142767
C 0.622649 1.038770 2.593229
C -0.254577 1.083750 3.671708
C -2.161897 1.127598 2.189764
H 1.690207 1.004549 2.751126
H -2.297245 1.161030 4.326167
I -1.792832 1.069073 -0.873262
H -3.231230 1.160692 2.030713
O 0.141542 1.087541 4.954261
C 1.536804 1.041981 5.226125
H 2.043281 1.912784 4.804839
H 1.980550 0.126984 4.828430
H 1.630362 1.053183 6.308458
H 2.884719 0.938051 0.969480

O 4.326518 0.830982 -1.305589
C 5.113877 0.820721 -0.121378
H 6.147987 0.772834 -0.451075
H 4.883646 -0.053574 0.490653
H 4.955867 1.732025 0.458745
SCF: -988.533474
ZPE: 0.227060
H: -988.290620
G: -988.346161

7_CF3_cation_conf1

H 2.535515 0.298610 -3.735986
C 2.552044 0.166226 -2.663453
C 2.582064 -0.173215 0.132224
C 1.405467 0.138477 -1.901372
C 3.741858 0.014988 -1.970787
C 3.759748 -0.153911 -0.588864
C 1.356309 -0.024908 -0.520210
H 4.704890 -0.272136 -0.073806
H 2.611977 -0.305139 1.205245
C 0.040230 -0.026861 0.119290
C -2.575106 0.006663 1.096940
C -1.076383 0.131480 -0.696152
C -0.204098 -0.173235 1.486244
C -1.499260 -0.154995 1.965948
C -2.384561 0.154457 -0.267225
H 0.620995 -0.299742 2.173778
H -1.678643 -0.267310 3.027925
I -0.514711 0.338375 -2.695641
H -3.216377 0.279161 -0.946452
C -3.965574 0.035873 1.672323
F -4.907179 0.083676 0.728831
F -4.209538 -1.045101 2.423465
F -4.144578 1.101970 2.464213
C 5.052744 0.027556 -2.709443
F 4.897566 0.207642 -4.021780
F 5.856330 1.003747 -2.267334
F 5.719074 -1.122450 -2.542825
SCF: -1433.651570
ZPE: 0.170572
H: -1433.462904
G: -1433.526763

7_CF3_cation_conf2

H 1.896330 0.076762 -3.417018
C 1.916147 0.048735 -2.336735
C 1.953629 -0.025610 0.478628
C 0.769961 0.050787 -1.573231
C 3.109648 0.005577 -1.634791
C 3.131022 -0.031432 -0.243125
C 0.724509 0.014931 -0.182718
H 4.078686 -0.066815 0.279447
H 1.986886 -0.055531 1.559246
C -0.591150 0.015279 0.457129
C -3.206888 0.006213 1.434249
C -1.712595 0.043763 -0.366489
C -0.830462 -0.014729 1.832464
C -2.125822 -0.018729 2.311497
C -3.021400 0.039070 0.061943
H -0.001292 -0.035202 2.526590
H -2.302071 -0.043040 3.379561
I -1.156377 0.094725 -2.378052
H -3.857994 0.058413 -0.622931
C -4.597601 -0.005748 2.009320
F -4.807877 1.048866 2.807727
F -5.540325 0.018634 1.065949
F -4.810205 -1.098391 2.754206
C 4.420096 -0.022332 -2.374385
F 4.265265 0.103816 -3.693313
F 5.233251 0.962845 -1.973609
F 5.076628 -1.170856 -2.161558
SCF: -1433.651584
ZPE: 0.170571
H: -1433.462952
G: -1433.526212

7_CN_cation_conf1

H -2.245536 0.000049 -3.535017
C -1.274872 0.007528 -3.058903
C 1.263781 0.032736 -1.831552
C -1.106773 0.009865 -1.696285
C -0.104579 0.015661 -3.815571
C 1.153141 0.031009 -3.208541
C 0.119703 0.017339 -1.033718
H 2.041864 0.041150 -3.824387
H 2.242476 0.047472 -1.370994
C 0.101978 0.010797 0.427054
C -0.187155 0.009340 3.202899

C -1.139629 0.013177 1.060972
C 1.226717 -0.000630 1.251224
C 1.084258 -0.000363 2.625100
C -1.339963 0.013664 2.419381
H 2.215321 -0.011542 0.812888
H 1.958563 -0.007525 3.261397
I -2.689934 0.009136 -0.335853
H -2.321903 0.016906 2.872002
C -0.318701 0.013140 4.631895
N -0.420172 0.017123 5.774221
C -0.207179 0.009807 -5.246907
N -0.287507 0.004160 -6.390904
SCF: -943.970029
ZPE: 0.158066
H: -943.797508
G: -943.850905

7_F_cation_conf1
H -2.383839 0.000000 -3.178565
C -1.401943 0.000000 -2.725734
C 1.176683 0.000000 -1.595094
C -1.178162 0.000000 -1.367061
C -0.259677 0.000000 -3.503044
C 1.017638 0.000000 -2.968031
C 0.068030 0.000000 -0.747315
H 1.872348 0.000000 -3.630752
H 2.172619 0.000000 -1.173473
C 0.106375 0.000000 0.714492
C -0.079977 0.000000 3.483157
C -1.106514 0.000000 1.397197
C 1.257920 0.000000 1.504287
C 1.168386 0.000000 2.883531
C -1.260215 0.000000 2.765608
H 2.232346 0.000000 1.033792
H 2.055037 0.000000 3.502722
I -2.706177 0.000000 0.054666
H -2.216667 0.000000 3.269613
F -0.155578 0.000000 4.817891
F -0.402535 0.000000 -4.832284
SCF: -957.975654
ZPE: 0.143760
H: -957.819292
G: -957.868339

7_NMe2_cation_conf1
H -1.228416 3.443578 -3.737134
C -0.717249 3.457093 -2.787024
C 0.595658 3.387929 -0.312569
C -0.597129 2.323458 -2.022624
C -0.141432 4.642463 -2.276845
C 0.513441 4.565148 -1.021818
C 0.034502 2.197853 -0.791793
H 0.964593 5.450461 -0.598976
H 1.106985 3.381913 0.642325
C 0.053468 0.895111 -0.144593
C -0.047430 -1.768713 0.907410
C -0.563073 -0.175547 -0.779698
C 0.638581 0.571044 1.085639
C 0.591588 -0.706844 1.595951
C -0.650336 -1.471448 -0.335844
H 1.141893 1.346850 1.649878
H 1.060754 -0.894759 2.550241
I -1.392075 0.466824 -2.599326
H -1.158157 -2.229927 -0.911559
N -0.082671 -3.025875 1.415999
C -0.777314 -4.076005 0.698632
C 0.493488 -3.297999 2.718968
H -1.841476 -3.847204 0.582888
H -0.682274 -5.004156 1.254086
H -0.348500 -4.225786 -0.296148
H 0.007853 -2.709415 3.502965
H 0.360401 -4.351450 2.946867
H 1.563396 -3.074616 2.734848
N -0.217999 5.806510 -2.968477
C -0.905851 5.845410 -4.243323
H -0.875168 6.859588 -4.629925
H -1.953527 5.547757 -4.139264
H -0.431203 5.182275 -4.972769
C 0.383963 7.011204 -2.430629
H 1.459736 6.885719 -2.280208
H -0.066485 7.290171 -1.473835
H 0.228862 7.823884 -3.133919
SCF: -1027.404535
ZPE: 0.307258
H: -1027.077429
G: -1027.142904

7_NMe2_cation_conf2

H 0.205794 2.920752 -2.229399
 C 0.688096 2.940194 -1.264330
 C 1.908764 2.888500 1.257515
 C 0.744472 1.821863 -0.470669
 C 1.286293 4.117817 -0.761848
 C 1.891899 4.049936 0.518212
 C 1.324853 1.706266 0.786079
 H 2.357444 4.929932 0.936517
 H 2.385868 2.889113 2.230041
 C 1.270499 0.421408 1.466287
 C 1.029427 -2.207928 2.580685
 C 0.642166 -0.643657 0.833296
 C 1.789445 0.110914 2.729259
 C 1.675662 -1.150450 3.269215
 C 0.489275 -1.923150 1.305902
 H 2.292954 0.884316 3.296494
 H 2.095670 -1.328174 4.248031
 I -0.086441 -0.022195 -1.035937
 H -0.021443 -2.678560 0.728557
 N 0.929352 -3.449149 3.118419
 C 0.239607 -4.497617 2.394055
 C 1.469342 -3.714598 4.438056
 H -0.808931 -4.238897 2.217058
 H 0.273989 -5.411304 2.979659
 H 0.713668 -4.690143 1.427277
 H 0.989967 -3.092749 5.199612
 H 1.293052 -4.757424 4.684524
 H 2.546399 -3.529466 4.471638
 N 1.276348 5.266339 -1.483836
 C 1.834923 6.480988 -0.921574
 H 1.721200 7.284975 -1.642706
 H 2.899300 6.363790 -0.702272
 H 1.323056 6.767845 0.001909
 C 0.607255 5.304859 -2.768660
 H -0.461411 5.087743 -2.672073
 H 1.043231 4.580898 -3.462491
 H 0.720062 6.296714 -3.195802
 SCF: -1027.404565
 ZPE: 0.307430
 H: -1027.077357
 G: -1027.142508

7_OMe_cation_conf1

H 3.178815 -0.000177 -1.863163

C 2.750675 -0.000097 -0.872100
 C 1.567336 0.000110 1.680462
 C 1.386889 -0.000067 -0.665384
 C 3.540466 -0.000016 0.276716
 C 2.935889 0.000086 1.542265
 C 0.730470 0.000034 0.556105
 H 3.574947 0.000143 2.415484
 H 1.132124 0.000184 2.671303
 C -0.728602 0.000050 0.558590
 C -3.539524 0.000050 0.288502
 C -1.389070 -0.000045 -0.660711
 C -1.561739 0.000154 1.685759
 C -2.930754 0.000154 1.552051
 C -2.753524 -0.000051 -0.862891
 H -1.123318 0.000233 2.675222
 H -3.566929 0.000232 2.427376
 I -0.003678 -0.000176 -2.229311
 H -3.184955 -0.000131 -1.852517
 O -4.880713 0.000056 0.272594
 C -5.534928 -0.000035 -0.990471
 H -5.276022 -0.894019 -1.561404
 H -5.275996 0.893850 -1.561547
 H -6.599837 -0.000002 -0.775480
 O 4.881589 -0.000032 0.256436
 C 5.531594 -0.000129 -1.008781
 H 5.270735 -0.894098 -1.578865
 H 6.597213 -0.000117 -0.797341
 H 5.270741 0.893756 -1.578999
 SCF: -988.532471
 ZPE: 0.226430
 H: -988.289986
 G: -988.346896

7_OMe_cation_conf2

H 3.168848 0.000001 -2.280982
 C 2.758525 0.000000 -1.282318
 C 1.622351 0.000000 1.291092
 C 1.398590 0.000001 -1.050505
 C 3.569356 0.000000 -0.148031
 C 2.988080 0.000000 1.128361
 C 0.764752 0.000000 0.182506
 H 3.643153 0.000000 1.989717
 H 1.204427 0.000000 2.289310
 C -0.694112 0.000000 0.214117

C -3.510585 0.000001 -0.002211
C -1.377581 0.000001 -1.000624
C -1.504697 0.000000 1.348224
C -2.885889 0.000000 1.248482
C -2.737347 0.000001 -1.167825
H -1.049315 0.000000 2.330398
H -3.475015 0.000000 2.153965
I -0.018885 0.000001 -2.593127
H -3.219623 0.000001 -2.135772
O -4.839447 0.000001 -0.188076
C -5.677340 0.000000 0.962235
H -5.507993 0.893639 1.565728
H -5.507993 -0.893638 1.565727
H -6.696777 0.000001 0.586479
O 4.909880 0.000000 -0.192323
C 5.536993 -0.000002 -1.469030
H 5.265630 -0.893942 -2.034409
H 6.606284 -0.000003 -1.276802
H 5.265632 0.893937 -2.034410
SCF: -988.532134
ZPE: 0.226411
H: -988.289712
G: -988.346153

7_OMe_cation_conf3

H 4.194495 0.963737 -1.149309
C 3.734616 0.951012 -0.170571
C 2.556731 0.914396 2.370570
C 2.378919 0.967556 0.026681
C 4.533157 0.916687 0.977480
C 3.935299 0.896650 2.241121
C 1.721654 0.954196 1.255386
H 4.542911 0.866928 3.133810
H 2.121802 0.895676 3.361704
C 0.262320 0.980044 1.257175
C -2.549735 1.022902 0.985678
C -0.397191 1.005429 0.029874
C -0.570753 0.983810 2.374602
C -1.949573 1.004293 2.248253
C -1.753268 1.026355 -0.164296
H -0.133941 0.972123 3.365044
H -2.555659 1.005605 3.142478
I 0.989362 1.011901 -1.539861
H -2.214994 1.043508 -1.142099

O -3.874786 1.039368 0.774139
C -4.734515 1.032804 1.908243
H -4.570049 1.918309 2.524990
H -4.582838 0.131265 2.504790
H -5.746638 1.044528 1.513394
O 5.857783 0.903436 0.763071
C 6.719625 0.879009 1.895337
H 6.569346 1.764285 2.516132
H 7.731009 0.877513 1.498426
H 6.556011 -0.022626 2.488464
SCF: -988.531743
ZPE: 0.226651
H: -988.289227
G: -988.344849

8_CF3_cation_conf1

C -2.400129 0.071080 2.345799
C 0.387153 -0.003036 2.532296
C -1.596936 0.045152 1.221180
C -1.778614 0.058599 3.586688
C -0.394025 0.023157 3.673101
C -0.204747 0.005777 1.268528
H -2.386109 0.077166 4.482992
H 0.078726 0.016274 4.645488
H 1.464221 -0.028364 2.624109
C 0.524218 -0.023350 -0.004007
C 1.726589 -0.076419 -2.535070
C -0.220961 -0.005710 -1.181438
C 1.913131 -0.070341 -0.132504
C 2.501358 -0.096184 -1.383971
C 0.342334 -0.030481 -2.443309
H 2.537399 -0.088441 0.750399
H 3.578740 -0.132757 -1.467818
H 2.191249 -0.096789 -3.513402
I -2.256682 0.063914 -0.752568
C -0.444542 -0.023474 -3.725635
F -0.256859 -1.142610 -4.423273
F -1.770544 0.081489 -3.506943
F -0.100567 0.994830 -4.510387
C -3.904621 0.091031 2.314575
F -4.383409 0.224013 1.061552
F -4.399669 1.099455 3.027253
F -4.421704 -1.034183 2.806364
SCF: -1433.646881

ZPE: 0.170279

H: -1433.458583

G: -1433.521308

8_CN_cation_conf1

C -2.624587 0.000000 -1.735988

C 0.127703 0.000000 -2.238336

C -1.685500 0.000000 -0.715291

C -2.152020 0.000000 -3.044524

C -0.782526 0.000000 -3.280668

C -0.313332 0.000000 -0.912256

H -2.861039 0.000000 -3.861221

H -0.423439 0.000000 -4.300477

H 1.189609 0.000000 -2.447245

C 0.534780 0.000000 0.278955

C 1.948641 0.000000 2.714047

C -0.099902 0.000000 1.511284

C 1.931983 0.000000 0.296143

C 2.619538 0.000000 1.497002

C 0.557510 0.000000 2.732646

H 2.476182 0.000000 -0.638934

H 3.700844 0.000000 1.490742

H 2.488435 0.000000 3.651022

I -2.174114 0.000000 1.310662

C -0.195307 0.000000 3.948201

N -0.865500 0.000000 4.879282

C -4.019908 0.000000 -1.423150

N -5.119252 0.000000 -1.095296

SCF: -943.961662

ZPE: 0.158193

H: -943.789014

G: -943.841954

8_F_cation_conf1

C -2.431310 0.000000 -1.777426

C 0.343134 0.000000 -1.975232

C -1.630202 0.000000 -0.660148

C -1.846335 0.000000 -3.025229

C -0.457041 0.000000 -3.107626

C -0.239425 0.000000 -0.709620

H -2.475279 0.000000 -3.905550

H 0.007474 0.000000 -4.084263

H 1.420702 0.000000 -2.067946

C 0.458614 0.000000 0.577050

C 1.523183 0.000000 3.186732

C -0.341705 0.000000 1.715659

C 1.837167 0.000000 0.778629

C 2.349908 0.000000 2.067153

C 0.158184 0.000000 2.996404

H 2.502720 0.000000 -0.074185

H 3.421849 0.000000 2.210516

H 1.917710 0.000000 4.194101

I -2.368515 0.000000 1.277281

F -0.693667 0.000000 4.022353

F -3.755870 0.000000 -1.623453

SCF: -957.969377

ZPE: 0.144756

H: -957.812136

G: -957.860405

8_NMe2_cation_conf1

C -0.707400 2.396701 -1.049518

C 1.234717 2.641614 0.996167

C -0.207370 1.326302 -0.335160

C -0.203895 3.644672 -0.687812

C 0.750733 3.752495 0.321947

C 0.747346 1.375291 0.670893

H -0.555868 4.531061 -1.199787

H 1.125734 4.733118 0.584725

H 1.969886 2.752746 1.782547

C 1.089041 0.099503 1.305023

C 1.435332 -2.484309 2.357396

C 0.416054 -1.019876 0.836393

C 1.979226 -0.114418 2.357925

C 2.134251 -1.393412 2.871147

C 0.547127 -2.314119 1.297447

H 2.529626 0.717162 2.778244

H 2.820173 -1.551515 3.693206

H 1.584297 -3.471138 2.776310

I -0.970870 -0.582753 -0.649334

N -0.213525 -3.331069 0.669794

C 0.477078 -3.899818 -0.494122

C -0.667457 -4.386213 1.570467

H -0.222250 -4.530593 -1.042111

H 1.339160 -4.504462 -0.186592

H 0.829621 -3.108867 -1.156292

H -1.390987 -5.002237 1.037143

H 0.153712 -5.032002 1.903652

H -1.152340 -3.944786 2.439985
N -1.667804 2.142730 -2.058270
C -1.047244 1.816141 -3.348078
H -0.578527 2.700741 -3.796616
H -1.816826 1.441332 -4.022166
H -0.283852 1.047761 -3.225106
C -2.668579 3.193080 -2.216153
H -3.100317 3.439451 -1.247116
H -3.456468 2.818586 -2.869117
H -2.251435 4.101198 -2.667261
SCF: -1027.400072
ZPE: 0.307477
H: -1027.073462
G: -1027.136280

8_NMe2_cation_conf2

C 0.381053 3.213571 -0.066416
C 2.071007 3.653550 2.161966
C 0.893661 2.200981 0.719227
C 0.734690 4.505578 0.317477
C 1.566216 4.709067 1.417509
C 1.730509 2.345212 1.816473
H 0.363770 5.351871 -0.246424
H 1.826679 5.722010 1.695766
H 2.709116 3.839072 3.016075
C 2.112423 1.111639 2.508535
C 2.563980 -1.417280 3.648811
C 1.593565 -0.068558 1.994420
C 2.897615 0.991112 3.655605
C 3.105485 -0.262505 4.210626
C 1.785068 -1.340758 2.495816
H 3.323867 1.873097 4.115574
H 3.707590 -0.349027 5.105749
H 2.751379 -2.381089 4.104247
I 0.335745 0.229896 0.365240
N 1.186044 -2.428950 1.816043
C 0.750314 -3.518416 2.684057
C 2.027444 -2.936999 0.725509
H 1.593591 -4.084163 3.098048
H 0.138791 -4.200631 2.094145
H 0.149197 -3.120964 3.500617
H 2.906710 -3.463392 1.116758
H 1.439133 -3.627433 0.121916
H 2.370110 -2.120155 0.090349

N -0.439063 2.859730 -1.165460
C 0.345200 2.584572 -2.375745
H 0.775584 3.506358 -2.786217
H -0.308938 2.134670 -3.121927
H 1.158535 1.892263 -2.157923
C -1.511644 3.808139 -1.447852
H -2.065825 4.020366 -0.534663
H -2.185985 3.354648 -2.173751
H -1.135615 4.748118 -1.868881
SCF: -1027.400073
ZPE: 0.307412
H: -1027.073511
G: -1027.136396

8_NMe2_cation_conf3

C 0.589425 3.473541 -0.048416
C 1.989964 3.776880 2.393243
C 1.028757 2.414503 0.720306
C 0.865075 4.739434 0.464383
C 1.554454 4.875714 1.668058
C 1.723848 2.491825 1.918887
H 0.544503 5.618357 -0.080138
H 1.756139 5.869764 2.045602
H 2.515651 3.910102 3.329790
C 2.046931 1.217370 2.565631
C 2.413227 -1.380825 3.574393
C 1.623425 0.069911 1.909864
C 2.687434 1.025466 3.790427
C 2.853804 -0.261645 4.278644
C 1.782818 -1.232302 2.340620
H 3.033269 1.878386 4.359783
H 3.342641 -0.403876 5.233723
H 2.564163 -2.372278 3.981723
I 0.566412 0.465587 0.163273
N 1.301526 -2.277017 1.515411
C 0.798762 -3.438379 2.242007
C 2.283094 -2.682511 0.501624
H 1.603967 -4.015502 2.712184
H 0.283281 -4.086745 1.534028
H 0.092796 -3.117526 3.006740
H 3.124357 -3.218190 0.958352
H 1.792957 -3.337532 -0.217997
H 2.674872 -1.812354 -0.025220
N -0.090034 3.189390 -1.258235

C -1.149024 4.137043 -1.590835
H -1.723668 3.728567 -2.421702
H -0.753716 5.113844 -1.894151
H -1.809186 4.266901 -0.734454
C 0.832679 3.021107 -2.387607
H 1.634208 2.329079 -2.129171
H 1.281880 3.978946 -2.677702
H 0.279008 2.616968 -3.234568
SCF: -1027.400056
ZPE: 0.307292
H: -1027.073568
G: -1027.136513

8_OMe_cation_conf1

C 2.794815 0.004940 -0.206675
C 1.499495 0.019170 2.302723
C 1.406231 0.003073 -0.089374
C 3.518019 0.012680 0.989757
C 2.883462 0.021306 2.213772
C 0.735331 0.007353 1.143578
H 4.597675 0.013365 0.913069
H 3.477544 0.029804 3.117976
H 1.022848 0.029186 3.271794
C -0.735332 0.001207 1.143575
C -3.518020 -0.003439 0.989758
C -1.406234 0.006770 -0.089370
C -1.499494 -0.011620 2.302710
C -2.883462 -0.013376 2.213763
C -2.794819 0.005280 -0.206669
H -1.022840 -0.022648 3.271767
H -3.477543 -0.022608 3.117961
H -4.597677 -0.003816 0.913073
I -0.000002 0.005713 -1.632094
O -3.552596 0.010593 -1.315339
C -2.992988 0.027220 -2.617103
H -2.420799 -0.883079 -2.815896
H -2.414818 0.938797 -2.790650
H -3.837426 0.039355 -3.301743
O 3.552587 0.001012 -1.315354
C 2.992991 -0.016755 -2.617110
H 2.415037 -0.928592 -2.789962
H 3.837433 -0.029152 -3.301738
H 2.420580 0.893258 -2.816603
SCF: -988.513114

ZPE: 0.226206
H: -988.270935
G: -988.327411

8_OMe_cation_conf2

C 3.013833 0.000000 -0.486969
C 1.881057 0.000000 2.104258
C 1.636489 0.000000 -0.285249
C 3.809940 0.000000 0.664888
C 3.257533 0.000000 1.927759
C 1.049449 0.000000 0.995406
H 4.882585 0.000000 0.519513
H 3.909776 0.000000 2.791069
H 1.453288 0.000000 3.096923
C -0.414626 0.000000 1.082403
C -3.230981 0.000000 0.921154
C -1.111179 0.000000 -0.110569
C -1.185019 0.000000 2.247842
C -2.566389 0.000000 2.147226
C -2.488454 0.000000 -0.253738
H -0.708460 0.000000 3.218527
H -3.158818 0.000000 3.052837
H -4.311394 0.000000 0.885288
I 0.130094 0.000000 -1.752689
O -2.956041 0.000000 -1.510986
C -4.373214 0.000000 -1.690084
H -4.811786 0.894697 -1.246569
H -4.811786 -0.894697 -1.246569
H -4.536065 0.000000 -2.763771
O 3.705199 0.000000 -1.638027
C 3.074529 0.000000 -2.907910
H 2.489516 -0.910434 -3.062661
H 3.881214 0.000000 -3.636742
H 2.489516 0.910434 -3.062661
SCF: -988.525516
ZPE: 0.226441
H: -988.282990
G: -988.340646

8_OMe_cation_conf3

C 2.711938 0.000000 -0.507148
C 1.576749 0.000000 2.078280
C 1.347209 0.000000 -0.277201
C 3.528487 0.000000 0.619705

C 2.949154 0.000000 1.887189
C 0.733713 0.000000 0.966738
H 4.604032 0.000000 0.512291
H 3.601085 0.000000 2.751032
H 1.159003 0.000000 3.075874
C -0.731030 0.000000 0.968848
C -3.526797 0.000000 0.629663
C -1.348036 0.000000 -0.273340
C -1.570947 0.000000 2.082778
C -2.943890 0.000000 1.895517
C -2.713396 0.000000 -0.499461
H -1.150425 0.000000 3.079222
H -3.593396 0.000000 2.761183
H -4.602646 0.000000 0.525218
I -0.002661 0.000000 -1.852185
O -3.109478 0.000000 -1.780748
C -4.514395 0.000000 -2.039031
H -4.977396 0.894665 -1.620857
H -4.977396 -0.894665 -1.620857
H -4.616406 0.000000 -3.120098
O 3.104528 0.000000 -1.789516
C 4.508757 0.000000 -2.051535
H 4.972868 0.894669 -1.634598
H 4.607905 0.000000 -3.132863
H 4.972868 -0.894669 -1.634598
SCF: -988.537863
ZPE: 0.226685
H: -988.295059
G: -988.351453

9_cation_conf1

H 0.000000 0.013323 0.108206
C 0.000000 0.054694 1.188455
C 0.000000 0.137713 4.002671
C 0.000000 -1.076017 1.970470
C 0.000000 1.269042 1.863246
C 0.000000 1.302594 3.252269
C 0.000000 -1.105586 3.365919
H 0.000000 2.187578 1.292135
H 0.000000 2.255838 3.763427
H 0.000000 0.193354 5.080478
C 0.000000 -2.422104 4.004151
C 0.000000 -5.079093 4.956343
C 0.000000 -3.536118 3.165166

C 0.000000 -2.701370 5.365973
C 0.000000 -4.004992 5.832165
C 0.000000 -4.840318 3.594639
I 0.000000 -3.016301 1.170513
F 0.000000 -5.843253 2.730881
F 0.000000 -6.313464 5.422841
F 0.000000 -4.234390 7.132785
F 0.000000 -1.730731 6.268666
SCF: -1156.443714
ZPE: 0.128528
H: -1156.300816
G: -1156.353248

10_CCF2_cation_conf1

H 2.766438 -0.878919 2.511299
C 1.875420 -0.338012 2.222123
C -0.420907 1.047303 1.433363
C 0.874752 -0.926092 1.475259
C 1.694188 0.987261 2.593582
C 0.551626 1.670615 2.199945
C -0.287940 -0.290597 1.058739
H 2.455849 1.480642 3.182261
H 0.419805 2.706644 2.482705
H -1.295311 1.596702 1.109234
I 1.066589 -2.944595 0.925654
C 0.166431 -2.642214 -0.947744
C -1.059247 -2.242413 -3.337059
C -0.880949 -1.730624 -0.979195
C 0.629870 -3.355104 -2.034944
C -0.010693 -3.148052 -3.248989
C -1.482720 -1.534072 -2.222994
H 1.455311 -4.049393 -1.952612
H 0.322646 -3.691555 -4.122854
H -2.284264 -0.811774 -2.308071
H -1.548179 -2.075696 -4.287792
C -1.301099 -0.978113 0.225345
C -2.586526 -0.905085 0.546911
F -3.064033 -0.273364 1.586813
F -3.557959 -1.476494 -0.115178
SCF: -1035.369103
ZPE: 0.179251
H: -1035.175448
G: -1035.228101

10_CH2_2_cation_conf1

C 3.002717 -1.969700 -0.337976
C 1.752570 -1.350867 -0.326598
C 1.767148 -0.003662 -0.010522
C 2.894685 0.739858 0.283929
C 4.117690 0.082851 0.250201
C 4.167063 -1.267788 -0.061425
C 0.493099 -2.117854 -0.599699
C -0.492360 -2.119031 0.597015
C -1.752026 -1.351641 0.325842
C -3.002169 -1.970510 0.338235
C -4.166923 -1.268412 0.063969
C -4.118036 0.082578 -0.246206
C -2.895117 0.739678 -0.280750
C -1.767108 -0.004075 0.011345
I -0.000072 1.179063 -0.000904
H 3.046334 -3.026681 -0.570941
H 2.845981 1.792118 0.535618
H 5.020399 0.635163 0.474589
H 5.118774 -1.782325 -0.083881
H 0.764020 -3.141550 -0.848460
H 0.004313 -1.701201 -1.485320
H -0.003492 -1.704057 1.483361
H -0.763175 -3.143226 0.843836
H -3.045418 -3.027732 0.570173
H -5.118564 -1.783045 0.087114
H -5.021059 0.635103 -0.468802
H -2.846881 1.792245 -0.531264
SCF: -838.083262
ZPE: 0.218244
H: -837.852643
G: -837.900067

10_CH2_2_cation_conf2

C 2.756689 -1.887606 0.639066
C 1.695560 -1.254163 -0.006982
C 1.600347 0.113902 0.206582
C 2.463361 0.866014 0.982438
C 3.513641 0.196274 1.594582
C 3.653021 -1.174739 1.422985
C 0.711371 -2.025244 -0.839693
C -0.575069 -2.395020 -0.099838
C -1.571600 -1.347416 0.364905
C -2.689126 -1.858772 1.041661

C -3.712375 -1.059995 1.514416
C -3.662280 0.317574 1.340941
C -2.573865 0.877149 0.698106
C -1.571035 0.034079 0.230942
I -0.005783 1.084169 -0.731015
H 2.875726 -2.956896 0.511604
H 2.330053 1.931321 1.114488
H 4.213362 0.750094 2.206133
H 4.470288 -1.695741 1.904750
H 1.178830 -2.965449 -1.130797
H 0.491673 -1.496657 -1.769249
H -0.300524 -2.972596 0.786380
H -1.134183 -3.079100 -0.741774
H -2.737057 -2.932352 1.184527
H -4.552602 -1.513871 2.023645
H -4.453079 0.956655 1.710192
H -2.508821 1.949794 0.572019
SCF: -838.086186
ZPE: 0.218481
H: -837.854581
G: -837.904499

10_CH2_2_cation_conf3

C 2.428270 -1.836479 1.111907
C 1.534797 -1.262090 0.207938
C 1.483624 0.127191 0.238345
C 2.237217 0.941930 1.060543
C 3.129182 0.323738 1.927563
C 3.213266 -1.060487 1.954751
C 0.772205 -2.115253 -0.772119
C -0.788938 -2.117115 -0.750254
C -1.527436 -1.262276 0.246971
C -2.397640 -1.835575 1.174040
C -3.163955 -1.058498 2.032919
C -3.084242 0.325823 1.998893
C -2.214399 0.943100 1.109002
C -1.478311 0.127249 0.272248
I -0.011098 1.032311 -0.942594
H 2.512924 -2.916019 1.136055
H 2.136549 2.018591 1.039817
H 3.741598 0.929474 2.582060
H 3.899707 -1.544938 2.637144
H 1.107500 -3.140056 -0.629640
H 1.096254 -1.824666 -1.774343

H -1.117807 -3.142216 -0.595385
H -1.141108 -1.830890 -1.744194
H -2.479578 -2.915185 1.203780
H -3.832696 -1.542270 2.733141
H -3.682645 0.932210 2.665624
H -2.116605 2.019976 1.081997
SCF: -838.083822
ZPE: 0.218466
H: -837.852953
G: -837.900930

10_CH2_3_cation_conf1
C -3.093686 -1.739981 -0.592767
C -1.826665 -1.148715 -0.601570
C -1.767688 0.110849 -0.028432
C -2.842086 0.787859 0.526405
C -4.080543 0.165314 0.496669
C -4.201768 -1.098955 -0.063883
C -0.648244 -1.921686 -1.116207
C -0.000503 -2.753850 -0.001585
C 0.647369 -1.924080 1.114750
C 1.826154 -1.150534 0.601838
C 3.092954 -1.742262 0.591997
C 4.201353 -1.100560 0.064609
C 4.080694 0.164941 -0.493289
C 2.842476 0.788016 -0.521916
C 1.767739 0.110230 0.031320
I 0.000221 1.290872 0.002477
H -3.191925 -2.730536 -1.021349
H -2.735054 1.768596 0.972642
H -4.938608 0.671757 0.917918
H -5.165650 -1.590468 -0.085849
H 0.085113 -1.259429 -1.582510
H -0.996298 -2.596879 -1.897577
H 0.760052 -3.399732 -0.445169
H -0.761197 -3.400469 0.440682
H 0.995062 -2.600929 1.894843
H -0.085802 -1.262439 1.582228
H 3.190737 -2.733756 1.018510
H 5.165044 -1.592484 0.085679
H 4.939022 0.671951 -0.913318
H 2.735902 1.769756 -0.966053
SCF: -877.396487
ZPE: 0.247113

H: -877.135102
G: -877.187527

10_CH2_3_cation_conf2
C -2.860335 -1.376359 1.196218
C -1.878985 -1.063307 0.251169
C -1.545412 0.284238 0.181063
C -2.116427 1.288786 0.946183
C -3.094491 0.929085 1.860354
C -3.455847 -0.405669 1.986585
C -1.292407 -2.160852 -0.597340
C 0.004340 -2.812789 -0.081344
C 1.334499 -2.159810 -0.502440
C 1.856084 -1.063375 0.388641
C 2.760990 -1.378243 1.406491
C 3.293282 -0.408890 2.242254
C 2.943685 0.926307 2.089742
C 2.039891 1.287871 1.102753
C 1.529490 0.284318 0.294590
I 0.040562 0.867257 -1.077010
H -3.162538 -2.412311 1.293748
H -1.809595 2.320783 0.842795
H -3.561979 1.691026 2.469616
H -4.215157 -0.693463 2.702270
H -1.143358 -1.812119 -1.622243
H -2.049358 -2.943005 -0.651509
H 0.019228 -3.823987 -0.489111
H -0.034565 -2.914603 1.005694
H 1.259323 -1.809603 -1.534819
H 2.094043 -2.941451 -0.502522
H 3.053973 -2.414517 1.526079
H 3.993718 -0.698056 3.015151
H 3.362788 1.687041 2.734691
H 1.742825 2.320281 0.976472
SCF: -877.397218
ZPE: 0.247498
H: -877.135512
G: -877.187486

10_CH2_3_cation_conf3
C -3.153534 -1.478998 -0.799486
C -2.061170 -1.111063 -0.013194
C -1.615487 0.192665 -0.202142
C -2.172267 1.107516 -1.081201

C -3.261882 0.697734 -1.834942
C -3.747577 -0.593974 -1.688565
C -1.435405 -2.103959 0.931892
C 0.072690 -2.409462 0.732962
C 0.656207 -2.118449 -0.665742
C 1.737290 -1.066588 -0.730340
C 2.921830 -1.350148 -1.416838
C 3.943385 -0.422834 -1.551801
C 3.816610 0.846622 -1.008226
C 2.656863 1.183233 -0.326905
C 1.667696 0.219793 -0.203556
I 0.008746 0.868739 0.943898
H -3.537379 -2.487347 -0.705074
H -1.776184 2.109232 -1.179180
H -3.720979 1.388328 -2.529542
H -4.596337 -0.920092 -2.275948
H -2.001106 -3.028497 0.830714
H -1.591402 -1.759727 1.958290
H 0.207660 -3.469745 0.940344
H 0.662073 -1.898050 1.493980
H -0.135844 -1.831454 -1.362146
H 1.085647 -3.031482 -1.072923
H 3.031318 -2.336065 -1.852270
H 4.843223 -0.695367 -2.088074
H 4.606076 1.579028 -1.111291
H 2.539075 2.174847 0.090791
SCF: -877.390794
ZPE: 0.247732
H: -877.128772
G: -877.181063

10_CH2_cation_conf1

H 2.880170 -0.710414 2.355887
C 1.895654 -0.301988 2.171092
C -0.646644 0.730675 1.641744
C 0.895016 -1.045583 1.577139
C 1.585462 1.005418 2.519839
C 0.321352 1.514894 2.252731
C -0.383635 -0.592515 1.292803
H 2.339959 1.621340 2.990624
H 0.086775 2.537012 2.519914
H -1.629082 1.136011 1.433583
I 1.296950 -3.029382 0.996704
C 0.179900 -2.821260 -0.776439

C -1.283805 -2.467221 -3.029080
C -0.976959 -2.066701 -0.661711
C 0.646004 -3.402557 -1.939247
C -0.118092 -3.220144 -3.083871
C -1.703829 -1.893223 -1.837668
H 1.565112 -3.972060 -1.967063
H 0.209945 -3.661394 -4.015482
H -2.611887 -1.304122 -1.803253
H -1.871858 -2.321642 -3.925837
C -1.426694 -1.470041 0.647942
H -2.336509 -0.896020 0.489792
H -1.672305 -2.286783 1.337655
SCF: -798.785006
ZPE: 0.189746
H: -798.583423
G: -798.630108

10_CMe2_cation_conf1

H 2.935267 -0.705020 2.303967
C 1.950817 -0.284142 2.146278
C -0.569422 0.774036 1.660849
C 0.946424 -0.999837 1.521023
C 1.659692 1.007072 2.556728
C 0.401335 1.529216 2.303609
C -0.338875 -0.543717 1.251961
H 2.419548 1.595421 3.053270
H 0.165223 2.541474 2.604998
H -1.531999 1.228034 1.480674
I 1.466662 -2.926639 0.865155
C 0.228371 -2.772004 -0.824845
C -1.246330 -2.534622 -3.077610
C -0.939257 -2.026266 -0.711601
C 0.689345 -3.395218 -1.969848
C -0.078949 -3.280022 -3.117556
C -1.660714 -1.918572 -1.905189
H 1.620125 -3.947001 -1.980732
H 0.247997 -3.757992 -4.031203
H -2.574018 -1.343928 -1.926075
H -1.847839 -2.423869 -3.970453
C -1.440290 -1.397644 0.600190
C -1.884012 -2.512443 1.576304
H -1.099658 -3.209671 1.860416
H -2.686747 -3.086282 1.112073
H -2.264527 -2.050796 2.488052

C -2.691744 -0.555472 0.346607
H -2.507039 0.274901 -0.335591
H -3.064063 -0.161061 1.290738
H -3.477322 -1.185235 -0.067690
SCF: -877.392385
ZPE: 0.246461
H: -877.131522
G: -877.182934

10_CO_cation_conf1

H 2.655947 -0.968885 2.782290
C 1.797845 -0.408978 2.433899
C -0.419339 1.024661 1.538495
C 0.899995 -0.936644 1.528310
C 1.567445 0.883696 2.886532
C 0.463944 1.596090 2.438039
C -0.222016 -0.271658 1.058480
H 2.261127 1.327110 3.588503
H 0.290739 2.603840 2.791048
H -1.281505 1.573670 1.183756
I 1.230977 -2.917910 0.930798
C 0.167394 -2.745088 -0.867638
C -1.262252 -2.656116 -3.187691
C -0.842250 -1.799534 -0.962371
C 0.485426 -3.648864 -1.861049
C -0.247034 -3.590806 -3.039682
C -1.556218 -1.774362 -2.162055
H 1.277107 -4.376859 -1.741663
H -0.011841 -4.280068 -3.839721
H -2.345046 -1.041817 -2.270580
H -1.828231 -2.613583 -4.108492
C -1.227855 -0.792555 0.077976
O -2.340861 -0.327640 0.068415
SCF: -872.798741
ZPE: 0.170736
H: -872.615444
G: -872.664157

10_NAc_cation_conf1

H 2.776917 -0.760497 2.530090
C 1.858122 -0.274001 2.231781
C -0.520201 0.966288 1.406516
C 0.828088 -0.970366 1.632120
C 1.661786 1.083867 2.440769

C 0.482047 1.693398 2.030286
C -0.361778 -0.399689 1.204778
H 2.441437 1.663187 2.916804
H 0.343944 2.754870 2.188328
H -1.432136 1.442795 1.073900
I 0.985692 -3.026381 1.252746
C 0.053307 -2.802743 -0.609806
C -1.214806 -2.341433 -2.968968
C -0.987648 -1.882921 -0.618316
C 0.494509 -3.491486 -1.720580
C -0.174093 -3.259557 -2.915420
C -1.610052 -1.642734 -1.837702
H 1.322516 -4.185609 -1.669059
H 0.135748 -3.789960 -3.805786
H -2.401387 -0.905612 -1.885498
H -1.716456 -2.151898 -3.908693
N -1.357434 -1.193581 0.568965
C -2.639274 -1.256109 1.126366
O -2.907431 -0.595344 2.102358
C -3.617426 -2.194310 0.481033
H -3.149938 -3.133886 0.189340
H -4.044217 -1.731595 -0.409760
H -4.414635 -2.378291 1.196107
SCF: -967.479372
ZPE: 0.215397
H: -967.248873
G: -967.302837

10_NH_cation_conf1

H 3.098419 -0.218967 1.996187
C 2.029467 -0.050917 1.991187
C -0.736616 0.346121 1.957928
C 1.161748 -0.953793 1.403366
C 1.480393 1.066094 2.599236
C 0.100561 1.248572 2.588271
C -0.216155 -0.793720 1.339238
H 2.128958 1.783916 3.082288
H -0.329946 2.119357 3.065405
H -1.807048 0.509962 1.925524
I 1.878354 -2.740500 0.591388
C 0.449314 -2.723180 -0.932222
C -1.538944 -2.826611 -2.780480
C -0.796437 -2.235375 -0.560184
C 0.754907 -3.217394 -2.187540

C -0.265699 -3.273218 -3.122416
C -1.802118 -2.301750 -1.528388
H 1.750588 -3.567284 -2.426598
H -0.065624 -3.669128 -4.108567
H -2.786662 -1.925734 -1.276992
H -2.337783 -2.872956 -3.509267
N -1.061566 -1.711407 0.708474
H -2.041907 -1.487887 0.838361
SCF: -814.831199
ZPE: 0.178202
H: -814.641239
G: -814.687845

10_O_cation_conf1

H 0.211812 0.493862 0.055599
C 0.062686 0.295147 1.108699
C -0.331993 -0.250063 3.834404
C -0.770099 -0.717351 1.543450
C 0.694699 1.059450 2.079633
C 0.492931 0.788307 3.427724
C -0.978801 -1.017410 2.879775
H 1.346508 1.866787 1.774733
H 0.991853 1.388944 4.176729
H -0.488271 -0.478122 4.880792
O -1.834572 -2.014495 3.285266
C -1.620752 -3.288983 2.815845
C -1.266462 -5.888400 1.881751
C -1.576551 -3.582329 1.462661
C -1.488411 -4.330972 3.718783
C -1.321635 -5.624156 3.245150
C -1.388158 -4.855742 0.962458
H -1.521094 -4.110816 4.777908
H -1.224584 -6.436162 3.953655
H -1.346494 -5.045082 -0.101948
H -1.127738 -6.899854 1.524865
I -1.827272 -1.929663 0.211267
SCF: -834.681596
ZPE: 0.164855
H: -834.505090
G: -834.551595

10_SO2_cation_conf1

H 3.080063 -0.381585 2.029763
C 2.031243 -0.117067 2.047693

C -0.679903 0.605935 2.027257
C 1.053500 -0.983728 1.613660
C 1.623033 1.134578 2.503676
C 0.285265 1.492906 2.489282
C -0.294681 -0.654620 1.601026
H 2.371941 1.831691 2.855079
H -0.016596 2.472292 2.834931
H -1.726771 0.878889 2.007087
I 1.637781 -2.868586 0.883742
C 0.276433 -2.839776 -0.720075
C -1.477725 -2.714132 -2.817000
C -0.994356 -2.325866 -0.503721
C 0.701268 -3.292949 -1.948740
C -0.208162 -3.235894 -3.002723
C -1.874824 -2.245877 -1.570037
H 1.703352 -3.670058 -2.104324
H 0.099759 -3.590594 -3.977275
H -2.862598 -1.831767 -1.415159
H -2.169224 -2.664407 -3.647233
S -1.535260 -1.820349 1.106432
O -2.786530 -1.137851 0.978816
O -1.422710 -2.960785 1.975044
SCF: -1308.078331
ZPE: 0.171766
H: -1307.892729
G: -1307.943722

10_SO_cation_conf1

H 3.085938 -0.437918 1.956085
C 2.029223 -0.208653 1.984885
C -0.717375 0.389780 2.010496
C 1.072822 -1.128226 1.608688
C 1.576541 1.039310 2.400968
C 0.220776 1.335715 2.405958
C -0.282500 -0.861848 1.610000
H 2.299184 1.782098 2.711171
H -0.114682 2.314465 2.722306
H -1.778181 0.606777 2.012886
I 1.657979 -3.018350 0.890933
C 0.331569 -2.909036 -0.739862
C -1.424151 -2.619238 -2.805086
C -0.940105 -2.441653 -0.470734
C 0.771071 -3.232834 -2.006324
C -0.141434 -3.090785 -3.046774

C -1.832423 -2.290282 -1.518119
H 1.779917 -3.576825 -2.191284
H 0.166700 -3.343395 -4.052505
H -2.831195 -1.924200 -1.315426
H -2.119109 -2.505243 -3.626434
S -1.503225 -2.124531 1.210321
O -2.815941 -1.457131 1.118849
SCF: -1232.844847
ZPE: 0.165705
H: -1232.665862
G: -1232.715820

11_cation_conf1

H 0.225629 0.509465 0.053985
C 0.057817 0.287711 1.099719
C -0.333268 -0.256214 3.831322
C -0.780066 -0.717230 1.540916
C 0.679734 1.025988 2.088078
C 0.499146 0.777275 3.436690
C -0.988584 -1.017235 2.875994
H 1.015685 1.387021 4.165837
H -0.487596 -0.482628 4.878154
O -1.853043 -2.008976 3.276498
C -1.629714 -3.283828 2.812209
C -1.261312 -5.852355 1.892618
C -1.584478 -3.576886 1.460226
C -1.488557 -4.324970 3.716245
C -1.312691 -5.618572 3.254961
C -1.386665 -4.846154 0.954125
H -1.521951 -4.107205 4.775617
H -1.206233 -6.446429 3.943112
H -1.338839 -5.065752 -0.104227
I -1.839142 -1.926180 0.209466
F -1.080356 -7.103949 1.457081
F 1.492584 2.021004 1.716375
SCF: -1033.177961
ZPE: 0.148230
H: -1033.016383
G: -1033.066978

Ph2I_cation_conf1

H 1.270832 1.356482 -2.048308
C 1.628880 1.436286 -1.030665
C 2.556473 1.618500 1.603735

C 1.804635 0.321728 -0.228748
C 1.929431 2.673127 -0.475777
C 2.390125 2.761195 0.831897
C 2.262175 0.367393 1.076768
H 1.802374 3.565908 -1.073771
H 2.622789 3.730531 1.253390
H 2.386976 -0.528540 1.670046
H 2.915835 1.692010 2.621686
I 1.329358 -1.557589 -1.040710
H -1.247802 -0.807893 -2.560213
C -1.599364 -1.145192 -1.594582
C -2.487220 -2.017622 0.912271
C -0.728421 -1.582192 -0.611579
C -2.955176 -1.153337 -1.292969
C -3.393545 -1.586050 -0.048167
C -1.125838 -2.023800 0.638681
H -3.664351 -0.818219 -2.038281
H -4.452397 -1.588017 0.175811
H -0.412500 -2.360022 1.379038
H -2.833372 -2.354689 1.880446
SCF: -760.664723
ZPE: 0.181871
H: -760.470532
G: -760.520558

acetonitrile_bromide_conf1

N 0.051291 -0.015854 0.968636
C 0.065850 -0.071760 -0.177016
C 0.077007 -0.136038 -1.627672
H 1.055799 0.169036 -1.995599
H -0.692460 0.536796 -2.015077
H -0.130116 -1.157084 -1.945721
Br -2.733370 2.371904 -2.316350
SCF: -2707.131026
ZPE: 0.046018
H: -2707.078162
G: -2707.114652

acetonitrile_conf1

N -0.000103 -0.000077 0.945694
C 0.000087 0.000084 -0.200979
C 0.000087 0.000003 -1.653855
H 1.027077 0.000006 -2.015963
H -0.513516 0.889509 -2.015892

H -0.513532 -0.889525 -2.015806
SCF: -132.757539
ZPE: 0.045552
H: -132.707477
G: -132.732939

1_CF3_cis_adduct_conf1

C -0.083271 1.887697 -1.641851
C 0.059236 1.831377 1.138326
C -0.036853 0.681933 -0.956475
C -0.055388 3.072738 -0.926376
C 0.018005 3.036217 0.463138
C 0.031756 0.626338 0.429744
H -0.090907 4.019444 -1.447909
H 0.040790 3.963676 1.019071
H 0.112699 1.826246 2.219024
C 0.064923 -0.709500 1.032403
C 0.106654 -3.346815 1.977987
C 0.020411 -1.814254 0.184210
C 0.135435 -0.972568 2.401548
C 0.155643 -2.277076 2.864654
C 0.038578 -3.123879 0.608521
H 0.174455 -0.151655 3.105173
H 0.210085 -2.462985 3.929284
H 0.001573 -3.943977 -0.094686
H 0.121874 -4.364082 2.346380
I -0.065596 -1.243787 -1.839693
Br -0.103520 -4.067150 -2.753258
C -0.187047 1.897759 -3.139959
F -0.104077 3.117515 -3.657796
F 0.782104 1.154539 -3.705565
F -1.347761 1.362349 -3.555892
SCF: -3670.962953
ZPE: 0.166268
H: -3670.779997
G: -3670.840317

1_CF3_trans_adduct_conf1

H -0.090907 2.246723 -3.240348
C -0.024624 2.332483 -2.164909
C 0.149491 2.515012 0.625697
C -0.019207 1.218406 -1.355952
C 0.059399 3.570780 -1.541097
C 0.147047 3.657410 -0.156332

C 0.063710 1.253008 0.034795
H 0.057091 4.467502 -2.146664
H 0.214436 4.627179 0.318957
H 0.219781 2.601918 1.701702
C 0.052565 -0.021541 0.759446
C 0.001167 -2.560436 1.936810
C -0.032364 -1.174275 -0.011231
C 0.114496 -0.160524 2.149518
C 0.090754 -1.416587 2.724785
C -0.061399 -2.439221 0.558916
H 0.179179 0.714695 2.782212
H 0.140009 -1.515070 3.800742
H -0.020188 -3.539697 2.395182
I -0.118957 -0.752848 -2.085469
Br -0.238544 0.171731 -4.903536
C -0.187322 -3.655054 -0.313717
F -1.370987 -3.682146 -0.950396
F 0.748899 -3.666851 -1.280501
F -0.073824 -4.792696 0.361394
SCF: -3670.962928
ZPE: 0.166122
H: -3670.780074
G: -3670.840686

1_CF3_trans_adduct_conf2

H 0.870121 3.314165 -2.236161
C 0.952339 3.379874 -1.160518
C 1.168324 3.512488 1.628832
C 0.959024 2.249611 -0.372259
C 1.056283 4.606248 -0.517484
C 1.165212 4.668259 0.867331
C 1.061139 2.261976 1.016913
H 1.053512 5.513334 -1.107412
H 1.249400 5.628876 1.358328
H 1.257194 3.580215 2.704779
C 1.050111 0.977011 1.723742
C 1.014060 -1.555196 2.894682
C 0.951886 -0.173225 0.940648
C 1.127137 0.836962 3.109661
C 1.109398 -0.420360 3.686509
C 0.934411 -1.435811 1.512681
H 1.198500 1.712299 3.741234
H 1.170084 -0.521075 4.761626
H 1.000114 -2.539858 3.346061

I 0.829896 0.295112 -1.125072
Br 0.656051 1.270845 -3.933214
C 0.815231 -2.714353 0.730089
F 0.869698 -2.519384 -0.598218
F 1.791923 -3.573540 1.033955
F -0.339948 -3.341273 0.978367
SCF: -3670.962446
ZPE: 0.165823
H: -3670.779849
G: -3670.840667

1_CN_cis_adduct_conf1

C -0.099360 2.065380 -1.911277
C 0.134955 1.993388 0.861697
C -0.079092 0.855380 -1.226736
C -0.000214 3.253501 -1.192761
C 0.116151 3.204415 0.190287
C 0.037103 0.792315 0.153899
H -0.015287 4.198405 -1.718771
H 0.192887 4.127056 0.749310
H 0.226667 1.983375 1.939933
C 0.045624 -0.551327 0.739545
C 0.038978 -3.201075 1.648083
C -0.062127 -1.642609 -0.121514
C 0.153686 -0.834916 2.101694
C 0.149890 -2.146043 2.546555
C -0.069528 -2.957515 0.284427
H 0.240561 -0.024448 2.813303
H 0.234060 -2.348706 3.606177
H -0.156142 -3.766345 -0.427438
H 0.036332 -4.223394 2.002448
I -0.213779 -1.043211 -2.137903
Br -0.369295 -3.837991 -3.079912
C -0.221433 2.074133 -3.339280
N -0.320536 2.030233 -4.481964
SCF: -3426.122401
ZPE: 0.160195
H: -3425.947319
G: -3426.002749

1_CN_trans_adduct_conf1

H -0.229771 1.925592 -3.259146
C -0.120230 2.007648 -2.186924
C 0.163206 2.182529 0.596036

C -0.094054 0.892353 -1.381133
C 0.000281 3.243706 -1.563896
C 0.141320 3.326632 -0.183450
C 0.043389 0.923313 0.006184
H -0.016250 4.141696 -2.167356
H 0.235747 4.294814 0.290491
H 0.274843 2.264788 1.669081
C 0.052130 -0.353704 0.726355
C 0.046255 -2.913300 1.877868
C -0.075133 -1.493880 -0.053260
C 0.176230 -0.513800 2.109301
C 0.172983 -1.779953 2.670423
C -0.079944 -2.769778 0.499099
H 0.275608 0.352012 2.750694
H 0.270833 -1.890245 3.741885
H 0.044121 -3.903017 2.314169
I -0.256437 -1.078239 -2.113880
Br -0.489713 -0.148989 -4.908616
C -0.213203 -3.913493 -0.354481
N -0.322313 -4.796687 -1.079442
SCF: -3426.122388
ZPE: 0.160210
H: -3425.947279
G: -3426.002816

1_F_cis_adduct_conf1

C -0.117532 1.824487 -2.180890
C 0.116195 1.991264 0.577717
C -0.091294 0.682752 -1.406513
C -0.026332 3.064506 -1.583492
C 0.091223 3.135890 -0.201081
C 0.023881 0.732665 -0.015758
H -0.047890 3.948929 -2.206530
H 0.164197 4.105671 0.272553
H 0.208304 2.072924 1.652040
C 0.037097 -0.547161 0.695681
C 0.038295 -3.114882 1.807561
C -0.063703 -1.696578 -0.082060
C 0.140424 -0.714969 2.077680
C 0.140668 -1.989046 2.620353
C -0.066586 -2.978950 0.429934
H 0.219710 0.147696 2.726169
H 0.221667 -2.109374 3.692693
H -0.146718 -3.849192 -0.208539

H 0.039663 -4.104403 2.245516
I -0.210652 -1.266841 -2.139153
Br -0.439614 -1.064706 -5.271719
F -0.231003 1.729118 -3.502163
SCF: -3433.113564
ZPE: 0.153333
H: -3432.946154
G: -3433.000508

1_F_trans_adduct_conf1

H -0.215211 1.694564 -3.309575
C -0.148629 1.781378 -2.234079
C 0.024981 1.967891 0.557384
C -0.093836 0.667774 -1.427059
C -0.114284 3.021393 -1.608004
C -0.028055 3.110226 -0.223151
C -0.006893 0.704572 -0.035391
H -0.154844 3.918063 -2.212300
H -0.001927 4.081763 0.252658
H 0.091825 2.051331 1.634229
C 0.044721 -0.569923 0.687115
C 0.129621 -3.143202 1.805021
C 0.001978 -1.708501 -0.109222
C 0.131260 -0.733581 2.070271
C 0.172552 -2.008837 2.611713
C 0.043720 -2.968983 0.440746
H 0.165967 0.128630 2.722523
H 0.239795 -2.130551 3.684645
H 0.161330 -4.142595 2.218540
I -0.129401 -1.310047 -2.165752
Br -0.314190 -0.380204 -4.981389
F -0.000478 -4.031260 -0.378722
SCF: -3433.124835
ZPE: 0.153485
H: -3432.957478
G: -3433.010450

1_H_adduct_conf1

H -0.224955 1.938254 -3.257046
C -0.117894 2.023025 -2.184427
C 0.158890 2.191848 0.599599
C -0.091503 0.906295 -1.379482
C -0.001184 3.258086 -1.559469
C 0.136188 3.337377 -0.177788

C 0.043447 0.932070 0.008280
H -0.017822 4.157828 -2.160388
H 0.227071 4.304865 0.298526
H 0.267493 2.272231 1.673225
C 0.053817 -0.346704 0.724586
C 0.047718 -2.908106 1.850373
C -0.071008 -1.496286 -0.049931
C 0.177218 -0.508278 2.106088
C 0.173717 -1.779413 2.656203
C -0.077748 -2.775062 0.474271
H 0.275334 0.356040 2.749945
H 0.270469 -1.895097 3.727918
H 0.046766 -3.895539 2.293385
I -0.249692 -1.062566 -2.102361
Br -0.492210 -0.108119 -4.970041
H -0.176711 -3.647745 -0.158766
SCF: -3333.874823
ZPE: 0.161657
H: -3333.700144
G: -3333.751312

1_NMe2_cis_adduct_conf1

C -0.216618 1.242481 -1.080720
C 0.268862 1.592737 1.686946
C -0.094742 0.192001 -0.186023
C -0.109370 2.516778 -0.525055
C 0.127816 2.677807 0.837885
C 0.150453 0.298694 1.175467
H -0.204714 3.384589 -1.164492
H 0.207934 3.679031 1.241149
H 0.447279 1.743430 2.743494
C 0.206220 -0.950651 1.935198
C 0.252609 -3.468454 3.159020
C -0.023947 -2.131314 1.229309
C 0.464776 -1.065376 3.301134
C 0.486637 -2.313962 3.900543
C -0.008487 -3.388926 1.797312
H 0.650266 -0.175820 3.889283
H 0.689699 -2.391121 4.960645
H -0.191334 -4.281518 1.213742
H 0.272942 -4.437897 3.639202
I -0.401895 -1.775984 -0.808625
Br -1.057413 -2.627991 -3.981736
N -0.450429 0.959826 -2.440165

C -1.210117 1.970413 -3.162756
C 0.763834 0.596145 -3.176143
H -2.101322 2.239745 -2.597324
H -1.514846 1.545194 -4.119319
H -0.621844 2.875136 -3.361462
H 1.350958 -0.137510 -2.624238
H 0.474919 0.153786 -4.128281
H 1.391974 1.478631 -3.354087
SCF: -3467.824975
ZPE: 0.234689
H: -3467.572976
G: -3467.633969

1_NMe2_cis_adduct_conf2

C 1.010447 1.991422 -0.155851
C 1.743848 2.431647 2.543803
C 0.991782 1.001801 0.813285
C 1.397793 3.255543 0.287683
C 1.754531 3.461799 1.618107
C 1.347125 1.153383 2.145883
H 1.424291 4.079011 -0.414072
H 2.050793 4.453850 1.933739
H 2.015360 2.616656 3.574782
C 1.216476 -0.025683 3.002047
C 0.861414 -2.406668 4.430015
C 0.712342 -1.184397 2.411939
C 1.547162 -0.090912 4.355533
C 1.368871 -1.272077 5.056683
C 0.524070 -2.375627 3.083039
H 1.945782 0.783932 4.853151
H 1.629011 -1.312068 6.106306
H 0.130550 -3.254857 2.590260
H 0.726814 -3.323465 4.988795
I 0.269056 -0.906636 0.374914
Br -0.748720 -1.833620 -2.676446
N 0.631082 1.667776 -1.472600
C 0.030993 2.756419 -2.230915
C 1.696630 1.021369 -2.243835
H -0.747252 3.236442 -1.638965
H -0.419598 2.335025 -3.129796
H 0.767236 3.510084 -2.537462
H 1.260822 0.580328 -3.138926
H 2.469028 1.747776 -2.528181
H 2.169358 0.225952 -1.668113

SCF: -3467.824934
ZPE: 0.234469
H: -3467.573078
G: -3467.634407

1_NMe2_trans_adduct_conf1

H -0.165499 2.912723 -3.256102
C -0.068331 3.039601 -2.186446
C 0.189362 3.323509 0.591071
C 0.000810 1.952630 -1.343429
C -0.005538 4.300742 -1.606481
C 0.122843 4.437971 -0.228376
C 0.127200 2.041134 0.044171
H -0.057054 5.176523 -2.240023
H 0.170782 5.425859 0.210881
H 0.288201 3.442823 1.662420
C 0.186774 0.791191 0.807465
C 0.357580 -1.751491 1.967505
C 0.070086 -0.375469 0.068996
C 0.392181 0.666003 2.183411
C 0.484860 -0.598342 2.740866
C 0.132279 -1.657101 0.596155
H 0.499365 1.545107 2.804868
H 0.658306 -0.696854 3.804849
H 0.430775 -2.724284 2.435950
I -0.068318 -0.050107 -1.991350
Br -0.182530 0.809797 -4.931324
N -0.020160 -2.756517 -0.283168
C -1.423443 -3.045219 -0.595468
C 0.672901 -3.970668 0.126700
H -1.958780 -2.135064 -0.864696
H -1.933337 -3.500302 0.263553
H -1.463954 -3.736322 -1.437277
H 0.198357 -4.453320 0.990339
H 0.654983 -4.673273 -0.706374
H 1.709302 -3.741181 0.371217
SCF: -3467.834610
ZPE: 0.234802
H: -3467.582604
G: -3467.642960

1_NMe2_trans_adduct_conf2

H 0.321656 3.873630 -2.182186
C 0.564720 4.007297 -1.136937

C 1.202755 4.310628 1.576348
C 0.785597 2.926269 -0.312542
C 0.669529 5.272094 -0.571054
C 0.986521 5.419314 0.775236
C 1.103787 3.025164 1.042977
H 0.500994 6.143146 -1.190660
H 1.065017 6.410062 1.203487
H 1.447965 4.434641 2.623308
C 1.310011 1.782262 1.791275
C 1.725361 -0.744957 2.920464
C 1.127409 0.608192 1.078541
C 1.712090 1.673586 3.124453
C 1.923384 0.416575 3.665947
C 1.305373 -0.667355 1.594470
H 1.877969 2.560467 3.721858
H 2.248224 0.330441 4.694965
H 1.895188 -1.711784 3.376176
I 0.686483 0.918693 -0.941859
Br 0.123714 1.759874 -3.836131
N 1.067342 -1.777616 0.748588
C -0.355491 -2.113186 0.635946
C 1.849835 -2.966155 1.061159
H -0.726338 -2.576109 1.559651
H -0.490447 -2.813036 -0.188581
H -0.952280 -1.223078 0.439254
H 1.516024 -3.457104 1.983963
H 1.738714 -3.675199 0.240886
H 2.902297 -2.702355 1.157996
SCF: -3467.834580
ZPE: 0.234669
H: -3467.582708
G: -3467.642980

1_OMe_cis_adduct_conf1

C -0.040723 1.440331 -1.450653
C 0.144855 1.542216 1.359457
C -0.034252 0.303133 -0.655872
C 0.046676 2.665014 -0.794960
C 0.137348 2.695863 0.594651
C 0.057220 0.299440 0.728446
H 0.045202 3.585773 -1.361224
H 0.204998 3.657072 1.087434
H 0.218087 1.598917 2.436994
C 0.055205 -1.009853 1.382071

C 0.037550 -3.623296 2.384799
C -0.038776 -2.128224 0.555672
C 0.141578 -1.237417 2.755913
C 0.132486 -2.533098 3.245272
C -0.050899 -3.430535 1.012465
H 0.215545 -0.399238 3.436838
H 0.200517 -2.698808 4.312450
H -0.125069 -4.272293 0.336777
H 0.032166 -4.630524 2.780173
I -0.165051 -1.606079 -1.478753
Br -0.458570 -1.850560 -4.749931
O -0.128633 1.246986 -2.771010
C -0.143340 2.391483 -3.618056
H 0.777362 2.965854 -3.503147
H -1.007168 3.020765 -3.397704
H -0.215413 2.006079 -4.631104
SCF: -3448.393607
ZPE: 0.194381
H: -3448.183347
G: -3448.241868

1_OMe_trans_adduct_conf1

H 0.210059 2.951052 -2.957776
C 0.156772 2.902609 -1.878918
C 0.016765 2.733736 0.916311
C 0.097870 1.694734 -1.220474
C 0.144864 4.052949 -1.099547
C 0.075109 3.965712 0.286721
C 0.027266 1.556892 0.166531
H 0.190255 5.019128 -1.584665
H 0.066240 4.869188 0.882335
H -0.037779 2.677348 1.995769
C -0.029728 0.201399 0.720987
C -0.123989 -2.498977 1.475810
C -0.009800 -0.824698 -0.207642
C -0.099851 -0.140864 2.073967
C -0.145121 -1.478360 2.426738
C -0.055589 -2.170795 0.126318
H -0.117894 0.626164 2.836451
H -0.198910 -1.748416 3.473581
H -0.160909 -3.532340 1.790785
I 0.102310 -0.176055 -2.190667
Br 0.278569 1.132113 -4.925639
O -0.028882 -3.039726 -0.902556

C -0.076152 -4.429842 -0.595472
H -0.046243 -4.947965 -1.549808
H -1.000395 -4.675911 -0.069732
H 0.784967 -4.719071 0.009492
SCF: -3448.405020
ZPE: 0.194657
H: -3448.194729
G: -3448.251629

1_OMe_trans_adduct_conf2

H -0.181296 2.436482 -3.393319
C -0.120835 2.563044 -2.321105
C 0.038268 2.846853 0.463771
C -0.078362 1.477029 -1.475588
C -0.082052 3.824073 -1.738913
C -0.002935 3.961286 -0.357179
C 0.000561 1.564202 -0.084862
H -0.113245 4.699653 -2.374042
H 0.026983 4.949165 0.083649
H 0.100581 2.965969 1.537676
C 0.038419 0.315103 0.681237
C 0.098021 -2.230693 1.859912
C -0.007018 -0.846642 -0.069609
C 0.114681 0.193358 2.071306
C 0.143499 -1.070761 2.633989
C 0.019667 -2.122341 0.475910
H 0.150332 1.072108 2.700852
H 0.203277 -1.170263 3.710187
H 0.123557 -3.199923 2.337705
I -0.122049 -0.525262 -2.130899
Br -0.281808 0.326079 -5.040492
O -0.033517 -3.143571 -0.400740
C -0.012049 -4.468123 0.122602
H -0.874469 -4.639661 0.768982
H 0.910940 -4.647429 0.676666
H -0.059250 -5.129835 -0.737695
SCF: -3448.405015
ZPE: 0.194599
H: -3448.194749
G: -3448.251789

2_CF3_cis_adduct_conf1

C -0.059870 1.185208 -1.912666
C 0.048357 1.390261 0.880079

C -0.040678 0.078186 -1.100115
C -0.025525 2.424813 -1.286147
C 0.031119 2.531175 0.096613
C 0.010904 0.125093 0.294801
H 0.059485 3.504205 0.567248
H 0.090312 1.486077 1.956432
C 0.021173 -1.146279 1.023200
C 0.032050 -3.695212 2.169465
C -0.017304 -2.303869 0.252039
C 0.064958 -1.291038 2.411191
C 0.070053 -2.557400 2.971551
C -0.012876 -3.577908 0.786952
H 0.094041 -0.419319 3.051790
H 0.103980 -2.662344 4.048032
H -0.042793 -4.458707 0.158041
H 0.036777 -4.678682 2.621119
I -0.086055 -1.894956 -1.813730
Br -0.178618 -0.946945 -4.666785
H -0.100258 1.095020 -2.991217
C -0.026951 3.649605 -2.155825
F -0.196099 4.773560 -1.454896
F 1.125114 3.781266 -2.832381
F -1.001495 3.608093 -3.075091
SCF: -3670.964153
ZPE: 0.166432
H: -3670.781052
G: -3670.841615

2_CF3_cis_adduct_conf2

C 0.929548 2.186295 -0.911056
C 1.098621 2.389111 1.878610
C 0.941413 1.079253 -0.098808
C 1.005689 3.425001 -0.286091
C 1.089121 3.530431 1.095146
C 1.023355 1.125156 1.294831
H 1.148152 4.502327 1.565121
H 1.166308 2.484041 2.953749
C 1.025107 -0.146389 2.023039
C 1.011498 -2.695113 3.169661
C 0.947575 -1.302965 1.253226
C 1.096169 -0.292102 3.409791
C 1.089149 -1.558377 3.970352
C 0.938678 -2.576878 1.788382
H 1.155697 0.578875 4.049264

H 1.144753 -1.664048 5.045869
H 0.877980 -3.456938 1.160687
H 1.007193 -3.678550 3.621404
I 0.844144 -0.892535 -0.810903
Br 0.714167 0.057432 -3.662872
H 0.864400 2.097461 -1.988578
C 0.979177 4.648473 -1.157359
F 1.180713 5.773119 -0.466795
F 1.917823 4.599775 -2.113555
F -0.196931 4.783044 -1.790015
SCF: -3670.964144
ZPE: 0.166335
H: -3670.781108
G: -3670.841896

2_CF3_trans_adduct_conf1

H -0.290729 2.284473 -3.649178
C -0.168250 2.372567 -2.578685
C 0.147909 2.557427 0.200594
C -0.133804 1.260068 -1.768959
C -0.039243 3.610531 -1.961583
C 0.117603 3.698462 -0.582771
C 0.020515 1.295753 -0.383393
H -0.061905 4.506680 -2.567630
H 0.217568 4.668443 -0.113678
H 0.271307 2.643953 1.271988
C 0.036515 0.021758 0.340498
C 0.034522 -2.517164 1.477830
C -0.105447 -1.129026 -0.427218
C 0.181289 -0.127104 1.722476
C 0.180804 -1.389233 2.282947
C -0.110764 -2.404605 0.105168
H 0.294017 0.739092 2.360307
I -0.309568 -0.711679 -2.482383
Br -0.571315 0.216072 -5.315909
H 0.294276 -1.503763 3.353925
H -0.223838 -3.283241 -0.516544
C 0.048824 -3.866836 2.135215
F -0.197716 -4.860687 1.278042
F 1.234537 -4.128620 2.707435
F -0.867204 -3.953424 3.111304
SCF: -3670.964775
ZPE: 0.166350
H: -3670.781750

G: -3670.842201

2_CF3_trans_adduct_conf2

H 0.801352 3.281798 -2.656485
C 0.877895 3.371640 -1.581862
C 1.077261 3.560931 1.208061
C 0.904963 2.259430 -0.771403
C 0.953934 4.611608 -0.959994
C 1.053450 4.701715 0.424016
C 1.001906 2.297160 0.619401
H 0.935993 5.507614 -1.566448
H 1.113576 5.673305 0.896552
H 1.155998 3.649184 2.283523
C 1.019812 1.022933 1.342974
C 1.043260 -1.517672 2.476812
C 0.944182 -0.129782 0.568995
C 1.106345 0.875246 2.730075
C 1.117498 -0.387638 3.288942
C 0.953965 -1.406120 1.099345
H 1.164660 1.742994 3.373149
I 0.810829 0.284737 -1.492354
Br 0.624738 1.207446 -4.333120
H 1.185125 -0.501592 4.363879
H 0.896584 -2.286040 0.471979
C 1.058688 -2.868153 3.132793
F 1.015003 -3.869961 2.250593
F 2.161517 -3.047360 3.875431
F 0.015868 -3.030424 3.961544
SCF: -3670.964780
ZPE: 0.166348
H: -3670.781742
G: -3670.842387

2_CN_cis_adduct_conf1

C -0.125320 1.518728 -2.112717
C 0.160507 1.717480 0.673505
C -0.103441 0.411984 -1.300143
C 0.000313 2.758028 -1.488322
C 0.143321 2.858194 -0.103338
C 0.034801 0.455153 0.088819
H 0.240249 3.832618 0.355741
H 0.273109 1.807721 1.745181
C 0.037114 -0.815810 0.815677
C 0.014066 -3.364391 1.960336

C -0.096425 -1.969320 0.048356
C 0.159981 -0.964369 2.198771
C 0.148021 -2.230851 2.758213
C -0.111419 -3.243176 0.583032
H 0.263916 -0.096020 2.836014
H 0.244265 -2.339439 3.830547
H -0.216633 -4.121089 -0.041758
H 0.006755 -4.348104 2.411444
I -0.275373 -1.554713 -2.009843
Br -0.508976 -0.598677 -4.846925
H -0.235202 1.437477 -3.185759
C -0.018966 3.947203 -2.289724
N -0.034465 4.901372 -2.927009
SCF: -3426.124328
ZPE: 0.160235
H: -3425.949228
G: -3426.004813

2_CN_trans_adduct_conf1

H -0.248654 1.922799 -3.457134
C -0.143678 2.012991 -2.385072
C 0.128566 2.205149 0.398442
C -0.113796 0.902051 -1.573432
C -0.032745 3.252892 -1.768040
C 0.102794 3.344522 -0.387296
C 0.018422 0.941598 -0.185424
H -0.052038 4.147795 -2.376070
H 0.189891 4.315965 0.081255
H 0.235965 2.294656 1.471259
C 0.033480 -0.329941 0.541367
C 0.044383 -2.866807 1.685326
C -0.081615 -1.484326 -0.230189
C 0.153174 -0.473334 1.925439
C 0.158780 -1.732240 2.492999
C -0.079403 -2.755605 0.301831
H 0.242256 0.395303 2.563563
I -0.259454 -1.071887 -2.290051
Br -0.495564 -0.153602 -5.117074
H 0.252352 -1.847024 3.564310
H -0.168765 -3.642095 -0.312812
C 0.053858 -4.168745 2.287105
N 0.061789 -5.210017 2.769696
SCF: -3426.124996
ZPE: 0.160254

H: -3425.949881

G: -3426.005404

2_F_cis_adduct_conf1

C -0.138844 1.741223 -2.256111
C 0.125945 1.950457 0.530480
C -0.105910 0.637443 -1.434256
C -0.033385 2.962860 -1.620980
C 0.098650 3.091429 -0.249544
C 0.022465 0.682523 -0.046899
H 0.177998 4.076552 0.190220
H 0.229682 2.046381 1.603009
C 0.038785 -0.587394 0.683902
C 0.045909 -3.137340 1.835447
C -0.072755 -1.745771 -0.079096
C 0.155169 -0.733644 2.067532
C 0.158171 -1.999377 2.630148
C -0.072420 -3.019317 0.457340
H 0.242676 0.137808 2.703321
H 0.249364 -2.103249 3.703536
H -0.160432 -3.899122 -0.167519
H 0.050010 -4.120094 2.288584
I -0.242799 -1.335042 -2.138176
Br -0.467223 -0.389291 -4.996484
H -0.240375 1.671261 -3.331034
F -0.060581 4.071606 -2.373419
SCF: -3433.125474
ZPE: 0.153246
H: -3432.958341
G: -3433.011538

2_F_trans_adduct_conf1

H -0.249590 1.695273 -3.322578
C -0.135905 1.783467 -2.251063
C 0.157162 1.964039 0.530111
C -0.110780 0.670615 -1.441034
C -0.009289 3.021006 -1.632978
C 0.136400 3.105931 -0.252654
C 0.031361 0.702074 -0.054251
H -0.024787 3.917725 -2.238330
H 0.235289 4.075006 0.218766
H 0.272333 2.049383 1.602651
C 0.037494 -0.572803 0.668069
C 0.021349 -3.095814 1.793934

C -0.098169 -1.723761 -0.101687
C 0.166428 -0.727553 2.050532
C 0.159001 -1.989518 2.615982
C -0.110862 -3.001952 0.422969
H 0.272889 0.137427 2.691696
I -0.283192 -1.301516 -2.157180
Br -0.523595 -0.370704 -5.000187
H 0.258163 -2.129073 3.684173
H -0.216991 -3.894346 -0.180480
F 0.015291 -4.314708 2.353636
SCF: -3433.125986
ZPE: 0.153347
H: -3432.958770
G: -3433.011882

2_NMe2_cis_adduct_conf1

C 0.141090 0.388020 -1.483348
C -0.283041 0.698929 1.261325
C 0.189282 -0.658052 -0.601568
C -0.139083 1.674126 -0.967752
C -0.346250 1.793548 0.428445
C -0.011667 -0.584709 0.774076
H -0.558975 2.760213 0.860513
H -0.447681 0.838236 2.322834
C 0.077142 -1.809396 1.561513
C 0.306767 -4.292882 2.843595
C 0.367283 -2.983063 0.868380
C -0.102518 -1.911377 2.943487
C 0.012421 -3.141585 3.569894
C 0.488159 -4.221369 1.468483
H -0.333294 -1.027634 3.524600
H -0.129610 -3.206866 4.640998
H 0.716564 -5.110373 0.894310
H 0.394876 -5.247307 3.345803
I 0.592272 -2.639898 -1.196752
Br 0.852270 -1.800105 -4.137213
H 0.312623 0.221783 -2.535960
N -0.204025 2.747999 -1.792615
C -0.490687 4.062812 -1.252755
C 0.028584 2.580947 -3.213814
H -1.462282 4.084029 -0.751590
H -0.509853 4.779816 -2.068133
H 0.272740 4.375595 -0.534711
H -0.697751 1.893669 -3.658121

H -0.066576 3.545441 -3.703583
H 1.031421 2.189257 -3.410445
SCF: -3467.838910
ZPE: 0.234760
H: -3467.586581
G: -3467.648410

2_NMe2_cis_adduct_conf2

C 1.517018 1.370915 -0.480504
C 0.418341 1.604375 2.078348
C 1.504017 0.338601 0.418664
C 0.943431 2.600380 -0.083113
C 0.399319 2.682512 1.222308
C 0.975345 0.375680 1.705861
H -0.043760 3.606152 1.564212
H -0.008800 1.712670 3.067795
C 1.045600 -0.827093 2.527773
C 1.305405 -3.258912 3.899504
C 1.652432 -1.944320 1.957042
C 0.559014 -0.959591 3.830884
C 0.691261 -2.163956 4.502497
C 1.796771 -3.156028 2.604601
H 0.077259 -0.119809 4.315374
H 0.310542 -2.253364 5.511829
H 2.275309 -4.001406 2.126929
H 1.402491 -4.193954 4.435404
I 2.317648 -1.560573 -0.003557
Br 3.165783 -0.670767 -2.817647
H 1.955170 1.236942 -1.457806
N 0.922140 3.657129 -0.932165
C 0.347160 4.919023 -0.508421
C 1.495422 3.528719 -2.257446
H -0.709904 4.808941 -0.250909
H 0.428811 5.633120 -1.322542
H 0.871646 5.324857 0.361313
H 0.994477 2.744561 -2.833079
H 1.378002 4.470210 -2.785634
H 2.561854 3.287491 -2.210012
SCF: -3467.838929
ZPE: 0.234703
H: -3467.586627
G: -3467.648576

2_NMe2_cis_adduct_conf3

C 1.548256 1.557124 -0.292139
C 0.495723 1.670499 2.293971
C 1.514585 0.473622 0.543937
C 1.024147 2.778898 0.188328
C 0.498977 2.798205 1.503872
C 1.009036 0.449837 1.840839
H 0.088339 3.712262 1.906709
H 0.083730 1.733089 3.293580
C 1.055891 -0.801853 2.588481
C 1.263190 -3.319503 3.806376
C 1.611638 -1.902147 1.938145
C 0.595790 -0.996492 3.893576
C 0.701579 -2.242998 4.488540
C 1.728692 -3.154964 2.508211
H 0.156150 -0.171955 4.440199
H 0.341513 -2.380164 5.500112
H 2.166929 -3.985472 1.969244
H 1.339927 -4.287745 4.283353
I 2.250137 -1.422500 -0.009930
Br 3.068726 -0.395680 -2.785657
H 1.965150 1.467046 -1.283641
N 1.029911 3.886194 -0.593763
C 1.568456 3.817272 -1.938079
C 0.493836 5.135344 -0.088997
H 2.624940 3.532356 -1.930649
H 1.478315 4.793486 -2.404879
H 1.024335 3.090020 -2.548402
H 1.031448 5.467522 0.803477
H 0.598077 5.897608 -0.855498
H -0.566121 5.041993 0.163885
SCF: -3467.838918
ZPE: 0.234739
H: -3467.586605
G: -3467.648393

2_NMe2_trans_adduct_conf1
H -0.660063 2.895353 -4.147220
C -0.320265 3.019837 -3.128053
C 0.551358 3.287606 -0.477578
C -0.278601 1.955848 -2.255662
C 0.092209 4.254887 -2.642759
C 0.523923 4.381409 -1.326097
C 0.144651 2.028047 -0.927611
H 0.074353 5.114847 -3.299161

H 0.844081 5.347361 -0.957219
H 0.890383 3.402762 0.543965
C 0.129741 0.805987 -0.132558
C 0.006978 -1.711139 1.194193
C -0.305765 -0.357690 -0.756169
C 0.512393 0.677165 1.206963
C 0.454248 -0.537363 1.852833
C -0.381716 -1.594606 -0.159720
H 0.862165 1.544199 1.753967
I -0.850264 -0.005885 -2.761548
Br -1.549841 0.828243 -5.620288
H 0.760669 -0.586682 2.887117
H -0.729290 -2.455077 -0.712319
N -0.047409 -2.904320 1.837331
C -0.505051 -4.085831 1.133673
C 0.338929 -2.998999 3.231779
H -1.535973 -3.969766 0.785965
H -0.463514 -4.936044 1.808017
H 0.126154 -4.302175 0.266941
H -0.277243 -2.351215 3.861553
H 0.205971 -4.024617 3.562820
H 1.386990 -2.722144 3.376542
SCF: -3467.838092
ZPE: 0.234792
H: -3467.585748
G: -3467.647539

2_NMe2_trans_adduct_conf2
H -0.382384 4.031030 -2.782323
C 0.288885 4.088385 -1.936342
C 2.014141 4.185692 0.270813
C 0.442986 3.025808 -1.074906
C 1.030971 5.232839 -1.671231
C 1.885721 5.274969 -0.574037
C 1.285228 3.015478 0.038148
H 0.936956 6.088634 -2.326536
H 2.459594 6.171003 -0.375434
H 2.683906 4.235017 1.119868
C 1.336495 1.806748 0.851970
C 1.255531 -0.665932 2.263171
C 0.537406 0.738177 0.461859
C 2.112843 1.604508 1.998040
C 2.076603 0.411428 2.683871
C 0.462362 -0.473099 1.109100

H 2.756551 2.396732 2.360112
I -0.571660 1.191861 -1.271137
Br -2.031393 2.150122 -3.783859
H 2.693466 0.303951 3.563636
H -0.186871 -1.255844 0.744030
N 1.230080 -1.840083 2.942063
C 0.366789 -2.914947 2.495539
C 2.031993 -2.008183 4.138613
H -0.685813 -2.616557 2.512556
H 0.493114 -3.766606 3.157134
H 0.617023 -3.228591 1.478063
H 1.751269 -1.289134 4.913652
H 1.875697 -3.010292 4.526947
H 3.097110 -1.884217 3.925120
SCF: -3467.838090
ZPE: 0.234716
H: -3467.585737
G: -3467.648019

2_NMe2_trans_adduct_conf3
H 0.900570 3.907278 -3.246678
C 0.965964 4.033499 -2.174541
C 1.135863 4.302937 0.610150
C 0.973273 2.947601 -1.328564
C 1.046669 5.292270 -1.591884
C 1.130829 5.419400 -0.208851
C 1.055969 3.018804 0.062972
H 1.043789 6.170083 -2.224436
H 1.193700 6.404117 0.236082
H 1.202663 4.420300 1.684078
C 1.053600 1.770939 0.817613
C 1.033319 -0.798821 2.046192
C 0.969294 0.586345 0.094444
C 1.129210 1.635378 2.208095
C 1.119906 0.395429 2.806447
C 0.956008 -0.676033 0.640129
H 1.196025 2.517020 2.833738
I 0.862350 0.949136 -1.978364
Br 0.726112 1.802695 -4.913847
H 1.179992 0.341874 3.883350
H 0.890903 -1.551784 0.010689
N 1.024914 -2.016727 2.643618
C 0.933688 -3.217642 1.837466
C 1.119915 -2.121639 4.086839

H 0.013374 -3.231472 1.246406
H 0.932359 -4.083335 2.493037
H 1.782110 -3.304306 1.152048
H 0.279772 -1.625169 4.580374
H 1.107435 -3.171761 4.363038
H 2.047421 -1.678112 4.459461
SCF: -3467.838108
ZPE: 0.234888
H: -3467.585693
G: -3467.647400

2_OMe_cis_adduct_conf1
C -0.084607 1.121356 -1.634626
C 0.153718 1.317806 1.151567
C -0.058264 0.018614 -0.809594
C 0.011111 2.367295 -1.018244
C 0.131445 2.453597 0.374892
C 0.056497 0.044724 0.574048
H 0.205927 3.433528 0.828044
H 0.247657 1.411639 2.225746
C 0.065623 -1.227771 1.295623
C 0.058437 -3.787331 2.431851
C -0.040037 -2.382976 0.525348
C 0.169049 -1.384710 2.679424
C 0.165034 -2.654106 3.234120
C -0.046823 -3.659821 1.053313
H 0.251571 -0.516276 3.320205
H 0.245930 -2.764705 4.307732
H -0.130660 -4.535059 0.421622
H 0.056674 -4.772965 2.878599
I -0.192061 -1.953229 -1.529544
Br -0.403304 -0.972331 -4.408484
H -0.175887 1.007471 -2.704789
O -0.005048 3.529175 -1.693048
C -0.135524 3.472827 -3.108058
H -1.072112 2.988266 -3.393286
H 0.706070 2.939447 -3.555709
H -0.138316 4.504039 -3.450250
SCF: -3448.403387
ZPE: 0.194526
H: -3448.193263
G: -3448.250237

2_OMe_cis_adduct_conf2

C -0.113299 0.930955 -1.946076
C 0.135504 1.067578 0.831865
C -0.090292 -0.187522 -1.156276
C -0.009554 2.170353 -1.306951
C 0.118388 2.231659 0.082316
C 0.028547 -0.186740 0.234768
H 0.205108 3.182641 0.587106
H 0.234665 1.140096 1.907311
C 0.028862 -1.473421 0.931781
C 0.000010 -4.053675 2.019724
C -0.086489 -2.612268 0.139875
C 0.130950 -1.657428 2.312360
C 0.116257 -2.936831 2.843207
C -0.104115 -3.898685 0.643975
H 0.220047 -0.802114 2.969677
H 0.195875 -3.068218 3.914536
H -0.195939 -4.761026 -0.003964
H -0.010433 -5.047577 2.447572
I -0.235229 -2.146492 -1.909536
Br -0.429818 -1.143170 -4.766838
H -0.209150 0.877881 -3.022152
O -0.042448 3.245283 -2.113371
C 0.027669 4.531844 -1.511666
H 0.970429 4.661373 -0.976580
H -0.809694 4.687603 -0.828453
H -0.029349 5.246501 -2.328208
SCF: -3448.402180
ZPE: 0.194526
H: -3448.192017
G: -3448.249117

2_OMe_trans_adduct_conf1

H -0.277819 2.618863 -3.530203
C -0.199315 2.697023 -2.454572
C 0.005675 2.849184 0.336860
C -0.131956 1.574874 -1.659746
C -0.161961 3.929945 -1.815418
C -0.060295 4.000192 -0.429938
C -0.028543 1.590718 -0.268734
H -0.212412 4.834138 -2.407553
H -0.032027 4.965809 0.057986
H 0.084544 2.921846 1.413811
C 0.034624 0.308583 0.432028
C 0.133722 -2.272483 1.533190

C -0.012192 -0.837774 -0.346423
C 0.137348 0.128940 1.817734
C 0.185652 -1.136907 2.354931
C 0.033782 -2.128293 0.151033
H 0.178285 0.986644 2.476890
I -0.170085 -0.394584 -2.399911
Br -0.410734 0.568658 -5.260999
H 0.264094 -1.280434 3.424861
H -0.006149 -2.986030 -0.505299
O 0.185181 -3.460150 2.161469
C 0.129333 -4.637807 1.367682
H 0.976440 -4.684692 0.679884
H -0.805928 -4.684776 0.805747
H 0.178634 -5.471088 2.063394
SCF: -3448.402876
ZPE: 0.194630
H: -3448.192686
G: -3448.249478

2_OMe_trans_adduct_conf2

H -0.310567 2.354530 -3.957127
C -0.231574 2.462138 -2.884025
C -0.024501 2.687241 -0.098207
C -0.161878 1.361392 -2.060104
C -0.195582 3.711516 -2.277738
C -0.092676 3.817829 -0.894679
C -0.057845 1.413159 -0.670247
H -0.247531 4.599934 -2.893234
H -0.065140 4.795966 -0.432191
H 0.055865 2.788102 0.976422
C 0.007713 0.149632 0.063942
C 0.115939 -2.403089 1.230789
C -0.036217 -1.020213 -0.692126
C 0.109257 0.001890 1.445526
C 0.162880 -1.254546 2.026703
C 0.014665 -2.285531 -0.158280
H 0.146454 0.874996 2.084642
I -0.196273 -0.626043 -2.755123
Br -0.436364 0.268877 -5.638788
H 0.240818 -1.333223 3.101347
H -0.020682 -3.180877 -0.766099
O 0.161057 -3.658622 1.711015
C 0.253760 -3.833201 3.118913
H -0.609470 -3.394294 3.623400

H 1.173201 -3.390424 3.507176
H 0.267290 -4.906937 3.286287
SCF: -3448.402449
ZPE: 0.194522
H: -3448.192326
G: -3448.249249

2_OMe_trans_adduct_conf3

H -0.310567 2.354530 -3.957127
C -0.231574 2.462138 -2.884025
C -0.024501 2.687241 -0.098207
C -0.161878 1.361392 -2.060104
C -0.195582 3.711516 -2.277738
C -0.092676 3.817829 -0.894679
C -0.057845 1.413159 -0.670247
H -0.247531 4.599934 -2.893234
H -0.065140 4.795966 -0.432191
H 0.055865 2.788102 0.976422
C 0.007713 0.149632 0.063942
C 0.115939 -2.403089 1.230789
C -0.036217 -1.020213 -0.692126
C 0.109257 0.001890 1.445526
C 0.162880 -1.254546 2.026703
C 0.014665 -2.285531 -0.158280
H 0.146454 0.874996 2.084642
I -0.196273 -0.626043 -2.755123
Br -0.436364 0.268877 -5.638788
H 0.240818 -1.333223 3.101347
H -0.020682 -3.180877 -0.766099
O 0.161057 -3.658622 1.711015
C 0.253760 -3.833201 3.118913
H -0.609470 -3.394294 3.623400
H 1.173201 -3.390424 3.507176
H 0.267290 -4.906937 3.286287
SCF: -3448.402449
ZPE: 0.194522
H: -3448.192326
G: -3448.249249

2_OMe_trans_adduct_conf4

H -0.310567 2.354530 -3.957127
C -0.231574 2.462138 -2.884025
C -0.024501 2.687241 -0.098207
C -0.161878 1.361392 -2.060104

C -0.195582 3.711516 -2.277738
C -0.092676 3.817829 -0.894679
C -0.057845 1.413159 -0.670247
H -0.247531 4.599934 -2.893234
H -0.065140 4.795966 -0.432191
H 0.055865 2.788102 0.976422
C 0.007713 0.149632 0.063942
C 0.115939 -2.403089 1.230789
C -0.036217 -1.020213 -0.692126
C 0.109257 0.001890 1.445526
C 0.162880 -1.254546 2.026703
C 0.014665 -2.285531 -0.158280
H 0.146454 0.874996 2.084642
I -0.196273 -0.626043 -2.755123
Br -0.436364 0.268877 -5.638788
H 0.240818 -1.333223 3.101347
H -0.020682 -3.180877 -0.766099
O 0.161057 -3.658622 1.711015
C 0.253760 -3.833201 3.118913
H -0.609470 -3.394294 3.623400
H 1.173201 -3.390424 3.507176
H 0.267290 -4.906937 3.286287
SCF: -3448.402449
ZPE: 0.194522
H: -3448.192326
G: -3448.249249

3_CF3_cis_adduct_conf1

C -0.108412 1.164289 -2.326111
C 0.059542 1.349706 0.469449
C -0.088404 0.050936 -1.513651
C -0.042134 2.402503 -1.710127
C 0.041166 2.480930 -0.322910
C -0.006988 0.087020 -0.123137
H 0.125172 1.439853 1.544813
C 0.004279 -1.185723 0.602827
C 0.011894 -3.739847 1.739075
C -0.064224 -2.339908 -0.171275
C 0.076845 -1.336795 1.988928
C 0.080302 -2.605543 2.544065
C -0.062429 -3.616204 0.358491
H 0.129658 -0.468712 2.633028
H 0.137066 -2.714954 3.619176
H -0.116086 -4.493787 -0.273286

H 0.015889 -4.725111 2.186823
I -0.172720 -1.920286 -2.232479
Br -0.317850 -0.979800 -5.090371
H -0.172979 1.074915 -3.401578
H -0.055281 3.302674 -2.311664
C 0.113497 3.847265 0.299895
F 0.170678 3.806469 1.633040
F 1.192987 4.525061 -0.118322
F -0.951467 4.595245 -0.024697
SCF: -3670.964322
ZPE: 0.166389
H: -3670.781255
G: -3670.841851

3_CF3_cis_adduct_conf2
C 0.832200 2.166159 -1.321935
C 1.068655 2.349510 1.468825
C 0.872995 1.052211 -0.511142
C 0.912873 3.403912 -0.706766
C 1.029730 3.481359 0.678079
C 0.989133 1.087274 0.876903
H 1.160137 2.438720 2.542396
C 1.020181 -0.186055 1.601219
C 1.059936 -2.740980 2.734811
C 0.932223 -1.339643 0.828199
C 1.130044 -0.338154 2.984729
C 1.149287 -1.607307 3.538590
C 0.948910 -2.616301 1.356763
H 1.200121 0.529478 3.627749
H 1.235306 -1.717515 4.611689
H 0.879063 -3.493414 0.725994
H 1.076394 -3.726599 3.181482
I 0.770919 -0.918468 -1.229229
Br 0.548337 0.024121 -4.081677
H 0.740767 2.077516 -2.395494
H 0.884697 4.304534 -1.307079
C 1.117924 4.847232 1.299905
F 1.187789 4.806010 2.632417
F 2.198479 5.517001 0.871353
F 0.055501 5.602997 0.985521
SCF: -3670.964314
ZPE: 0.166321
H: -3670.781297
G: -3670.841972

3_CF3_trans_adduct_conf1
H -0.220667 1.919918 -3.907323
C -0.165741 2.019359 -2.832152
C -0.021871 2.232082 -0.040490
C -0.116987 0.913704 -2.013618
C -0.140605 3.264996 -2.217644
C -0.069387 3.366536 -0.832644
C -0.044445 0.962931 -0.621871
H -0.176456 4.156321 -2.830134
H -0.050546 4.342443 -0.365511
H 0.033224 2.330030 1.035688
C 0.004037 -0.306683 0.108271
C 0.091418 -2.856242 1.262096
C -0.025444 -1.467667 -0.655392
C 0.078740 -0.441043 1.495905
C 0.122005 -1.706375 2.049571
C 0.015957 -2.740714 -0.114844
H 0.103184 0.431999 2.133496
I -0.140120 -1.068328 -2.720926
Br -0.302960 -0.166693 -5.572172
H -0.008085 -3.625276 -0.738122
H 0.125729 -3.835605 1.723238
C 0.205851 -1.879148 3.540129
F -0.834142 -2.579363 4.018328
F 1.310219 -2.551247 3.900242
F 0.227193 -0.716235 4.195880
SCF: -3670.964909
ZPE: 0.166355
H: -3670.781863
G: -3670.843017

3_CF3_trans_adduct_conf2
H 0.772636 2.919535 -2.907127
C 0.840502 3.018923 -1.832721
C 1.017678 3.232172 0.956857
C 0.878870 1.913497 -1.013348
C 0.893510 4.264633 -1.220195
C 0.981658 4.366419 0.163784
C 0.966290 1.962953 0.377553
H 0.866334 5.155710 -1.833487
H 1.022974 5.342295 0.629495
H 1.086677 3.330646 2.032148
C 0.999655 0.693423 1.108806

C 1.054940 -1.856219 2.264447
C 0.943918 -0.467648 0.346673
C 1.084048 0.559057 2.495927
C 1.111360 -0.706355 3.050482
C 0.969033 -1.740743 0.888140
H 1.127998 1.432018 3.132537
I 0.817379 -0.068507 -1.718154
Br 0.643371 0.831464 -4.570007
H 0.924783 -2.625443 0.266158
H 1.077323 -2.835604 2.726255
C 1.206019 -0.879339 4.540403
F 0.160440 -1.564006 5.028605
F 2.303690 -1.567260 4.891126
F 1.250313 0.283581 5.195144
SCF: -3670.964903
ZPE: 0.166324
H: -3670.781875
G: -3670.843156

3_CN_cis_adduct_conf1

C -0.151179 1.516867 -2.295466
C 0.104828 1.701609 0.495755
C -0.118083 0.406548 -1.481020
C -0.053165 2.758394 -1.689914
C 0.073907 2.838042 -0.302764
C 0.006657 0.442675 -0.091444
H 0.205440 1.803610 1.567705
C 0.025902 -0.829622 0.635329
C 0.040375 -3.381606 1.773352
C -0.079793 -1.982880 -0.135438
C 0.140096 -0.979433 2.018595
C 0.146852 -2.247712 2.574716
C -0.075821 -3.258630 0.395508
H 0.223015 -0.111106 2.659144
H 0.236395 -2.357111 3.647595
H -0.159362 -4.136289 -0.232839
H 0.047355 -4.366476 2.221941
I -0.247439 -1.564512 -2.193763
Br -0.473515 -0.625849 -5.041893
H -0.249775 1.424298 -3.368079
H -0.074301 3.658572 -2.288608
C 0.175482 4.129255 0.318719
N 0.256133 5.161357 0.812971
SCF: -3426.124097

ZPE: 0.160344
H: -3425.948912
G: -3426.004424

3_CN_trans_adduct_conf1

H -0.201546 1.773814 -3.566926
C -0.130883 1.865511 -2.492072
C 0.053193 2.061365 0.298293
C -0.096686 0.754928 -1.679705
C -0.070079 3.107209 -1.872065
C 0.021856 3.200537 -0.487864
C -0.006739 0.796432 -0.288878
H -0.094028 4.001907 -2.480156
H 0.069854 4.173314 -0.016457
H 0.125455 2.152686 1.374002
C 0.019679 -0.477570 0.435438
C 0.057906 -3.044025 1.570838
C -0.041848 -1.635664 -0.334976
C 0.100081 -0.620158 1.818026
C 0.118024 -1.897227 2.366909
C -0.024404 -2.912426 0.195638
H 0.147734 0.242177 2.469232
I -0.168348 -1.222589 -2.397992
Br -0.345509 -0.307849 -5.234012
H -0.072704 -3.791748 -0.433620
H 0.074233 -4.023358 2.029317
C 0.199703 -2.040583 3.793671
N 0.264959 -2.156982 4.933258
SCF: -3426.124882
ZPE: 0.160356
H: -3425.949699
G: -3426.005091

3_F_cis_adduct_conf1

C -0.179623 1.745714 -2.259748
C 0.075077 1.942846 0.530587
C -0.123351 0.634299 -1.446835
C -0.106293 2.992066 -1.657113
C 0.019054 3.055012 -0.280417
C 0.002577 0.681103 -0.057784
H 0.174194 2.067107 1.600637
C 0.050707 -0.588074 0.672889
C 0.123226 -3.133668 1.824453
C -0.030877 -1.747611 -0.091787

C 0.170979 -0.728799 2.056486
C 0.206310 -1.993483 2.619752
C 0.002168 -3.020030 0.446192
H 0.236291 0.145550 2.691011
H 0.300140 -2.095193 3.693051
H -0.062759 -3.902385 -0.177741
H 0.152330 -4.115856 2.277973
I -0.210964 -1.340277 -2.150180
Br -0.466562 -0.414686 -5.014024
H -0.277512 1.651506 -3.332469
H -0.144776 3.901074 -2.241893
F 0.089666 4.263682 0.296958
SCF: -3433.126297
ZPE: 0.153369
H: -3432.959065
G: -3433.012180

3_F_trans_adduct_conf1
H -0.238702 1.674981 -3.335027
C -0.136117 1.766228 -2.262593
C 0.129286 1.957445 0.521457
C -0.106762 0.655013 -1.450528
C -0.028298 3.006194 -1.645533
C 0.103785 3.097152 -0.264201
C 0.022295 0.694104 -0.062540
H -0.047456 3.901324 -2.253210
H 0.188229 4.068569 0.205033
H 0.233712 2.045608 1.594904
C 0.036154 -0.579165 0.662552
C 0.039776 -3.138876 1.809082
C -0.077663 -1.734878 -0.104930
C 0.153145 -0.717110 2.045504
C 0.151356 -1.989198 2.573909
C -0.078349 -3.008487 0.434300
H 0.243311 0.135015 2.706087
I -0.249159 -1.319736 -2.160660
Br -0.479856 -0.392888 -5.018383
H -0.167751 -3.889758 -0.187886
H 0.045502 -4.109083 2.287328
F 0.263763 -2.122458 3.905435
SCF: -3433.126515
ZPE: 0.153375
H: -3432.959279
G: -3433.012376

3_NMe2_cis_adduct_conf1
C 0.282497 0.229567 -2.455410
C -0.027942 0.588112 0.300066
C 0.182540 -0.844233 -1.595944
C 0.228860 1.504489 -1.926787
C 0.076365 1.718345 -0.535623
C 0.026124 -0.699329 -0.217885
H -0.153246 0.712178 1.365074
C -0.070693 -1.923855 0.586363
C -0.230385 -4.395468 1.890957
C 0.000619 -3.131601 -0.101868
C -0.225857 -1.980279 1.972653
C -0.304907 -3.206509 2.612022
C -0.074426 -4.367744 0.511841
H -0.284683 -1.067662 2.551448
H -0.426486 -3.238869 3.686959
H -0.014088 -5.287075 -0.056607
H -0.293473 -5.347072 2.402494
I 0.236546 -2.855526 -2.175513
Br 0.582123 -2.099484 -5.108894
H 0.400389 0.081311 -3.520361
H 0.306925 2.341783 -2.604042
N 0.032740 2.976121 -0.022310
C -0.141573 3.172180 1.402635
C 0.099497 4.124105 -0.904986
H -1.093885 2.761326 1.752420
H -0.127925 4.236808 1.616781
H 0.663788 2.697472 1.970103
H -0.726682 4.127673 -1.622302
H 0.038889 5.029500 -0.308486
H 1.038645 4.143737 -1.464901
SCF: -3467.837419
ZPE: 0.234567
H: -3467.585167
G: -3467.647699

3_NMe2_cis_adduct_conf2
C 1.641034 1.224351 -1.202388
C 1.130375 1.455413 1.537511
C 1.395355 0.116010 -0.419334
C 1.630208 2.469237 -0.604276
C 1.372976 2.619030 0.779989
C 1.137892 0.197869 0.948452

H 0.933657 1.527525 2.596740
C 0.892499 -1.057091 1.669022
C 0.455545 -3.574237 2.811043
C 0.937871 -2.228739 0.919386
C 0.618451 -1.173399 3.032658
C 0.403132 -2.422273 3.591863
C 0.726828 -3.486411 1.452402
H 0.574479 -0.288699 3.654720
H 0.191095 -2.502024 4.650175
H 0.769125 -4.376862 0.838064
H 0.285114 -4.544081 3.260119
I 1.364861 -1.860889 -1.108800
Br 2.000049 -0.978146 -3.956083
H 1.838580 1.126005 -2.261285
H 1.823467 3.333826 -1.221463
N 1.360120 3.848149 1.359837
C 1.650787 5.028185 0.569307
C 1.122836 3.974457 2.783574
H 2.652546 4.982231 0.131782
H 1.597138 5.903018 1.210675
H 0.928518 5.152853 -0.242140
H 1.888935 3.453928 3.366728
H 1.142433 5.026353 3.052721
H 0.146694 3.567211 3.061805
SCF: -3467.837470
ZPE: 0.235068
H: -3467.584906
G: -3467.646489

3_NMe2_cis_adduct_conf3

C 1.689291 1.176263 -1.469481
C 1.066603 1.619351 1.220202
C 1.431280 0.130672 -0.608103
C 1.631560 2.465489 -0.977164
C 1.314456 2.722384 0.378446
C 1.119621 0.318097 0.737984
H 0.829335 1.775178 2.261722
C 0.871816 -0.879502 1.550117
C 0.449561 -3.305943 2.879784
C 0.973380 -2.107093 0.902204
C 0.544818 -0.891568 2.907229
C 0.337624 -2.095721 3.559588
C 0.771153 -3.321997 1.529413
H 0.451845 0.039116 3.451860

H 0.085289 -2.094064 4.612025
H 0.858867 -4.258198 0.992959
H 0.285662 -4.240180 3.400948
I 1.463190 -1.895963 -1.134351
Br 2.164268 -1.232567 -4.025942
H 1.933680 0.995738 -2.507534
H 1.837202 3.280359 -1.654913
N 1.251271 3.994643 0.853238
C 0.985047 4.230577 2.257941
C 1.554429 5.111832 -0.019670
H 0.011082 3.828828 2.550959
H 0.980881 5.300918 2.441385
H 1.748813 3.773190 2.894783
H 0.878291 5.139423 -0.878301
H 1.433271 6.036462 0.537089
H 2.581716 5.064974 -0.394115
SCF: -3467.837432
ZPE: 0.234886
H: -3467.584991
G: -3467.646893

3_NMe2_trans_adduct_conf1

H -0.153686 2.029993 -4.748014
C 0.003386 2.161940 -3.686107
C 0.402084 2.452174 -0.927218
C -0.102057 1.102572 -2.812557
C 0.318800 3.401556 -3.144287
C 0.515972 3.541357 -1.774469
C 0.085586 1.190084 -1.433665
H 0.409368 4.257402 -3.800203
H 0.761548 4.511871 -1.363308
H 0.560073 2.576796 0.136341
C -0.062121 -0.033484 -0.636961
C -0.399444 -2.476389 0.664475
C -0.381588 -1.190749 -1.340183
C 0.091489 -0.104444 0.741774
C -0.067281 -1.327283 1.423533
C -0.553316 -2.408251 -0.706417
H 0.335811 0.793105 1.289473
I -0.569411 -0.860879 -3.401278
Br -0.769615 -0.034685 -6.352693
H -0.806169 -3.303365 -1.260981
H -0.538425 -3.430562 1.150482
N 0.094247 -1.403148 2.773139

C -0.155936 -2.651898 3.465377
C 0.354781 -0.199652 3.536528
H -1.188438 -2.990223 3.331247
H 0.023143 -2.507190 4.526820
H 0.511211 -3.442445 3.112055
H -0.458686 0.526823 3.437795
H 0.456377 -0.462277 4.585506
H 1.282095 0.281048 3.213796
SCF: -3467.836703
ZPE: 0.234683
H: -3467.584381
G: -3467.646684

3_NMe2_trans_adduct_conf2
H 0.745773 3.020430 -3.801988
C 1.113084 3.118856 -2.789586
C 2.043332 3.325562 -0.154218
C 0.864657 2.149110 -1.844010
C 1.852718 4.223335 -2.386219
C 2.312065 4.322314 -1.077101
C 1.303030 2.200083 -0.521249
H 2.067012 5.006133 -3.101863
H 2.886843 5.187610 -0.773561
H 2.408604 3.418051 0.860243
C 0.955539 1.083276 0.365277
C 0.169373 -1.138237 1.856621
C 0.206475 0.057364 -0.202501
C 1.317303 0.990575 1.703319
C 0.939046 -0.124144 2.477530
C -0.191720 -1.048720 0.526469
H 1.895990 1.785839 2.148068
I -0.234317 0.397744 -2.222785
Br -0.705499 1.208978 -5.149559
H -0.779072 -1.839801 0.077104
H -0.149181 -2.002779 2.419627
N 1.303143 -0.224884 3.785777
C 0.824970 -1.332924 4.588669
C 2.005208 0.869724 4.424578
H -0.267968 -1.346359 4.653858
H 1.228330 -1.238294 5.592841
H 1.154706 -2.290577 4.178298
H 1.415886 1.792753 4.410758
H 2.205383 0.604081 5.458378
H 2.960887 1.067903 3.932325

SCF: -3467.836696
ZPE: 0.234623
H: -3467.584435
G: -3467.646718

3_OMe_cis_adduct_conf1
C -0.167855 0.855671 -2.188542
C 0.099181 1.066631 0.584517
C -0.139008 -0.253037 -1.377510
C -0.060248 2.107847 -1.596987
C 0.073411 2.211711 -0.211048
C -0.007447 -0.192625 0.013033
H 0.204775 1.184892 1.654973
C 0.008529 -1.458524 0.754055
C 0.016259 -3.997306 1.927969
C -0.106667 -2.622801 0.000489
C 0.128956 -1.592556 2.138379
C 0.132171 -2.852905 2.712833
C -0.105947 -3.891284 0.549196
H 0.219737 -0.715076 2.765413
H 0.226574 -2.947605 3.786774
H -0.196323 -4.776791 -0.067198
H 0.020698 -4.976136 2.389593
I -0.282474 -2.229796 -2.061385
Br -0.518371 -1.317232 -4.944897
H -0.271578 0.761323 -3.260923
H -0.081682 2.985410 -2.226170
O 0.183960 3.381330 0.446075
C 0.168951 4.580808 -0.316220
H -0.771953 4.686328 -0.860093
H 1.005702 4.608570 -1.017388
H 0.268053 5.391552 0.400665
SCF: -3448.402586
ZPE: 0.194577
H: -3448.192396
G: -3448.249378

3_OMe_cis_adduct_conf2
C -0.188400 1.089707 -2.530765
C 0.076250 1.238427 0.259014
C -0.163724 -0.042045 -1.738468
C -0.077721 2.314611 -1.906143
C 0.054744 2.393429 -0.513841
C -0.033923 -0.012206 -0.353940

H 0.177657 1.296190 1.332510
C -0.021336 -1.293502 0.360519
C -0.022579 -3.859611 1.477352
C -0.141187 -2.441118 -0.418141
C 0.100275 -1.460397 1.741602
C 0.099133 -2.733472 2.287245
C -0.145568 -3.721657 0.101622
H 0.195759 -0.599850 2.390788
H 0.194528 -2.852483 3.358680
H -0.240722 -4.592142 -0.534956
H -0.021820 -4.848603 1.916807
I -0.314455 -2.000861 -2.468739
Br -0.549009 -1.025995 -5.332495
H -0.290876 1.018934 -3.604914
H -0.091458 3.229103 -2.484478
O 0.155685 3.635828 -0.006897
C 0.296501 3.775337 1.399983
H 1.210354 3.290676 1.750223
H -0.566674 3.356640 1.921785
H 0.354767 4.843560 1.591047
SCF: -3448.402724
ZPE: 0.194195
H: -3448.192813
G: -3448.250216

3_OMe_trans_adduct_conf1

H -0.364489 2.310123 -4.003446
C -0.254758 2.376664 -2.929798
C 0.029943 2.501449 -0.144239
C -0.198733 1.246014 -2.146012
C -0.164039 3.602503 -2.282433
C -0.023493 3.660294 -0.900047
C -0.056516 1.250903 -0.758845
H -0.203839 4.512349 -2.866784
H 0.045760 4.620828 -0.406446
H 0.139892 2.563727 0.930553
C -0.008505 -0.040904 -0.066202
C 0.057779 -2.620829 1.021111
C -0.111566 -1.178396 -0.866736
C 0.130671 -0.213791 1.303487
C 0.163936 -1.497849 1.845976
C -0.081723 -2.456506 -0.350957
H 0.215530 0.631382 1.974186
I -0.315955 -0.712818 -2.904948

Br -0.615958 0.293886 -5.759625
H -0.163642 -3.327546 -0.988685
H 0.082168 -3.619683 1.431489
O 0.302095 -1.562753 3.184997
C 0.345546 -2.846891 3.791156
H 1.196170 -3.424680 3.423144
H -0.579828 -3.397169 3.608663
H 0.459652 -2.670606 4.857537
SCF: -3448.402268
ZPE: 0.194494
H: -3448.192127
G: -3448.249365

3_OMe_trans_adduct_conf2

H -0.393812 1.832945 -4.085614
C -0.278368 1.920183 -3.014034
C 0.019015 2.096758 -0.232701
C -0.215185 0.804465 -2.209747
C -0.187615 3.157978 -2.390169
C -0.040723 3.241196 -1.009741
C -0.066551 0.834234 -0.823118
H -0.232545 4.056905 -2.990813
H 0.028296 4.210779 -0.534124
H 0.132730 2.181879 0.839992
C -0.013256 -0.445368 -0.108572
C 0.058495 -2.994371 1.021558
C -0.117559 -1.591115 -0.884404
C 0.132637 -0.583308 1.274589
C 0.166211 -1.855574 1.832689
C -0.084068 -2.867544 -0.344286
H 0.218162 0.294815 1.897412
I -0.330865 -1.167159 -2.929611
Br -0.639919 -0.216055 -5.801533
H -0.167091 -3.749586 -0.966454
H 0.088320 -3.970939 1.487039
O 0.300062 -2.093132 3.151914
C 0.395091 -0.977744 4.025991
H -0.501186 -0.356253 3.965058
H 1.277037 -0.375711 3.797198
H 0.485585 -1.388777 5.027981
SCF: -3448.402550
ZPE: 0.194213
H: -3448.192666
G: -3448.249846

4_CF3_cis_adduct_conf1

C -0.126149 1.456321 -2.546823
C 0.044296 1.755025 0.226141
C -0.105481 0.381177 -1.686956
C -0.051747 2.719298 -1.992752
C 0.028172 2.857002 -0.616640
C -0.012511 0.439227 -0.289544
C 0.013182 -0.862071 0.423550
C 0.033992 -3.500239 1.447482
C -0.085512 -1.998156 -0.383805
C 0.136179 -1.108166 1.797541
C 0.144880 -2.402696 2.291114
C -0.081028 -3.298600 0.081683
H 0.231433 -0.312838 2.512642
H 0.241983 -2.551739 3.358490
H -0.162331 -4.138224 -0.597150
H 0.041223 -4.505797 1.846982
I -0.224862 -1.575691 -2.427054
Br -0.409388 -0.678681 -5.307644
H -0.197925 1.310458 -3.616154
H -0.061562 3.593340 -2.629275
H 0.075571 3.848833 -0.192801
C 0.114714 2.061668 1.703185
F -0.921794 1.543472 2.378875
F 1.238455 1.594228 2.269090
F 0.096308 3.372950 1.949718
SCF: -3670.952186
ZPE: 0.166659
H: -3670.769023
G: -3670.828974

4_CF3_trans_adduct_conf1

H -0.176051 1.478575 -3.772388
C -0.112406 1.630707 -2.703800
C 0.053095 1.953502 0.060487
C -0.087223 0.561864 -1.837941
C -0.052473 2.903700 -2.156657
C 0.030904 3.053810 -0.780853
C -0.007413 0.647126 -0.440668
H -0.069906 3.767006 -2.808588
H 0.079965 4.043565 -0.346409
H 0.119931 2.144444 1.115141
C 0.004725 -0.626692 0.320043

C 0.006106 -3.261777 1.378495
C -0.059003 -1.778676 -0.465946
C 0.069403 -0.860262 1.713501
C 0.069568 -2.154631 2.212891
C -0.060398 -3.075622 0.012574
I -0.162135 -1.413118 -2.528313
Br -0.300227 -0.595488 -5.408147
H -0.111752 -3.922662 -0.660421
H 0.008117 -4.258489 1.797978
H 0.120240 -2.309437 3.280306
C 0.140982 0.241311 2.742423
F 0.184283 -0.229199 3.990480
F 1.235925 1.003988 2.595272
F -0.924358 1.056354 2.690744
SCF: -3670.953212
ZPE: 0.166699
H: -3670.770032
G: -3670.829822

4_CN_cis_adduct_conf1

C -0.131667 1.650573 -2.380888
C 0.101046 1.888595 0.385742
C -0.107197 0.552776 -1.550765
C -0.035265 2.905999 -1.799711
C 0.079289 3.021829 -0.426231
C 0.008829 0.592997 -0.158529
C 0.020740 -0.689898 0.561076
C 0.012585 -3.283200 1.642122
C -0.091019 -1.833022 -0.230489
C 0.133010 -0.886999 1.941224
C 0.128057 -2.169175 2.465805
C -0.098887 -3.120444 0.268853
H 0.225026 -0.053133 2.618505
H 0.216121 -2.299443 3.536376
H -0.188224 -3.979519 -0.383952
H 0.009853 -4.278871 2.065994
I -0.245740 -1.408582 -2.280604
Br -0.453101 -0.479950 -5.133678
H -0.223342 1.533662 -3.452362
H -0.050655 3.789944 -2.422196
H 0.152755 3.996520 0.036995
C 0.220459 2.139598 1.792785
N 0.317325 2.409844 2.903929
SCF: -3426.118910

ZPE: 0.160225

H: -3425.943876

G: -3425.999220

4_CN_trans_adduct_conf1

H -0.187059 1.571060 -3.512237

C -0.123781 1.689969 -2.439530

C 0.042229 1.945868 0.340739

C -0.084289 0.597913 -1.604286

C -0.078452 2.947181 -1.851474

C 0.005507 3.067473 -0.471142

C -0.004237 0.661175 -0.209011

H -0.107391 3.827665 -2.479698

H 0.043174 4.048401 -0.016077

H 0.108734 2.082170 1.408343

C 0.025480 -0.611693 0.527216

C 0.073527 -3.213697 1.635968

C -0.017180 -1.767784 -0.248082

C 0.089645 -0.812101 1.919452

C 0.113618 -2.098477 2.457029

C 0.005290 -3.052340 0.261124

I -0.130601 -1.377682 -2.311906

Br -0.294080 -0.507996 -5.160978

H -0.028942 -3.916031 -0.391485

H 0.093380 -4.205195 2.067154

H 0.163822 -2.213227 3.531626

C 0.129566 0.260759 2.870336

N 0.162240 1.076691 3.676919

SCF: -3426.119867

ZPE: 0.160294

H: -3425.944780

G: -3426.000051

4_F_cis_adduct_conf1

C -0.101697 1.763869 -2.262865

C 0.108322 1.976924 0.491267

C -0.082032 0.661712 -1.440885

C -0.011487 3.011038 -1.656803

C 0.094223 3.120074 -0.278705

C 0.020576 0.693565 -0.046779

C 0.027822 -0.575581 0.687529

C 0.017496 -3.149313 1.801059

C -0.067803 -1.726840 -0.093440

C 0.119258 -0.747495 2.072746

C 0.113415 -2.024099 2.612606

C -0.075493 -3.007377 0.423201

H 0.194162 0.105926 2.728469

H 0.185117 -2.142443 3.685988

H -0.150650 -3.876579 -0.218069

H 0.014679 -4.139320 2.238213

I -0.201100 -1.310950 -2.151140

Br -0.377006 -0.396625 -5.019378

H -0.183526 1.661283 -3.335582

H -0.023394 3.902816 -2.268951

H 0.166617 4.081571 0.212151

F 0.212601 2.118042 1.819468

SCF: -3433.122449

ZPE: 0.153356

H: -3432.955225

G: -3433.008308

4_F_trans_adduct_conf1

H -0.202072 1.665665 -3.323159

C -0.133578 1.765220 -2.248726

C 0.045807 1.974900 0.539791

C -0.088984 0.659095 -1.432367

C -0.086379 3.011759 -1.636956

C 0.002824 3.109334 -0.254574

C 0.000059 0.702090 -0.037996

H -0.118968 3.903093 -2.249515

H 0.039738 4.083672 0.214827

H 0.115667 2.077321 1.611464

C 0.038067 -0.578942 0.672807

C 0.097727 -3.164104 1.789211

C -0.015076 -1.738056 -0.100319

C 0.122587 -0.787474 2.048309

C 0.153088 -2.045693 2.610420

C 0.011786 -3.019876 0.410803

I -0.143939 -1.313674 -2.158152

Br -0.325523 -0.396016 -5.009385

H -0.031571 -3.888325 -0.233477

H 0.121401 -4.153013 2.227299

H 0.220069 -2.135312 3.686605

F 0.177270 0.268532 2.873092

SCF: -3433.123139

ZPE: 0.153285

H: -3432.955972

G: -3433.009122

4_NMe2_cis_adduct_conf1

C 0.072453 0.933569 -2.994007
 C 0.198715 1.285418 -0.184082
 C -0.066313 -0.105810 -2.105105
 C 0.338335 2.178755 -2.443667
 C 0.387648 2.349690 -1.069920
 C 0.034547 -0.022757 -0.713728
 C 0.028945 -1.292547 0.036095
 C 0.027627 -3.874799 1.174118
 C -0.203560 -2.451132 -0.708209
 C 0.301258 -1.480709 1.398155
 C 0.302082 -2.753028 1.947830
 C -0.221963 -3.728252 -0.182719
 H 0.529086 -0.631982 2.023265
 H 0.519792 -2.868520 3.001819
 H -0.413181 -4.592464 -0.806595
 H 0.020522 -4.861244 1.618995
 I -0.435154 -2.071125 -2.755819
 Br -0.698942 -1.231300 -5.679311
 H -0.014163 0.782790 -4.060452
 H 0.475861 3.030685 -3.096988
 H 0.548502 3.342568 -0.675362
 N 0.179103 1.489387 1.200912
 C -1.112429 1.232266 1.836546
 C 0.767104 2.722145 1.696067
 H -1.790676 2.081900 1.687081
 H -0.966858 1.084745 2.907581
 H -1.582326 0.342726 1.424003
 H 0.149333 3.603600 1.480198
 H 0.867850 2.637815 2.778267
 H 1.756802 2.867709 1.265031
 SCF: -3467.827009
 ZPE: 0.235035
 H: -3467.574983
 G: -3467.634511

4_NMe2_cis_adduct_conf2

C 0.812251 1.879583 -1.937553
 C 0.777642 2.146893 0.884367
 C 0.854516 0.801577 -1.085668
 C 0.808522 3.131882 -1.340954
 C 0.779267 3.259167 0.038098
 C 0.893728 0.852364 0.310345

C 1.117746 -0.419714 1.021684
 C 1.597218 -2.990821 2.081540
 C 1.142638 -1.573555 0.235413
 C 1.381284 -0.599697 2.386492
 C 1.619783 -1.865731 2.897679
 C 1.363073 -2.847213 0.721689
 H 1.416258 0.253877 3.044542
 H 1.825237 -1.974022 3.954893
 H 1.365412 -3.708267 0.065193
 H 1.773523 -3.974668 2.496332
 I 0.900083 -1.173667 -1.806956
 Br 0.554408 -0.297471 -4.712136
 H 0.790870 1.753835 -3.010487
 H 0.795041 4.017496 -1.963139
 H 0.727803 4.249220 0.467627
 N 0.674288 2.291573 2.272898
 C -0.558403 1.759050 2.851885
 C 0.989271 3.596711 2.827810
 H -1.386635 2.464370 2.707701
 H -0.417538 1.598701 3.921746
 H -0.831020 0.812410 2.391536
 H 0.215377 4.345848 2.615632
 H 1.070601 3.493147 3.910005
 H 1.943156 3.951622 2.439786
 SCF: -3467.827044
 ZPE: 0.235208
 H: -3467.574903
 G: -3467.634186

4_NMe2_cis_adduct_conf3

C 0.767358 1.879757 -1.834613
 C 0.691264 1.924113 0.998881
 C 1.024462 0.770738 -1.064117
 C 0.405410 3.030581 -1.149855
 C 0.380668 3.052445 0.234962
 C 0.955971 0.698904 0.329782
 C 1.094986 -0.635984 0.940291
 C 1.355690 -3.311509 1.797681
 C 1.410936 -1.684315 0.073477
 C 0.874900 -0.989033 2.278770
 C 1.001414 -2.306444 2.690248
 C 1.556662 -3.001997 0.460309
 H 0.587459 -0.234411 2.993616
 H 0.821206 -2.550728 3.729205

H 1.807633 -3.774947 -0.254992
H 1.462188 -4.334132 2.135234
I 1.552341 -1.073512 -1.926398
Br 1.653830 0.090505 -4.746790
H 0.837334 1.849664 -2.912464
H 0.172264 3.929470 -1.706003
H 0.141595 3.979172 0.736214
N 0.734376 1.983842 2.396738
C 2.060732 1.775548 2.976174
C 0.057585 3.101270 3.032467
H 1.958701 1.501404 4.027129
H 2.658371 2.693379 2.908240
H 2.593979 0.980846 2.460065
H 0.001019 2.897656 4.101944
H 0.588341 4.052382 2.895172
H -0.954871 3.200137 2.643128
SCF: -3467.827047
ZPE: 0.235239
H: -3467.574852
G: -3467.634291

4_NMe2_trans_adduct_conf1
H 0.061480 1.205145 -4.415291
C -0.047356 1.385928 -3.354578
C -0.351448 1.780724 -0.603753
C 0.002209 0.349264 -2.451371
C -0.254580 2.663123 -2.850848
C -0.420113 2.847826 -1.484795
C -0.119634 0.476834 -1.062745
H -0.298272 3.503275 -3.531338
H -0.604401 3.840294 -1.094164
H -0.495738 1.950469 0.451548
C -0.070834 -0.753008 -0.251897
C -0.283952 -3.283257 0.952295
C -0.033812 -1.946943 -0.970319
C -0.124161 -0.860088 1.162949
C -0.270496 -2.131274 1.725379
C -0.130620 -3.210091 -0.423277
I 0.182405 -1.655547 -3.039817
Br 0.537371 -0.907244 -5.970157
H -0.102385 -4.102363 -1.034723
H -0.385755 -4.248175 1.432394
H -0.346780 -2.227066 2.798860
N -0.037279 0.284244 1.965951

C -0.512926 0.169999 3.333852
C 1.256138 0.964689 1.915655
H -1.506703 -0.275739 3.351078
H -0.574019 1.173491 3.755555
H 0.157015 -0.424945 3.968345
H 1.643921 0.995225 0.900144
H 1.142822 1.987940 2.276475
H 1.988003 0.447171 2.548892
SCF: -3467.827482
ZPE: 0.235096
H: -3467.575420
G: -3467.634901

4_NMe2_trans_adduct_conf2
H 0.707451 2.173164 -3.548985
C 0.818299 2.381455 -2.493598
C 1.129913 2.848354 0.244970
C 0.790803 1.366443 -1.565188
C 1.006520 3.673877 -2.022304
C 1.176015 3.894626 -0.662131
C 0.917578 1.529966 -0.180719
H 1.032753 4.497849 -2.723196
H 1.345599 4.899260 -0.296766
H 1.276858 3.046341 1.294925
C 0.893626 0.319834 0.660318
C 1.155011 -2.176497 1.924529
C 0.872383 -0.891810 -0.028459
C 0.956701 0.248298 2.077095
C 1.127507 -1.006290 2.669232
C 0.992515 -2.139528 0.548585
I 0.642306 -0.655174 -2.103322
Br 0.265229 0.010209 -5.051478
H 0.974772 -3.046719 -0.040847
H 1.275175 -3.127621 2.427403
H 1.212170 -1.074659 3.744107
N 0.855669 1.409967 2.852994
C -0.448454 2.069125 2.793534
C 1.339363 1.335623 4.220887
H -0.842451 2.068555 1.779971
H -0.348843 3.102567 3.128476
H -1.168608 1.556242 3.443736
H 2.340172 0.906170 4.243827
H 1.386351 2.349630 4.618499
H 0.681715 0.745343 4.872410

SCF: -3467.827481

ZPE: 0.235116

H: -3467.575398

G: -3467.634891

4_OMe_cis_adduct_conf1

C -0.329623 1.539925 -2.557259

C 0.354582 1.575085 0.159296

C -0.195047 0.391047 -1.815355

C -0.111747 2.744349 -1.898857

C 0.228218 2.757948 -0.556247

C 0.136996 0.332315 -0.457834

C 0.222637 -0.991001 0.176525

C 0.292758 -3.645102 1.102222

C -0.042189 -2.083595 -0.649988

C 0.534076 -1.272389 1.512240

C 0.565741 -2.584291 1.958719

C -0.016674 -3.398208 -0.227969

H 0.757545 -0.469979 2.196922

H 0.808626 -2.781308 2.994880

H -0.230429 -4.214231 -0.906662

H 0.320813 -4.663876 1.466044

I -0.483877 -1.526804 -2.626503

Br -1.067529 -0.418860 -5.390722

H -0.590878 1.504823 -3.605426

H -0.203717 3.673391 -2.445818

H 0.410398 3.691875 -0.039274

O 0.729331 1.627660 1.467757

C -0.329646 1.986671 2.359609

H 0.091658 1.978258 3.362435

H -1.145483 1.262139 2.294343

H -0.706640 2.984461 2.126719

SCF: -3448.393884

ZPE: 0.193859

H: -3448.184177

G: -3448.242243

4_OMe_cis_adduct_conf2

C -0.751891 1.643277 -2.403191

C -0.003234 1.606579 0.295812

C -0.660139 0.479125 -1.678727

C -0.454016 2.825764 -1.736594

C -0.084162 2.803605 -0.401912

C -0.291839 0.384135 -0.332778

C -0.246377 -0.951852 0.278704

C -0.247372 -3.622974 1.156566

C -0.575714 -2.018801 -0.558000

C 0.087782 -1.268006 1.601092

C 0.084705 -2.588109 2.023809

C -0.586152 -3.340904 -0.159392

H 0.340586 -0.485315 2.298290

H 0.345197 -2.812072 3.050163

H -0.849761 -4.135904 -0.845395

H -0.245004 -4.648601 1.501656

I -1.066766 -1.409606 -2.507300

Br -1.717862 -0.223706 -5.223645

H -1.045315 1.635490 -3.443397

H -0.517422 3.766084 -2.268076

H 0.143412 3.720667 0.127158

O 0.331458 1.633408 1.616391

C 1.739236 1.733641 1.848392

H 1.879618 1.716237 2.926934

H 2.128241 2.668714 1.440238

H 2.262889 0.889023 1.393003

SCF: -3448.393902

ZPE: 0.193858

H: -3448.184194

G: -3448.242315

4_OMe_trans_adduct_conf1

H -0.331643 1.679846 -3.987178

C -0.225207 1.775562 -2.915364

C 0.049646 1.963075 -0.136360

C -0.183146 0.665946 -2.103985

C -0.125759 3.018619 -2.303342

C 0.009926 3.102634 -0.924680

C -0.046841 0.688903 -0.710666

H -0.155059 3.913596 -2.910718

H 0.086946 4.072166 -0.449785

H 0.155847 2.057374 0.931321

C -0.020843 -0.602558 -0.010415

C -0.006965 -3.207367 1.040171

C -0.135848 -1.742016 -0.801052

C 0.108646 -0.814032 1.380578

C 0.112657 -2.112122 1.885547

C -0.133886 -3.039803 -0.329365

I -0.320266 -1.293245 -2.845394

Br -0.581039 -0.344265 -5.713726

H -0.226621 -3.890094 -0.991661
H -0.000304 -4.204556 1.461113
H 0.209298 -2.277864 2.948224
O 0.224022 0.274882 2.159720
C 0.365422 0.096346 3.564216
H 1.266901 -0.474107 3.795191
H -0.509419 -0.404233 3.982754
H 0.448535 1.096314 3.981256
SCF: -3448.399535
ZPE: 0.194599
H: -3448.189362
G: -3448.246295

4_OMe_trans_adduct_conf2

H -0.376633 1.399638 -3.904670
C -0.132938 1.529789 -2.859234
C 0.498315 1.810308 -0.145728
C -0.113262 0.459523 -1.995002
C 0.174123 2.778764 -2.334884
C 0.489196 2.909966 -0.988887
C 0.188652 0.534286 -0.631409
H 0.168160 3.643134 -2.985812
H 0.733713 3.884271 -0.586088
H 0.756706 1.935880 0.893745
C 0.158637 -0.715906 0.139993
C 0.045092 -3.257421 1.346002
C -0.150446 -1.878195 -0.566849
C 0.411119 -0.874657 1.512123
C 0.352998 -2.131899 2.096670
C -0.215983 -3.140046 -0.012674
I -0.527271 -1.508017 -2.602564
Br -1.018951 -0.664374 -5.467139
H -0.457766 -4.011080 -0.608095
H 0.008720 -4.229986 1.819102
H 0.559912 -2.212132 3.156568
O 0.744906 0.196645 2.287694
C -0.370008 0.770203 2.975608
H -0.802117 0.047100 3.670595
H -1.134394 1.095870 2.265055
H 0.009718 1.628336 3.525880
SCF: -3448.394269
ZPE: 0.193943
H: -3448.184537
G: -3448.242157

5_CF3_adduct_conf1

H 0.477608 1.458454 -3.676281
C 0.344294 1.628747 -2.616759
C -0.202824 2.007508 0.089332
C 0.123136 0.581471 -1.754755
C 0.362361 2.907686 -2.082809
C 0.026617 3.088118 -0.753297
C -0.033548 0.685275 -0.363929
H 0.557426 3.758503 -2.720924
H -0.096257 4.091751 -0.365685
C -0.081253 -0.599295 0.383337
C -0.522669 -3.180659 1.459952
C -0.440882 -1.704572 -0.392727
C 0.259841 -0.902024 1.715421
C 0.003805 -2.162949 2.239192
C -0.681407 -2.970894 0.100257
I -0.265148 -1.357715 -2.459710
Br 0.252677 -0.605212 -5.282516
H -0.966718 -3.783746 -0.555924
H -0.727875 -4.149993 1.893340
H 0.261846 -2.362911 3.271837
C 1.102152 -0.030763 2.617374
F 2.203516 -0.704810 2.989719
F 1.534397 1.085773 2.028873
F 0.487325 0.319321 3.752630
C -0.840608 2.395196 1.404054
F -1.256706 1.355633 2.127758
F -0.050872 3.143628 2.181598
F -1.932433 3.140779 1.163745
SCF: -4008.021165
ZPE: 0.170634
H: -4007.830488
G: -4007.897886

5_CF3_adduct_conf2

H 1.428459 2.236119 -2.902238
C 1.304552 2.397447 -1.840179
C 0.781754 2.751814 0.873892
C 1.103254 1.341958 -0.983346
C 1.315394 3.672753 -1.297409
C 0.991791 3.840555 0.036777
C 0.959687 1.434558 0.409672
H 1.495292 4.529899 -1.931489

H 0.863321 4.840167 0.432862
C 0.933092 0.144627 1.148565
C 0.530520 -2.448642 2.211700
C 0.577106 -0.959074 0.368613
C 1.291160 -0.163462 2.474971
C 1.053907 -1.430601 2.992592
C 0.355602 -2.231335 0.855190
I 0.728782 -0.596582 -1.697597
Br 1.211593 0.179898 -4.520089
H 0.072402 -3.042707 0.196298
H 0.340473 -3.423182 2.640297
H 1.324629 -1.634648 4.021192
C 2.133577 0.710643 3.374148
F 3.243357 0.044025 3.734693
F 2.551851 1.833134 2.786764
F 1.525488 1.051064 4.515926
C 0.153962 3.123776 2.197836
F -0.245570 2.075018 2.917562
F 0.944953 3.873198 2.973137
F -0.946788 3.861480 1.974458
SCF: -4008.021159
ZPE: 0.170646
H: -4007.830476
G: -4007.897912

5_CN_adduct_conf1

H 0.052500 1.585451 -3.464224
C 0.011729 1.704760 -2.390142
C -0.241665 1.958465 0.373886
C -0.021438 0.610072 -1.557588
C -0.030236 2.964573 -1.808798
C -0.203618 3.088231 -0.442000
C -0.055198 0.669055 -0.161701
H 0.008678 3.845458 -2.434639
H -0.345348 4.061778 0.007519
C 0.017990 -0.604077 0.565941
C -0.060630 -3.191214 1.682136
C -0.220325 -1.744751 -0.196073
C 0.379994 -0.824676 1.909794
C 0.310815 -2.104800 2.457951
C -0.277382 -3.023685 0.322561
I -0.229250 -1.354738 -2.268207
Br -0.045436 -0.487434 -5.080100
H -0.471972 -3.879412 -0.312121

H -0.117088 -4.176764 2.123677
H 0.589226 -2.243285 3.494013
C 1.021039 0.173584 2.715481
N 1.614844 0.910744 3.364219
C -0.675385 2.169148 1.724069
N -1.107545 2.382519 2.765344
SCF: -3518.355239
ZPE: 0.158679
H: -3518.180032
G: -3518.238963

5_F_adduct_conf1

H 0.949354 0.065147 3.762239
C 1.265157 0.038213 2.729270
C 2.012467 -0.082361 0.066604
C 0.347282 0.019439 1.707684
C 2.609492 0.013040 2.382684
C 2.979344 -0.058297 1.052351
C 0.641696 -0.011323 0.334828
H 3.364052 0.031783 3.157460
H 4.017500 -0.108726 0.751903
C -0.495908 -0.000449 -0.604980
C -2.909089 -0.031716 -2.096068
C -1.766361 -0.063976 -0.021286
C -0.514921 0.097877 -2.000298
C -1.684395 0.070087 -2.734692
C -2.960249 -0.084983 -0.710788
H -3.822010 -0.051301 -2.675991
I -1.716013 -0.036869 2.077573
H -3.909736 -0.134502 -0.193674
H -1.611402 0.142725 -3.811788
F 0.613669 0.252791 -2.697072
F 2.450182 -0.205235 -1.187817
Br -1.353014 0.065938 5.047060
SCF: -3532.365422
ZPE: 0.144882
H: -3532.205758
G: -3532.261390

5_NMe2_adduct_conf1

H -1.467459 0.674044 -4.397721
C -1.170125 0.864671 -3.376856
C -0.135360 1.370886 -0.778642
C -0.608442 -0.107763 -2.591196

C -1.319491 2.114133 -2.777255
C -0.793786 2.367121 -1.526292
C -0.198014 0.027031 -1.258750
H -1.789380 2.916204 -3.332007
H -0.831877 3.375597 -1.139865
C 0.157122 -1.206538 -0.537985
C 1.237767 -3.600353 0.462674
C 0.455906 -2.311280 -1.340907
C 0.193280 -1.429437 0.871507
C 0.826612 -2.603211 1.326839
C 0.992293 -3.500699 -0.904240
I -0.154338 -2.025834 -3.330795
Br -1.251550 -1.380302 -6.132907
H 1.211617 -4.317252 -1.578970
H 1.693633 -4.497067 0.863050
H 0.937876 -2.761852 2.389911
N -0.370345 -0.549587 1.759209
C -1.690671 0.001384 1.510532
C -0.040242 -0.632835 3.165501
H -2.005248 -0.179827 0.486961
H -1.705680 1.076880 1.698947
H -2.417973 -0.477968 2.175567
H 1.034576 -0.749025 3.302623
H -0.346481 0.299132 3.642230
H -0.554634 -1.460900 3.670041
N 0.541704 1.689180 0.368317
C 1.864263 1.145904 0.621777
H 2.103062 0.351937 -0.079952
H 1.937779 0.752661 1.637989
H 2.611546 1.937889 0.500380
C 0.306935 2.960876 1.017460
H 0.682864 2.895828 2.039338
H -0.759310 3.180505 1.058919
H 0.821571 3.789566 0.514569
SCF: -3601.776031
ZPE: 0.308104
H: -3601.446755
G: -3601.514701

5_OMe_adduct_conf1

H 0.072024 1.087345 -4.284000
C 0.041372 1.221701 -3.212606
C -0.234398 1.523889 -0.427492
C -0.071687 0.153554 -2.355409

C 0.098925 2.478511 -2.624023
C -0.062878 2.633084 -1.256600
C -0.107086 0.219719 -0.960157
H 0.216130 3.353363 -3.250256
H -0.100398 3.628153 -0.837329
C -0.120804 -1.048451 -0.217167
C -0.370057 -3.602878 0.924642
C -0.421535 -2.189357 -0.959373
C 0.245744 -1.267920 1.131579
C 0.052370 -2.529967 1.696415
C -0.562585 -3.460541 -0.442107
I -0.402235 -1.811379 -3.028386
Br -0.163785 -1.001571 -5.942520
H -0.801967 -4.310361 -1.067487
H -0.498141 -4.572575 1.388325
H 0.275357 -2.689452 2.741268
O 0.845899 -0.264547 1.782857
C 1.083681 -0.395019 3.176129
H 1.807017 -1.187216 3.380671
H 0.154444 -0.596245 3.713376
H 1.491561 0.560078 3.497226
O -0.602056 1.623591 0.854577
C -0.485154 2.879322 1.506597
H 0.527357 3.275842 1.406480
H -0.702533 2.690419 2.554923
H -1.204683 3.598707 1.109944
SCF: -3562.912012
ZPE: 0.227086
H: -3562.666670
G: -3562.729731

5_OMe_adduct_conf2

H -0.456892 0.974058 -4.029769
C -0.399603 1.116631 -2.960464
C -0.400680 1.428416 -0.168347
C -0.377922 0.050360 -2.093221
C -0.359782 2.380568 -2.388838
C -0.382417 2.537610 -1.013242
C -0.293447 0.121599 -0.699302
H -0.356522 3.254090 -3.027713
H -0.419849 3.532003 -0.593000
C -0.199350 -1.146197 0.053423
C -0.339523 -3.750913 1.162847
C -0.492324 -2.297108 -0.690971

C 0.185654 -1.389016 1.393500
C 0.063723 -2.670980 1.926947
C -0.579523 -3.578340 -0.193812
I -0.630355 -1.924791 -2.753534
Br -0.658969 -1.117284 -5.675562
H -0.817800 -4.420202 -0.830933
H -0.415796 -4.734295 1.607961
H 0.334446 -2.800450 2.966922
O 0.691125 -0.457577 2.237597
C 1.891896 0.180543 1.817656
H 1.799128 0.635430 0.831094
H 2.710546 -0.543934 1.802040
H 2.103352 0.954902 2.551765
O -0.564862 1.527539 1.155086
C -0.432871 2.800117 1.771786
H 0.522801 3.260736 1.511957
H -0.471928 2.614131 2.842164
H -1.252355 3.462548 1.485962
SCF: -3562.909627
ZPE: 0.226908
H: -3562.664488
G: -3562.727104

5_OMe_adduct_conf3

H 0.020129 2.142575 -2.858717
C 0.283822 2.263418 -1.817592
C 1.093662 2.512494 0.853170
C 0.573240 1.179537 -1.026040
C 0.359535 3.516519 -1.223822
C 0.784265 3.631126 0.086260
C 0.916914 1.209782 0.335246
H 0.127986 4.400052 -1.803824
H 0.912632 4.601815 0.547480
C 1.094399 -0.093485 1.013910
C 1.585218 -2.735676 1.917986
C 1.145321 -1.208393 0.168568
C 1.178785 -0.391155 2.392780
C 1.454658 -1.688653 2.813612
C 1.388981 -2.505906 0.563780
I 0.654462 -0.761772 -1.821148
Br -0.199533 0.139292 -4.583750
H 1.419436 -3.318913 -0.150159
H 1.794775 -3.735425 2.275162
H 1.537798 -1.857462 3.879511

O 1.008599 0.530426 3.373247
C -0.312752 1.055728 3.478791
H -0.995997 0.270272 3.812295
H -0.664227 1.463281 2.529957
H -0.273205 1.850876 4.218950
O 1.556907 2.751970 2.104731
C 2.927278 2.414909 2.311330
H 3.131949 1.374723 2.053562
H 3.128910 2.570382 3.368157
H 3.563053 3.070362 1.710467
SCF: -3562.906460
ZPE: 0.226550
H: -3562.661674
G: -3562.723998

6_CF3_adduct_conf2

H 0.834597 2.401171 -2.895464
C 0.867307 2.483981 -1.818078
C 0.950869 2.658774 0.982506
C 0.921410 1.367092 -1.012504
C 0.856204 3.719381 -1.192800
C 0.897747 3.792998 0.196265
C 0.965481 1.399727 0.379684
H 0.815150 4.621848 -1.789637
H 0.981213 2.745407 2.059813
C 1.023709 0.123319 1.096824
C 1.130625 -2.438336 2.215780
C 1.028528 -1.025964 0.315848
C 1.074353 -0.027364 2.483603
C 1.126065 -1.299679 3.019873
C 1.080938 -2.305464 0.839345
H 1.073426 0.836225 3.134474
I 0.946506 -0.601351 -1.747325
Br 0.823092 0.341783 -4.567993
H 1.083129 -3.181602 0.203894
H 1.171772 -3.423341 2.664017
C 1.186335 -1.492804 4.509197
F 0.189326 -2.275545 4.947898
F 2.327900 -2.089528 4.885484
F 1.106592 -0.343597 5.183706
C 0.883913 5.157414 0.828020
F -0.213853 5.848176 0.486897
F 1.932834 5.894128 0.433262
F 0.918333 5.110850 2.161412

SCF: -4008.054033

ZPE: 0.171094

H: -4007.862589

G: -4007.932820

6_CF3_adduct_conf3

H 0.918930 2.391416 -2.914120

C 0.918703 2.477578 -1.836515

C 0.916014 2.662146 0.961216

C 0.973799 1.367104 -1.028053

C 0.861066 3.719223 -1.217397

C 0.860294 3.796763 0.167608

C 0.976265 1.404317 0.367989

H 0.816811 4.614195 -1.822132

H 0.911148 2.757449 2.040213

C 1.040129 0.130204 1.089164

C 1.166797 -2.426344 2.216888

C 1.088112 -1.020088 0.311370

C 1.057822 -0.016438 2.477097

C 1.120801 -1.286421 3.017859

C 1.150511 -2.297276 0.839264

H 1.024546 0.848924 3.124822

I 1.059897 -0.602754 -1.755417

Br 1.006468 0.329772 -4.581969

H 1.185654 -3.174509 0.206267

H 1.215256 -3.409549 2.668343

C 1.149644 -1.475586 4.508667

F 0.152808 -2.269377 4.927269

F 2.289614 -2.057413 4.911911

F 1.041004 -0.325801 5.178454

C 0.789828 5.131538 0.856754

F -0.315705 5.242823 1.608137

F 0.782507 6.153237 -0.002034

F 1.829578 5.319368 1.682344

SCF: -4008.053923

ZPE: 0.171180

H: -4007.862446

G: -4007.932175

6_CN_adduct_conf1

H -0.206654 1.792983 -3.553539

C -0.133531 1.880016 -2.478535

C 0.056448 2.060640 0.318422

C -0.098732 0.767166 -1.668268

C -0.070250 3.120640 -1.866378

C 0.025179 3.199144 -0.476938

C -0.007256 0.803762 -0.276376

H -0.093414 4.022038 -2.463168

H 0.131463 2.161451 1.392560

C 0.018248 -0.471665 0.445555

C 0.055708 -3.040469 1.566964

C -0.043516 -1.624010 -0.331948

C 0.097632 -0.618260 1.827400

C 0.115270 -1.898024 2.369415

C -0.026206 -2.903204 0.192343

H 0.144607 0.240592 2.483303

I -0.168773 -1.203527 -2.395626

Br -0.335560 -0.271050 -5.203258

H -0.074352 -3.779760 -0.440763

H 0.071957 -4.022059 2.020682

C 0.196150 -2.048971 3.795525

N 0.260803 -2.171936 4.934333

C 0.093187 4.489874 0.150026

N 0.147490 5.521430 0.648669

SCF: -3518.373549

ZPE: 0.159102

H: -3518.197805

G: -3518.257494

6_F_adduct_conf1

H -0.258103 1.682683 -3.329885

C -0.146748 1.769220 -2.257933

C 0.141305 1.949551 0.530486

C -0.115035 0.653232 -1.450074

C -0.031229 3.010519 -1.651582

C 0.109766 3.065870 -0.276114

C 0.025373 0.693759 -0.062426

H -0.049268 3.922171 -2.233274

H 0.255279 2.066483 1.599934

C 0.041274 -0.578861 0.663245

C 0.046797 -3.136310 1.807663

C -0.082319 -1.732321 -0.105235

C 0.169147 -0.715370 2.045005

C 0.167992 -1.987624 2.572886

C -0.082274 -3.005946 0.433938

H 0.267120 0.137026 2.704274

I -0.269794 -1.314982 -2.160042

Br -0.521129 -0.376706 -5.001336

H -0.179519 -3.887017 -0.187345
H 0.053608 -4.106710 2.285576
F 0.290774 -2.122284 3.902802
F 0.221685 4.269522 0.303938
SCF: -3532.377804
ZPE: 0.145098
H: -3532.217988
G: -3532.273118

6_NMe2_adduct_conf1

H -0.693641 1.099868 -4.461024
C -0.448976 1.159913 -3.408887
C 0.177647 1.287565 -0.687658
C -0.495476 0.040443 -2.604794
C -0.083744 2.364930 -2.840892
C 0.243470 2.460031 -1.466995
C -0.192543 0.069869 -1.243832
H -0.050650 3.239130 -3.473796
H 0.415734 1.324734 0.364656
C -0.292203 -1.194044 -0.498478
C -0.562596 -3.697992 0.703769
C -0.675281 -2.313471 -1.231149
C -0.041500 -1.337536 0.860614
C -0.161206 -2.591517 1.490742
C -0.815442 -3.559494 -0.647256
H 0.245470 -0.469970 1.435280
I -1.023907 -1.878633 -3.251136
Br -1.455718 -0.886453 -6.144852
H -1.121014 -4.423113 -1.225109
H -0.679840 -4.673415 1.151714
N 0.101767 -2.737094 2.821093
C -0.175318 -4.000306 3.476493
C 0.371281 -1.565909 3.630728
H -1.234759 -4.271061 3.411422
H 0.096332 -3.918478 4.525073
H 0.412097 -4.809672 3.037196
H -0.473024 -0.867422 3.633152
H 0.562518 -1.880703 4.652617
H 1.253828 -1.032813 3.269706
N 0.609995 3.648464 -0.916453
C 0.900557 3.731614 0.500469
H 1.724828 3.067941 0.775303
H 0.029900 3.465266 1.108626
H 1.190638 4.750068 0.741545

C 0.587252 4.856336 -1.717722
H 0.885008 5.695885 -1.096348
H -0.412769 5.057433 -2.114284
H 1.281386 4.789710 -2.559733
SCF: -3601.799114
ZPE: 0.308306
H: -3601.468764
G: -3601.540974

6_NMe2_adduct_conf2

H 0.022641 2.172331 -3.394433
C 0.383366 2.211173 -2.375328
C 1.305676 2.283654 0.262284
C 0.375483 1.086420 -1.577417
C 0.862091 3.393070 -1.844160
C 1.340534 3.459679 -0.513660
C 0.824868 1.088733 -0.257364
H 0.863776 4.271929 -2.471449
H 1.658461 2.299411 1.282385
C 0.754104 -0.177866 0.486509
C 0.535382 -2.686955 1.688384
C 0.246943 -1.272841 -0.206786
C 1.153390 -0.347252 1.806391
C 1.047940 -1.601319 2.439613
C 0.135693 -2.522273 0.376384
H 1.546611 0.499778 2.347902
I -0.298376 -0.802863 -2.174989
Br -0.983354 0.235319 -5.005605
H -0.254093 -3.370101 -0.173491
H 0.448923 -3.666610 2.134239
N 1.427327 -1.766553 3.737566
C 2.041355 -0.667601 4.454858
C 1.398124 -3.085272 4.338294
H 2.966667 -0.334940 3.972493
H 2.276459 -0.992844 5.464145
H 1.365199 0.188770 4.522221
H 2.058710 -3.785378 3.816230
H 1.725889 -3.008311 5.370975
H 0.387284 -3.500375 4.332514
N 1.819462 4.624415 -0.000073
C 2.246171 4.684809 1.383284
H 3.065426 3.986958 1.576623
H 1.426537 4.448095 2.069547
H 2.597413 5.689432 1.599663

C 1.782666 5.836799 -0.793936
H 2.204448 6.650593 -0.211341
H 0.759296 6.105486 -1.074191
H 2.370806 5.730794 -1.709281
SCF: -3601.799080
ZPE: 0.307959
H: -3601.468941
G: -3601.542009

6_NMe2_adduct_conf3

H 0.755260 1.933238 -3.622891
C 0.908813 2.034961 -2.556782
C 1.293544 2.272662 0.201705
C 0.752459 0.956706 -1.711436
C 1.264142 3.253664 -2.012006
C 1.469665 3.404187 -0.619667
C 0.935088 1.041118 -0.331503
H 1.382348 4.095585 -2.677548
H 1.437467 2.351955 1.268769
C 0.729463 -0.183337 0.456778
C 0.282472 -2.623413 1.736806
C 0.366820 -1.322011 -0.256745
C 0.869449 -0.273993 1.835978
C 0.650205 -1.493323 2.507413
C 0.142313 -2.536863 0.365447
H 1.149724 0.606287 2.394422
I 0.209609 -0.972130 -2.316537
Br 0.075012 -0.104179 -5.279239
H -0.139699 -3.416616 -0.199507
H 0.105009 -3.575743 2.213948
N 0.787626 -1.583927 3.858607
C 0.559757 -2.847848 4.529717
C 1.161134 -0.414873 4.627757
H -0.463951 -3.203516 4.379811
H 0.722451 -2.714862 5.595349
H 1.245300 -3.621477 4.171431
H 0.426106 0.388440 4.518533
H 1.217223 -0.686248 5.677913
H 2.137092 -0.027463 4.319831
N 1.825959 4.606430 -0.091617
C 1.950844 4.758717 1.343955
H 2.718437 4.093212 1.747790
H 1.007773 4.544118 1.857497
H 2.238701 5.782270 1.565777

C 1.911937 5.774693 -0.945487
H 2.200572 6.630211 -0.342045
H 0.953531 5.996757 -1.425650
H 2.662845 5.640015 -1.728076
SCF: -3601.799114
ZPE: 0.307928
H: -3601.468956
G: -3601.544026

6_NMe2_adduct_conf4

H 0.703995 1.961770 -3.612932
C 0.861527 2.046973 -2.546020
C 1.261247 2.238122 0.214203
C 0.787608 0.939154 -1.728113
C 1.140130 3.272338 -1.972661
C 1.351053 3.400066 -0.578726
C 0.978419 0.999832 -0.347963
H 1.194088 4.137544 -2.616325
H 1.415598 2.299297 1.280976
C 0.864227 -0.256103 0.408837
C 0.590912 -2.752505 1.627106
C 0.578129 -1.398596 -0.332644
C 1.015348 -0.371982 1.785097
C 0.890362 -1.621179 2.424707
C 0.437951 -2.641045 0.258842
H 1.229633 0.512358 2.366013
I 0.385185 -1.007708 -2.381927
Br 0.181177 -0.075952 -5.322724
H 0.209825 -3.522748 -0.327288
H 0.476846 -3.725957 2.080203
N 1.053126 -1.738839 3.772069
C 0.818898 -3.012925 4.422288
C 1.278318 -0.555590 4.576786
H -0.207456 -3.363097 4.271626
H 0.990305 -2.899815 5.488917
H 1.500241 -3.781223 4.047725
H 0.440521 0.146854 4.510745
H 1.397991 -0.852346 5.614722
H 2.186433 -0.032858 4.265367
N 1.631920 4.608724 -0.022936
C 1.821906 4.723447 1.408649
H 2.660739 4.110210 1.750695
H 0.927199 4.415148 1.958469
H 2.034610 5.759894 1.653753

C 1.696376 5.793128 -0.855819
H 1.932597 6.649630 -0.231348
H 0.743004 5.984344 -1.357431
H 2.472208 5.701433 -1.621142
SCF: -3601.799091
ZPE: 0.308012
H: -3601.468911
G: -3601.541906

6_OMe_adduct_conf1
H -0.370531 1.404901 -3.889047
C -0.256041 1.481162 -2.816324
C 0.039194 1.645830 -0.043169
C -0.207571 0.358277 -2.025843
C -0.154191 2.723774 -2.203644
C -0.007151 2.804695 -0.817551
C -0.060118 0.396273 -0.636194
H -0.190838 3.612114 -2.816841
H 0.154932 1.745940 1.028193
C -0.021009 -0.883317 0.081831
C 0.027825 -3.441860 1.217955
C -0.136218 -2.034523 -0.697001
C 0.121030 -1.030725 1.453937
C 0.146250 -2.304384 2.020945
C -0.114898 -3.302634 -0.156648
H 0.214913 -0.173196 2.107660
I -0.342047 -1.607509 -2.744539
Br -0.631770 -0.640480 -5.616397
H -0.205947 -4.185113 -0.777320
H 0.045010 -4.432828 1.647444
O 0.289461 -2.344928 3.360396
C 0.329421 -3.617812 3.989967
H 1.175021 -4.206828 3.628169
H -0.599733 -4.166497 3.822575
H 0.450088 -3.422466 5.052295
O 0.097894 3.963347 -0.140470
C 0.066131 5.176164 -0.880803
H 0.896900 5.223756 -1.587967
H 0.163966 5.974766 -0.150220
H -0.879973 5.283103 -1.415288
SCF: -3562.930016
ZPE: 0.227457
H: -3562.684325
G: -3562.747333

6_OMe_adduct_conf2
H -0.402731 1.013311 -3.933980
C -0.281496 1.102077 -2.862957
C 0.029513 1.297027 -0.093666
C -0.225943 -0.011960 -2.060604
C -0.178021 2.351428 -2.264755
C -0.022763 2.447209 -0.880545
C -0.070684 0.040237 -0.671879
H -0.219767 3.233042 -2.887250
H 0.150606 1.411730 0.975501
C -0.025701 -1.232428 0.058050
C 0.031353 -3.768584 1.216437
C -0.141201 -2.385558 -0.704950
C 0.122756 -1.355642 1.442079
C 0.149018 -2.621686 2.014585
C -0.114652 -3.655961 -0.150340
H 0.215825 -0.471256 2.054967
I -0.359522 -1.984572 -2.755376
Br -0.668930 -1.050944 -5.635328
H -0.205496 -4.544407 -0.762314
H 0.056199 -4.740145 1.692611
O 0.284719 -2.845056 3.336108
C 0.392124 -1.720215 4.196611
H -0.499067 -1.091907 4.131291
H 1.278366 -1.128477 3.957750
H 0.482626 -2.120151 5.203080
O 0.085030 3.613325 -0.216715
C 0.050651 4.817781 -0.970512
H 0.877808 4.856454 -1.682451
H 0.153204 5.624410 -0.249478
H -0.898124 4.919817 -1.501173
SCF: -3562.930321
ZPE: 0.227188
H: -3562.684873
G: -3562.747861

6_OMe_adduct_conf4
H 0.531247 2.029546 -2.904753
C 0.713371 2.087262 -1.840361
C 1.180859 2.201455 0.924248
C 0.774942 0.946574 -1.063122
C 0.891950 3.303208 -1.213695
C 1.125956 3.365033 0.166030

C 1.004412 0.960328 0.308420
H 0.853136 4.223977 -1.780820
H 1.358378 2.245241 1.988563
C 1.042268 -0.329121 1.008537
C 1.061781 -2.904294 2.110686
C 0.836892 -1.465244 0.225507
C 1.262263 -0.501622 2.367602
C 1.271817 -1.782890 2.917582
C 0.842599 -2.740564 0.748993
H 1.430193 0.340638 3.026098
I 0.531458 -1.001037 -1.799719
Br 0.140847 0.017179 -4.642868
H 0.680120 -3.610249 0.124883
H 1.066924 -3.901238 2.526508
O 1.492344 -1.845923 4.245650
C 1.513751 -3.126572 4.860013
H 2.312438 -3.745704 4.445922
H 0.554509 -3.634416 4.739617
H 1.701318 -2.949007 5.915724
O 1.286341 4.599830 0.676264
C 1.534073 4.720544 2.070127
H 0.701613 4.317498 2.650936
H 1.633005 5.784895 2.265899
H 2.458797 4.209771 2.347429
SCF: -3562.930226
ZPE: 0.227398
H: -3562.684653
G: -3562.747214

7_CF3_adduct_conf1

H -0.334315 2.308824 -3.638652
C -0.188419 2.390500 -2.570282
C 0.189188 2.568431 0.204524
C -0.150665 1.275652 -1.763544
C -0.031308 3.616781 -1.946108
C 0.156570 3.710562 -0.570300
C 0.033301 1.310176 -0.382812
H 0.277772 4.681485 -0.105911
H 0.336548 2.653055 1.272452
C 0.047927 0.034411 0.338010
C 0.032979 -2.505410 1.465580
C -0.126270 -1.110054 -0.431818
C 0.219395 -0.119073 1.716156
C 0.212347 -1.383198 2.271925

C -0.138861 -2.387204 0.096598
H 0.357780 0.743003 2.354404
I -0.368243 -0.684877 -2.482659
Br -0.672774 0.283164 -5.279515
H 0.346174 -1.503753 3.339862
H -0.277227 -3.262378 -0.524874
C 0.038147 -3.857797 2.119385
F -0.221891 -4.846231 1.260434
F 1.224108 -4.130716 2.684494
F -0.874239 -3.937518 3.099033
C -0.064359 4.883366 -2.753976
F -0.224717 4.656613 -4.059336
F -1.064239 5.690203 -2.368851
F 1.066888 5.589581 -2.612419
SCF: -4008.053862
ZPE: 0.171071
H: -4007.862437
G: -4007.932349

7_CF3_adduct_conf2

H 0.579915 2.720247 -2.293917
C 0.774350 2.798377 -1.232980
C 1.276321 2.966469 1.522596
C 0.818185 1.682895 -0.427425
C 0.989193 4.020306 -0.617462
C 1.238994 4.109105 0.748767
C 1.062866 1.712661 0.943972
H 1.404649 5.076446 1.206854
H 1.472038 3.047053 2.583035
C 1.073850 0.437237 1.665409
C 1.033331 -2.100385 2.797401
C 0.834513 -0.702149 0.905786
C 1.299741 0.279685 3.035230
C 1.279360 -0.983268 3.593275
C 0.807545 -1.977970 1.436676
H 1.490745 1.137916 3.665090
I 0.516118 -0.271129 -1.133372
Br 0.117892 0.706439 -3.914461
H 1.454752 -1.106869 4.654854
H 0.618034 -2.849093 0.823136
C 1.021874 -3.451564 3.453628
F 0.731988 -4.436300 2.600013
F 2.209602 -3.745616 4.003889
F 0.120671 -3.512807 4.445164

C 0.951256 5.287616 -1.423997
F 0.728120 5.065319 -2.720677
F -0.011301 6.117926 -0.995497
F 2.104097 5.966750 -1.332588
SCF: -4008.053913
ZPE: 0.171243
H: -4007.862371
G: -4007.931924

7_CF3_adduct_conf3

H 0.735204 2.709676 -2.314264
C 0.849325 2.793535 -1.242208
C 1.146557 2.977075 1.542058
C 0.880738 1.679438 -0.434249
C 0.971985 4.021943 -0.614583
C 1.120543 4.118543 0.765842
C 1.024534 1.716731 0.951284
H 1.216851 5.091110 1.232564
H 1.264285 3.063701 2.613509
C 1.039282 0.440986 1.672299
C 1.049269 -2.100819 2.796511
C 0.915659 -0.705990 0.896551
C 1.166306 0.289188 3.055456
C 1.170539 -0.975718 3.609763
C 0.917526 -1.983863 1.422976
H 1.261450 1.153266 3.698920
I 0.721500 -0.284127 -1.159855
Br 0.459491 0.678839 -3.961817
H 1.269540 -1.094520 4.681700
H 0.822118 -2.860642 0.795959
C 1.055470 -3.454645 3.447668
F 0.998395 -4.452118 2.561857
F 2.159533 -3.645713 4.184452
F 0.014425 -3.609144 4.279749
C 0.946642 5.287555 -1.424051
F 0.814296 5.058850 -2.732161
F -0.065880 6.088182 -1.059766
F 2.070316 6.001282 -1.260260
SCF: -4008.053824
ZPE: 0.170978
H: -4007.862427
G: -4007.933045

7_CN_adduct_conf1

H -0.246441 1.946788 -3.456699
C -0.141684 2.023286 -2.383058
C 0.131957 2.216594 0.404975
C -0.112172 0.913509 -1.575172
C -0.029890 3.261242 -1.753404
C 0.107264 3.359770 -0.368320
C 0.020226 0.956391 -0.185840
H 0.193972 4.333559 0.093910
H 0.240232 2.305515 1.477082
C 0.033806 -0.316559 0.538114
C 0.042488 -2.853946 1.671918
C -0.080793 -1.466483 -0.239244
C 0.151159 -0.461975 1.921871
C 0.155658 -1.723028 2.484589
C -0.079601 -2.739460 0.288702
H 0.238938 0.403931 2.563709
I -0.258619 -1.051417 -2.300743
Br -0.493919 -0.101690 -5.091615
H 0.247339 -1.842024 3.555500
H -0.168492 -3.624365 -0.328295
C 0.051238 -4.158338 2.269474
N 0.058615 -5.201073 2.748414
C -0.056652 4.452737 -2.552084
N -0.078030 5.408233 -3.186884
SCF: -3518.373593
ZPE: 0.158818
H: -3518.198054
G: -3518.258085

7_F_adduct_conf1

H -0.249449 1.714237 -3.331840
C -0.136685 1.776599 -2.257706
C 0.157646 1.966699 0.526714
C -0.110436 0.668015 -1.442256
C -0.009258 2.993402 -1.617427
C 0.137624 3.112254 -0.246780
C 0.031847 0.703316 -0.056190
H 0.234088 4.093603 0.197997
H 0.273241 2.055877 1.598625
C 0.037954 -0.570534 0.667212
C 0.021067 -3.094307 1.791772
C -0.097187 -1.721187 -0.102644
C 0.165846 -0.725689 2.049587
C 0.158015 -1.988181 2.614077

C -0.110265 -2.999763 0.420777
H 0.271645 0.138909 2.691441
I -0.282213 -1.299050 -2.159420
Br -0.520697 -0.344703 -4.982462
H 0.256314 -2.128060 3.682309
H -0.216096 -3.891731 -0.183419
F 0.014619 -4.313440 2.350996
F -0.029421 4.106435 -2.363764
SCF: -3532.376532
ZPE: 0.144961
H: -3532.216833
G: -3532.272002

7_NMe2_adduct_conf1

H -1.076889 3.158487 -3.768013
C -0.582288 3.241120 -2.812154
C 0.652017 3.329266 -0.308809
C -0.462831 2.142534 -2.000793
C -0.044041 4.462409 -2.353129
C 0.565395 4.471311 -1.076518
C 0.138042 2.103864 -0.746425
H 0.977117 5.388412 -0.681780
H 1.129658 3.384139 0.661873
C 0.170039 0.838220 -0.024591
C 0.093084 -1.753105 1.165852
C -0.410477 -0.264287 -0.640744
C 0.720529 0.606274 1.239604
C 0.682658 -0.644240 1.819901
C -0.476344 -1.531458 -0.106373
H 1.184369 1.421826 1.781481
I -1.206449 0.239637 -2.525863
Br -2.270037 1.303933 -5.229975
H 1.116869 -0.768494 2.800878
H -0.951488 -2.334898 -0.649704
N 0.075099 -2.990196 1.738955
C -0.673732 -4.058900 1.108909
C 0.535967 -3.157962 3.103170
H -1.737159 -3.811743 1.015321
H -0.579398 -4.957482 1.711788
H -0.284628 -4.277404 0.111510
H -0.056857 -2.568849 3.811458
H 0.455442 -4.207237 3.373170
H 1.582475 -2.862166 3.203466
N -0.115516 5.585110 -3.121777

C -0.866358 5.553777 -4.360910
H -0.798290 6.526799 -4.838868
H -1.923553 5.318427 -4.192584
H -0.458028 4.808402 -5.047986
C 0.293198 6.861198 -2.568537
H 1.348878 6.848823 -2.288395
H -0.293884 7.128819 -1.683351
H 0.153307 7.630935 -3.322258
SCF: -3601.800036
ZPE: 0.307751
H: -3601.470111
G: -3601.542685

7_NMe2_adduct_conf2

H -0.408541 2.881516 -1.794256
C 0.301431 2.916785 -0.981738
C 2.094270 2.885977 1.159485
C 0.495214 1.816274 -0.187406
C 1.056321 4.075419 -0.699298
C 1.947380 4.026048 0.398226
C 1.366935 1.721052 0.892827
H 2.532378 4.896308 0.656612
H 2.790180 2.895181 1.989739
C 1.436365 0.464417 1.627568
C 1.380944 -2.096965 2.881531
C 0.617289 -0.573694 1.199435
C 2.241300 0.184301 2.735869
C 2.215027 -1.051628 3.346763
C 0.550542 -1.823559 1.773525
H 2.899101 0.949924 3.129418
I -0.541160 -0.000175 -0.464704
Br -2.084217 1.152926 -2.886139
H 2.853933 -1.214679 4.201968
H -0.121722 -2.573809 1.383438
N 1.379524 -3.323342 3.478246
C 0.410674 -4.318151 3.064996
C 2.109675 -3.521357 4.715086
H -0.618981 -3.982865 3.234062
H 0.576670 -5.228603 3.633901
H 0.522772 -4.556630 2.004926
H 1.750185 -2.862044 5.512690
H 1.982953 -4.551827 5.034642
H 3.177485 -3.339432 4.575586
N 0.922543 5.195160 -1.464073

C -0.111174 5.245701 -2.478557
H -0.071108 6.210975 -2.975275
H -1.110902 5.114241 -2.049056
H 0.039082 4.468694 -3.232423
C 1.592987 6.418055 -1.069092
H 2.675238 6.277047 -1.030420
H 1.257231 6.770163 -0.087497
H 1.379575 7.188192 -1.804801
SCF: -3601.800042
ZPE: 0.307959
H: -3601.469974
G: -3601.542041

7_NMe2_adduct_conf3

H 0.230231 2.752095 -2.168416
C 0.689600 2.839928 -1.195573
C 1.871762 2.930498 1.332758
C 0.764913 1.749370 -0.368289
C 1.227663 4.059107 -0.731145
C 1.827582 4.064784 0.549859
C 1.333156 1.713553 0.901343
H 2.265454 4.973543 0.935866
H 2.340542 2.983640 2.307868
C 1.322380 0.455625 1.637273
C 1.169274 -2.121199 2.851344
C 0.741716 -0.644007 1.016050
C 1.831568 0.228748 2.919603
C 1.757487 -1.014819 3.511024
C 0.640343 -1.904375 1.560754
H 2.291609 1.043105 3.466455
I 0.011610 -0.148203 -0.897604
Br -0.940624 0.898380 -3.649882
H 2.160757 -1.135535 4.505595
H 0.168246 -2.706235 1.012212
N 1.114286 -3.350916 3.436474
C 0.379228 -4.418944 2.789758
C 1.543269 -3.514939 4.811378
H -0.676603 -4.161010 2.651367
H 0.438732 -5.310910 3.406654
H 0.804581 -4.653839 1.810857
H 0.948501 -2.906172 5.500979
H 1.434029 -4.559387 5.089743
H 2.593695 -3.240430 4.931401
N 1.164917 5.183190 -1.499197

C 1.866610 6.379615 -1.077775
H 1.695460 7.162676 -1.811022
H 2.945742 6.211732 -0.991316
H 1.496624 6.732468 -0.112743
C 0.675309 5.089550 -2.860162
H -0.354292 4.723940 -2.882532
H 1.288864 4.416462 -3.470121
H 0.692883 6.078411 -3.309337
SCF: -3601.800010
ZPE: 0.307735
H: -3601.470115
G: -3601.542655

7_NMe2_adduct_conf4

H -0.597873 3.244297 -1.416449
C 0.265511 3.111856 -0.782386
C 2.438294 2.657644 0.912190
C 0.415633 1.959361 -0.055214
C 1.267285 4.099540 -0.668139
C 2.347396 3.839297 0.207820
C 1.466676 1.656540 0.804632
H 3.126954 4.575752 0.335779
H 3.285361 2.501834 1.569337
C 1.458949 0.372615 1.494150
C 1.198889 -2.194364 2.710565
C 0.387456 -0.478708 1.250623
C 2.427875 -0.110006 2.378982
C 2.307249 -1.351474 2.966834
C 0.219412 -1.726307 1.808647
H 3.295372 0.497067 2.608768
I -0.978674 0.377402 -0.107179
Br -2.778272 1.916909 -2.099604
H 3.086121 -1.679098 3.639353
H -0.641668 -2.329385 1.560284
N 1.079109 -3.412600 3.311927
C 2.178108 -3.935516 4.099708
C 0.011703 -4.306027 2.909675
H 3.089112 -4.055167 3.503036
H 1.893574 -4.906232 4.495669
H 2.405063 -3.279327 4.942618
H 0.077380 -4.569968 1.848030
H 0.074640 -5.217286 3.497590
H -0.966576 -3.854341 3.089875
N 1.185832 5.256915 -1.381177

C 0.003985 5.525326 -2.175616
H 0.123489 6.483034 -2.674268
H -0.901681 5.561970 -1.559675
H -0.137500 4.757958 -2.941453
C 2.146933 6.316005 -1.145859
H 3.164204 5.979138 -1.358227
H 2.113209 6.674561 -0.111504
H 1.921172 7.147385 -1.807342
SCF: -3601.800058
ZPE: 0.308116
H: -3601.469891
G: -3601.541856

7_OMe_adduct_conf1

H -0.232816 2.536629 -3.546993
C -0.161058 2.646859 -2.474991
C 0.027302 2.832494 0.315592
C -0.098705 1.540279 -1.656151
C -0.127878 3.891074 -1.849737
C -0.032131 3.971891 -0.454670
C -0.005565 1.560043 -0.270865
H -0.007353 4.950898 0.006076
H 0.099824 2.921573 1.392008
C 0.047023 0.284659 0.440122
C 0.124440 -2.291659 1.559190
C 0.002621 -0.867778 -0.329848
C 0.135360 0.112429 1.827509
C 0.173022 -1.150931 2.373130
C 0.038405 -2.155783 0.175624
H 0.172970 0.975064 2.480688
I -0.135302 -0.432994 -2.386032
Br -0.342803 0.547126 -5.260967
H 0.240063 -1.287427 3.444799
H 0.000757 -3.017123 -0.476153
O 0.164547 -3.476905 2.196166
C 0.110262 -4.657724 1.408063
H 0.963032 -4.712439 0.727715
H -0.820086 -4.703647 0.837705
H 0.149453 -5.488185 2.107887
O -0.183801 5.057537 -2.517751
C -0.294247 5.004274 -3.933954
H 0.573070 4.507184 -4.374531
H -0.333743 6.036495 -4.271139
H -1.207365 4.484786 -4.234090

SCF: -3562.930903
ZPE: 0.227536
H: -3562.685241
G: -3562.747741

7_OMe_adduct_conf3

H 0.760087 2.875338 -1.995226
C 0.852226 3.007172 -0.927181
C 1.093961 3.250166 1.854473
C 0.943643 1.917835 -0.088242
C 0.883783 4.263979 -0.327411
C 1.006128 4.373468 1.063564
C 1.064013 1.966026 1.294085
H 1.029379 5.361553 1.504570
H 1.187959 3.361070 2.927287
C 1.146508 0.705849 2.029694
C 1.281763 -1.847478 3.197010
C 1.102105 -0.465889 1.276058
C 1.262727 0.558365 3.409803
C 1.329733 -0.698329 3.990959
C 1.165912 -1.731042 1.809297
H 1.300367 1.432867 4.047170
I 0.917086 -0.069656 -0.783995
Br 0.636734 0.854826 -3.670599
H 1.418679 -0.775439 5.064870
H 1.129246 -2.626359 1.201597
O 1.338918 -3.104183 3.677566
C 1.443702 -3.276256 5.084190
H 0.582248 -2.841552 5.595501
H 2.363591 -2.828050 5.465304
H 1.464502 -4.349616 5.253482
O 0.802172 5.416295 -1.016990
C 0.671460 5.334263 -2.430071
H 1.536661 4.836073 -2.873586
H 0.617941 6.359319 -2.786632
H -0.241232 4.801185 -2.706744
SCF: -3562.930502
ZPE: 0.227476
H: -3562.684870
G: -3562.747462

7_OMe_adduct_conf4

H 0.838597 3.052911 -1.849252
C 0.923692 3.085924 -0.771319

C 1.143252 3.170088 2.011153
C 0.970597 1.952175 -0.004070
C 0.988095 4.313893 -0.106163
C 1.100921 4.349097 1.284906
C 1.077683 1.925816 1.387654
H 1.155475 5.291356 1.810321
H 1.229017 3.221572 3.089151
C 1.109265 0.625672 2.054662
C 1.142629 -1.987144 3.087557
C 1.032947 -0.498728 1.247494
C 1.206569 0.405653 3.434663
C 1.222425 -0.875469 3.938273
C 1.046199 -1.803268 1.710213
H 1.268623 1.245201 4.115503
I 0.886483 0.003739 -0.794847
Br 0.677499 1.055322 -3.630676
H 1.296395 -1.048513 5.004212
H 0.983942 -2.641832 1.031062
O 1.164935 -3.193715 3.684362
C 1.084972 -4.345954 2.857310
H 1.931105 -4.391094 2.167984
H 0.149280 -4.357853 2.293961
H 1.116451 -5.200243 3.528251
O 0.933644 5.405504 -0.891720
C 0.967718 6.679280 -0.262114
H 0.121830 6.800536 0.417850
H 0.899569 7.410577 -1.063115
H 1.902891 6.820396 0.283634
SCF: -3562.929693
ZPE: 0.227403
H: -3562.684107
G: -3562.746739

7_OMe_adduct_conf5

H 0.664294 3.041974 -1.852720
C 0.746179 3.100275 -0.775613
C 0.958415 3.248110 2.004393
C 0.855649 1.985407 0.012669
C 0.741179 4.342181 -0.133743
C 0.850395 4.409265 1.256493
C 0.962700 1.990567 1.404448
H 0.850900 5.362822 1.764038
H 1.040844 3.323885 3.081307
C 1.064459 0.706990 2.096616

C 1.235887 -1.881543 3.178216
C 1.050666 -0.438273 1.302994
C 1.169284 0.514631 3.472129
C 1.254131 -0.759537 4.011182
C 1.132769 -1.719551 1.794135
H 1.183585 1.367534 4.139191
I 0.879770 0.021027 -0.747245
Br 0.617935 1.009702 -3.599841
H 1.333166 -0.872003 5.082740
H 1.119035 -2.594607 1.156578
O 1.310897 -3.152634 3.616736
C 1.401446 -3.370184 5.018087
H 0.525747 -2.968731 5.532451
H 2.308005 -2.918378 5.426071
H 1.439968 -4.448106 5.151387
O 0.626626 5.414099 -0.939579
C 0.602623 6.700242 -0.335015
H -0.245725 6.795094 0.346055
H 0.497397 7.411480 -1.149935
H 1.532172 6.895763 0.203774
SCF: -3562.929302
ZPE: 0.227434
H: -3562.683705
G: -3562.746303

8_CF3_adduct_conf1

C -0.030500 2.249912 -1.613655
C 0.085826 2.337739 1.173435
C -0.004470 1.092574 -0.852251
C 0.002138 3.467238 -0.955925
C 0.061266 3.503274 0.433722
C 0.052903 1.092849 0.537310
H -0.017317 4.384542 -1.527939
H 0.088104 4.458669 0.939436
H 0.131456 2.390241 2.252918
C 0.069519 -0.205586 1.212987
C 0.062104 -2.792648 2.292475
C 0.033789 -1.340650 0.409998
C 0.110672 -0.400348 2.596413
C 0.109335 -1.677767 3.122488
C 0.024359 -2.629608 0.917418
H 0.142462 0.452042 3.261662
H 0.142098 -1.815278 4.194564
H 0.053229 -3.789077 2.713037

I -0.017996 -0.855906 -1.631444
Br -0.190721 -2.046399 -4.674713
C -0.085619 -3.828238 0.016229
F -1.342096 -4.001311 -0.416141
F 0.671391 -3.685452 -1.087901
F 0.291754 -4.950408 0.613860
C -0.095189 2.180934 -3.113485
F -1.215690 1.566470 -3.522879
F -0.060364 3.377545 -3.683652
F 0.927565 1.464645 -3.607966
SCF: -4008.034227
ZPE: 0.170709
H: -4007.842835
G: -4007.915100

8_CF3_adduct_conf2

C 0.966810 3.262968 -0.619308
C 1.085848 3.330763 2.166899
C 0.975722 2.098597 0.132972
C 1.018388 4.475328 0.045728
C 1.077488 4.501529 1.435574
C 1.034980 2.090593 1.522396
H 1.013062 5.396404 -0.520413
H 1.117934 5.452967 1.947840
H 1.133103 3.376747 3.246500
C 1.043880 0.788808 2.193307
C 1.058169 -1.789095 3.278623
C 0.993409 -0.347425 1.385828
C 1.101155 0.599374 3.574321
C 1.107545 -0.677286 4.106521
C 0.999619 -1.631904 1.899846
H 1.140682 1.453208 4.237013
H 1.152399 -0.811635 5.178535
H 1.065293 -2.787723 3.698166
I 0.904264 0.156446 -0.650260
Br 0.663356 -0.855257 -3.759123
C 0.955007 -2.883945 1.066185
F 0.881973 -2.623359 -0.251338
F 2.041995 -3.634997 1.251107
F -0.100649 -3.640281 1.369336
C 0.901944 3.207041 -2.119537
F -0.222164 2.602686 -2.532842
F 0.941716 4.409187 -2.679338
F 1.921568 2.492164 -2.620736

SCF: -4008.034496
ZPE: 0.170666
H: -4007.843220
G: -4007.914573

8_CF3_adduct_conf3

C 0.940507 3.239562 -0.615675
C 1.007247 3.328005 2.172951
C 0.984307 2.082027 0.144908
C 0.929306 4.456436 0.043713
C 0.962808 4.493239 1.434039
C 1.020561 2.083516 1.535507
H 0.894824 5.373277 -0.528264
H 0.953450 5.448563 1.940499
H 1.030161 3.379707 3.253191
C 1.058827 0.787090 2.213792
C 1.083708 -1.796497 3.298818
C 1.051185 -0.349204 1.412078
C 1.094118 0.596695 3.597779
C 1.109584 -0.679502 4.126814
C 1.055972 -1.636835 1.922969
H 1.109974 1.451166 4.260946
H 1.137753 -0.814261 5.199375
H 1.083997 -2.792258 3.721236
I 1.029790 0.131904 -0.631126
Br 1.037736 -0.909916 -3.726466
C 0.963024 -2.840605 1.026886
F -0.295399 -3.049139 0.617404
F 1.696961 -2.682114 -0.091299
F 1.380475 -3.950510 1.620878
C 0.908654 3.174087 -2.116732
F -0.156920 2.482394 -2.548628
F 0.863896 4.374261 -2.680118
F 1.990194 2.540313 -2.595074
SCF: -4008.034242
ZPE: 0.170762
H: -4007.842853
G: -4007.914619

8_CN_adduct_conf1

C -0.224963 2.010372 -2.204592
C 0.353052 2.167330 0.523241
C -0.025477 0.862483 -1.442352
C -0.058572 3.247925 -1.580928

C 0.265313 3.318622 -0.235366
C 0.186884 0.911976 -0.065448
H -0.216294 4.146442 -2.162185
H 0.402191 4.284475 0.231267
H 0.542114 2.239075 1.585794
C 0.139177 -0.351818 0.677920
C -0.090875 -2.875566 1.879774
C -0.116242 -1.487970 -0.073416
C 0.275368 -0.495637 2.061214
C 0.159630 -1.745206 2.646848
C -0.221146 -2.749456 0.499728
H 0.468323 0.367366 2.684694
H 0.264774 -1.844511 3.718579
H -0.186200 -3.850859 2.337610
I -0.056586 -1.115384 -2.149237
Br 0.904759 -0.439991 -4.854516
C -0.463404 -3.891026 -0.331873
N -0.651119 -4.772463 -1.042540
C -0.767707 2.035313 -3.531729
N -1.302304 2.173406 -4.536886
SCF: -3518.353683
ZPE: 0.158574
H: -3518.178341
G: -3518.238179

8_F_adduct_conf1

C -0.131776 1.837852 -2.179321
C 0.016381 1.992160 0.585993
C -0.091109 0.688429 -1.415306
C -0.101721 3.075089 -1.568120
C -0.028865 3.142210 -0.183473
C -0.012446 0.737533 -0.020414
H -0.134267 3.962069 -2.187163
H -0.005497 4.110331 0.298439
H 0.075762 2.064336 1.663343
C 0.040161 -0.542536 0.689914
C 0.135158 -3.130389 1.774189
C 0.007538 -1.672324 -0.117471
C 0.121800 -0.723460 2.070898
C 0.167976 -2.005720 2.594930
C 0.053538 -2.941412 0.411804
H 0.149275 0.130575 2.734056
H 0.231533 -2.140907 3.666390
H 0.171558 -4.134558 2.175553

I -0.128887 -1.267554 -2.171883
Br -0.376129 -0.956236 -5.194450
F 0.018187 -3.989183 -0.423966
F -0.196769 1.761496 -3.503941
SCF: -3532.362613
ZPE: 0.145218
H: -3532.202487
G: -3532.258540

8_NMe2_adduct_conf1

C -0.275100 3.263772 -1.984959
C 0.116273 3.448004 0.813300
C -0.195171 2.158634 -1.153573
C -0.125870 4.501447 -1.359692
C 0.066972 4.581069 0.017569
C -0.011759 2.189697 0.223602
H -0.165698 5.405544 -1.953183
H 0.178446 5.555284 0.475893
H 0.274482 3.530545 1.880727
C 0.087202 0.893298 0.897177
C 0.338470 -1.730494 1.856147
C -0.011667 -0.224904 0.081030
C 0.322319 0.665926 2.253973
C 0.452263 -0.635787 2.711600
C 0.088883 -1.540907 0.498246
H 0.421488 1.500571 2.935819
H 0.645542 -0.810178 3.762241
H 0.440948 -2.734384 2.247376
I -0.221632 0.223457 -1.943616
Br -0.583247 -0.603552 -5.198369
N -0.052718 -2.566469 -0.467183
C -1.455306 -2.898239 -0.741648
C 0.717242 -3.773896 -0.193592
H -2.041097 -1.996289 -0.917632
H -1.904519 -3.441699 0.099223
H -1.500719 -3.523228 -1.633283
H 1.749933 -3.510785 0.031535
H 0.302882 -4.353910 0.640293
H 0.699101 -4.400173 -1.085281
N -0.475746 3.065030 -3.366479
C -1.876183 2.813739 -3.719178
H -1.917589 2.431263 -4.738019
H -2.469059 3.735066 -3.650434
H -2.319237 2.071067 -3.056359

C 0.097695 4.089159 -4.228662
H 1.133646 4.273741 -3.947346
H -0.460733 5.032808 -4.187125
H 0.071162 3.722774 -5.255040
SCF: -3601.785713
ZPE: 0.307965
H: -3601.456229
G: -3601.526931

8_NMe2_adduct_conf2

C 1.049063 3.287797 -0.086270
C 1.758245 3.609236 2.636212
C 1.046940 2.247747 0.828569
C 1.453983 4.526767 0.409637
C 1.803294 4.673434 1.750080
C 1.374916 2.348864 2.175406
H 1.489807 5.380218 -0.254747
H 2.114323 5.646758 2.107133
H 2.040424 3.743906 3.672364
C 1.326277 1.107686 2.951624
C 1.076884 -1.416888 4.149466
C 1.016386 -0.042801 2.239364
C 1.517438 0.965445 4.326819
C 1.381455 -0.286419 4.905804
C 0.896059 -1.314861 2.771422
H 1.747420 1.830065 4.935560
H 1.518006 -0.392378 5.974333
H 0.984000 -2.381022 4.632418
I 0.626592 0.293949 0.219938
Br -0.221736 -0.765523 -2.869175
N 0.594809 -2.386295 1.896936
C 1.783634 -2.922453 1.224464
C -0.187046 -3.461145 2.495996
H 2.390437 -2.118707 0.807674
H 1.464436 -3.575612 0.412592
H 2.406639 -3.496836 1.921731
H -1.056056 -3.046530 3.005171
H -0.527383 -4.121688 1.698842
H 0.397867 -4.056609 3.207829
N 0.669904 3.024639 -1.419003
C -0.782779 2.978116 -1.610916
H -0.993916 2.539597 -2.585340
H -1.217180 3.985089 -1.563004
H -1.259631 2.363343 -0.847982

C 1.295105 3.878675 -2.419664
H 2.371537 3.913845 -2.256806
H 0.895347 4.900462 -2.407770
H 1.101402 3.448530 -3.402408
SCF: -3601.785551
ZPE: 0.307640
H: -3601.456244
G: -3601.528247

8_NMe2_adduct_conf3

C 0.686075 3.201166 -0.108477
C 1.425143 3.565987 2.599616
C 0.880310 2.153013 0.774203
C 0.902494 4.476900 0.410535
C 1.268079 4.645163 1.744503
C 1.233767 2.272567 2.112591
H 0.779252 5.340857 -0.229378
H 1.429204 5.647020 2.121191
H 1.715808 3.717172 3.631146
C 1.408246 1.019852 2.850204
C 1.605430 -1.542830 3.974296
C 1.253380 -0.146892 2.113596
C 1.673864 0.873918 4.212227
C 1.758712 -0.398552 4.755357
C 1.355393 -1.435280 2.607376
H 1.790706 1.749148 4.838217
H 1.953024 -0.509524 5.814387
H 1.686312 -2.521987 4.428346
I 0.742875 0.176263 0.118683
Br 0.019400 -1.268848 -2.847843
N 1.193153 -2.517002 1.708789
C 2.429920 -2.849349 0.992796
C 0.600881 -3.712741 2.296172
H 2.891781 -1.954033 0.576693
H 2.190851 -3.529311 0.175477
H 3.155215 -3.332483 1.659808
H -0.305159 -3.447623 2.839491
H 0.340642 -4.397096 1.488968
H 1.289983 -4.229729 2.975283
N 0.302361 2.908777 -1.437278
C -1.141449 2.689581 -1.576037
H -1.695488 3.630287 -1.463060
H -1.503759 1.986199 -0.826342
H -1.340363 2.276526 -2.564420

C 0.776396 3.860840 -2.434135
H 1.844019 4.032464 -2.303406
H 0.247939 4.820758 -2.380773
H 0.606302 3.432720 -3.421908
SCF: -3601.785604
ZPE: 0.307714
H: -3601.456308
G: -3601.527178

8_OMe_adduct_conf1

C 0.035234 2.236152 -1.511448
C 0.422385 2.350045 1.278592
C 0.019763 1.107318 -0.705832
C 0.252380 3.457403 -0.879497
C 0.441020 3.494861 0.500310
C 0.206432 1.112696 0.670102
H 0.275238 4.371125 -1.456569
H 0.608243 4.453828 0.973462
H 0.573989 2.406545 2.348136
C 0.158744 -0.188943 1.338165
C 0.017696 -2.819206 2.313279
C -0.066592 -1.280487 0.513664
C 0.316846 -0.435180 2.703046
C 0.244327 -1.738442 3.165041
C -0.143942 -2.593995 0.950110
H 0.492588 0.384012 3.387347
H 0.366651 -1.932514 4.222793
H -0.031877 -3.822389 2.712667
I -0.296622 -0.797012 -1.499733
Br -0.851004 -1.225474 -4.743999
O -0.368566 -3.523596 0.005532
C -0.454597 -4.885234 0.420803
H 0.481849 -5.204682 0.880984
H -0.637052 -5.460417 -0.482289
H -1.281316 -5.019958 1.119950
O -0.159910 2.039094 -2.820950
C -0.154109 3.175713 -3.679644
H -0.955137 3.865242 -3.408263
H -0.322559 2.788446 -4.680506
H 0.809899 3.685048 -3.635252
SCF: -3562.923914
ZPE: 0.227096
H: -3562.678228
G: -3562.743193

8_OMe_adduct_conf2

C 0.700354 3.120160 -0.268558
C 1.183008 3.456955 2.488397
C 0.806214 2.051915 0.609777
C 0.843198 4.395333 0.271374
C 1.081446 4.542967 1.635888
C 1.042798 2.167398 1.973186
H 0.770684 5.266103 -0.364891
H 1.190270 5.542598 2.036261
H 1.369850 3.599416 3.544313
C 1.120838 0.916293 2.729126
C 1.213037 -1.640564 3.886647
C 0.947610 -0.243942 1.990365
C 1.348776 0.780202 4.099525
C 1.390864 -0.488649 4.652239
C 0.985337 -1.524781 2.519291
H 1.490318 1.656036 4.718339
H 1.567827 -0.597429 5.714477
H 1.252693 -2.614103 4.354542
I 0.615750 0.077713 -0.041801
Br 0.052022 -0.462364 -3.252356
O 0.796988 -2.534564 1.652021
C 0.829061 -3.863747 2.167493
H 0.039446 -4.005770 2.907036
H 1.802059 -4.077788 2.612630
H 0.660037 -4.516975 1.316369
O 0.470777 2.818235 -1.551561
C 0.371254 3.887645 -2.486739
H -0.467591 4.539331 -2.237095
H 0.200362 3.418387 -3.451460
H 1.298114 4.463290 -2.512037
SCF: -3562.923950
ZPE: 0.227139
H: -3562.678234
G: -3562.742862

8_OMe_adduct_conf3

C 0.829750 2.978028 -0.433119
C 1.167239 3.375999 2.332409
C 0.852974 1.919005 0.463722
C 0.987234 4.257795 0.087814
C 1.153675 4.447398 1.453322
C 1.021792 2.081589 1.839915

H 0.975940 5.094854 -0.598500
H 1.272301 5.452744 1.835671
H 1.301552 3.539878 3.393280
C 1.064873 0.857243 2.641619
C 1.128945 -1.652332 3.912803
C 0.960503 -0.340385 1.951074
C 1.208343 0.776377 4.028261
C 1.238040 -0.466776 4.636718
C 0.984313 -1.600340 2.529882
H 1.294607 1.678325 4.618541
H 1.349840 -0.526274 5.711571
H 1.155663 -2.605865 4.421179
I 0.742852 -0.095964 -0.104381
Br 0.477709 -2.659310 -2.155348
O 0.865605 -2.642609 1.698142
C 0.881840 -3.952125 2.259732
H 0.048914 -4.081567 2.952668
H 1.827590 -4.137463 2.771460
H 0.775014 -4.633453 1.420504
O 0.727896 2.823619 -1.775158
C -0.408863 2.119537 -2.290263
H -0.130549 1.110938 -2.607661
H -0.750149 2.666636 -3.166987
H -1.214443 2.082098 -1.555468
SCF: -3562.913851
ZPE: 0.226706
H: -3562.668409
G: -3562.733441

9_adduct_conf1

H 0.073462 0.032984 0.118149
C 0.050095 0.066916 1.198123
C -0.012305 0.124706 3.998601
C 0.044726 -1.083407 1.951289
C 0.023776 1.277825 1.879850
C -0.007144 1.301282 3.267429
C 0.013716 -1.111734 3.348027
H 0.027222 2.200473 1.314808
H -0.027924 2.248247 3.790416
H -0.037294 0.166021 5.076697
C 0.008701 -2.426693 3.994703
C 0.002309 -5.066176 4.954721
C 0.030703 -3.526449 3.140469
C -0.015471 -2.693285 5.358514

C -0.018761 -3.993939 5.830498
C 0.027869 -4.820653 3.594860
I 0.078930 -3.014702 1.095032
F 0.049845 -5.844630 2.742099
F -0.001559 -6.304599 5.424427
F -0.042694 -4.221513 7.136333
F -0.035744 -1.719849 6.266229
Br 0.157540 -1.967726 -1.612775
SCF: -3730.850427
ZPE: 0.129042
H: -3730.704748
G: -3730.763794

9_adduct_conf2

H 0.063699 0.038706 0.143788
C 0.038332 0.073276 1.225243
C -0.026327 0.148271 4.031173
C 0.038316 -1.076334 1.987887
C 0.003844 1.287643 1.897177
C -0.028743 1.317132 3.287038
C 0.008268 -1.088668 3.380396
H 0.002065 2.209825 1.331202
H -0.056433 2.268290 3.802038
H -0.051955 0.203780 5.108290
C 0.013595 -2.414557 4.003203
C 0.017499 -5.044467 4.992104
C 0.042929 -3.531186 3.156650
C -0.009994 -2.676059 5.367556
C -0.007687 -3.968554 5.857833
C 0.042905 -4.826514 3.625477
I 0.088651 -3.005236 1.141147
F 0.065346 -5.872237 2.820316
F 0.017262 -6.279191 5.466832
F -0.031785 -4.180069 7.163467
F -0.036052 -1.691444 6.259932
Br 0.200666 -5.679706 -0.371649
SCF: -3730.836552
ZPE: 0.129021
H: -3730.690752
G: -3730.750785

10_CCF2_adduct_conf1

H 2.790482 -0.716918 2.454988
C 1.877890 -0.204598 2.176626

C -0.468278 1.109117 1.437354
C 0.885111 -0.850034 1.461018
C 1.678447 1.122220 2.535225
C 0.507868 1.772010 2.166515
C -0.299139 -0.228531 1.080047
H 2.442609 1.645230 3.095161
H 0.356590 2.808482 2.438793
H -1.367049 1.629857 1.131944
I 1.116111 -2.908300 1.016035
C 0.214511 -2.611052 -0.863958
C -0.992507 -2.215518 -3.279945
C -0.853365 -1.722075 -0.914541
C 0.707268 -3.290559 -1.959955
C 0.084987 -3.085853 -3.183618
C -1.449507 -1.534309 -2.163392
H 1.538192 -3.975011 -1.863824
H 0.451274 -3.606849 -4.058321
H -2.272115 -0.835898 -2.249289
H -1.474574 -2.054861 -4.235427
C -1.302708 -0.961505 0.274383
C -2.588298 -0.921236 0.593434
F -3.089296 -0.278209 1.619147
F -3.545470 -1.539304 -0.053380
Br 1.346064 -5.888392 0.331278
SCF: -3609.764193
ZPE: 0.179659
H: -3609.567725
G: -3609.627699

10_CH2_2_adduct_conf1

C 2.527898 -1.881742 -0.634977
C 1.500623 -1.417318 0.201866
C 1.501351 -0.043592 0.408667
C 2.423644 0.830989 -0.153809
C 3.421155 0.322432 -0.964330
C 3.469689 -1.045865 -1.202456
C 0.596871 -2.503137 0.761300
C -0.745803 -2.185135 1.425874
C -1.672508 -1.366294 0.572440
C -2.694194 -1.957771 -0.168079
C -3.540810 -1.194059 -0.960954
C -3.384179 0.183352 -1.037964
C -2.367475 0.802742 -0.322422
C -1.540201 0.014400 0.459809

I 0.014786 0.926605 1.563089
H 2.571673 -2.947235 -0.829622
H 2.367834 1.892034 0.046077
H 4.144731 0.992587 -1.409206
H 4.241178 -1.461570 -1.837842
H 1.194742 -3.070067 1.479778
H 0.401573 -3.184204 -0.069458
H -0.595863 -1.703030 2.392862
H -1.220349 -3.144011 1.634979
H -2.826894 -3.031767 -0.110091
H -4.330897 -1.678872 -1.520182
H -4.045312 0.778765 -1.653997
H -2.227535 1.874576 -0.381224
Br 2.394615 2.182796 3.179872
SCF: -3412.477692
ZPE: 0.219073
H: -3412.243085
G: -3412.300491

10_CH2_2_adduct_conf2

C 2.664970 -1.878125 0.669898
C 1.629042 -1.265362 -0.038319
C 1.527922 0.110071 0.109972
C 2.370864 0.883029 0.887826
C 3.390777 0.237461 1.570956
C 3.532780 -1.140802 1.460561
C 0.678520 -2.072669 -0.875284
C -0.609018 -2.455064 -0.144489
C -1.572285 -1.397585 0.365146
C -2.653175 -1.896425 1.105596
C -3.645700 -1.083496 1.620671
C -3.590231 0.290108 1.422473
C -2.530285 0.824850 0.712329
C -1.545998 -0.015618 0.195992
I -0.055311 1.053630 -0.892493
H 2.785969 -2.951514 0.583834
H 2.246364 1.955167 0.954953
H 4.068781 0.813841 2.186500
H 4.329463 -1.644565 1.992825
H 1.171970 -3.005504 -1.148362
H 0.457526 -1.558376 -1.811988
H -0.336200 -3.068678 0.717893
H -1.181970 -3.108652 -0.806742
H -2.702912 -2.967504 1.267558

H -4.462001 -1.521894 2.180402
H -4.354993 0.942267 1.823332
H -2.468309 1.896498 0.568250
Br 2.181270 2.629293 -2.351149
SCF: -3412.478868
ZPE: 0.219096
H: -3412.244276
G: -3412.301553

10_CH2_2_adduct_conf3

C 2.673040 -1.907560 0.733554
C 1.667984 -1.280986 -0.001034
C 1.535497 0.093590 0.170509
C 2.348212 0.844463 1.003381
C 3.348547 0.191047 1.711695
C 3.503993 -1.182160 1.577174
C 0.758100 -2.058893 -0.909185
C -0.597497 -2.405346 -0.286713
C -1.512782 -1.344380 0.300939
C -2.558820 -1.844638 1.092738
C -3.513200 -1.034175 1.675701
C -3.459184 0.343366 1.500304
C -2.443226 0.886591 0.736599
C -1.508482 0.037270 0.156293
I 0.003112 1.057592 -0.920376
H 2.804957 -2.978325 0.630759
H 2.209867 1.913280 1.106267
H 3.998045 0.756575 2.367027
H 4.281143 -1.693415 2.130993
H 1.236479 -3.007718 -1.152609
H 0.627270 -1.533219 -1.855979
H -0.419440 -3.122547 0.517046
H -1.180404 -2.939462 -1.041722
H -2.607111 -2.917686 1.238621
H -4.299110 -1.477298 2.273762
H -4.192919 0.993713 1.957767
H -2.383677 1.955263 0.584610
Br -2.343256 2.395789 -2.521141
SCF: -3412.477704
ZPE: 0.219084
H: -3412.243106
G: -3412.300430

10_CH2_2_adduct_conf4

C 2.685330 -1.803543 1.135228
C 1.576486 -1.281268 0.455062
C 1.514352 0.108093 0.383423
C 2.490759 0.934730 0.935579
C 3.579269 0.378098 1.583135
C 3.670899 -1.004081 1.683752
C 0.626497 -2.324187 -0.106978
C -0.691114 -1.925031 -0.772661
C -1.634228 -1.201082 0.144780
C -2.633841 -1.886638 0.838300
C -3.492551 -1.226991 1.704034
C -3.377242 0.143207 1.906726
C -2.393744 0.859313 1.240533
C -1.559071 0.162968 0.385421
I -0.027620 1.209885 -0.595396
H 2.763468 -2.881730 1.220954
H 2.400573 2.011988 0.868878
H 4.338115 1.019533 2.011591
H 4.509974 -1.460195 2.193414
H 0.393995 -3.007097 0.714065
H 1.196369 -2.911160 -0.831408
H -1.170575 -2.849200 -1.095171
H -0.510818 -1.342818 -1.677709
H -2.732993 -2.954243 0.681055
H -4.260943 -1.785291 2.223383
H -4.047957 0.658636 2.581502
H -2.290956 1.926704 1.380037
Br -2.340223 2.816590 -1.892966
SCF: -3412.478845
ZPE: 0.218969
H: -3412.244338
G: -3412.301875

10_CH2_3_adduct_conf1

C -3.046716 -1.777186 -0.661122
C -1.773290 -1.213735 -0.521070
C -1.735412 0.074998 -0.003732
C -2.876691 0.785602 0.348678
C -4.119840 0.196111 0.184717
C -4.201548 -1.094404 -0.319387
C -0.577086 -2.042883 -0.897044
C 0.021967 -2.798325 0.295017
C 0.729893 -1.900381 1.320962
C 1.841170 -1.148108 0.651533

C 3.072170 -1.778584 0.449401
C 4.083472 -1.187326 -0.288996
C 3.889432 0.058577 -0.872694
C 2.684857 0.720396 -0.697069
C 1.706325 0.102977 0.066850
I -0.014378 1.286369 0.405660
H -3.113450 -2.782833 -1.060113
H -2.815479 1.791695 0.749476
H -5.011869 0.746303 0.453800
H -5.165871 -1.568292 -0.450095
H 0.182451 -1.426732 -1.381641
H -0.899937 -2.774170 -1.637997
H 0.745532 -3.522637 -0.085516
H -0.767790 -3.359700 0.799018
H 1.147812 -2.527343 2.108687
H 0.016560 -1.224955 1.797507
H 3.218734 -2.760177 0.885170
H 5.025814 -1.704249 -0.417692
H 4.669949 0.522041 -1.461432
H 2.525855 1.697536 -1.130672
Br 2.055104 3.539934 1.383215
SCF: -3451.784976
ZPE: 0.247907
H: -3451.520440
G: -3451.580423

10_CH2_3_adduct_conf2

C -3.074821 -1.710552 -0.458138
C -1.837079 -1.087888 -0.642215
C -1.684627 0.138990 -0.012285
C -2.651850 0.739094 0.779173
C -3.863448 0.085443 0.936313
C -4.075398 -1.135099 0.306992
C -0.736672 -1.828322 -1.342047
C -0.037210 -2.770730 -0.350666
C 0.569163 -2.066853 0.869007
C 1.775684 -1.237907 0.526745
C 3.042344 -1.820070 0.651184
C 4.206006 -1.138235 0.338752
C 4.140566 0.170587 -0.118345
C 2.904599 0.779412 -0.265106
C 1.754056 0.069250 0.056761
I 0.048053 1.312420 -0.319323
H -3.235501 -2.673206 -0.929738

H -2.478742 1.697461 1.247948
H -4.635450 0.535503 1.546308
H -5.023402 -1.645093 0.420896
H -0.016496 -1.144600 -1.795872
H -1.163739 -2.421595 -2.150671
H 0.746776 -3.320886 -0.875636
H -0.768057 -3.501422 0.002839
H 0.882336 -2.829219 1.582248
H -0.183857 -1.460595 1.375731
H 3.096518 -2.840078 1.013977
H 5.164494 -1.627290 0.455774
H 5.039642 0.720219 -0.364109
H 2.855840 1.799983 -0.629411
Br -2.007951 3.600600 -1.231495
SCF: -3451.784981
ZPE: 0.248099
H: -3451.520305
G: -3451.579899

10_CH2_3_adduct_conf3

C -2.814396 -1.397129 1.274181
C -1.876847 -1.090801 0.284247
C -1.527804 0.252980 0.168047
C -2.074550 1.254728 0.958184
C -3.010386 0.913199 1.923421
C -3.371117 -0.417985 2.083226
C -1.332825 -2.203039 -0.576930
C -0.023806 -2.860207 -0.104519
C 1.292835 -2.181813 -0.523573
C 1.783587 -1.068088 0.364130
C 2.665449 -1.364509 1.408461
C 3.173493 -0.380892 2.241943
C 2.821127 0.949712 2.055836
C 1.942198 1.288657 1.038681
C 1.451607 0.274083 0.232736
I 0.000838 0.830642 -1.184999
H -3.115244 -2.431275 1.396470
H -1.773971 2.287120 0.831425
H -3.447438 1.683323 2.545487
H -4.096998 -0.695560 2.836971
H -1.214081 -1.864210 -1.609004
H -2.095972 -2.981571 -0.598401
H -0.006220 -3.859732 -0.541411
H -0.043999 -2.993219 0.980245

H 1.213814 -1.836589 -1.557613
H 2.069287 -2.947313 -0.516136
H 2.960259 -2.397702 1.550525
H 3.856085 -0.653406 3.036662
H 3.221590 1.723975 2.696871
H 1.650349 2.318702 0.881897
Br 2.480618 1.569091 -2.938364
SCF: -3451.789415
ZPE: 0.247832
H: -3451.524922
G: -3451.584643

10_CH2_3_adduct_conf4

C -3.064279 -1.455115 -0.835281
C -2.009776 -1.090822 0.003615
C -1.544330 0.208358 -0.153783
C -2.052223 1.122632 -1.060677
C -3.103024 0.720813 -1.872437
C -3.606753 -0.567295 -1.753506
C -1.428981 -2.081912 0.976864
C 0.068870 -2.440084 0.781069
C 0.660281 -2.175680 -0.617834
C 1.702021 -1.084271 -0.726459
C 2.853178 -1.348824 -1.475386
C 3.851098 -0.405401 -1.664606
C 3.728849 0.858764 -1.108237
C 2.598516 1.165390 -0.366181
C 1.615900 0.199460 -0.184053
I 0.026082 0.858898 1.072938
H -3.458710 -2.461186 -0.758925
H -1.651240 2.124935 -1.131124
H -3.521973 1.415612 -2.588245
H -4.427199 -0.886312 -2.383601
H -2.024946 -2.989696 0.897409
H -1.573432 -1.704243 1.993228
H 0.167750 -3.503848 0.992591
H 0.676149 -1.942207 1.536974
H -0.137770 -1.955464 -1.332269
H 1.130749 -3.087694 -0.981043
H 2.960393 -2.332908 -1.916266
H 4.726210 -0.661535 -2.248199
H 4.499303 1.605574 -1.248233
H 2.490510 2.154666 0.061563
Br -2.339345 1.852083 2.880673

SCF: -3451.782634
ZPE: 0.248017
H: -3451.517867
G: -3451.577961

10_CH2_3_adduct_conf5

C -3.063242 -1.463850 -0.871781
C -2.021040 -1.100397 -0.018446
C -1.527171 0.192873 -0.171291
C -2.021498 1.099536 -1.097271
C -3.062177 0.704365 -1.925619
C -3.580173 -0.578003 -1.807249
C -1.471306 -2.093578 0.974700
C 0.035778 -2.438332 0.844943
C 0.669497 -2.195854 -0.536581
C 1.673892 -1.071840 -0.676110
C 2.794706 -1.311502 -1.483479
C 3.755182 -0.348190 -1.736031
C 3.633540 0.920120 -1.185355
C 2.545348 1.206763 -0.379253
C 1.607674 0.211684 -0.140811
I 0.017833 0.836114 1.114334
H -3.470092 -2.465147 -0.795893
H -1.608032 2.096998 -1.174757
H -3.461848 1.396851 -2.654742
H -4.391690 -0.894216 -2.450384
H -2.052445 -3.007674 0.861724
H -1.664688 -1.730628 1.987933
H 0.135511 -3.498357 1.074529
H 0.613834 -1.927181 1.615156
H -0.110239 -2.040044 -1.287851
H 1.190761 -3.100180 -0.845669
H 2.900095 -2.297320 -1.920275
H 4.602259 -0.589831 -2.365249
H 4.375030 1.684696 -1.375524
H 2.439005 2.185406 0.067580
Br 2.285785 1.684149 3.171670
SCF: -3451.781131
ZPE: 0.248061
H: -3451.516362
G: -3451.576222

10_CH2_adduct_conf1

H 2.754884 -0.738823 2.473064

C 1.856213 -0.215786 2.170711
C -0.451362 1.120393 1.357304
C 0.838186 -0.866286 1.495539
C 1.699265 1.136029 2.449479
C 0.549214 1.798611 2.040786
C -0.328128 -0.238145 1.078817
H 2.480400 1.667158 2.977549
H 0.430895 2.853595 2.252569
H -1.344940 1.642677 1.037131
I 1.024057 -2.935291 1.076830
C 0.169464 -2.612890 -0.825065
C -0.921141 -2.104710 -3.266853
C -0.876418 -1.702750 -0.878887
C 0.697313 -3.268044 -1.920236
C 0.131166 -3.004919 -3.160167
C -1.413737 -1.459278 -2.142485
H 1.511939 -3.970534 -1.813176
H 0.521122 -3.502876 -4.038125
H -2.231617 -0.754467 -2.230353
H -1.360107 -1.900372 -4.234965
Br 1.197468 -5.949606 0.363036
C -1.402472 -1.002282 0.347654
H -1.826498 -1.752395 1.026476
H -2.207265 -0.327911 0.064267
SCF: -3373.178561
ZPE: 0.190192
H: -3372.974161
G: -3373.028093

10_CMe2_adduct_conf1

H 2.810325 -0.746444 2.409689
C 1.896782 -0.223705 2.153396
C -0.432355 1.096566 1.442681
C 0.881408 -0.861532 1.459221
C 1.730224 1.105918 2.509725
C 0.564406 1.760411 2.145501
C -0.312462 -0.249477 1.085465
H 2.510906 1.621212 3.053640
H 0.423121 2.801772 2.405180
H -1.320620 1.648964 1.175164
I 1.232365 -2.886443 0.969706
C 0.207252 -2.603750 -0.851032
C -0.956974 -2.204729 -3.273688
C -0.869959 -1.720636 -0.882597

C 0.721471 -3.271105 -1.947294
C 0.119612 -3.071170 -3.179694
C -1.433441 -1.543660 -2.151274
H 1.565115 -3.939105 -1.844507
H 0.502473 -3.583297 -4.052479
H -2.270222 -0.873137 -2.273177
H -1.434460 -2.032256 -4.229706
Br 1.653204 -5.888408 0.264342
C -1.436630 -0.998096 0.351599
C -2.102136 -2.019804 1.302399
H -1.433442 -2.786117 1.685874
H -2.913384 -2.520817 0.772521
H -2.520864 -1.486078 2.156623
C -2.553193 -0.032609 -0.051333
H -2.206857 0.751995 -0.724992
H -2.972773 0.431474 0.839987
H -3.359494 -0.581734 -0.535239
SCF: -3451.785691
ZPE: 0.247013
H: -3451.521877
G: -3451.580701

10_CO_adduct_conf1

H 2.733388 -0.745916 2.581543
C 1.845001 -0.212866 2.265013
C -0.445179 1.158529 1.473128
C 0.926504 -0.794812 1.409022
C 1.613307 1.081910 2.711968
C 0.470374 1.765006 2.316579
C -0.227902 -0.137771 1.004674
H 2.332190 1.553618 3.369296
H 0.293487 2.773472 2.666431
H -1.338589 1.681182 1.156972
I 1.247813 -2.827351 0.909714
C 0.250536 -2.571941 -0.929006
C -1.092777 -2.341101 -3.308718
C -0.793957 -1.657930 -1.005380
C 0.647272 -3.359606 -1.990418
C -0.032753 -3.228846 -3.194739
C -1.467473 -1.566388 -2.224994
H 1.457753 -4.066957 -1.888631
H 0.275931 -3.828240 -4.041205
H -2.285416 -0.862393 -2.303571
H -1.624857 -2.246662 -4.246002

C -1.238705 -0.713733 0.070542
Br 1.618291 -5.785735 0.315020
O -2.386741 -0.338574 0.104061
SCF: -3447.195166
ZPE: 0.171305
H: -3447.008964
G: -3447.064679

10_NAc_adduct_conf1

H 3.155115 0.141904 2.695872
C 2.365847 0.765474 2.294924
C 0.335507 2.367043 1.225578
C 1.307772 0.214702 1.593032
C 2.388880 2.141652 2.476725
C 1.377232 2.933414 1.945092
C 0.292162 0.989276 1.052610
H 3.202956 2.594106 3.027551
H 1.404731 4.006418 2.083385
H -0.446620 2.980102 0.798746
I 1.143218 -1.879970 1.323579
C 0.507074 -1.519482 -0.643406
C -0.324058 -0.891032 -3.169592
C -0.342790 -0.432240 -0.806602
C 0.964702 -2.290431 -1.692624
C 0.527135 -1.970670 -2.970652
C -0.744565 -0.115946 -2.100240
H 1.627218 -3.126864 -1.519193
H 0.865119 -2.563804 -3.809973
H -1.385520 0.742915 -2.252173
H -0.651241 -0.638402 -4.169594
Br 0.804810 -4.840679 0.756329
N -0.745922 0.355770 0.306697
C -2.071847 0.504320 0.700472
O -2.357360 1.225358 1.631366
C -3.102221 -0.286600 -0.055606
H -2.758605 -1.294842 -0.283128
H -3.339400 0.214705 -0.995068
H -3.999429 -0.326291 0.556192
SCF: -3541.876221
ZPE: 0.215849
H: -3541.642888
G: -3541.703960

10_NH_adduct_conf1

H 2.798397 0.468084 2.501793
C 1.865340 0.946294 2.229632
C -0.546897 2.149751 1.522779
C 0.920264 0.269578 1.475578
C 1.586900 2.237524 2.651067
C 0.374240 2.825503 2.304352
C -0.282131 0.848800 1.089994
H 2.308429 2.775999 3.250570
H 0.148932 3.831532 2.634427
H -1.478681 2.619322 1.230725
I 1.193634 -1.765581 1.006760
C 0.249718 -1.452064 -0.837059
C -1.135653 -1.112640 -3.165991
C -0.819270 -0.562522 -0.833029
C 0.676986 -2.128948 -1.965100
C -0.029335 -1.956577 -3.144163
C -1.518686 -0.415497 -2.035647
H 1.519406 -2.804480 -1.912645
H 0.278168 -2.487594 -4.034762
H -2.361249 0.265344 -2.063096
H -1.697516 -0.982222 -4.081931
Br 1.477879 -4.738318 0.279347
N -1.210512 0.160990 0.298129
H -2.057862 0.693722 0.140970
SCF: -3389.225966
ZPE: 0.178787
H: -3389.033056
G: -3389.086878

10_O_adduct_conf1

H 0.802034 0.147975 0.125183
C 0.452732 0.035533 1.142153
C -0.498719 -0.262406 3.754742
C -0.500727 -0.913212 1.458718
C 0.921627 0.856489 2.157574
C 0.439378 0.711916 3.452985
C -0.974561 -1.092253 2.749915
H 1.662626 1.610700 1.929470
H 0.804194 1.358147 4.240596
H -0.875279 -0.397706 4.760353
O -1.923452 -2.031913 3.071991
C -1.648082 -3.346449 2.756307
C -1.157008 -6.004630 2.140270
C -1.308018 -3.721178 1.468210

C -1.751325 -4.305492 3.750628
C -1.512345 -5.634822 3.432217
C -1.048368 -5.042425 1.144968
H -2.017277 -4.000085 4.754362
H -1.596814 -6.387816 4.204988
H -0.775471 -5.323518 0.135177
H -0.964360 -7.042481 1.903289
I -1.299723 -2.193336 0.006580
Br -1.263365 0.115961 -1.926376
SCF: -3409.079562
ZPE: 0.165528
H: -3408.900083
G: -3408.953494

10_SO2_adduct_conf1
H 2.803264 0.386921 2.382562
C 1.875755 0.905375 2.172879
C -0.489730 2.282173 1.592150
C 0.815532 0.254739 1.572189
C 1.740388 2.252934 2.498118
C 0.570215 2.936846 2.207238
C -0.363171 0.934859 1.294594
H 2.567087 2.767553 2.970175
H 0.478405 3.986119 2.453902
H -1.406676 2.804038 1.351555
I 1.039019 -1.819757 1.105943
C 0.122631 -1.502327 -0.767740
C -1.003094 -1.011901 -3.231258
C -0.985969 -0.670215 -0.858887
C 0.687823 -2.084047 -1.881654
C 0.105779 -1.835340 -3.121410
C -1.547019 -0.416371 -2.101409
H 1.556928 -2.721008 -1.797132
H 0.540473 -2.286688 -4.003506
H -2.405639 0.238129 -2.171408
H -1.446365 -0.822363 -4.199629
Br 1.290383 -4.685110 0.355083
S -1.725031 0.071907 0.571466
O -2.710090 1.021366 0.139741
O -2.110899 -0.987931 1.466436
SCF: -3882.478325
ZPE: 0.172222
H: -3882.289921
G: -3882.347876

10_SO_adduct_conf1
H 2.711636 0.303373 2.423014
C 1.794704 0.831381 2.192027
C -0.561211 2.213051 1.563391
C 0.703957 0.170380 1.656902
C 1.692636 2.199654 2.424167
C 0.527252 2.884266 2.108008
C -0.460203 0.850242 1.344798
H 2.535847 2.729314 2.847752
H 0.461268 3.949652 2.285797
H -1.478048 2.730314 1.309902
I 0.806173 -1.925199 1.272469
C 0.007493 -1.565958 -0.645222
C -1.008060 -0.956400 -3.116206
C -1.074641 -0.711601 -0.737962
C 0.613181 -2.118035 -1.755336
C 0.084445 -1.805576 -3.002769
C -1.594278 -0.404542 -1.985079
H 1.464183 -2.778133 -1.659213
H 0.539672 -2.229972 -3.887802
H -2.447076 0.259292 -2.052397
H -1.409093 -0.719631 -4.092925
Br 0.855316 -4.821526 0.529145
S -1.889325 -0.042435 0.721260
O -2.876030 0.958092 0.256281
SCF: -3807.243893
ZPE: 0.166407
H: -3807.061932
G: -3807.118649

10_SO_adduct_conf2
H 2.661689 0.391275 2.425752
C 1.750587 0.923658 2.181592
C -0.575645 2.324529 1.522582
C 0.682781 0.278287 1.588516
C 1.645245 2.287090 2.449165
C 0.495125 2.984590 2.115341
C -0.478764 0.965256 1.267098
H 2.477563 2.800365 2.912814
H 0.423401 4.044408 2.320768
H -1.483772 2.859127 1.270299
I 0.859612 -1.800656 1.161774
C -0.016451 -1.467514 -0.724781

C -1.072719 -0.916698 -3.202764
C -1.098780 -0.606170 -0.820257
C 0.553900 -2.058045 -1.831998
C 0.008578 -1.774763 -3.081428
C -1.630107 -0.331630 -2.072894
H 1.399313 -2.724835 -1.734836
H 0.446891 -2.229404 -3.960095
H -2.483606 0.330229 -2.157189
H -1.490583 -0.702772 -4.177490
Br 1.062819 -4.708138 0.407507
S -1.914334 0.123993 0.601557
O -2.222742 -0.992184 1.538966
SCF: -3807.241025
ZPE: 0.166551
H: -3807.058905
G: -3807.115627

11_adduct_conf1
H 0.347371 0.406718 0.041625
C 0.146921 0.202397 1.084436
C -0.372256 -0.270456 3.795829
C -0.737683 -0.776883 1.492069
C 0.748565 0.944549 2.080196
C 0.501622 0.736128 3.424370
C -0.998935 -1.042148 2.827449
H 0.996664 1.350783 4.164200
H -0.583152 -0.471336 4.837988
O -1.882333 -2.013581 3.230747
C -1.633034 -3.301214 2.801243
C -1.194355 -5.871417 1.967359
C -1.492270 -3.589263 1.455845
C -1.557828 -4.317598 3.740104
C -1.344359 -5.620426 3.318366
C -1.258559 -4.878335 1.009371
H -1.668319 -4.080692 4.790197
H -1.284560 -6.436770 4.025755
H -1.138022 -5.122965 -0.038563
I -1.742606 -1.977408 0.101827
F -0.977129 -7.133838 1.564823
F 1.606874 1.910533 1.721272
Br -2.027516 0.425223 -1.622205
SCF: -3607.578912
ZPE: 0.148905
H: -3607.414378

G: -3607.471596

Ph2I_adduct_conf1
C -1.699059 0.042197 0.616906
C -1.755995 0.098347 3.362026
C -1.540411 -1.147365 1.312029
C -1.891162 1.257744 1.255261
C -1.918947 1.276228 2.644701
C -1.566971 -1.108873 2.699952
H -1.397197 -2.086000 0.791634
H -2.015604 2.174010 0.692265
H -2.067172 2.215247 3.162236
H -1.442492 -2.026002 3.261147
H -1.777966 0.120178 4.444110
I -1.655207 0.003622 -1.500621
C 0.441476 -0.038605 -1.593573
C 3.170965 -0.095348 -1.671607
C 1.063426 -1.258004 -1.792669
C 1.124090 1.153430 -1.432046
C 2.512392 1.111165 -1.472747
C 2.452060 -1.273352 -1.830661
H 0.495293 -2.169577 -1.921138
H 0.602668 2.089549 -1.281854
H 3.073810 2.028369 -1.351301
H 2.967154 -2.212414 -1.985927
H 4.252610 -0.117771 -1.704258
Br -1.425763 -0.036579 -4.617567
SCF: -3335.056678
ZPE: 0.182191
H: -3334.859696
G: -3334.917915

1_CF3_cis_TS_conf1
C 0.201077 1.574819 -1.847917
C 0.053268 1.707149 0.932509
C -0.028925 0.454711 -1.077383
C 0.298271 2.799206 -1.188612
C 0.207828 2.869518 0.191201
C -0.046350 0.463528 0.312663
H 0.439206 3.696046 -1.779905
H 0.288371 3.824747 0.690597
H 0.040621 1.747221 2.015105
C -0.087632 -0.811305 1.031634
C -0.020508 -3.312373 2.292229

C 0.407493 -1.951617 0.397786
C -0.566445 -0.963326 2.331430
C -0.532054 -2.202475 2.952705
C 0.458207 -3.196175 0.992345
H -0.981625 -0.106566 2.847270
H -0.913643 -2.303936 3.960219
H 0.004792 -4.277073 2.781587
I 1.086191 -1.631494 -1.550758
Br -2.191570 -0.555324 -1.858351
H 0.854293 -4.056824 0.470804
C 0.242472 1.556462 -3.346361
F -0.918413 1.933106 -3.895503
F 1.173209 2.397288 -3.815674
F 0.531665 0.344886 -3.839723
SCF: -3670.910247
ZPE: 0.164681
H: -3670.729397
G: -3670.787367

1_CF3_trans_TS_conf1

C -0.054049 2.384725 -2.317166
C -0.025769 2.491438 0.488760
C -0.197517 1.284643 -1.514315
C 0.062558 3.599330 -1.647114
C 0.063604 3.654672 -0.256289
C -0.142579 1.244867 -0.137480
C -0.140384 -0.042689 0.556249
C -0.056597 -2.547125 1.801418
C 0.321145 -1.173348 -0.120343
C -0.567009 -0.198940 1.875140
C -0.524067 -1.436321 2.489644
C 0.370488 -2.421275 0.486993
I 0.934450 -0.824200 -2.089320
Br -2.406517 0.163916 -2.240053
H -0.080245 2.326569 -3.395403
H 0.146160 4.505550 -2.233764
H 0.159639 4.607509 0.246170
H 0.026210 2.524622 1.570471
H -0.950723 0.660379 2.410361
H -0.863676 -1.543603 3.510840
H -0.026450 -3.514722 2.282296
C 0.863329 -3.637289 -0.251225
F 0.084023 -3.932277 -1.302814
F 2.102920 -3.458531 -0.736468

F 0.900855 -4.718105 0.523313
SCF: -3670.906934
ZPE: 0.164482
H: -3670.726177
G: -3670.785063

1_CN_cis_TS_conf1

C 0.145818 1.718613 -2.157104
C 0.004489 1.869708 0.619493
C -0.056817 0.589811 -1.373153
C 0.206508 2.958265 -1.512244
C 0.114595 3.032025 -0.133899
C -0.055944 0.616020 0.016001
H 0.324490 3.848168 -2.116769
H 0.164211 3.992652 0.358874
H -0.004761 1.921189 1.701839
C -0.044200 -0.659722 0.731674
C 0.116627 -3.172077 1.961338
C 0.463415 -1.782066 0.075236
C -0.484796 -0.837012 2.041364
C -0.402989 -2.081679 2.647273
C 0.559268 -3.031721 0.650697
H -0.907353 0.003931 2.576956
H -0.754703 -2.203133 3.663373
H 0.177866 -4.140949 2.439037
I 1.106946 -1.421915 -1.884861
Br -2.191212 -0.437715 -2.126858
H 0.961298 -3.877398 0.109804
C 0.231963 1.607432 -3.574907
N 0.324982 1.487374 -4.713363
SCF: -3426.070093
ZPE: 0.158259
H: -3425.897325
G: -3425.951494

1_CN_trans_TS_conf1

C -0.003957 2.033270 -2.358743
C 0.044149 2.166411 0.447663
C -0.136755 0.943742 -1.542467
C 0.114555 3.254499 -1.699814
C 0.124587 3.322315 -0.309782
C -0.072137 0.913666 -0.165894
C -0.057556 -0.369111 0.535342
C 0.071034 -2.881244 1.784123

C 0.384197 -1.496283 -0.154386
C -0.443107 -0.531613 1.866013
C -0.379317 -1.771606 2.480410
C 0.458177 -2.746697 0.451470
I 0.945582 -1.190954 -2.134552
Br -2.390974 -0.169061 -2.221274
H -0.039608 1.964821 -3.436069
H 0.191376 4.155394 -2.295446
H 0.220613 4.280264 0.182848
H 0.101955 2.209384 1.528743
H -0.810920 0.325182 2.416486
H -0.688663 -1.876824 3.511305
H 0.125498 -3.853793 2.253873
C 0.929368 -3.888362 -0.273594
N 1.311805 -4.793395 -0.866358
SCF: -3426.067496
ZPE: 0.158221
H: -3425.894727
G: -3425.949184

1_F_cis_TS_conf1
H -0.473664 1.708520 -3.454668
C -0.378588 1.788112 -2.381657
C -0.083857 1.951796 0.407536
C -0.124032 0.711395 -1.577673
C -0.441746 3.014504 -1.724090
C -0.280875 3.097530 -0.344281
C -0.018700 0.693701 -0.203274
H -0.611992 3.906697 -2.313477
H -0.334700 4.058945 0.148092
H -0.007213 2.005004 1.487079
C 0.075612 -0.580677 0.507876
C 0.125871 -3.101030 1.748657
C -0.427855 -1.716129 -0.130908
C 0.612441 -0.733414 1.783234
C 0.634932 -1.980467 2.390947
C -0.405586 -2.949228 0.483604
H 1.027656 0.127062 2.291370
H 1.060710 -2.085896 3.379800
H 0.135218 -4.081688 2.205596
I -1.228571 -1.464206 -2.024123
Br 2.055772 -0.362069 -2.519712
F -0.911031 -4.008363 -0.159626
SCF: -3433.070061

ZPE: 0.151442
H: -3432.905059
G: -3432.957169
1_F_trans_TS_conf1
C 0.065929 1.803925 -2.398398
C 0.077309 1.951812 0.406787
C -0.070416 0.718378 -1.577750
C 0.170197 3.029639 -1.745053
C 0.160971 3.104505 -0.355428
C -0.023330 0.694246 -0.200252
C -0.005567 -0.584094 0.509665
C 0.149889 -3.107988 1.734587
C 0.452876 -1.704124 -0.187683
C -0.391935 -0.754344 1.836276
C -0.313662 -2.003086 2.435747
C 0.532517 -2.938702 0.418960
I 1.032237 -1.425074 -2.156650
Br -2.311137 -0.406348 -2.283955
H 0.043478 1.729232 -3.475639
H 0.250457 3.927633 -2.344611
H 0.244412 4.065565 0.133514
H 0.119403 1.999471 1.488430
H -0.769480 0.093007 2.393670
H -0.623502 -2.122075 3.465374
H 0.217591 -4.089572 2.184551
F 0.991759 -3.982006 -0.282140
SCF: -3433.070056
ZPE: 0.151398
H: -3432.905085
G: -3432.957225

1_H_TS_conf1
C 0.068137 1.708672 -2.183857
C 0.035056 1.862212 0.618602
C -0.074004 0.620936 -1.365090
C 0.152453 2.936838 -1.533053
C 0.121441 3.014804 -0.143887
C -0.048017 0.602478 0.013533
H 0.234972 3.834138 -2.133397
H 0.190389 3.977320 0.344525
H 0.062245 1.912698 1.700709
C -0.032633 -0.672988 0.728958
C 0.107458 -3.173375 1.983889

C 0.456629 -1.805351 0.073991
C -0.462741 -0.832100 2.044791
C -0.392185 -2.070547 2.664367
C 0.539810 -3.048769 0.668511
H -0.869499 0.019829 2.575354
H -0.736207 -2.176705 3.684873
H 0.161168 -4.138664 2.469900
I 1.093026 -1.497178 -1.893112
Br -2.263120 -0.533394 -2.118247
H 0.927714 -3.904882 0.133598
H 0.064006 1.631532 -3.261158
SCF: -3333.820752
ZPE: 0.159602
H: -3333.648474
G: -3333.698502

1_NMe2_cis_TS_conf1

C 0.247792 1.349037 -1.232797
C -0.102247 1.575112 1.582116
C 0.121290 0.274391 -0.370746
C 0.157095 2.591247 -0.580509
C -0.028480 2.706346 0.785515
C -0.018076 0.306433 1.004540
H 0.231895 3.475403 -1.203170
H -0.086932 3.688395 1.235545
H -0.191816 1.655835 2.657866
C -0.034889 -0.934800 1.784569
C 0.061493 -3.347862 3.208718
C 0.587740 -2.073210 1.273494
C -0.630281 -1.044609 3.040797
C -0.580914 -2.238391 3.743739
C 0.654934 -3.273508 1.954763
H -1.149524 -0.191665 3.459024
H -1.054115 -2.304999 4.714660
H 0.098798 -4.278352 3.759814
I 1.428908 -1.848568 -0.616931
Br -1.914636 -1.025567 -1.332734
H 1.151229 -4.134701 1.528433
N 0.384946 1.322128 -2.625222
C -0.728116 1.878720 -3.389306
C 0.978778 0.162825 -3.257939
H -1.526160 1.139605 -3.527644
H -0.364361 2.193114 -4.368271
H -1.140797 2.746329 -2.879293

H 0.344127 -0.731687 -3.215525
H 1.143021 0.405709 -4.308116
H 1.959095 -0.042506 -2.825391
SCF: -3467.774382
ZPE: 0.233003
H: -3467.524581
G: -3467.582948

1_NMe2_trans_TS_conf1

C -0.213488 3.058944 -2.393931
C -0.129825 3.308739 0.398076
C -0.339918 1.996439 -1.537176
C -0.083426 4.307033 -1.791700
C -0.056713 4.433944 -0.406020
C -0.258119 2.031261 -0.159076
C -0.225535 0.780497 0.600766
C 0.006038 -1.667928 1.932976
C 0.213160 -0.374689 -0.043903
C -0.554614 0.681614 1.951851
C -0.426566 -0.532669 2.605762
C 0.330584 -1.614763 0.575992
I 0.826529 -0.144706 -2.024440
Br -2.515609 0.827968 -2.181748
H -0.260746 2.946139 -3.467141
H -0.011129 5.181749 -2.425875
H 0.047403 5.411183 0.045610
H -0.055084 3.397991 1.475245
H -0.908781 1.555643 2.482970
H -0.679870 -0.603094 3.655799
H 0.084835 -2.609045 2.460588
N 0.770067 -2.733801 -0.167609
C -0.293560 -3.331386 -0.978757
C 1.465337 -3.756586 0.600723
H -1.004114 -3.883399 -0.349538
H 0.151221 -4.020968 -1.696523
H -0.843370 -2.565656 -1.524267
H 0.790573 -4.334510 1.245252
H 1.935496 -4.447472 -0.099387
H 2.239420 -3.298570 1.215277
SCF: -3467.779069
ZPE: 0.232888
H: -3467.529406
G: -3467.588150

1_OMe_cis_TS_conf1

C 0.120642 1.388076 -1.614702
C -0.202650 1.473481 1.184162
C -0.112951 0.262675 -0.839441
C 0.107804 2.601097 -0.933778
C -0.071627 2.636352 0.450647
C -0.198587 0.231976 0.532507
H 0.236241 3.522159 -1.486473
H -0.072448 3.593512 0.954591
H -0.268435 1.498558 2.264672
C -0.169909 -1.071342 1.198149
C 0.041805 -3.611068 2.362811
C 0.442246 -2.141998 0.540090
C -0.685432 -1.314861 2.469571
C -0.579759 -2.572579 3.044183
C 0.562817 -3.402163 1.090643
H -1.184475 -0.512882 2.999156
H -0.991215 -2.744687 4.030223
H 0.123514 -4.591042 2.814351
I 1.203487 -1.710593 -1.364499
Br -2.129799 -0.859651 -1.825514
H 1.046931 -4.207749 0.555581
O 0.320903 1.209144 -2.929873
C 0.567821 2.370258 -3.714328
H 1.461434 2.892121 -3.366012
H -0.290263 3.044825 -3.686549
H 0.721804 2.016281 -4.729970
SCF: -3448.347053
ZPE: 0.192780
H: -3448.139004
G: -3448.194747

1_OMe_trans_TS_conf1

C -0.745338 2.828417 -2.109767
C -0.182316 2.738968 0.637996
C -0.666590 1.665448 -1.390371
C -0.569020 3.998883 -1.376711
C -0.305506 3.956155 -0.010839
C -0.343282 1.533635 -0.055345
C -0.114572 0.205395 0.515339
C 0.426363 -2.386349 1.441431
C 0.275203 -0.815598 -0.346136
C -0.238045 -0.096039 1.870879
C 0.030513 -1.380012 2.314547

C 0.557384 -2.108683 0.081963
I 0.454111 -0.333165 -2.358082
Br -2.900763 0.456785 -1.782941
H -0.979725 2.845910 -3.164034
H -0.650681 4.947554 -1.892309
H -0.171091 4.875795 0.542341
H 0.074115 2.698326 1.690004
H -0.559585 0.669626 2.564268
H -0.073597 -1.613107 3.366372
H 0.629005 -3.379123 1.817126
O 0.941020 -2.992956 -0.855592
C 1.222202 -4.325077 -0.438968
H 0.339444 -4.783704 0.009864
H 2.052568 -4.341921 0.269174
H 1.498084 -4.865462 -1.340211
SCF: -3448.349558
ZPE: 0.192634
H: -3448.141652
G: -3448.197434

2_CF3_cis_TS_conf1

C -0.007135 1.195174 -2.070994
C 0.070330 1.362127 0.729409
C -0.148596 0.102331 -1.249470
C 0.126878 2.414403 -1.423945
C 0.150329 2.510383 -0.034528
C -0.061241 0.105182 0.129948
H 0.258991 3.475891 0.442128
H 0.139106 1.418818 1.808682
C -0.040704 -1.167427 0.849968
C 0.114571 -3.669564 2.096864
C 0.393288 -2.309241 0.173218
C -0.407350 -1.317553 2.185721
C -0.329933 -2.557857 2.800673
C 0.484202 -3.554224 0.761446
H -0.769925 -0.458455 2.736359
H -0.624831 -2.658303 3.836938
H 0.173667 -4.635753 2.580397
I 0.935718 -2.002591 -1.822937
Br -2.375370 -0.945895 -1.894468
H 0.828204 -4.417782 0.208911
H -0.048599 1.117724 -3.147487
C 0.251546 3.676717 -2.229981
F -0.708098 4.560432 -1.919121

F 1.420963 4.294518 -2.002890
F 0.173887 3.460845 -3.545140
SCF: -3670.910368
ZPE: 0.164416
H: -3670.729607
G: -3670.789504

2_CF3_trans_TS_conf1

C -0.180803 2.376951 -2.734257
C 0.234313 2.534162 0.039502
C -0.271093 1.302104 -1.891333
C 0.091910 3.594936 -2.117380
C 0.284142 3.676062 -0.741129
C -0.031719 1.284514 -0.532878
C -0.002403 0.011211 0.183939
C 0.134730 -2.484433 1.418090
C 0.287627 -1.153950 -0.534987
C -0.231717 -0.117124 1.550076
C -0.163403 -1.357165 2.166522
C 0.365225 -2.398426 0.048558
I 0.622912 -0.889658 -2.576896
Br -2.639862 0.318225 -2.257665
H 0.597066 -3.286125 -0.526221
H -0.358608 2.301685 -3.797020
H 0.144313 4.483830 -2.733429
H 0.497924 4.631339 -0.281333
H 0.432911 2.584003 1.103455
H -0.481770 0.759495 2.133496
H -0.350492 -1.439635 3.228250
C 0.227875 -3.839444 2.059176
F 1.464108 -4.352908 1.956936
F -0.077504 -3.814975 3.358232
F -0.595781 -4.724573 1.478198
SCF: -3670.910374
ZPE: 0.164398
H: -3670.729604
G: -3670.789699

2_CN_cis_TS_conf1

C 0.058250 1.536225 -2.267078
C 0.044447 1.700586 0.535760
C -0.090141 0.439722 -1.456879
C 0.149699 2.764366 -1.610574
C 0.126091 2.856201 -0.217525

C -0.043566 0.445488 -0.071723
H 0.199866 3.822297 0.261131
H 0.078490 1.754352 1.616762
C -0.019930 -0.828397 0.645268
C 0.145332 -3.331233 1.888226
C 0.453433 -1.959899 -0.022377
C -0.421142 -0.989341 1.969834
C -0.338930 -2.230287 2.582666
C 0.550792 -3.204883 0.564161
H -0.815075 -0.139152 2.512559
H -0.661304 -2.339906 3.609735
H 0.207839 -4.297979 2.370199
I 1.047296 -1.636028 -2.000979
Br -2.276109 -0.643453 -2.154297
H 0.925845 -4.060143 0.019000
H 0.054652 1.471842 -3.345426
C 0.265216 3.956947 -2.399916
N 0.358851 4.912575 -3.028428
SCF: -3426.070376
ZPE: 0.158319
H: -3425.897561
G: -3425.951971

2_CN_trans_TS_conf1

C 0.029604 2.040595 -2.539057
C 0.067001 2.185716 0.266281
C -0.094160 0.948640 -1.722319
C 0.132829 3.264804 -1.884760
C 0.137284 3.339297 -0.494429
C -0.031970 0.929136 -0.343772
C -0.003753 -0.347807 0.363541
C 0.155129 -2.844510 1.593839
C 0.453287 -1.479882 -0.320094
C -0.390223 -0.507231 1.693207
C -0.312472 -1.742708 2.308259
C 0.545189 -2.725137 0.259441
I 1.028371 -1.163636 -2.299445
Br -2.318458 -0.182722 -2.402311
H 0.904003 -3.588871 -0.282910
H -0.002015 1.968976 -3.616305
H 0.202119 4.164309 -2.483487
H 0.220845 4.300348 -0.005672
H 0.120368 2.232771 1.347365
H -0.769985 0.343121 2.244442

H -0.618515 -1.860527 3.338799
C 0.238787 -4.125460 2.232798
N 0.306735 -5.149324 2.746691
SCF: -3426.070636
ZPE: 0.158262
H: -3425.897846
G: -3425.952386

2_F_cis_TS_conf1

C 0.066529 1.774328 -2.405579
C 0.062613 1.930437 0.395014
C -0.074093 0.677745 -1.591355
C 0.158035 2.980532 -1.734645
C 0.143566 3.090678 -0.354072
C -0.027372 0.672728 -0.208511
H 0.223532 4.063336 0.110491
H 0.101034 1.983367 1.476365
C 0.000553 -0.602370 0.506132
C 0.164113 -3.112185 1.743145
C 0.477619 -1.732204 -0.161267
C -0.404402 -0.770048 1.828995
C -0.321098 -2.012440 2.439189
C 0.571353 -2.980305 0.420458
H -0.800988 0.078158 2.373160
H -0.645022 -2.124444 3.465648
H 0.226336 -4.080213 2.222533
I 1.080781 -1.398329 -2.135996
Br -2.255466 -0.433066 -2.306019
H 0.947886 -3.832990 -0.127869
H 0.046529 1.730790 -3.484888
F 0.257658 4.096495 -2.471031
SCF: -3433.071590
ZPE: 0.151331
H: -3432.906748
G: -3432.958756

2_F_trans_TS_conf1

C 0.062105 1.805351 -2.414335
C 0.081448 1.950976 0.389427
C -0.065592 0.717900 -1.594273
C 0.158990 3.031895 -1.761564
C 0.154017 3.105306 -0.371964
C -0.014195 0.692757 -0.217075
C 0.008621 -0.585953 0.491585

C 0.151871 -3.063622 1.716390
C 0.471852 -1.718009 -0.182253
C -0.390293 -0.748665 1.817172
C -0.320978 -1.984666 2.437617
C 0.558044 -2.967528 0.398088
I 1.070382 -1.408401 -2.156726
Br -2.285239 -0.431652 -2.305026
H 0.919244 -3.842041 -0.125375
H 0.037746 1.730376 -3.491515
H 0.230345 3.930782 -2.360882
H 0.232319 4.066354 0.117935
H 0.128257 1.999358 1.470926
H -0.774988 0.102084 2.365126
H -0.634595 -2.119775 3.463977
F 0.220742 -4.262731 2.312641
SCF: -3433.071469
ZPE: 0.151270
H: -3432.906647
G: -3432.958806

2_NMe2_cis_TS_conf1

C 0.222469 0.373368 -1.618040
C -0.319153 0.686616 1.105053
C 0.090213 -0.651510 -0.735124
C 0.056905 1.677624 -1.085634
C -0.243068 1.796457 0.295234
C -0.119110 -0.618369 0.624205
H -0.386359 2.771503 0.735227
H -0.495781 0.815768 2.167049
C -0.047659 -1.826385 1.434957
C 0.185877 -4.218589 2.887652
C 0.678314 -2.921562 0.957742
C -0.661676 -1.969719 2.680109
C -0.542352 -3.150234 3.396914
C 0.807234 -4.110421 1.649213
H -1.249581 -1.151172 3.076645
H -1.030874 -3.240836 4.358463
H 0.273938 -5.139986 3.448085
I 1.610059 -2.633977 -0.889786
Br -1.766910 -2.190179 -1.769646
H 1.378621 -4.935579 1.245897
H 0.353089 0.197500 -2.673744
N 0.157154 2.766090 -1.887062
C -0.196278 4.076850 -1.373085

C 0.462555 2.606207 -3.294772
H -1.223892 4.095107 -0.999152
H -0.107901 4.802839 -2.175921
H 0.470788 4.378045 -0.561583
H 1.387456 2.040739 -3.430180
H -0.340354 2.086411 -3.828203
H 0.596073 3.587596 -3.740311
SCF: -3467.784371
ZPE: 0.232749
H: -3467.534331
G: -3467.595302

2_NMe2_trans_TS_conf1

C -0.368413 2.992961 -3.308291
C 0.541516 3.234140 -0.665908
C -0.448604 1.994403 -2.378247
C 0.165576 4.193855 -2.844409
C 0.600538 4.316510 -1.528672
C 0.019458 2.001278 -1.081247
C 0.012772 0.777242 -0.288687
C 0.044680 -1.703524 1.120689
C 0.010504 -0.459311 -0.932994
C 0.028645 0.730742 1.106894
C 0.043501 -0.462041 1.797720
C 0.028245 -1.676950 -0.293405
I 0.030776 -0.369136 -3.025437
Br -2.957357 1.321305 -2.309356
H 0.034556 -2.594340 -0.861319
H -0.739084 2.883372 -4.316859
H 0.225559 5.031472 -3.527766
H 1.012059 5.254928 -1.181964
H 0.928908 3.313725 0.343145
H 0.010545 1.659653 1.664407
H 0.044778 -0.434782 2.877190
N 0.059659 -2.881421 1.795090
C 0.045621 -4.135008 1.068012
C 0.114497 -2.886594 3.243812
H -0.840796 -4.215288 0.432435
H 0.030669 -4.955001 1.779840
H 0.931830 -4.242181 0.434932
H -0.766155 -2.406677 3.680251
H 0.150769 -3.915584 3.589178
H 1.004745 -2.367947 3.610869
SCF: -3467.783492

ZPE: 0.232728
H: -3467.533455
G: -3467.595027

2_OMe_cis_TS_conf1

C 0.390441 1.193570 -1.698100
C 0.125315 1.226613 1.091940
C -0.008920 0.114644 -0.952415
C 0.626705 2.363658 -0.972339
C 0.477256 2.375927 0.422358
C -0.113609 0.019277 0.415497
H 0.669557 3.295577 0.957878
H 0.058455 1.231043 2.173630
C -0.371081 -1.269312 1.050987
C -0.761819 -3.818930 2.152514
C -0.024421 -2.437363 0.367261
C -0.931848 -1.418992 2.318618
C -1.122441 -2.680344 2.862049
C -0.204793 -3.704963 0.884016
H -1.232912 -0.537331 2.870591
H -1.563420 -2.775588 3.845745
H -0.912816 -4.801818 2.579168
I 0.834101 -2.140514 -1.515621
Br -2.271244 -0.598059 -1.971795
H 0.079074 -4.586746 0.325752
H 0.449379 1.153624 -2.774526
O 0.987192 3.523446 -1.545938
C 1.167669 3.549078 -2.955555
H 0.233264 3.317223 -3.471404
H 1.944113 2.844353 -3.260689
H 1.476802 4.561829 -3.199423
SCF: -3448.348967
ZPE: 0.192557
H: -3448.141159
G: -3448.197017

2_OMe_cis_TS_conf2

C -0.006735 0.950665 -2.094521
C 0.041715 1.054705 0.694595
C -0.150853 -0.143404 -1.295945
C 0.129892 2.178176 -1.431231
C 0.136616 2.228891 -0.034335
C -0.085402 -0.194293 0.084422
H 0.242717 3.168475 0.486319

H 0.101690 1.093150 1.776164
C -0.070232 -1.480750 0.775191
C 0.051924 -4.014794 1.970902
C 0.367250 -2.611353 0.081354
C -0.453837 -1.660571 2.103437
C -0.390056 -2.913668 2.693423
C 0.437243 -3.870740 0.643120
H -0.817820 -0.811087 2.668139
H -0.696079 -3.033126 3.724599
H 0.097792 -4.991886 2.433499
I 0.955177 -2.267253 -1.895373
Br -2.382190 -1.239148 -1.999795
H 0.782165 -4.723411 0.074192
H -0.057129 0.913595 -3.172989
O 0.236955 3.253349 -2.230391
C 0.358711 4.530597 -1.616118
H 1.261902 4.584127 -1.005266
H -0.516866 4.752607 -1.002988
H 0.425451 5.247147 -2.430401
SCF: -3448.348207
ZPE: 0.192526
H: -3448.140407
G: -3448.196306

2_OMe_trans_TS_conf1

C -0.063103 2.748858 -2.594787
C 0.010539 2.815536 0.209922
C -0.200821 1.643003 -1.801848
C 0.073758 3.955267 -1.911490
C 0.094327 3.989288 -0.520718
C -0.123214 1.575514 -0.427159
C -0.106837 0.278884 0.245459
C 0.035321 -2.272777 1.420808
C 0.320387 -0.843881 -0.455344
C -0.474124 0.078985 1.579592
C -0.405916 -1.169314 2.158235
C 0.406313 -2.114201 0.085380
I 0.888087 -0.498422 -2.437388
Br -2.448629 0.558177 -2.514144
H 0.748472 -2.949536 -0.506809
H -0.109450 2.703641 -3.672952
H 0.154983 4.868439 -2.487485
H 0.202124 4.934340 -0.005730
H 0.078970 2.833043 1.291313

H -0.832412 0.919062 2.161685
H -0.698562 -1.318349 3.189354
O 0.070761 -3.449981 2.070279
C 0.512763 -4.595558 1.354696
H 1.541622 -4.467492 1.011245
H -0.139122 -4.798060 0.502045
H 0.463665 -5.424268 2.055942
SCF: -3448.348275
ZPE: 0.192527
H: -3448.140486
G: -3448.196406

2_OMe_trans_TS_conf2

C 0.006392 2.485525 -3.032488
C 0.082778 2.663070 -0.232932
C -0.095152 1.407787 -2.196747
C 0.106455 3.721262 -2.397039
C 0.128472 3.809652 -1.008654
C -0.013734 1.395608 -0.820791
C 0.036241 0.126028 -0.099534
C 0.226520 -2.380425 1.163797
C 0.492337 -1.015440 -0.767102
C -0.326372 -0.038288 1.232421
C -0.236624 -1.269087 1.866134
C 0.598934 -2.252304 -0.179397
I 1.056898 -0.721576 -2.757683
Br -2.312799 0.225552 -2.855043
H 0.957374 -3.122534 -0.712190
H -0.039650 2.396830 -4.107906
H 0.158244 4.613500 -3.008152
H 0.207607 4.776756 -0.530758
H 0.151449 2.724771 0.846750
H -0.703872 0.812321 1.786677
H -0.536507 -1.352033 2.900536
O 0.349689 -3.614114 1.685635
C -0.009257 -3.798820 3.048572
H -1.063595 -3.564972 3.209247
H 0.609611 -3.180152 3.701788
H 0.168558 -4.848912 3.264856
SCF: -3448.348155
ZPE: 0.192419
H: -3448.140424
G: -3448.196525

3_CF3_cis_TS_conf1

C -0.009513 1.184156 -2.487667
C 0.002917 1.340466 0.313656
C -0.130814 0.084798 -1.672835
C 0.064366 2.415489 -1.851112
C 0.051827 2.489331 -0.463018
C -0.067952 0.086803 -0.286120
H 0.050227 1.405018 1.395209
C -0.009852 -1.187014 0.430905
C 0.218135 -3.690999 1.664775
C 0.479318 -2.307226 -0.243421
C -0.393499 -1.360153 1.758979
C -0.279560 -2.601078 2.367239
C 0.606670 -3.552476 0.337083
H -0.797694 -0.519657 2.309297
H -0.588406 -2.719525 3.397524
H 0.304511 -4.657620 2.143300
I 1.043895 -1.962384 -2.226848
Br -2.301185 -1.047126 -2.331737
H 0.993020 -4.397903 -0.215596
H -0.024764 1.108370 -3.564999
H 0.124636 3.312260 -2.453060
C 0.142089 3.811213 0.234936
F -0.875110 3.999341 1.091895
F 1.265716 3.922147 0.965059
F 0.131024 4.843772 -0.613545
SCF: -3670.911793
ZPE: 0.164315
H: -3670.731159
G: -3670.790518

3_CF3_trans_TS_conf1

C 0.059525 1.796173 -2.406031
C 0.094319 1.931658 0.398994
C -0.064950 0.703057 -1.591724
C 0.161385 3.019080 -1.748222
C 0.164345 3.088379 -0.358068
C -0.005422 0.677279 -0.214131
C 0.019570 -0.604399 0.488172
C 0.170745 -3.126914 1.711301
C 0.476885 -1.737746 -0.192656
C -0.369509 -0.770074 1.811241
C -0.288549 -2.020622 2.407510
C 0.561992 -2.986929 0.384901

H 0.227165 -4.096584 2.185890
I 1.062104 -1.414220 -2.169336
Br -2.287536 -0.433979 -2.285797
H 0.921564 -3.843556 -0.167952
H 0.029394 1.727050 -3.483476
H 0.230752 3.920406 -2.344160
H 0.246663 4.047647 0.134495
H 0.146990 1.975571 1.480394
H -0.749376 0.077112 2.370356
C -0.731043 -2.144151 3.838344
F -0.550341 -3.372258 4.329433
F -2.032516 -1.851503 3.983373
F -0.063653 -1.299279 4.638947
SCF: -3670.910577
ZPE: 0.164303
H: -3670.729916
G: -3670.789653

3_CN_cis_TS_conf1

C 0.071305 1.538292 -2.446789
C 0.020861 1.683758 0.360252
C -0.085371 0.431070 -1.638050
C 0.139952 2.763385 -1.811197
C 0.095394 2.838320 -0.414223
C -0.046881 0.435962 -0.247657
H 0.044140 1.749480 1.440960
C -0.012800 -0.840345 0.466311
C 0.177213 -3.353340 1.688610
C 0.478292 -1.961006 -0.205235
C -0.419444 -1.018136 1.786855
C -0.323704 -2.263523 2.389151
C 0.587663 -3.210969 0.367862
H -0.826665 -0.177901 2.335338
H -0.649765 -2.385763 3.413664
H 0.248782 -4.323125 2.163077
I 1.073809 -1.598597 -2.177081
Br -2.244255 -0.637507 -2.330295
H 0.975528 -4.056124 -0.184166
H 0.083286 1.463653 -3.524385
H 0.223150 3.666235 -2.401810
C 0.166986 4.115097 0.227545
N 0.222527 5.140985 0.741361
SCF: -3426.073205
ZPE: 0.158277

H: -3425.900448

G: -3425.954743

3_CN_trans_TS_conf1

C 0.096178 1.887510 -2.639422

C 0.124783 2.045142 0.165076

C -0.024507 0.800289 -1.816849

C 0.190411 3.115808 -1.990657

C 0.190423 3.196049 -0.601049

C 0.032822 0.785845 -0.438964

C 0.062429 -0.490728 0.272220

C 0.223982 -3.010059 1.507812

C 0.524646 -1.626539 -0.399537

C -0.329501 -0.645244 1.596151

C -0.244582 -1.895569 2.200635

C 0.615004 -2.874731 0.185145

H 0.280185 -3.972748 1.996900

I 1.108866 -1.315209 -2.377222

Br -2.243900 -0.352075 -2.501926

H 0.978693 -3.732509 -0.363141

H 0.068604 1.809964 -3.716353

H 0.256179 4.012855 -2.593411

H 0.266906 4.159589 -0.116005

H 0.174692 2.097782 1.246163

H -0.713772 0.199488 2.153099

C -0.655964 -2.039343 3.568674

N -0.982578 -2.155468 4.662361

SCF: -3426.070563

ZPE: 0.158213

H: -3425.897820

G: -3425.952361

3_F_cis_TS_conf1

C 0.049688 1.784372 -2.412260

C 0.075899 1.921661 0.396540

C -0.079944 0.686473 -1.600203

C 0.154282 3.012438 -1.770875

C 0.148051 3.052144 -0.386879

C -0.022884 0.671402 -0.220375

H 0.130616 2.000182 1.475219

C 0.003850 -0.605743 0.492061

C 0.164978 -3.109762 1.733573

C 0.472063 -1.737028 -0.179373

C -0.392736 -0.766405 1.817883

C -0.312161 -2.007499 2.430791

C 0.565256 -2.982676 0.408206

H -0.780563 0.085819 2.362121

H -0.630101 -2.115946 3.459427

H 0.226553 -4.077077 2.214579

I 1.064350 -1.422757 -2.159648

Br -2.277236 -0.441807 -2.310092

H 0.935664 -3.838716 -0.139034

H 0.024176 1.714180 -3.489786

H 0.231485 3.927741 -2.342948

F 0.248614 4.248906 0.220674

SCF: -3433.070038

ZPE: 0.151311

H: -3432.905180

G: -3432.957276

3_F_trans_TS_conf1

C 0.057025 1.791348 -2.422224

C 0.067564 1.941791 0.381307

C -0.068787 0.700573 -1.604230

C 0.147469 3.018323 -1.770613

C 0.137871 3.095258 -0.380850

C -0.019293 0.683589 -0.225630

C 0.012170 -0.593287 0.485532

C 0.180499 -3.106145 1.730620

C 0.487753 -1.724220 -0.183968

C -0.389297 -0.744911 1.809352

C -0.293865 -1.990780 2.393500

C 0.581040 -2.968593 0.408760

H 0.232204 -4.060208 2.237303

I 1.085834 -1.409928 -2.157828

Br -2.270721 -0.450620 -2.312606

H 0.955596 -3.826098 -0.133003

H 0.035705 1.716547 -3.499513

H 0.217389 3.916755 -2.370875

H 0.210669 4.057561 0.107292

H 0.110093 1.990732 1.462948

H -0.786868 0.087408 2.375875

F -0.690048 -2.124996 3.668751

SCF: -3433.072237

ZPE: 0.151271

H: -3432.907421

G: -3432.959544

3_NMe2_cis_TS_conf1

C 0.555894 0.286096 -2.544210
C 0.013989 0.572047 0.187393
C 0.320882 -0.769719 -1.711386
C 0.485297 1.547738 -1.967747
C 0.211480 1.721902 -0.594205
C 0.084702 -0.711946 -0.360125
H -0.155777 0.648834 1.251902
C -0.003273 -1.946187 0.423120
C -0.047585 -4.364225 1.837763
C 0.632701 -3.094679 -0.053862
C -0.677201 -2.046799 1.638718
C -0.698383 -3.244022 2.337842
C 0.628776 -4.297491 0.625257
H -1.201655 -1.182171 2.025986
H -1.232802 -3.304316 3.276884
H -0.064942 -5.297815 2.384632
I 1.631134 -2.897476 -1.880256
Br -1.653211 -2.083880 -2.822559
H 1.134850 -5.167665 0.229925
H 0.740537 0.166989 -3.601992
H 0.642590 2.398749 -2.613922
N 0.171409 2.978384 -0.032042
C -0.378326 3.120577 1.302141
C 0.110008 4.130919 -0.910437
H -1.406775 2.744191 1.368764
H -0.374937 4.173182 1.572327
H 0.229480 2.586503 2.034907
H -0.773126 4.112241 -1.561043
H 0.075740 5.031599 -0.303096
H 0.998724 4.188343 -1.540777
SCF: -3467.778363
ZPE: 0.233193
H: -3467.528110
G: -3467.587981

3_NMe2_trans_TS_conf1

C 0.466358 2.269477 -3.697129
C 0.847295 2.385774 -0.920720
C 0.190962 1.230325 -2.848790
C 0.917006 3.436560 -3.086078
C 1.092054 3.499374 -1.707033
C 0.396426 1.186698 -1.485530
C 0.219552 -0.071898 -0.756278

C -0.049870 -2.542933 0.516747
C 0.359097 -1.269665 -1.460505
C -0.065822 -0.127278 0.599921
C -0.197013 -1.359256 1.273722
C 0.227626 -2.496093 -0.837465
H -0.157277 -3.510500 0.983637
I 0.783654 -1.090799 -3.493389
Br -2.274892 0.612729 -3.294477
H 0.334906 -3.419970 -1.390343
H 0.299030 2.210998 -4.762593
H 1.122412 4.299085 -3.707659
H 1.445330 4.412987 -1.248383
H 1.033004 2.414820 0.146545
H -0.209507 0.803117 1.129499
N -0.464241 -1.405385 2.608747
C -0.745389 -2.678737 3.242136
C -0.728817 -0.178934 3.334164
H -1.616995 -3.170682 2.797375
H -0.944792 -2.509986 4.296382
H 0.107470 -3.356854 3.162132
H -1.611926 0.341807 2.948159
H -0.898048 -0.418330 4.380111
H 0.122604 0.503350 3.276794
SCF: -3467.782937
ZPE: 0.232832
H: -3467.532846
G: -3467.593719

3_OMe_cis_TS_conf1

C -0.086986 0.906269 -2.331478
C 0.145557 1.037965 0.454051
C -0.246226 -0.172736 -1.513452
C 0.166563 2.126125 -1.703713
C 0.266289 2.194350 -0.313899
C -0.102162 -0.196378 -0.140653
H 0.283535 1.099490 1.526828
C -0.137683 -1.470976 0.578233
C -0.112973 -3.973347 1.834422
C 0.191006 -2.641010 -0.109418
C -0.465174 -1.591126 1.927079
C -0.452680 -2.831015 2.547574
C 0.214494 -3.886821 0.486191
H -0.745950 -0.705784 2.483996
H -0.716026 -2.906606 3.594465

H -0.104023 -4.940021 2.320643
I 0.678492 -2.400614 -2.127994
Br -2.589501 -1.143484 -2.080438
H 0.478080 -4.773842 -0.073719
H -0.195838 0.845020 -3.404466
H 0.272590 3.005951 -2.322103
O 0.507151 3.335021 0.372428
C 0.657131 4.533812 -0.371438
H -0.249575 4.760670 -0.937226
H 1.508370 4.469124 -1.053654
H 0.835736 5.320066 0.357544
SCF: -3448.344949
ZPE: 0.192691
H: -3448.137011
G: -3448.192895

3_OMe_cis_TS_conf2

C 0.007001 1.147808 -2.668699
C 0.047326 1.230307 0.140375
C -0.118366 0.033261 -1.877835
C 0.118873 2.353683 -1.999015
C 0.122896 2.402193 -0.599167
C -0.060130 -0.010583 -0.507092
H 0.106251 1.240417 1.220065
C -0.038583 -1.301267 0.182235
C 0.110886 -3.828027 1.383355
C 0.427112 -2.423516 -0.507105
C -0.440036 -1.484831 1.504037
C -0.365068 -2.735986 2.097081
C 0.513892 -3.678970 0.061250
H -0.829404 -0.642170 2.061745
H -0.686909 -2.860120 3.122782
H 0.168721 -4.803470 1.848194
I 1.023811 -2.089868 -2.482491
Br -2.325125 -1.089773 -2.641966
H 0.882556 -4.526770 -0.499944
H -0.024467 1.102223 -3.747494
H 0.195489 3.276384 -2.560234
O 0.229511 3.635216 -0.054220
C 0.232068 3.730688 1.360955
H 1.094412 3.213249 1.788177
H -0.688056 3.319061 1.782739
H 0.295235 4.790962 1.592172
SCF: -3448.345225

ZPE: 0.192472
H: -3448.137424
G: -3448.193663

3_OMe_cis_TS_conf3

C -0.013239 1.173775 -2.657790
C 0.088966 1.226484 0.150319
C -0.162299 0.056509 -1.874819
C 0.156206 2.368036 -1.979585
C 0.191592 2.402266 -0.579741
C -0.077023 -0.003268 -0.506122
H 0.171984 1.223513 1.228450
C -0.086281 -1.300652 0.170936
C 0.003867 -3.841961 1.347118
C 0.325709 -2.431639 -0.538096
C -0.465048 -1.482860 1.499647
C -0.419517 -2.741210 2.080308
C 0.382604 -3.694443 0.017697
H -0.813384 -0.632607 2.072827
H -0.723019 -2.863883 3.111758
H 0.038934 -4.823065 1.802253
I 0.889350 -2.100433 -2.523527
Br -2.423489 -0.976515 -2.605125
H 0.710377 -4.548944 -0.558502
H -0.068451 1.140131 -3.736053
H 0.254848 3.292945 -2.533702
O 0.354704 3.625091 -0.025810
C 0.408863 3.703814 1.389357
H 1.264706 3.148308 1.780640
H -0.511281 3.322403 1.838520
H 0.520426 4.758100 1.629340
SCF: -3448.345252
ZPE: 0.192623
H: -3448.137364
G: -3448.193303

3_OMe_trans_TS_conf1

C 0.087445 2.417637 -3.055158
C 0.174228 2.485018 -0.251009
C -0.020025 1.303999 -2.265765
C 0.200660 3.625218 -2.371380
C 0.228920 3.660687 -0.980378
C 0.064769 1.244700 -0.890443
C 0.110773 -0.053443 -0.216340

C 0.302202 -2.593957 0.957171
C 0.572383 -1.163516 -0.934424
C -0.260389 -0.245435 1.103761
C -0.165689 -1.507192 1.693859
C 0.674176 -2.416197 -0.371351
H 0.380026 -3.578129 1.395069
I 1.127169 -0.792402 -2.910395
Br -2.235919 0.172623 -2.960235
H 1.036405 -3.261415 -0.941061
H 0.037550 2.373756 -4.133242
H 0.259074 4.540417 -2.947049
H 0.319447 4.607788 -0.466014
H 0.247104 2.501987 0.830049
H -0.645454 0.578142 1.692007
O -0.556346 -1.580964 2.980783
C -0.491611 -2.845409 3.625208
H 0.535109 -3.216217 3.656047
H -1.131385 -3.573458 3.122026
H -0.850616 -2.684040 4.638265
SCF: -3448.348389
ZPE: 0.192566
H: -3448.140566
G: -3448.196418

3_OMe_trans_TS_conf2

C 1.034102 3.397462 -2.134701
C 1.214459 3.550384 0.661273
C 0.949648 2.308900 -1.308427
C 1.173022 4.625161 -1.492789
C 1.247551 4.703037 -0.105353
C 1.080849 2.291054 0.064784
C 1.151803 1.013983 0.776413
C 1.398099 -1.473286 2.023614
C 1.593867 -0.110356 0.083846
C 0.819024 0.873565 2.123600
C 0.941607 -0.365456 2.744674
C 1.725550 -1.349949 0.687571
H 1.485849 -2.427735 2.525903
I 2.071844 0.190592 -1.923977
Br -1.289679 1.165856 -1.893348
H 2.076160 -2.211557 0.135756
H 0.948099 3.320751 -3.208662
H 1.214094 5.522121 -2.097913
H 1.357651 5.664986 0.376648

H 1.325661 3.601932 1.737880
H 0.450441 1.733553 2.664420
O 0.635698 -0.589722 4.036823
C 0.162499 0.503443 4.810845
H -0.767963 0.900018 4.398749
H 0.910460 1.297709 4.863314
H -0.019798 0.108648 5.806861
SCF: -3448.348419
ZPE: 0.192506
H: -3448.140640
G: -3448.196549

4_CF3_cis_TS_conf1

C -0.012831 1.518906 -2.664278
C 0.018939 1.743871 0.129282
C -0.057140 0.438280 -1.817428
C -0.021334 2.762886 -2.057495
C -0.003489 2.874638 -0.672094
C -0.024424 0.450708 -0.431832
C 0.025554 -0.856774 0.245449
C 0.221366 -3.439200 1.343457
C 0.640191 -1.917759 -0.427803
C -0.543491 -1.156170 1.482454
C -0.442407 -2.428894 2.023949
C 0.763667 -3.190845 0.088430
H -1.095415 -0.398782 2.018654
H -0.897637 -2.632259 2.984289
H 0.302215 -4.429907 1.770884
I 1.300222 -1.485437 -2.359999
Br -2.138258 -0.897567 -2.526780
H 1.253749 -3.979025 -0.466533
H -0.010353 1.406345 -3.738839
H -0.023898 3.651429 -2.675101
H 0.026717 3.854435 -0.218979
C 0.147355 1.965148 1.618260
F -1.023956 1.828781 2.262355
F 1.012124 1.120105 2.191425
F 0.582436 3.197086 1.898573
SCF: -3670.902135
ZPE: 0.164780
H: -3670.721235
G: -3670.779220

4_CF3_trans_TS_conf1

C 0.128005 1.675567 -2.787499
C 0.398942 1.899562 -0.007244
C 0.009776 0.613869 -1.927192
C 0.348279 2.911278 -2.191953
C 0.485060 3.021768 -0.811321
C 0.147319 0.632781 -0.551865
C 0.140592 -0.643991 0.177053
C 0.390886 -3.188762 1.377772
C 0.619259 -1.768605 -0.507261
C -0.293332 -0.875046 1.491434
C -0.152860 -2.126457 2.079382
C 0.762197 -3.021187 0.052923
H -0.490600 -2.277271 3.095060
H 0.497873 -4.155602 1.850075
I 1.074655 -1.475306 -2.521054
Br -2.285122 -0.489307 -2.435529
H 1.147128 -3.853224 -0.520942
H 0.027199 1.565911 -3.857455
H 0.423775 3.786120 -2.825366
H 0.684171 3.985176 -0.362226
H 0.563121 1.992036 1.056752
C -0.981908 0.186120 2.316789
F -1.747659 -0.356501 3.269172
F -0.113497 0.991585 2.952263
F -1.783361 0.969590 1.588230
SCF: -3670.902643
ZPE: 0.164588
H: -3670.721898
G: -3670.780000

4_CN_cis_TS_conf1

C 0.042356 1.688102 -2.525852
C 0.077545 1.877748 0.260181
C -0.075012 0.594261 -1.700856
C 0.120154 2.926323 -1.904858
C 0.131922 3.028431 -0.520826
C -0.026256 0.597432 -0.317309
C -0.005954 -0.688584 0.384995
C 0.154450 -3.232624 1.558058
C 0.519646 -1.794045 -0.291846
C -0.490657 -0.911315 1.672945
C -0.406666 -2.169795 2.250965
C 0.619529 -3.053512 0.259901
H -0.964344 -0.106282 2.217115

H -0.793763 -2.320405 3.250050
H 0.219957 -4.211647 2.014055
I 1.125450 -1.425704 -2.255993
Br -2.244050 -0.563672 -2.386643
H 1.036715 -3.882205 -0.295691
H 0.033044 1.594553 -3.602402
H 0.178399 3.817183 -2.516145
H 0.213888 3.992743 -0.039484
C 0.206563 2.038102 1.680325
N 0.326986 2.204910 2.809419
SCF: -3426.067000
ZPE: 0.158383
H: -3425.894156
G: -3425.948265

4_CN_trans_TS_conf1

C 0.070773 1.708746 -2.569648
C 0.247802 1.915038 0.224672
C -0.042838 0.636572 -1.724409
C 0.232917 2.944607 -1.952465
C 0.317482 3.047834 -0.567391
C 0.064471 0.648522 -0.345725
C 0.075378 -0.627138 0.370385
C 0.249115 -3.163388 1.596546
C 0.539049 -1.760269 -0.302891
C -0.349080 -0.831409 1.691774
C -0.256076 -2.084175 2.298006
C 0.641738 -3.010431 0.272797
H -0.595744 -2.200971 3.318209
H 0.323130 -4.132897 2.069492
I 1.053340 -1.457373 -2.300711
Br -2.306496 -0.492720 -2.291658
H 1.013676 -3.857191 -0.287973
H -0.000840 1.610668 -3.643025
H 0.297301 3.828215 -2.574900
H 0.464720 4.014291 -0.105136
H 0.377276 1.996866 1.295671
C -0.956685 0.224953 2.449444
N -1.460309 1.041747 3.078833
SCF: -3426.067032
ZPE: 0.158233
H: -3425.894286
G: -3425.948677

4_F_cis_TS_conf1

C 0.052750 1.785300 -2.418215
C 0.090032 1.959936 0.354137
C -0.075972 0.696425 -1.593875
C 0.155335 3.015570 -1.778850
C 0.167274 3.115648 -0.393068
C -0.021213 0.687783 -0.209225
C 0.006812 -0.585919 0.510462
C 0.159642 -3.115078 1.714644
C 0.498689 -1.707242 -0.165213
C -0.428919 -0.777517 1.821461
C -0.350429 -2.029879 2.413158
C 0.589006 -2.961704 0.401188
H -0.848538 0.053057 2.370673
H -0.698480 -2.158152 3.429717
H 0.220001 -4.089237 2.181692
I 1.097871 -1.365201 -2.137230
Br -2.260661 -0.456607 -2.268722
H 0.976452 -3.805049 -0.153883
H 0.026003 1.702479 -3.494433
H 0.222266 3.910818 -2.383699
H 0.258252 4.068071 0.110123
F 0.163827 2.056601 1.688954
SCF: -3433.069197
ZPE: 0.151561
H: -3432.904139
G: -3432.955981

4_F_trans_TS_conf1

C 0.057806 1.780170 -2.411853
C 0.095981 1.959745 0.390629
C -0.065428 0.698844 -1.581672
C 0.158650 3.013816 -1.775392
C 0.168378 3.103052 -0.387249
C -0.010658 0.693573 -0.200778
C 0.018322 -0.589484 0.499181
C 0.162331 -3.121435 1.721744
C 0.499257 -1.722552 -0.165282
C -0.402620 -0.806301 1.806705
C -0.339536 -2.038147 2.425181
C 0.586727 -2.974897 0.405701
H -0.690229 -2.133413 3.444189
H 0.219139 -4.092036 2.195767
I 1.097989 -1.392079 -2.136845

Br -2.271648 -0.474645 -2.264699
H 0.968102 -3.822003 -0.146846
H 0.031926 1.692143 -3.488050
H 0.225933 3.905710 -2.385564
H 0.255285 4.069089 0.091145
H 0.151684 2.028441 1.468237
F -0.917492 0.222311 2.495551
SCF: -3433.069213
ZPE: 0.151482
H: -3432.904204
G: -3432.956173

4_NMe2_cis_TS_conf1

C 0.117207 0.989570 -3.079357
C 0.072657 1.252357 -0.261493
C -0.012731 -0.059869 -2.211206
C 0.224431 2.235044 -2.473583
C 0.192331 2.363389 -1.092486
C 0.012370 -0.048434 -0.829428
C 0.092123 -1.333261 -0.115180
C 0.386600 -3.878990 1.077040
C 0.645046 -2.431343 -0.790271
C -0.324889 -1.575284 1.196580
C -0.177896 -2.826403 1.779760
C 0.804426 -3.683994 -0.233313
H -0.777042 -0.784766 1.770136
H -0.517064 -2.975178 2.796694
H 0.500572 -4.852697 1.535082
I 1.262261 -2.096168 -2.754303
Br -2.151986 -1.322678 -2.926646
H 1.241212 -4.496156 -0.798177
H 0.103086 0.866446 -4.151824
H 0.308335 3.113140 -3.101814
H 0.254010 3.347495 -0.648626
N 0.016220 1.391991 1.146199
C -1.357418 1.556093 1.620656
C 0.884497 2.419377 1.705697
H -1.745670 2.553723 1.373348
H -1.382680 1.428432 2.704286
H -2.011723 0.814832 1.162050
H 0.525426 3.438026 1.510493
H 0.925468 2.280599 2.786913
H 1.891019 2.314506 1.302473
SCF: -3467.771088

ZPE: 0.232946

H: -3467.521408

G: -3467.580330

4_NMe2_trans_TS_conf1

C 0.110092 1.231264 -3.441415
C 0.603850 1.705235 -0.723514
C 0.036567 0.264305 -2.472906
C 0.416292 2.509547 -2.987858
C 0.657781 2.743443 -1.637034
C 0.296616 0.395552 -1.124809
C 0.356701 -0.798202 -0.271027
C 0.889377 -3.121634 1.203871
C 0.769119 -1.994085 -0.861977
C 0.110207 -0.817550 1.125311
C 0.424068 -1.983351 1.838691
C 1.043255 -3.159275 -0.175728
H 0.268536 -2.009213 2.907384
H 1.105853 -4.007562 1.787220
I 1.005387 -1.944001 -2.939771
Br -2.308957 -0.804735 -2.684632
H 1.367461 -4.057903 -0.680653
H -0.091856 1.025960 -4.482458
H 0.460490 3.318572 -3.706141
H 0.903339 3.740674 -1.297384
H 0.812956 1.880624 0.323723
N -0.403905 0.302615 1.761985
C -1.629015 0.898076 1.237340
C -0.346045 0.357244 3.209726
H -1.573117 1.987818 1.281850
H -2.486221 0.569085 1.835850
H -1.805299 0.598253 0.207370
H -1.063654 -0.323806 3.685543
H 0.656994 0.118905 3.561684
H -0.586874 1.374243 3.519457

SCF: -3467.776173

ZPE: 0.232889

H: -3467.526447

G: -3467.585366

4_OMe_cis_TS_conf1

C -0.057151 1.517867 -2.669936
C -0.117668 1.437151 0.155783
C -0.077271 0.361649 -1.934962

C -0.115084 2.679310 -1.911022
C -0.152610 2.652906 -0.522209
C -0.064892 0.219028 -0.563686
C 0.079471 -1.118736 0.018248
C 0.453045 -3.746526 0.952170
C 0.725571 -2.102648 -0.739489
C -0.398199 -1.510397 1.270454
C -0.211927 -2.807289 1.727201
C 0.927410 -3.397253 -0.306686
H -0.930931 -0.796254 1.879625
H -0.597052 -3.085910 2.699503
H 0.599484 -4.755544 1.314652
I 1.370763 -1.498110 -2.631369
Br -2.083945 -0.994525 -2.840432
H 1.434997 -4.124548 -0.925562
H -0.050233 1.530352 -3.749063
H -0.139129 3.631628 -2.426254
H -0.192089 3.582312 0.024861
O -0.097403 1.333429 1.494745
C -0.080163 2.531056 2.263100
H -0.042646 2.214620 3.301951
H -0.984287 3.117010 2.089953
H 0.801742 3.129621 2.028418
SCF: -3448.345700
ZPE: 0.192778
H: -3448.137702
G: -3448.193294

4_OMe_trans_TS_conf1

C 0.034105 1.805677 -3.015701
C 0.346931 1.949530 -0.231919
C -0.027459 0.719335 -2.185368
C 0.222433 3.030879 -2.383116
C 0.370426 3.100546 -1.002162
C 0.155999 0.687831 -0.816016
C 0.232727 -0.607247 -0.134259
C 0.478848 -3.157978 1.006216
C 0.652222 -1.722024 -0.859435
C -0.096524 -0.823541 1.218555
C 0.033417 -2.093953 1.775951
C 0.791872 -2.991546 -0.334856
H -0.217798 -2.260383 2.812990
H 0.576325 -4.136663 1.457887
I 1.074738 -1.371510 -2.875165

Br -2.293613 -0.432435 -2.691554
H 1.126890 -3.823582 -0.937625
H -0.097755 1.727538 -4.084957
H 0.247976 3.928048 -2.988745
H 0.524290 4.058187 -0.523307
H 0.499992 2.004251 0.835843
O -0.550518 0.242279 1.902007
C -0.943115 0.060543 3.256839
H -0.099142 -0.265206 3.867744
H -1.757358 -0.662602 3.332175
H -1.286108 1.033726 3.597775
SCF: -3448.345507
ZPE: 0.192686
H: -3448.137574
G: -3448.193393

5_CF3_TS_conf1

C 0.041561 1.456103 -2.934102
C 0.297780 1.776780 -0.166550
C 0.054717 0.405941 -2.048532
C 0.082759 2.722831 -2.376852
C 0.237999 2.878684 -1.006251
C 0.143425 0.468837 -0.663448
C 0.174819 -0.837237 0.037338
C 0.550467 -3.412097 1.155729
C 0.871255 -1.867946 -0.611641
C -0.466088 -1.220477 1.222069
C -0.258648 -2.479358 1.776590
C 1.091494 -3.123338 -0.088766
H -0.762493 -2.737974 2.699660
H 0.713357 -4.382356 1.604394
I 1.401571 -1.459989 -2.585105
Br -2.086911 -1.004027 -2.574388
H 1.649702 -3.871889 -0.634364
H -0.015636 1.303295 -4.002261
H 0.041414 3.588326 -3.024924
H 0.355663 3.870363 -0.589306
C 0.676399 2.107747 1.258289
F -0.239088 2.870110 1.868213
F 0.882810 1.039303 2.029523
F 1.819808 2.810819 1.277267
C -1.533976 -0.408995 1.916617
F -1.229947 -0.144500 3.193602
F -1.809883 0.752492 1.323634

F -2.684129 -1.101343 1.943663
SCF: -4007.978887
ZPE: 0.169320
H: -4007.789952
G: -4007.855660

5_CN_TS_conf1

C -0.008564 1.686495 -2.513722
C 0.154115 1.909612 0.269076
C -0.098317 0.599419 -1.674006
C 0.091094 2.929988 -1.909339
C 0.185837 3.047979 -0.528621
C -0.026651 0.628779 -0.290474
C -0.023342 -0.654785 0.413328
C 0.199537 -3.199166 1.605403
C 0.554768 -1.746641 -0.238896
C -0.597065 -0.924738 1.664983
C -0.470484 -2.180940 2.258343
C 0.693804 -2.998282 0.322036
H -0.926286 -2.353051 3.223945
H 0.301302 -4.169086 2.072339
I 1.085497 -1.378598 -2.220116
Br -2.315920 -0.585299 -2.267198
H 1.161582 -3.809816 -0.218793
H -0.042885 1.580755 -3.588743
H 0.127719 3.814028 -2.532146
H 0.329331 4.014593 -0.066762
C 0.465380 2.067347 1.660691
N 0.766436 2.216819 2.757791
C -1.454711 0.029672 2.306233
N -2.185780 0.754914 2.812149
SCF: -3518.309778
ZPE: 0.156926
H: -3518.136598
G: -3518.194667

5_F_TS_conf1

C 0.015981 1.780920 -2.413075
C 0.154682 1.983710 0.357737
C -0.088632 0.700667 -1.575134
C 0.133213 3.018037 -1.789271
C 0.205330 3.130485 -0.407220
C -0.012453 0.710293 -0.189241
C 0.013922 -0.567671 0.520883

C 0.177523 -3.111187 1.716852
C 0.535054 -1.685774 -0.141475
C -0.482594 -0.817241 1.795741
C -0.396884 -2.055088 2.403543
C 0.637490 -2.941583 0.414794
H -0.799795 -2.176884 3.400188
H 0.247783 -4.083848 2.184765
I 1.089595 -1.325474 -2.119460
Br -2.302118 -0.494407 -2.182455
H 1.050434 -3.773875 -0.137599
H -0.028562 1.685718 -3.487755
H 0.182507 3.907073 -2.404880
H 0.334984 4.085980 0.081516
F 0.334305 2.093110 1.677724
F -1.116464 0.161539 2.449523
SCF: -3532.316377
ZPE: 0.143324
H: -3532.158704
G: -3532.212494

5_NMe2_TS_conf1

C -0.167182 1.059792 -3.581847
C 0.057523 1.448397 -0.755359
C 0.130849 0.087483 -2.677267
C -0.489359 2.279191 -2.980087
C -0.381207 2.473646 -1.616005
C 0.237685 0.140746 -1.306657
C 0.581186 -1.093113 -0.587447
C 1.670577 -3.318662 0.724060
C 1.496462 -1.961158 -1.193680
C 0.074995 -1.477446 0.682943
C 0.694365 -2.560948 1.338150
C 2.061388 -3.061541 -0.588576
H 0.361955 -2.838635 2.328365
H 2.105363 -4.157860 1.252245
I 1.972347 -1.503774 -3.180974
Br -1.552692 -1.892028 -3.230345
H 2.771892 -3.696735 -1.097584
H -0.189812 0.905330 -4.649036
H -0.780725 3.105300 -3.617483
H -0.564420 3.458741 -1.212131
N 0.281059 1.691687 0.573557
C -0.310105 2.853655 1.202256
C 1.463676 1.190659 1.250281

H 0.258731 3.771567 1.007386
H -0.329230 2.686013 2.279984
H -1.334747 2.993037 0.859234
H 2.074332 2.038267 1.577307
H 1.199543 0.595988 2.128821
H 2.068153 0.582877 0.582285
N -0.969719 -0.810960 1.265147
C -1.225191 -0.951219 2.682147
H -0.292607 -0.929030 3.245738
H -1.763117 -1.876659 2.923724
H -1.836523 -0.107432 3.004218
C -2.111394 -0.361347 0.489543
H -3.017734 -0.820204 0.895510
H -2.019248 -0.669463 -0.550201
H -2.227169 0.725837 0.531981
SCF: -3601.730531
ZPE: 0.306031
H: -3601.403543
G: -3601.470399

5_NMe2_TS_conf2

C 0.555968 1.845213 -2.520703
C 1.030763 2.434018 0.239265
C 0.957333 0.943242 -1.583678
C 0.262915 3.098225 -1.976175
C 0.492047 3.389368 -0.644669
C 1.187953 1.093690 -0.235454
C 1.623547 -0.081619 0.530995
C 2.877396 -2.196264 1.879859
C 2.496060 -0.976329 -0.099165
C 1.248221 -0.383833 1.867460
C 1.948523 -1.411105 2.531772
C 3.137701 -2.024565 0.521803
H 1.716949 -1.624467 3.565649
H 3.376392 -2.991245 2.419536
I 2.778787 -0.648644 -2.147385
Br -0.725251 -1.095265 -1.848344
H 3.810505 -2.682567 -0.009022
H 0.439061 1.616285 -3.568246
H -0.104755 3.872816 -2.638343
H 0.324770 4.397221 -0.293769
N 1.371292 2.773734 1.521464
C 0.817217 3.968624 2.121585
C 2.623424 2.341398 2.115317

H 1.347295 4.878333 1.812329
H 0.901268 3.876676 3.205339
H -0.237416 4.069744 1.867405
H 3.245976 3.219145 2.316360
H 2.456449 1.813789 3.058205
H 3.172449 1.691189 1.439527
N 0.250747 0.307474 2.501738
C 0.133379 0.259947 3.942933
H 1.114345 0.332146 4.412149
H -0.361423 -0.653957 4.295206
H -0.460907 1.115613 4.265601
C -0.969713 0.684666 1.812111
H -1.822793 0.239751 2.332876
H -0.970647 0.308098 0.791124
H -1.105427 1.770154 1.793942
SCF: -3601.730558
ZPE: 0.306082
H: -3601.403535
G: -3601.470325

5_NMe2_TS_conf3

C 1.005084 2.158476 -2.482652
C 1.201613 2.504476 0.346755
C 1.156027 1.117991 -1.593924
C 0.844496 3.412389 -1.890958
C 0.940959 3.587928 -0.514591
C 1.221498 1.185288 -0.208340
C 1.429748 -0.074488 0.517140
C 2.294007 -2.388225 1.866480
C 2.291367 -1.017888 -0.070373
C 0.851838 -0.418960 1.772473
C 1.354674 -1.550645 2.448779
C 2.746432 -2.162830 0.563980
H 0.959801 -1.801076 3.430253
H 2.642851 -3.262886 2.411768
I 2.860793 -0.616779 -2.056606
Br -0.682299 -0.560178 -2.208762
H 3.424008 -2.855404 0.072682
H 0.971739 2.012011 -3.557250
H 0.684441 4.277761 -2.532116
H 0.886151 4.593257 -0.106258
N 1.399903 2.705649 1.701570
C 2.550937 2.133885 2.377251
C 0.933370 3.926955 2.319627

H 2.260782 1.686955 3.338998
H 3.299821 2.918206 2.575666
H 3.030209 1.363326 1.768816
H -0.064552 4.193403 1.955075
H 0.865436 3.763308 3.402717
H 1.612025 4.782020 2.150238
N -0.151730 0.341321 2.327523
C -1.229204 0.895725 1.532371
H -1.141918 0.596270 0.482929
H -1.253949 1.995087 1.586743
H -2.190426 0.514825 1.909112
C -0.422654 0.294881 3.746038
H 0.505038 0.209284 4.321967
H -1.091023 -0.536388 4.029546
H -0.911891 1.233370 4.037734
SCF: -3601.729084
ZPE: 0.304816
H: -3601.403957
G: -3601.468853

5_OMe_TS_conf1

C -0.178516 1.398076 -2.905913
C 0.335169 1.423741 -0.128518
C -0.113595 0.270614 -2.129031
C -0.042796 2.589129 -2.203364
C 0.215177 2.616424 -0.838275
C 0.116415 0.185160 -0.772808
C 0.283351 -1.132868 -0.153493
C 0.961764 -3.669507 0.861445
C 0.881032 -2.136700 -0.931671
C -0.101549 -1.512464 1.144189
C 0.286903 -2.756942 1.646290
C 1.234405 -3.384493 -0.474867
H 0.003444 -3.000244 2.662130
H 1.239030 -4.632953 1.268820
I 1.148677 -1.628666 -2.941403
Br -2.313252 -1.072106 -2.606921
H 1.699092 -4.117992 -1.118285
H -0.354670 1.370722 -3.970269
H -0.119930 3.521309 -2.749318
H 0.359361 3.564313 -0.342231
O 0.699292 1.349139 1.159852
C 0.811020 2.558168 1.899223
H 1.041589 2.261484 2.918909

H -0.129416 3.113091 1.880380
H 1.616359 3.182643 1.507449
O -0.857962 -0.759824 1.968808
C -1.960802 -0.035107 1.427286
H -1.719687 1.023337 1.330684
H -2.781649 -0.149395 2.133962
H -2.258263 -0.437992 0.457139
SCF: -3562.864097
ZPE: 0.225375
H: -3562.620942
G: -3562.681825

5_OMe_TS_conf2

C -0.413775 1.690651 -2.847334
C 0.347341 1.742261 -0.125603
C -0.294149 0.581785 -2.060770
C -0.217221 2.894919 -2.174162
C 0.160082 2.922581 -0.842770
C 0.063707 0.495600 -0.726147
C 0.156155 -0.844628 -0.132780
C 0.457159 -3.483682 0.799746
C 0.566043 -1.900765 -0.956393
C -0.201521 -1.191588 1.178207
C -0.026084 -2.493894 1.636471
C 0.736299 -3.200623 -0.533357
H -0.297268 -2.712847 2.661214
H 0.586034 -4.492579 1.169060
I 0.815403 -1.396323 -2.968681
Br -2.572503 -0.697229 -2.288323
H 1.063219 -3.979428 -1.207976
H -0.678346 1.646271 -3.892797
H -0.332233 3.820822 -2.723857
H 0.368111 3.858743 -0.342994
O 0.799176 1.868594 1.139459
C 1.934652 1.097244 1.536395
H 2.600646 1.772979 2.071563
H 2.456294 0.693756 0.667415
H 1.632879 0.289412 2.200358
O -0.705984 -0.278369 2.048334
C -2.003278 0.224529 1.727622
H -2.033116 0.663432 0.729228
H -2.227331 0.988229 2.468719
H -2.740391 -0.579959 1.790150
SCF: -3562.857954

ZPE: 0.224255
H: -3562.615359
G: -3562.678183

5_OMe_TS_conf3

C -0.567088 1.720673 -2.906818
C 0.626280 1.896535 -0.347493
C -0.371144 0.660789 -2.072626
C -0.217747 2.952825 -2.353510
C 0.371611 3.040217 -1.105586
C 0.183746 0.634851 -0.803949
C 0.310567 -0.670832 -0.147526
C 0.582848 -3.241636 0.928913
C 0.537969 -1.797314 -0.936735
C 0.109219 -0.894497 1.225663
C 0.279110 -2.172463 1.757588
C 0.690016 -3.077766 -0.446036
H 0.150702 -2.341030 2.816699
H 0.706080 -4.228008 1.357008
I 0.500596 -1.432801 -2.992566
Br -2.721782 -0.528832 -1.877268
H 0.872576 -3.920990 -1.096726
H -0.991995 1.626610 -3.894499
H -0.381702 3.848746 -2.939305
H 0.702423 3.992267 -0.713521
O 1.316000 2.083135 0.796590
C 2.419024 1.226510 1.085946
H 3.209778 1.862635 1.481172
H 2.776327 0.728347 0.183522
H 2.150121 0.485308 1.837771
O -0.281100 0.168901 1.945568
C -0.381519 0.027546 3.355716
H -1.163349 -0.686276 3.622865
H -0.641530 1.012194 3.734920
H 0.571261 -0.291844 3.783917
SCF: -3562.862406
ZPE: 0.225056
H: -3562.619439
G: -3562.680771

5_OMe_TS_conf4

C -0.656536 1.696683 -2.795738
C 0.218845 1.819280 -0.106282
C -0.451940 0.600355 -2.002027

C -0.479032 2.911198 -2.143157
C -0.044602 2.984737 -0.826310
C -0.047779 0.554931 -0.684864
C 0.217548 -0.749922 -0.073755
C 0.877077 -3.290117 0.909708
C 0.698679 -1.775138 -0.887858
C -0.055399 -1.089434 1.265920
C 0.317805 -2.342904 1.753474
C 1.044758 -3.035122 -0.444831
H 0.143109 -2.594141 2.789440
H 1.152703 -4.258823 1.306070
I 0.748228 -1.302335 -2.921901
Br -2.667857 -0.825211 -2.173290
H 1.422214 -3.793465 -1.115596
H -0.965643 1.631216 -3.827490
H -0.664113 3.824850 -2.694640
H 0.129008 3.952401 -0.380647
O 0.792257 1.807952 1.103595
C 1.012469 3.049470 1.758472
H 1.435759 2.801591 2.728324
H 0.073251 3.589203 1.895122
H 1.716856 3.668510 1.199044
O -0.733663 -0.186785 1.987822
C -0.939584 -0.441522 3.369033
H -1.561623 -1.326748 3.517730
H -1.454007 0.433106 3.758636
H 0.012815 -0.568417 3.888201
SCF: -3562.866566
ZPE: 0.225435
H: -3562.623242
G: -3562.684996

6_CF3_TS_conf1

C 0.079192 1.495554 -2.948750
C 0.131196 1.639383 -0.145532
C -0.050033 0.394748 -2.137238
C 0.181126 2.721770 -2.306811
C 0.187798 2.790024 -0.918132
C 0.032228 0.390737 -0.751677
H 0.193101 1.698609 0.935617
C 0.073268 -0.888848 -0.045016
C 0.260798 -3.415476 1.163269
C 0.521730 -2.018185 -0.736914
C -0.288257 -1.060513 1.284822

C -0.189903 -2.313999 1.872656
C 0.626001 -3.269743 -0.170008
H -0.660178 -0.217965 1.856349
H 0.330061 -4.386756 1.632815
I 1.060930 -1.671135 -2.723300
Br -2.261718 -0.687362 -2.760131
H 0.978312 -4.122113 -0.734087
H 0.048310 1.425604 -4.026185
H 0.247977 3.620367 -2.905352
C 0.303810 4.108561 -0.216638
F -0.701021 4.305988 0.652273
F 1.437075 4.202192 0.500204
F 0.295720 5.143316 -1.062093
C -0.603500 -2.446461 3.311755
F -0.421572 -3.679805 3.788231
F -1.899227 -2.145541 3.485349
F 0.086971 -1.613049 4.104326
SCF: -4008.001186
ZPE: 0.169066
H: -4007.812144
G: -4007.880811

6_CF3_TS_conf2

C 1.085396 2.492360 -1.956766
C 1.116026 2.650617 0.845995
C 0.955412 1.395055 -1.140666
C 1.176979 3.722295 -1.320412
C 1.173327 3.797538 0.067914
C 1.027445 1.398334 0.245613
H 1.170051 2.715987 1.927189
C 1.072409 0.122600 0.958751
C 1.271924 -2.391656 2.182194
C 1.533358 -1.004307 0.278244
C 0.700591 -0.041176 2.291246
C 0.804576 -1.286564 2.884359
C 1.644660 -2.254731 0.854590
H 0.318979 0.803232 2.850036
H 1.344391 -3.358617 2.664158
I 2.081712 -0.667390 -1.707204
Br -1.245457 0.298428 -1.774862
H 2.007765 -3.107250 0.297732
H 1.062848 2.416644 -3.034007
H 1.243958 4.618179 -1.922994
C 1.280218 5.119887 0.763635

F 0.269583 5.317910 1.625614
F 2.408930 5.220995 1.486681
F 1.273563 6.150544 -0.086822
C 0.402954 -1.480969 4.319742
F -0.578273 -2.387386 4.441760
F -0.031216 -0.355595 4.891221
F 1.425792 -1.929364 5.063257
SCF: -4008.001218
ZPE: 0.169068
H: -4007.812163
G: -4007.881000

6_CN_TS_conf1

C 0.075238 1.529179 -2.438104
C 0.022089 1.687126 0.370302
C -0.079207 0.425261 -1.624823
C 0.139320 2.756252 -1.806307
C 0.093910 2.837344 -0.409383
C -0.041244 0.437628 -0.234765
H 0.043290 1.758028 1.450672
C -0.009004 -0.837498 0.479930
C 0.176635 -3.364201 1.696012
C 0.473057 -1.963208 -0.192645
C -0.410436 -1.006410 1.798989
C -0.313325 -2.261123 2.392664
C 0.578018 -3.215428 0.377645
H -0.810430 -0.171986 2.360419
H 0.240706 -4.329669 2.178572
I 1.060352 -1.604987 -2.162720
Br -2.252696 -0.643534 -2.302333
H 0.957324 -4.063538 -0.175152
H 0.088688 1.450578 -3.515415
H 0.220098 3.657144 -2.400237
C 0.161218 4.117545 0.226670
N 0.213175 5.145934 0.735396
C -0.735676 -2.422405 3.755673
N -1.071299 -2.553035 4.844840
SCF: -3518.322277
ZPE: 0.156907
H: -3518.149044
G: -3518.207788

6_F_TS_conf1

C 0.065447 1.783874 -2.407719

C 0.061509 1.921158 0.402018
C -0.068805 0.683791 -1.598519
C 0.158476 3.011406 -1.764454
C 0.137347 3.051767 -0.380288
C -0.024691 0.671654 -0.217806
H 0.103156 1.999125 1.481333
C 0.000909 -0.606119 0.492582
C 0.164915 -3.119650 1.732942
C 0.477068 -1.735462 -0.178371
C -0.403713 -0.758380 1.815004
C -0.310863 -2.005509 2.397008
C 0.569092 -2.980660 0.412349
H -0.801048 0.073864 2.381961
H 0.215096 -4.074568 2.238192
I 1.079950 -1.417489 -2.150570
Br -2.259476 -0.443234 -2.321317
H 0.944763 -3.837476 -0.129725
H 0.051446 1.714729 -3.485555
H 0.238252 3.927249 -2.335376
F 0.226311 4.248784 0.227523
F -0.709940 -2.141953 3.670584
SCF: -3532.321363
ZPE: 0.142994
H: -3532.163966
G: -3532.218084

6_NMe2_TS_conf2

C 1.558704 2.185768 -2.445561
C 1.467428 2.299935 0.347206
C 1.412032 1.081937 -1.655192
C 1.634123 3.407087 -1.788446
C 1.587310 3.494216 -0.381368
C 1.394412 1.053948 -0.282075
H 1.477204 2.310478 1.427869
C 1.384254 -0.230231 0.427475
C 1.489724 -2.719271 1.691880
C 1.904141 -1.351540 -0.222907
C 0.901903 -0.375199 1.720055
C 0.936742 -1.619063 2.383610
C 1.964050 -2.584365 0.399625
H 0.472576 0.488586 2.206666
H 1.546940 -3.690143 2.160734
I 2.606880 -1.063020 -2.164623
Br -0.753535 -0.084277 -2.528701

H 2.379204 -3.446104 -0.106395
H 1.568676 2.133368 -3.524542
H 1.723661 4.295081 -2.396536
N 1.689922 4.710688 0.259957
C 1.326797 4.780036 1.662296
C 1.541397 5.920840 -0.525605
H 0.299248 4.439045 1.841381
H 1.414649 5.810501 1.996393
H 1.999259 4.173805 2.271492
H 0.563832 5.980346 -1.020445
H 1.652030 6.779497 0.131687
H 2.316879 5.985404 -1.290101
N 0.446942 -1.754923 3.647128
C -0.013298 -0.588139 4.372482
H -0.851730 -0.108305 3.861084
H 0.782902 0.154095 4.494169
H -0.350396 -0.896229 5.357986
C 0.580230 -3.021447 4.338595
H 1.629801 -3.307638 4.464819
H 0.070970 -3.822544 3.797286
H 0.125932 -2.935520 5.321425
SCF: -3601.740215
ZPE: 0.306325
H: -3601.412209
G: -3601.483301

6_OMe_TS_conf1

C -0.009911 1.119131 -2.982694
C 0.309533 1.257000 -0.206700
C -0.154376 0.042985 -2.157585
C 0.274503 2.338415 -2.367380
C 0.417719 2.409959 -0.981661
C 0.032167 0.023189 -0.789274
H 0.482239 1.321784 0.860894
C 0.010304 -1.251148 -0.067025
C 0.062146 -3.739623 1.198273
C 0.313452 -2.417416 -0.764307
C -0.280963 -1.347240 1.293350
C -0.255334 -2.587230 1.923929
C 0.347134 -3.659021 -0.150648
H -0.542358 -0.450515 1.837015
H 0.075942 -4.694278 1.707584
I 0.737924 -2.190370 -2.794156
Br -2.519043 -0.906725 -2.646113

H 0.589860 -4.555030 -0.705886
H -0.152199 1.056146 -4.051686
H 0.370087 3.215366 -2.991536
O 0.690725 3.550370 -0.306722
C 0.831769 4.744795 -1.059289
H -0.089484 4.981010 -1.597140
H 1.660116 4.667156 -1.767840
H 1.043040 5.531227 -0.339284
O -0.529739 -2.770618 3.229575
C -0.863753 -1.630564 4.008590
H -0.042040 -0.910947 4.020964
H -1.040663 -1.997471 5.016164
H -1.768798 -1.150334 3.630189
SCF: -3562.872609
ZPE: 0.225708
H: -3562.629090
G: -3562.690758

6_OMe_TS_conf2

C -0.249402 1.527124 -2.926881
C 0.250648 1.611802 -0.174788
C -0.335392 0.434553 -2.115519
C 0.070400 2.735202 -2.306636
C 0.303471 2.780332 -0.932021
C -0.059775 0.388978 -0.763111
H 0.490435 1.654859 0.880879
C -0.034210 -0.899434 -0.066526
C 0.087351 -3.427432 1.140120
C 0.221267 -2.057275 -0.811036
C -0.234316 -1.035292 1.296737
C -0.174164 -2.291250 1.903691
C 0.286961 -3.304810 -0.230951
H -0.457716 -0.169852 1.908176
H 0.135666 -4.408429 1.589336
I 0.522601 -1.780195 -2.856695
Br -2.723949 -0.522133 -2.460982
H 0.490257 -4.189105 -0.819786
H -0.460425 1.484757 -3.985514
H 0.122397 3.624876 -2.917753
O 0.615376 3.908888 -0.254041
C 0.703561 5.118100 -0.990906
H -0.252000 5.361813 -1.461324
H 1.482563 5.056333 -1.754778
H 0.961306 5.891099 -0.271467

O -0.388343 -2.308972 3.233406
C -0.348303 -3.564079 3.897807
H -1.115786 -4.236608 3.508599
H -0.545049 -3.354715 4.945937
H 0.634667 -4.028934 3.795922
SCF: -3562.872534
ZPE: 0.225504
H: -3562.629118
G: -3562.691210

6_OMe_TS_conf3

C -0.008676 1.341280 -3.271272
C 0.256404 1.439802 -0.475859
C -0.124779 0.238149 -2.462621
C 0.212687 2.544765 -2.625209
C 0.329054 2.602130 -1.230624
C 0.039264 0.201241 -1.099781
H 0.404090 1.455300 0.595155
C 0.058464 -1.086071 -0.401880
C 0.200312 -3.595973 0.816432
C 0.422860 -2.225016 -1.115995
C -0.249765 -1.223192 0.951623
C -0.178291 -2.473102 1.558635
C 0.501017 -3.475878 -0.526202
H -0.560603 -0.351089 1.509144
H 0.248737 -4.559028 1.307466
I 0.870477 -1.938164 -3.133189
Br -2.432127 -0.778227 -3.042516
H 0.789829 -4.349451 -1.094803
H -0.126977 1.290330 -4.343777
H 0.289079 3.459037 -3.200108
O 0.536961 3.832195 -0.708133
C 0.659294 3.936209 0.701093
H 1.526281 3.377680 1.062315
H -0.243189 3.574686 1.200120
H 0.794405 4.993271 0.915423
O -0.463003 -2.693980 2.856346
C -0.860934 -1.586101 3.651405
H -0.072749 -0.830948 3.692344
H -1.038295 -1.981047 4.648263
H -1.780027 -1.139010 3.266302
SCF: -3562.872880
ZPE: 0.225624
H: -3562.629424

G: -3562.691082

6_OMe_TS_conf4

C 0.923607 2.172344 -1.896924
C 1.252314 2.194189 0.893745
C 0.804390 1.051193 -1.113868
C 1.182434 3.354323 -1.225590
C 1.330677 3.373940 0.167125
C 0.998066 0.976764 0.243334
H 1.421004 2.178006 1.961763
C 1.003434 -0.327893 0.908229
C 1.101252 -2.885696 2.056305
C 1.322123 -1.462585 0.151526
C 0.727461 -0.503866 2.253820
C 0.776360 -1.774055 2.831392
C 1.376086 -2.723760 0.702303
H 0.452069 0.340085 2.874056
H 1.141890 -3.876973 2.483284
I 1.741934 -1.125101 -1.863920
Br -1.535273 0.091352 -1.665840
H 1.627390 -3.588580 0.103052
H 0.780747 2.151553 -2.967439
H 1.264462 4.281401 -1.778806
O 1.573589 4.586252 0.715264
C 1.729856 4.652079 2.123480
H 2.593866 4.068371 2.450480
H 0.832110 4.295000 2.634127
H 1.890218 5.700648 2.360790
O 0.487465 -1.829669 4.145930
C 0.518957 -3.100043 4.780951
H -0.207391 -3.780094 4.330719
H 0.255839 -2.922327 5.820349
H 1.517464 -3.539060 4.726366
SCF: -3562.872890
ZPE: 0.225593
H: -3562.629431
G: -3562.691287

7_CF3_TS_conf1

C 0.015651 1.184358 -2.066716
C 0.047908 1.360812 0.735837
C -0.127915 0.091586 -1.244653
C 0.127649 2.405446 -1.420253
C 0.129094 2.506632 -0.030557

C -0.061455 0.101847 0.136069
H 0.221475 3.474831 0.443928
H 0.098758 1.421042 1.815845
C -0.040444 -1.168445 0.858529
C 0.127350 -3.653061 2.108221
C 0.410608 -2.307616 0.183107
C -0.419538 -1.317939 2.188325
C -0.336342 -2.553491 2.812247
C 0.507750 -3.546577 0.773825
H -0.796314 -0.463940 2.736218
H -0.638360 -2.653494 3.845547
I 0.967166 -1.998653 -1.804368
Br -2.347057 -0.970094 -1.907288
H 0.864960 -4.413086 0.232005
H -0.007556 1.104156 -3.143588
C 0.252894 3.667485 -2.227971
F -0.720801 4.541038 -1.934409
F 1.412105 4.296452 -1.982586
F 0.198952 3.447180 -3.543221
C 0.237024 -5.002446 2.759893
F 1.492811 -5.473012 2.714153
F -0.127064 -4.983363 4.043432
F -0.530407 -5.916045 2.146826
SCF: -4007.999469
ZPE: 0.169164
H: -4007.810277
G: -4007.879759

7_CF3_TS_conf2

C 0.947948 2.791469 -1.399341
C 1.042243 2.951914 1.402634
C 0.808815 1.695613 -0.580399
C 1.088712 4.007502 -0.749011
C 1.120431 4.100962 0.640819
C 0.906150 1.697562 0.798684
H 1.234473 5.065197 1.118647
H 1.117313 3.005901 2.481531
C 0.932655 0.423372 1.513923
C 1.117957 -2.066680 2.748761
C 1.358037 -0.714306 0.826144
C 0.583924 0.272427 2.855346
C 0.675223 -0.963397 3.468600
C 1.463894 -1.960287 1.409760
H 0.226983 1.127476 3.414680

H 0.398284 -1.071212 4.509861
I 1.866666 -0.404771 -1.173947
Br -1.435840 0.666108 -1.199843
H 1.803432 -2.822806 0.853704
H 0.900267 2.717849 -2.475913
C 1.213906 5.272293 -1.552446
F 0.259037 6.157678 -1.233567
F 2.386826 5.883760 -1.328572
F 1.128961 5.060164 -2.867453
C 1.197744 -3.394063 3.447755
F 1.794761 -4.330661 2.706601
F 1.880548 -3.307089 4.597872
F -0.019145 -3.862280 3.764970
SCF: -4007.999565
ZPE: 0.169119
H: -4007.810426
G: -4007.879642

7_CN_TS_conf1

C 0.065601 1.521994 -2.261473
C 0.040265 1.690934 0.543283
C -0.080112 0.424125 -1.451163
C 0.147200 2.749758 -1.604998
C 0.118432 2.844709 -0.211656
C -0.037112 0.435486 -0.065467
H 0.185061 3.812226 0.264948
H 0.069255 1.746581 1.624221
C -0.011094 -0.836885 0.650983
C 0.158580 -3.327887 1.887306
C 0.461410 -1.966760 -0.024552
C -0.409168 -0.994964 1.976849
C -0.326848 -2.229212 2.594295
C 0.561548 -3.209878 0.556507
H -0.802144 -0.147336 2.522882
H -0.642535 -2.348054 3.621738
I 1.046117 -1.639993 -2.000165
Br -2.273239 -0.654709 -2.137267
H 0.933045 -4.071785 0.019899
H 0.066930 1.457227 -3.339847
C 0.258573 3.942691 -2.395329
N 0.348838 4.898265 -3.024016
C 0.246752 -4.606757 2.530645
N 0.318247 -5.628574 3.047677
SCF: -3518.319365

ZPE: 0.156952

H: -3518.146070

G: -3518.204926

7_F_TS_conf1

C 0.072571 1.771699 -2.404306
C 0.062598 1.929795 0.396700
C -0.066582 0.677608 -1.587837
C 0.158581 2.979043 -1.734120
C 0.141008 3.089361 -0.353693
C -0.022655 0.671103 -0.205682
H 0.216486 4.062550 0.110524
H 0.098186 1.984491 1.478054
C 0.003988 -0.604634 0.507375
C 0.159120 -3.085670 1.727682
C 0.475844 -1.733842 -0.164144
C -0.397595 -0.772991 1.831582
C -0.321358 -2.010052 2.449220
C 0.567874 -2.985110 0.410524
H -0.789273 0.073918 2.380632
H -0.636444 -2.148968 3.474648
I 1.078687 -1.403110 -2.135122
Br -2.258269 -0.439874 -2.302950
H 0.935207 -3.856005 -0.114712
H 0.055001 1.726209 -3.483587
F 0.255739 4.094571 -2.470957
F 0.233288 -4.285193 2.322372
SCF: -3532.322128
ZPE: 0.143029
H: -3532.164723
G: -3532.218794

7_NMe2_TS_conf1

C 0.361917 0.495827 -1.664172
C -0.469595 0.610607 0.998047
C 0.192622 -0.584197 -0.856088
C 0.073613 1.755055 -1.081207
C -0.372769 1.771926 0.262518
C -0.155494 -0.653421 0.470991
H -0.616647 2.708826 0.740069
H -0.759307 0.666533 2.041692
C -0.105832 -1.906761 1.210855
C 0.092267 -4.424043 2.546988
C 0.713837 -2.941150 0.762385

C -0.840220 -2.181377 2.366165
C -0.752162 -3.394589 3.018142
C 0.833133 -4.170525 1.372128
H -1.515369 -1.426203 2.751399
H -1.356740 -3.551000 3.899109
I 1.829596 -2.498686 -0.951815
Br -1.456339 -2.153993 -2.191435
H 1.487466 -4.921965 0.958002
H 0.610037 0.388831 -2.707808
N 0.198321 2.898419 -1.808095
C -0.335176 4.141556 -1.282669
C 0.573735 2.824834 -3.205431
H -1.407277 4.066226 -1.074015
H -0.179046 4.927075 -2.016556
H 0.175042 4.430449 -0.361292
H -0.181780 2.305266 -3.805858
H 0.691580 3.833039 -3.591973
H 1.525209 2.302266 -3.323913
N 0.194216 -5.619671 3.196979
C 0.924135 -6.708992 2.579467
H 1.973683 -6.444831 2.431564
H 0.499730 -6.987327 1.608145
H 0.885503 -7.574137 3.235386
C -0.704673 -5.912142 4.296168
H -0.464017 -6.894517 4.692721
H -1.753974 -5.909506 3.980468
H -0.587725 -5.184302 5.101542
SCF: -3601.745463
ZPE: 0.306030
H: -3601.417682
G: -3601.488689

7_NMe2_TS_conf2

C 1.608904 3.159960 -0.812541
C 0.753625 3.245484 1.842947
C 1.470095 2.074407 -0.005881
C 1.274425 4.408495 -0.231592
C 0.816057 4.409524 1.108108
C 1.115260 1.993069 1.318656
H 0.535914 5.337199 1.583705
H 0.454250 3.291533 2.884289
C 1.204573 0.743163 2.060597
C 1.489521 -1.760116 3.407339
C 2.063726 -0.261925 1.619504

C 0.474603 0.445212 3.213075
C 0.604275 -0.761477 3.870059
C 2.225552 -1.483801 2.234539
H -0.229740 1.176241 3.592561
H 0.001635 -0.937086 4.748749
I 3.171757 0.216155 -0.090455
Br -0.117005 0.453591 -1.353392
H 2.909317 -2.212145 1.826792
H 1.867634 3.061357 -1.854421
N 1.367673 5.556471 -0.956619
C 1.754364 5.496238 -2.351524
C 0.775452 6.777009 -0.440818
H 2.718580 4.996597 -2.464092
H 1.851609 6.508370 -2.733692
H 1.015752 4.961180 -2.959522
H 1.257246 7.085201 0.489411
H 0.914061 7.568505 -1.171855
H -0.296541 6.659255 -0.251769
N 1.634557 -2.947576 4.063123
C 0.750519 -3.266386 5.166825
H -0.298766 -3.307187 4.853889
H 0.840867 -2.528473 5.966540
H 1.030310 -4.235622 5.569822
C 2.416991 -4.007808 3.459754
H 2.407088 -4.870885 4.119475
H 3.456057 -3.699876 3.321738
H 2.015802 -4.308354 2.485281
SCF: -3601.745454
ZPE: 0.305932
H: -3601.417737
G: -3601.488955

7_OMe_TS_conf1

C 0.457073 1.877261 -2.315340
C 0.321151 1.970179 0.481517
C 0.119725 0.810332 -1.524263
C 0.696971 3.070561 -1.629527
C 0.611032 3.111942 -0.230730
C 0.080930 0.740098 -0.152552
H 0.803253 4.048565 0.274679
H 0.304099 2.000102 1.564832
C -0.117076 -0.539065 0.521265
C -0.409724 -3.083736 1.690999
C 0.215817 -1.718149 -0.153452

C -0.607265 -0.686302 1.814116
C -0.754358 -1.935034 2.401200
C 0.085306 -2.974527 0.386985
H -0.894917 0.195911 2.372956
H -1.144587 -2.001545 3.406272
I 0.980917 -1.449960 -2.079600
Br -2.180132 0.018158 -2.426315
H 0.352181 -3.871867 -0.154706
H 0.465577 1.811436 -3.392190
O 1.001056 4.224953 -2.247386
C 1.125520 4.215358 -3.662800
H 0.178319 3.945505 -4.135181
H 1.907667 3.521931 -3.979620
H 1.398390 5.228194 -3.946643
O -0.516664 -4.337467 2.170691
C -1.024898 -4.502187 3.487430
H -0.383240 -4.006045 4.218723
H -1.030050 -5.572749 3.674316
H -2.041972 -4.111955 3.564528
SCF: -3562.875931
ZPE: 0.225620
H: -3562.632512
G: -3562.694085

7_OMe_TS_conf2

C 0.373463 2.075398 -1.970327
C 0.174294 2.097286 0.824347
C 0.017524 0.988814 -1.214963
C 0.598508 3.250626 -1.248917
C 0.480532 3.256558 0.148122
C -0.051165 0.883972 0.153579
H 0.660911 4.179966 0.681417
H 0.132749 2.100154 1.907383
C -0.259070 -0.412005 0.790707
C -0.563119 -2.982757 1.897444
C 0.087546 -1.570025 0.102782
C -0.775516 -0.586669 2.078537
C -0.924378 -1.843434 2.623445
C -0.046122 -2.850933 0.609019
H -1.075826 0.282901 2.649944
H -1.330603 -1.970624 3.618457
I 0.889153 -1.258815 -1.803434
Br -2.258888 0.224127 -2.189459
H 0.242564 -3.713022 0.026539

H 0.405685 2.037322 -3.048020
O 0.916585 4.420369 -1.829767
C 1.066698 4.449258 -3.242451
H 0.127656 4.194468 -3.738958
H 1.853415 3.763288 -3.564088
H 1.346137 5.468959 -3.493376
O -0.746333 -4.166425 2.512099
C -0.397738 -5.346990 1.803309
H -0.985718 -5.440181 0.887497
H -0.626310 -6.175210 2.468686
H 0.667165 -5.356378 1.560448
SCF: -3562.876057
ZPE: 0.225539
H: -3562.632686
G: -3562.694341

7_OMe_TS_conf3

C 0.308671 1.764091 -2.576182
C 0.261210 1.787376 0.214402
C 0.037120 0.669405 -1.813463
C 0.528197 2.956742 -1.872491
C 0.487986 2.967665 -0.475900
C 0.044285 0.570837 -0.435052
H 0.658826 3.879627 0.076071
H 0.282217 1.792566 1.298245
C -0.089913 -0.730685 0.212474
C -0.270955 -3.311665 1.323750
C 0.262970 -1.881111 -0.499884
C -0.542248 -0.925687 1.512667
C -0.633889 -2.192590 2.071217
C 0.187096 -3.154218 0.011124
H -0.845239 -0.067318 2.099844
H -0.996888 -2.296877 3.083197
I 0.962818 -1.540574 -2.439960
Br -2.265738 -0.205268 -2.631887
H 0.467600 -4.028582 -0.560459
H 0.294809 1.759209 -3.656501
O 0.758020 4.040259 -2.635639
C 0.952448 5.286471 -1.978888
H 1.833151 5.254785 -1.334196
H 0.073340 5.557859 -1.391017
H 1.104246 6.018406 -2.767683
O -0.327187 -4.579716 1.773670
C -0.795860 -4.792658 3.098207

H -0.150216 -4.295888 3.825548
H -0.765146 -5.867245 3.257522
H -1.821527 -4.435218 3.211266
SCF: -3562.875219
ZPE: 0.225543
H: -3562.631834
G: -3562.693593

7_OMe_TS_conf4

C 1.285951 3.143603 -0.856260
C 1.140837 3.088464 1.930293
C 0.955162 2.036071 -0.136641
C 1.515106 4.308559 -0.110363
C 1.425017 4.280975 1.283632
C 0.912907 1.897808 1.237887
H 1.601593 5.170905 1.868714
H 1.124327 3.062679 3.013836
C 0.726772 0.582786 1.843286
C 0.455054 -2.019691 2.882396
C 1.068922 -0.553289 1.118235
C 0.232535 0.369162 3.133931
C 0.099738 -0.903104 3.645816
C 0.951267 -1.848760 1.590429
H -0.064051 1.220526 3.733982
H -0.290318 -1.060141 4.643016
I 1.833408 -0.185623 -0.793561
Br -1.339542 1.263384 -1.062891
H 1.235856 -2.692267 0.979330
H 1.308364 3.171143 -1.936065
O 1.801905 5.406107 -0.832880
C 2.003266 6.628311 -0.134232
H 2.858486 6.555748 0.540804
H 1.110119 6.905972 0.429095
H 2.202192 7.377502 -0.895844
O 0.286152 -3.221042 3.465866
C 0.622372 -4.379881 2.716323
H 0.017665 -4.446476 1.809188
H 0.406124 -5.227589 3.360980
H 1.682619 -4.381144 2.453897
SCF: -3562.875341
ZPE: 0.225484
H: -3562.632026
G: -3562.693667

8_CF3_TS_conf1

C 0.220143 1.582611 -1.842911
C 0.067635 1.693715 0.938955
C -0.021404 0.457380 -1.082261
C 0.323029 2.800216 -1.173356
C 0.230790 2.860400 0.207182
C -0.038885 0.456573 0.307149
H 0.471077 3.701026 -1.756799
H 0.317030 3.811003 0.714205
H 0.054424 1.726889 2.021606
C -0.094027 -0.824405 1.014357
C -0.086267 -3.321222 2.281361
C 0.395262 -1.963360 0.375452
C -0.590720 -0.968705 2.310217
C -0.584735 -2.202052 2.934528
C 0.408794 -3.207373 0.990417
H -0.998393 -0.104534 2.818992
H -0.977998 -2.299955 3.937220
H -0.085556 -4.285167 2.770740
I 1.089575 -1.616500 -1.564648
Br -2.177889 -0.541839 -1.874635
C 0.270745 1.571344 -3.341069
F -0.889515 1.936528 -3.897437
F 1.196688 2.420933 -3.801510
F 0.575299 0.361920 -3.834068
C 0.927794 -4.427276 0.278121
F 0.953511 -5.499839 1.062438
F 2.177292 -4.241641 -0.180071
F 0.176701 -4.734273 -0.790580
SCF: -4007.996326
ZPE: 0.169426
H: -4007.807091
G: -4007.874007

8_CF3_TS_conf2

C 1.134217 3.104597 -0.837535
C 1.006561 3.219469 1.945348
C 0.875881 1.984828 -0.074406
C 1.267305 4.320077 -0.169457
C 1.187386 4.382401 1.211766
C 0.869920 1.984504 1.315066
H 1.429157 5.217543 -0.754380
H 1.296831 5.331193 1.717729
H 1.002775 3.253523 3.028024

C 0.794216 0.705011 2.023088
C 0.758769 -1.791512 3.290128
C 1.252592 -0.444355 1.379842
C 0.307110 0.571609 3.323748
C 0.291782 -0.661626 3.948083
C 1.244117 -1.688513 1.994624
H -0.075905 1.444582 3.836599
H -0.093738 -0.750909 4.954575
H 0.742751 -2.755288 3.779539
I 1.939133 -0.112281 -0.565544
Br -1.307370 1.030521 -0.848897
C 1.172693 3.091542 -2.336021
F 0.015367 3.479028 -2.883393
F 2.111339 3.922600 -2.804392
F 1.449554 1.876099 -2.830583
C 1.730538 -2.919325 1.278169
F 1.733072 -3.993671 2.060485
F 2.982400 -2.762986 0.815559
F 0.968345 -3.206262 0.211732
SCF: -4007.996334
ZPE: 0.169433
H: -4007.807093
G: -4007.874022

8_CN_TS_conf1

C 0.152930 1.708736 -2.159422
C 0.011378 1.857618 0.620240
C -0.056309 0.582617 -1.374829
C 0.220224 2.946006 -1.511836
C 0.128803 3.018418 -0.132698
C -0.054976 0.605536 0.012872
H 0.343238 3.836423 -2.114590
H 0.184536 3.978348 0.360632
H 0.001259 1.908417 1.702515
C -0.049704 -0.672962 0.722669
C 0.100545 -3.188316 1.965497
C 0.442655 -1.788057 0.050970
C -0.479090 -0.850779 2.038025
C -0.404524 -2.092521 2.647600
C 0.531516 -3.040120 0.648160
H -0.888212 -0.006346 2.578279
H -0.747952 -2.211015 3.666152
H 0.164616 -4.160203 2.435248
I 1.056316 -1.441655 -1.910450

Br -2.227332 -0.421637 -2.120619
C 0.238737 1.594822 -3.577160
N 0.331775 1.466905 -4.714576
C 1.062810 -4.157829 -0.071865
N 1.496062 -5.035106 -0.671210
SCF: -3518.315649
ZPE: 0.156833
H: -3518.142406
G: -3518.201141

8_F_TS_conf1

C 0.093720 1.769297 -2.356226
C 0.034306 1.949584 0.409156
C -0.090483 0.653060 -1.571495
C 0.189532 3.004712 -1.753757
C 0.144248 3.092111 -0.363808
C -0.059683 0.688953 -0.189221
H 0.289267 3.881089 -2.382199
H 0.222926 4.060159 0.111072
H 0.056806 2.010576 1.490020
C -0.031379 -0.586819 0.527328
C 0.178356 -3.112126 1.745321
C 0.451055 -1.697151 -0.168857
C -0.414248 -0.769071 1.853285
C -0.309007 -2.018169 2.448264
C 0.558673 -2.932461 0.430456
H -0.808368 0.069290 2.412834
H -0.616203 -2.146664 3.477539
H 0.266945 -4.092718 2.193798
I 1.029312 -1.391983 -2.138848
Br -2.260750 -0.348145 -2.367724
F 0.129528 1.640755 -3.685128
F 1.042347 -3.960177 -0.276009
SCF: -3532.316947
ZPE: 0.143440
H: -3532.159101
G: -3532.212979

8_F_TS_conf2

C 0.087736 1.780501 -2.362466
C 0.028751 1.960140 0.402968
C -0.096126 0.664049 -1.577961
C 0.183415 3.015796 -1.759728
C 0.138343 3.102866 -0.369752

C -0.065093 0.699628 -0.195683
H 0.282878 3.892337 -2.387986
H 0.216913 4.070820 0.105338
H 0.051415 2.020890 1.483841
C -0.036413 -0.576305 0.520565
C 0.174024 -3.101866 1.737919
C 0.446100 -1.686382 -0.175972
C -0.418994 -0.758945 1.846552
C -0.313407 -2.008165 2.441215
C 0.554059 -2.921816 0.423025
H -0.813158 0.079208 2.406380
H -0.620382 -2.136960 3.470518
H 0.262879 -4.082550 2.186145
I 1.023959 -1.380652 -2.145991
Br -2.266338 -0.337389 -2.374044
F 1.037788 -3.949272 -0.283778
F 0.123351 1.652268 -3.691403
SCF: -3532.316947
ZPE: 0.143440
H: -3532.159100
G: -3532.212978

8_NMe2_TS_conf1

C 0.806704 1.152609 -3.437410
C 0.319962 1.326566 -0.688581
C 0.668018 0.060089 -2.630300
C 0.662958 2.391119 -2.825172
C 0.413386 2.508343 -1.441535
C 0.463922 0.064903 -1.272339
H 0.177356 1.363527 0.382069
C 0.486506 -1.194400 -0.520424
C 0.647221 -3.631329 0.834857
C 1.200645 -2.271209 -1.049943
C -0.157652 -1.357465 0.697394
C -0.085479 -2.570925 1.411739
C 1.284258 -3.479417 -0.383556
H -0.740723 -0.533104 1.081355
H 0.719018 -4.585551 1.334884
I 2.134389 -1.959753 -2.887957
Br -1.229306 -1.354086 -3.732509
H 1.837982 -4.310224 -0.800841
H 0.971447 1.074388 -4.502213
H 0.742096 3.267788 -3.451004
N 0.297076 3.743705 -0.842190

C -0.239075 3.809040 0.503560
C 0.137403 4.912208 -1.686329
H -1.232409 3.348792 0.576520
H -0.316414 4.851731 0.800042
H 0.422390 3.309299 1.213863
H -0.753176 4.847730 -2.323807
H 0.048896 5.791154 -1.053120
H 1.008796 5.051792 -2.328223
N -0.707246 -2.715931 2.616468
C -0.751573 -4.019650 3.248838
H 0.254397 -4.388683 3.460972
H -1.263381 -4.759679 2.623940
H -1.284718 -3.934827 4.191483
C -1.566342 -1.660123 3.113863
H -2.412576 -1.470799 2.444129
H -1.011635 -0.726830 3.235255
H -1.953123 -1.950699 4.086423
SCF: -3601.740237
ZPE: 0.306274
H: -3601.412281
G: -3601.483137

8_NMe2_TS_conf2

C 1.117764 3.425681 -0.379860
C 0.734655 3.631639 2.453087
C 0.877601 2.349008 0.472487
C 1.169954 4.653759 0.314442
C 0.965751 4.753692 1.682625
C 0.709579 2.373371 1.839045
H 1.365776 5.554067 -0.249000
H 1.012320 5.729278 2.148537
H 0.614143 3.699560 3.526011
C 0.578947 1.122220 2.595191
C 0.519703 -1.306426 3.985090
C 1.139239 -0.041173 2.076265
C -0.028932 1.042181 3.847991
C -0.043957 -0.161255 4.533019
C 1.120715 -1.271961 2.725994
H -0.487864 1.921941 4.279534
H -0.514427 -0.215351 5.506375
H 0.484079 -2.238942 4.532307
I 2.123750 0.163893 0.258776
Br -1.181341 1.117869 -0.534413
N 1.203229 3.365819 -1.754731

C 1.706483 2.168746 -2.405917
C 1.491575 4.602304 -2.460542
H 2.773149 1.999353 -2.208513
H 1.581876 2.290007 -3.479947
H 1.121758 1.300137 -2.112869
H 2.485858 5.000982 -2.223358
H 1.443794 4.402794 -3.528122
H 0.745807 5.361351 -2.226165
N 1.700484 -2.402344 2.103749
C 0.821175 -3.012472 1.103288
H 0.397370 -2.256091 0.444174
H -0.005120 -3.552609 1.584081
H 1.399182 -3.714972 0.502449
C 2.218410 -3.414325 3.013580
H 2.818677 -4.117277 2.435561
H 1.422953 -3.980700 3.514826
H 2.852181 -2.948157 3.767048
SCF: -3601.736218
ZPE: 0.306981
H: -3601.408449
G: -3601.475365

8_OMe_TS_conf1

C -0.768018 2.030721 -1.741207
C -0.262943 2.300839 1.017500
C -0.683498 0.950901 -0.874762
C -0.667940 3.287346 -1.153410
C -0.438118 3.413555 0.218351
C -0.358342 1.017899 0.460344
H -0.771288 4.171651 -1.768008
H -0.361472 4.403258 0.648205
H -0.010176 2.399707 2.065706
C -0.025188 -0.227527 1.155734
C 0.762285 -2.657740 2.314813
C 0.453481 -1.287044 0.388454
C -0.111464 -0.407992 2.535429
C 0.278397 -1.613543 3.094494
C 0.859487 -2.500445 0.933304
H -0.495798 0.390199 3.156824
H 0.203488 -1.753918 4.165137
H 1.061706 -3.585859 2.780101
I 0.578274 -0.984426 -1.667624
Br -2.792497 -0.349151 -1.159324
O -0.947087 1.769341 -3.046178

C -1.018693 2.882031 -3.929431
H -0.103161 3.475248 -3.883174
H -1.879359 3.509808 -3.691078
H -1.135583 2.464738 -4.925855
O 1.323248 -3.430197 0.079130
C 1.745074 -4.678329 0.618971
H 2.573176 -4.537846 1.315959
H 2.075432 -5.271543 -0.229172
H 0.916775 -5.181682 1.120564
SCF: -3562.875829
ZPE: 0.225747
H: -3562.632191
G: -3562.693733

8_OMe_TS_conf2

C -1.161426 1.727173 -1.847234
C -0.976593 2.136018 0.934470
C -0.840666 0.718607 -0.950775
C -1.469814 2.961385 -1.284759
C -1.395758 3.150981 0.096961
C -0.657126 0.878744 0.403089
H -1.772022 3.777564 -1.927258
H -1.638668 4.122195 0.506778
H -0.849050 2.303308 1.996597
C -0.042066 -0.217554 1.154152
C 1.298171 -2.322487 2.434327
C 0.775647 -1.101326 0.454175
C -0.184905 -0.408228 2.527576
C 0.480702 -1.452862 3.146921
C 1.459155 -2.149711 1.060511
H -0.826235 0.253048 3.095238
H 0.362219 -1.603854 4.212196
H 1.806337 -3.127487 2.945498
I 0.976409 -0.780749 -1.593189
Br -2.464489 -1.128966 -1.368917
O -1.158096 1.421879 -3.154786
C -1.491714 2.461385 -4.066629
H -0.791767 3.294860 -3.979796
H -2.510560 2.813794 -3.894164
H -1.418843 2.023269 -5.058268
O 2.231751 -2.915650 0.269607
C 2.928663 -4.001303 0.872023
H 3.628451 -3.639768 1.627393
H 3.474417 -4.486334 0.067555

H 2.228072 -4.707927 1.320408
SCF: -3562.875842
ZPE: 0.225797
H: -3562.632187
G: -3562.693569

8_OMe_TS_conf3

C -0.092979 2.163005 -1.747822
C -0.294210 2.276238 1.060629
C -0.331822 1.048461 -0.957462
C -0.032789 3.379452 -1.075968
C -0.153490 3.429900 0.314541
C -0.359648 1.032010 0.417817
H 0.106057 4.291982 -1.640260
H -0.099485 4.389415 0.811078
H -0.313693 2.308550 2.142856
C -0.336184 -0.265953 1.095938
C -0.107777 -2.806512 2.263248
C 0.225325 -1.341343 0.411887
C -0.796801 -0.486590 2.393046
C -0.679633 -1.746125 2.956736
C 0.359855 -2.610170 0.964828
H -1.256144 0.324373 2.942679
H -1.044305 -1.916333 3.961565
H -0.027758 -3.777398 2.730847
I 0.905735 -0.978893 -1.522036
Br -2.406995 -0.010545 -1.852730
O 0.043196 1.971234 -3.069926
C 0.282604 3.120662 -3.872906
H 1.205903 3.620261 -3.572617
H -0.554510 3.818667 -3.807391
H 0.377226 2.757578 -4.892631
O 0.939670 -3.552325 0.199941
C 1.078369 -4.859808 0.746149
H 1.709057 -4.841792 1.636694
H 1.553455 -5.455784 -0.028104
H 0.101770 -5.282023 0.989374
SCF: -3562.875844
ZPE: 0.225775
H: -3562.632192
G: -3562.693642

8_OMe_TS_conf4

C -0.204284 2.176911 -1.764312

C -0.637255 2.304702 1.016970
C -0.173796 1.062846 -0.938517
C -0.543722 3.377113 -1.148796
C -0.777018 3.428964 0.227142
C -0.296897 1.077019 0.431685
H -0.627310 4.274952 -1.746355
H -1.036252 4.376567 0.679967
H -0.745869 2.360805 2.092796
C 0.047152 -0.140198 1.170387
C 0.908415 -2.473670 2.468052
C 0.941870 -1.025700 0.573933
C -0.424326 -0.449582 2.445347
C 0.007324 -1.605685 3.073909
C 1.393802 -2.185833 1.193568
H -1.135279 0.208486 2.927474
H -0.365712 -1.846951 4.060945
H 1.229606 -3.366843 2.984507
I 1.630738 -0.534282 -1.328141
Br -1.787516 -0.574592 -1.906194
O 0.080394 1.997149 -3.064388
C 0.051365 3.146881 -3.901638
H 0.769352 3.895299 -3.560169
H -0.950537 3.579804 -3.928138
H 0.326867 2.800207 -4.893860
O 2.273998 -2.940393 0.511796
C 2.752026 -4.129824 1.131484
H 3.280815 -3.897684 2.057734
H 3.438762 -4.579314 0.419583
H 1.929089 -4.817358 1.334128
SCF: -3562.875839
ZPE: 0.225864
H: -3562.632159
G: -3562.693294

9_TS_conf1

C 0.085990 1.687655 -2.180530
C 0.036612 1.895513 0.624241
C -0.053081 0.617252 -1.341764
C 0.156400 2.927612 -1.550788
C 0.122776 3.030324 -0.164056
C -0.039914 0.624509 0.039533
H 0.235132 3.814331 -2.166984
H 0.186724 4.001957 0.306297
H 0.058297 1.975547 1.702386

C -0.027020 -0.653219 0.747739
C 0.104298 -3.181335 1.965246
C 0.462162 -1.776959 0.072524
C -0.462654 -0.850025 2.048916
C -0.399005 -2.094489 2.653732
C 0.536109 -3.017380 0.659670
I 1.079408 -1.490599 -1.878203
Br -2.282922 -0.562539 -2.047111
H 0.093925 1.589636 -3.256178
F -0.983689 0.148521 2.756085
F -0.828650 -2.247804 3.896786
F 0.169715 -4.367442 2.549232
F 1.018087 -4.064965 0.001328
SCF: -3730.794570
ZPE: 0.127307
H: -3730.650933
G: -3730.709207

9_TS_conf2

C 0.068601 1.670168 -2.151184
C 0.022128 1.874994 0.604215
C -0.118434 0.559618 -1.357318
C 0.170086 2.906889 -1.548188
C 0.136270 3.014495 -0.166380
C -0.086920 0.611180 0.033310
C -0.058017 -0.657326 0.762979
C 0.132623 -3.180643 1.971407
C 0.447986 -1.774728 0.092682
C -0.490571 -0.850425 2.074227
C -0.392040 -2.100758 2.667439
C 0.558145 -3.027303 0.656259
H -0.923182 -0.024839 2.621226
H -0.736817 -2.232047 3.684630
H 0.207744 -4.152133 2.441597
I 1.043235 -1.415730 -1.883651
Br -2.251942 -0.434958 -2.127381
H 0.956362 -3.866567 0.102616
F 0.092160 1.568152 -3.476502
F 0.290364 3.998924 -2.290151
F 0.250718 4.209790 0.406566
F 0.074403 2.015249 1.927300
SCF: -3730.793314
ZPE: 0.127569
H: -3730.649480

G: -3730.707385

10_CCF2_TS_conf1

H 3.114400 0.771458 2.260070
C 2.123290 1.140360 2.032106
C -0.431618 2.075718 1.435161
C 1.161676 0.307971 1.483964
C 1.783386 2.459286 2.297441
C 0.506429 2.920905 2.006381
C -0.125059 0.740587 1.165568
H 2.521361 3.121635 2.730614
H 0.242524 3.950022 2.212388
H -1.416310 2.447076 1.179986
I 1.607080 -1.719234 1.220841
C 0.184788 -1.880618 -0.809189
C -0.445159 -0.773247 -3.201062
C -0.649748 -0.787029 -0.782100
C 0.793793 -2.411699 -1.922243
C 0.447279 -1.839202 -3.139617
C -0.972567 -0.247741 -2.034568
H 1.468324 -3.253328 -1.863227
H 0.883843 -2.245855 -4.043260
H -1.637464 0.607794 -2.059674
H -0.709696 -0.339783 -4.155998
C -1.095446 -0.140228 0.474961
C -2.338128 -0.283425 0.899219
F -2.832464 0.259725 1.986887
F -3.261054 -0.989687 0.294385
Br -0.923462 -3.891460 0.330967
SCF: -3609.713303
ZPE: 0.177703
H: -3609.519075
G: -3609.578287

10_CH2_2_TS_conf1

C 1.804693 -0.952868 -0.729738
C 1.412320 -0.513189 0.541662
C 1.651788 0.822282 0.766490
C 2.165190 1.742169 -0.114442
C 2.532340 1.248468 -1.362310
C 2.356233 -0.095817 -1.668834
C 0.769923 -1.433937 1.537736
C -0.793187 -1.455959 1.532652
C -1.483218 -0.573061 0.523506

C -2.199455 -1.135006 -0.532774
C -2.872256 -0.347758 -1.457783
C -2.844208 1.035478 -1.354183
C -2.130501 1.632877 -0.323959
C -1.473065 0.821343 0.587001
I -0.277759 1.709887 2.057072
H 1.655166 -2.001513 -0.962962
H 2.298477 2.781452 0.147792
H 2.958355 1.932520 -2.085530
H 2.643071 -0.473265 -2.641301
H 1.123794 -1.155037 2.531014
H 1.125726 -2.442738 1.334966
H -1.148960 -1.184729 2.528694
H -1.121546 -2.477603 1.351821
H -2.229649 -2.214591 -0.620202
H -3.421469 -0.819525 -2.262581
H -3.367099 1.653967 -2.071923
H -2.088375 2.710378 -0.237526
Br 2.953673 1.185779 2.985639
SCF: -3412.437003
ZPE: 0.217298
H: -3412.204552
G: -3412.260464

10_CH2_2_TS_conf2

C 1.878698 -0.888317 0.603777
C 1.396201 -0.436973 -0.632111
C 1.565190 0.912681 -0.835079
C 2.087680 1.833681 0.039202
C 2.546124 1.327674 1.251529
C 2.445580 -0.029882 1.532485
C 0.739819 -1.362609 -1.614560
C -0.818993 -1.448806 -1.530928
C -1.487140 -0.624940 -0.459232
C -2.115706 -1.245038 0.620093
C -2.761850 -0.511986 1.606577
C -2.794049 0.873587 1.543398
C -2.168825 1.528313 0.490686
C -1.536930 0.769924 -0.481983
I -0.469341 1.746615 -1.994355
H 1.788250 -1.947735 0.817861
H 2.160951 2.883714 -0.203042
H 2.982636 2.012893 1.967347
H 2.803094 -0.416978 2.477344

H 1.145837 -2.359756 -1.452577
H 1.030397 -1.049171 -2.618089
H -1.096499 -2.488245 -1.366826
H -1.237036 -1.162324 -2.497991
H -2.097674 -2.326935 0.676674
H -3.242915 -1.027750 2.427833
H -3.296081 1.449810 2.309566
H -2.174358 2.608665 0.434924
Br 2.726941 1.379891 -3.112524
SCF: -3412.437066
ZPE: 0.217414
H: -3412.204544
G: -3412.260221

10_CH2_2_TS_conf3

C 2.184959 -1.165551 0.526845
C 1.494086 -0.553923 -0.518690
C 1.485699 0.841990 -0.517207
C 2.119980 1.609237 0.446935
C 2.808343 0.963348 1.465143
C 2.834973 -0.423235 1.503832
C 0.824912 -1.386708 -1.582933
C -0.738026 -1.363080 -1.616222
C -1.399254 -0.483843 -0.595214
C -1.819286 -0.977738 0.647198
C -2.388624 -0.161216 1.611437
C -2.554847 1.195925 1.361034
C -2.160247 1.742884 0.144145
C -1.631024 0.860949 -0.765736
I 0.327186 1.799831 -1.973441
H 2.213285 -2.248076 0.564034
H 2.079257 2.689689 0.410904
H 3.313158 1.546880 2.223911
H 3.365012 -0.932684 2.298461
H 1.149521 -2.416445 -1.446217
H 1.199663 -1.067481 -2.557525
H -1.097988 -2.378870 -1.461237
H -1.072776 -1.043797 -2.603979
H -1.676743 -2.036072 0.836974
H -2.696451 -0.580238 2.560172
H -2.993889 1.848981 2.104827
H -2.284702 2.793193 -0.074824
Br -2.886174 1.326054 -2.992626
SCF: -3412.437053

ZPE: 0.217347
H: -3412.204579
G: -3412.260346

10_CH2_2_TS_conf4

C 2.158559 -1.231791 0.475050
C 1.486746 -0.554147 -0.541788
C 1.503046 0.839720 -0.467465
C 2.142044 1.544403 0.540329
C 2.810484 0.833909 1.528429
C 2.813217 -0.553088 1.494281
C 0.808967 -1.317780 -1.651465
C -0.753300 -1.265193 -1.688286
C -1.402940 -0.426474 -0.626424
C -1.838092 -0.975252 0.587353
C -2.395917 -0.198592 1.590496
C -2.534677 1.172665 1.409922
C -2.124030 1.773685 0.224220
C -1.608246 0.929596 -0.728437
I 0.371752 1.891733 -1.879470
H 2.167545 -2.315124 0.455714
H 2.119770 2.625877 0.560516
H 3.318697 1.367819 2.320702
H 3.327996 -1.112528 2.265000
H 1.115096 -2.358892 -1.568612
H 1.193228 -0.953758 -2.606436
H -1.131158 -2.280994 -1.584732
H -1.078715 -0.891885 -2.660169
H -1.716713 -2.044489 0.722954
H -2.716032 -0.660097 2.515146
H -2.964132 1.794904 2.185065
H -2.227110 2.836243 0.059586
Br -2.846085 1.529529 -2.931478
SCF: -3412.437083
ZPE: 0.217445
H: -3412.204569
G: -3412.260024

10_CH2_3_TS_conf1

C -3.122091 -0.971405 -0.245125
C -1.926829 -0.379626 -0.661888
C -1.841820 1.001557 -0.502116
C -2.857505 1.772151 0.050837
C -4.027161 1.145980 0.451033

C -4.158393 -0.228492 0.297054
C -0.809826 -1.260623 -1.150623
C -0.049736 -1.904546 0.017155
C 0.601578 -0.908337 0.978478
C 1.795706 -0.184911 0.419917
C 3.026397 -0.841048 0.260318
C 4.164370 -0.191967 -0.189465
C 4.116268 1.163497 -0.491264
C 2.925331 1.870912 -0.354725
C 1.853883 1.146925 0.102702
I -0.142628 2.038748 -1.160960
H -3.225755 -2.045253 -0.352767
H -2.740538 2.841356 0.166564
H -4.828570 1.733633 0.879299
H -5.070467 -0.724104 0.604326
H -0.117405 -0.706352 -1.786138
H -1.237631 -2.055348 -1.763331
H 0.711129 -2.575959 -0.387279
H -0.748443 -2.519292 0.589642
H 0.938992 -1.455177 1.861407
H -0.124732 -0.172958 1.327027
H 3.062982 -1.892978 0.524358
H 5.090642 -0.740258 -0.298079
H 4.996007 1.690155 -0.839017
H 2.865664 2.926207 -0.581672
Br 0.880585 2.427515 2.234333
SCF: -3451.744254
ZPE: 0.246028
H: -3451.481997
G: -3451.540057

10_CH2_3_TS_conf2

C -3.036202 -0.790546 -0.294841
C -1.797985 -0.142134 -0.425105
C -1.839796 1.173441 -0.044072
C -2.901691 1.886979 0.450565
C -4.100838 1.188063 0.555212
C -4.165612 -0.150518 0.188143
C -0.613825 -0.852024 -1.021112
C 0.025690 -1.901766 -0.110198
C 0.794038 -1.323011 1.085854
C 1.921831 -0.433701 0.638628
C 3.108765 -1.020624 0.192196
C 4.155153 -0.266372 -0.313738

C 4.042765 1.115641 -0.399968
C 2.881598 1.737360 0.030626
C 1.855389 0.954591 0.546037
I 0.169986 1.982595 1.253739
H -3.085819 -1.827833 -0.609686
H -2.829138 2.929183 0.728416
H -4.973541 1.707516 0.930403
H -5.098190 -0.692409 0.272029
H 0.121390 -0.109649 -1.334386
H -0.959338 -1.350596 -1.929134
H 0.716161 -2.497174 -0.712313
H -0.743362 -2.582028 0.262806
H 1.212184 -2.150674 1.660406
H 0.108365 -0.791006 1.747162
H 3.197591 -2.099771 0.246949
H 5.060300 -0.758752 -0.645639
H 4.852261 1.712627 -0.799177
H 2.779208 2.812373 -0.033116
Br -0.857336 2.540219 -2.116684
SCF: -3451.744231
ZPE: 0.246004
H: -3451.481995
G: -3451.540059

10_CH2_3_TS_conf3

C -2.404128 -0.792348 0.788799
C -1.733895 -0.441515 -0.387102
C -1.497180 0.920321 -0.573654
C -1.896652 1.892677 0.336507
C -2.564463 1.504082 1.486936
C -2.811708 0.155828 1.713064
C -1.336936 -1.537269 -1.344398
C -0.008439 -2.239354 -1.028007
C 1.267532 -1.464905 -1.380989
C 1.615025 -0.342510 -0.441462
C 1.984436 -0.607573 0.886333
C 2.324032 0.396605 1.776788
C 2.312243 1.724078 1.361666
C 1.957888 2.048410 0.057371
C 1.646312 0.991574 -0.766296
I -0.310157 1.549614 -2.177635
H -2.611123 -1.841633 0.966417
H -1.686486 2.938330 0.153840
H -2.883901 2.252282 2.200515

H -3.330370 -0.157415 2.610256
H -1.315958 -1.166195 -2.370554
H -2.123511 -2.292483 -1.303248
H 0.008759 -3.167544 -1.602294
H 0.010721 -2.522396 0.028065
H 1.206137 -1.078442 -2.399556
H 2.102043 -2.169933 -1.364315
H 2.000328 -1.646137 1.200014
H 2.598048 0.146920 2.793211
H 2.573567 2.523336 2.043745
H 1.938806 3.071920 -0.287699
Br 2.969031 1.351677 -2.976319
SCF: -3451.750633
ZPE: 0.246040
H: -3451.488380
G: -3451.546198

10_CH2_3_TS_conf4

C -2.931563 -0.930308 -0.370731
C -2.080897 -0.422225 0.624400
C -1.984399 0.941939 0.588490
C -2.533097 1.826768 -0.299997
C -3.356428 1.258386 -1.268857
C -3.562359 -0.115263 -1.296567
C -1.323066 -1.332291 1.545660
C 0.161171 -1.597675 1.146641
C 0.593107 -1.164934 -0.276002
C 1.843612 -0.325005 -0.325010
C 2.980019 -0.785890 -0.989940
C 4.131546 -0.017050 -1.089579
C 4.173095 1.250323 -0.527789
C 3.059550 1.742699 0.140772
C 1.926178 0.949083 0.237572
I 0.324696 1.725824 1.385350
H -3.067365 -2.005779 -0.401850
H -2.370941 2.892722 -0.241503
H -3.834809 1.910432 -1.988726
H -4.206566 -0.552496 -2.047752
H -1.861664 -2.278158 1.576780
H -1.352241 -0.906289 2.550582
H 0.339747 -2.667431 1.245903
H 0.811656 -1.124499 1.880732
H -0.199921 -0.597154 -0.766589
H 0.752506 -2.046002 -0.896156

H 2.949116 -1.770803 -1.440772
H 4.994973 -0.408621 -1.612247
H 5.063294 1.861005 -0.605368
H 3.083921 2.732369 0.578943
Br -2.522872 1.956323 2.943609
SCF: -3451.739243
ZPE: 0.246067
H: -3451.476789
G: -3451.535213

10_CH2_3_TS_conf5

C -2.424753 -0.743781 -0.803627
C -1.789174 -0.385132 0.387136
C -1.448034 0.962124 0.509523
C -1.704360 1.912186 -0.467817
C -2.343870 1.514796 -1.633595
C -2.698044 0.183546 -1.799247
C -1.556106 -1.434521 1.449032
C -0.105712 -1.761119 1.858190
C 0.926382 -1.776073 0.738431
C 1.401712 -0.474028 0.130405
C 1.848700 -0.497531 -1.204679
C 2.444232 0.586048 -1.823553
C 2.632238 1.767663 -1.116193
C 2.201132 1.861572 0.200047
C 1.617491 0.737842 0.740428
I -0.270069 1.534408 2.136061
H -2.709602 -1.779889 -0.942869
H -1.405439 2.942835 -0.329679
H -2.552795 2.243651 -2.405623
H -3.190403 -0.137272 -2.708463
H -2.018891 -2.351007 1.082574
H -2.108425 -1.147866 2.348980
H -0.125461 -2.769085 2.277306
H 0.241531 -1.123186 2.667398
H 0.568089 -2.402279 -0.081796
H 1.826457 -2.260520 1.130529
H 1.723980 -1.430029 -1.744674
H 2.762747 0.509360 -2.854692
H 3.095405 2.630635 -1.577481
H 2.318156 2.774137 0.765973
Br 2.842885 0.312515 3.071974
SCF: -3451.741142
ZPE: 0.246056

H: -3451.478775

G: -3451.536919

10_CH2_TS_conf1

H 1.678528 2.604648 -2.359275

C 1.340863 2.386262 -1.356809

C 0.411778 1.804971 1.216227

C 0.185610 1.692683 -1.098154

C 2.032322 2.831797 -0.234755

C 1.564227 2.554206 1.045686

C -0.320028 1.328246 0.121150

H 2.940286 3.403443 -0.380666

H 2.108176 2.910497 1.910259

H 0.051543 1.558723 2.209067

C -1.494087 0.399145 0.279883

C -1.015140 -1.028976 0.182986

C -0.015323 -3.653924 0.050414

C -0.395940 -1.530461 -0.959420

C -1.113257 -1.893088 1.272973

C -0.629385 -3.191156 1.207110

C 0.112295 -2.816623 -1.048566

H -1.582402 -1.532103 2.180335

H -0.727755 -3.843555 2.065214

H 0.594404 -3.164224 -1.952589

H 0.369397 -4.664039 -0.001831

I -0.263083 -0.261688 -2.619643

Br -1.640365 2.932105 -2.477733

H -1.963248 0.557493 1.248739

H -2.229419 0.615819 -0.500600

SCF: -3373.130506

ZPE: 0.188327

H: -3372.928324

G: -3372.981183

10_CMe2_TS_conf1

H 1.697805 2.573266 -2.392054

C 1.370428 2.388460 -1.379883

C 0.452161 1.876896 1.182522

C 0.204698 1.705733 -1.108449

C 2.076648 2.861554 -0.287497

C 1.604042 2.616224 0.997639

C -0.309412 1.354916 0.114618

H 2.986928 3.423494 -0.454049

H 2.143983 2.986874 1.858701

H 0.125309 1.674113 2.192048

C -1.492123 0.403621 0.380898

C -0.965429 -1.035940 0.220151

C 0.005179 -3.696700 0.006989

C -0.315879 -1.515133 -0.921364

C -1.112513 -1.968252 1.253214

C -0.648006 -3.271096 1.152248

C 0.176326 -2.807477 -1.041116

H -1.611722 -1.676841 2.164931

H -0.796957 -3.952392 1.980135

H 0.685508 -3.120643 -1.942993

H 0.381018 -4.707810 -0.078382

I -0.057997 -0.299983 -2.611907

Br -1.376237 2.940556 -2.746687

C -2.695199 0.636121 -0.550088

H -2.480562 0.530335 -1.607594

H -3.084928 1.642704 -0.396216

H -3.470947 -0.083408 -0.283421

C -2.034591 0.642181 1.795878

H -1.332355 0.381679 2.584867

H -2.939204 0.052936 1.943937

H -2.297671 1.695217 1.899726

SCF: -3451.733565

ZPE: 0.245424

H: -3451.471870

G: -3451.528728

10_CO_TS_conf1

H 1.516282 2.506109 -2.445114

C 1.307171 2.475827 -1.385423

C 0.755477 2.365887 1.344495

C 0.798212 1.344861 -0.779125

C 1.487909 3.588389 -0.581249

C 1.205767 3.540670 0.784977

C 0.556035 1.207040 0.571967

H 1.855307 4.500357 -1.035338

H 1.354078 4.415786 1.402521

H 0.545110 2.292768 2.403876

C 0.078086 -0.017625 1.269404

C -0.236296 -1.292050 0.533072

C -0.977659 -3.748413 -0.607048

C 0.369186 -1.779988 -0.619493

C -1.242698 -2.079261 1.096872

C -1.617252 -3.287408 0.534060

C 0.028431 -2.991972 -1.192552
H -1.731311 -1.716126 1.991097
H -2.407226 -3.869848 0.989347
H 0.523774 -3.343032 -2.087802
H -1.259245 -4.692804 -1.054295
I 1.858065 -0.682210 -1.590439
Br -1.292534 0.782065 -2.114282
O -0.104367 0.008978 2.466676
SCF: -3447.147815
ZPE: 0.169471
H: -3446.963874
G: -3447.018120

10_NAc_TS_conf1

H 1.343883 2.628147 -2.755356
C 1.319275 2.254639 -1.741892
C 1.227992 1.274628 0.873200
C 0.253539 1.519511 -1.267808
C 2.334905 2.538562 -0.840165
C 2.285777 2.067648 0.469688
C 0.181973 0.970842 -0.002123
H 3.169905 3.140083 -1.176863
H 3.084762 2.296722 1.161447
H 1.188377 0.850794 1.870243
C -0.540909 -1.313690 0.016437
C 0.199685 -3.910286 -0.697529
C -0.337436 -1.673517 -1.311773
C -0.367909 -2.288822 0.994882
C -0.014149 -3.578492 0.636344
C 0.047942 -2.951407 -1.686688
H -0.512881 -2.019479 2.032699
H 0.110789 -4.329064 1.405916
H 0.214581 -3.197889 -2.726750
H 0.489018 -4.916222 -0.971597
I -0.692297 -0.202889 -2.744092
Br -1.768979 2.925268 -1.897138
N -0.830846 0.036409 0.363398
C -1.886073 0.342946 1.208551
O -2.694880 -0.505869 1.518804
C -1.943367 1.755227 1.713578
H -1.739691 2.476745 0.923873
H -1.192529 1.881906 2.496774
H -2.930454 1.927649 2.134138
SCF: -3541.826992

ZPE: 0.213981
H: -3541.595866
G: -3541.655783

10_NAc_TS_conf2

H 1.722905 2.367728 -2.946629
C 1.307741 2.453251 -1.952992
C 0.134998 2.619628 0.574388
C 0.836892 1.361730 -1.271988
C 1.149750 3.685751 -1.329422
C 0.535771 3.768173 -0.084990
C 0.327595 1.352755 0.009914
H 1.484819 4.576600 -1.845117
H 0.383649 4.730908 0.384070
H -0.307072 2.672573 1.559153
C -0.445621 -0.988979 0.111850
C -1.419123 -3.310844 -1.082287
C 0.305158 -1.695725 -0.819965
C -1.717192 -1.451436 0.421272
C -2.198626 -2.609744 -0.170498
C -0.157615 -2.846927 -1.428684
H -2.314069 -0.897509 1.134998
H -3.189378 -2.965327 0.080219
H 0.439706 -3.364684 -2.166990
H -1.797565 -4.213604 -1.543561
I 2.104168 -0.827357 -1.401893
Br -0.803168 0.415758 -3.040821
N 0.085496 0.169240 0.756201
C 0.625486 0.058684 2.043977
O 1.206270 0.983876 2.564238
C 0.456048 -1.268593 2.730656
H 0.846393 -2.083242 2.119380
H -0.597991 -1.469670 2.923061
H 0.994878 -1.222914 3.672561
SCF: -3541.820018
ZPE: 0.214084
H: -3541.588920
G: -3541.648174

10_NH_TS_conf1

H 1.539924 2.777587 -2.282370
C 1.219894 2.497523 -1.289051
C 0.357894 1.740720 1.269488
C 0.123065 1.706477 -1.063043

C 1.890512 2.936879 -0.150249
C 1.464771 2.562286 1.119353
C -0.345485 1.277187 0.158235
H 2.756445 3.574451 -0.276255
H 1.999010 2.909651 1.993367
H 0.007862 1.433836 2.248418
C -1.031588 -0.984750 0.195969
C -0.133462 -3.633672 0.089769
C -0.386763 -1.498091 -0.929950
C -1.216747 -1.838442 1.276541
C -0.779374 -3.154216 1.221568
C 0.073728 -2.801550 -1.002563
H -1.709938 -1.447643 2.157550
H -0.938324 -3.806538 2.070343
H 0.577690 -3.168100 -1.887075
H 0.215341 -4.657199 0.049800
I -0.179342 -0.225058 -2.577222
Br -1.901871 2.802115 -2.276242
N -1.446474 0.384709 0.290102
H -2.156769 0.611936 -0.406587
SCF: -3389.162273
ZPE: 0.176254
H: -3388.972255
G: -3389.025015

10_NH_TS_conf2

H 1.527777 2.777292 -2.291767
C 1.227718 2.505768 -1.289887
C 0.401084 1.803358 1.277543
C 0.115727 1.731330 -1.053767
C 1.900844 2.989530 -0.174383
C 1.477133 2.658236 1.107846
C -0.306905 1.296582 0.183743
H 2.753983 3.638824 -0.324919
H 2.001405 3.042333 1.972443
H 0.088074 1.488818 2.267208
C -0.974442 -0.996560 0.255500
C -0.164713 -3.678508 0.067183
C -0.360227 -1.499898 -0.890394
C -1.196366 -1.886713 1.308400
C -0.810648 -3.212121 1.207265
C 0.067727 -2.815053 -0.991758
H -1.673138 -1.515252 2.208030
H -1.000648 -3.884295 2.034198

H 0.555382 -3.166513 -1.891621
H 0.151830 -4.710405 -0.004146
I -0.222982 -0.234199 -2.540853
Br -1.752690 2.856326 -2.349663
N -1.361260 0.354625 0.354636
H -1.851965 0.521596 1.226460
SCF: -3389.168016
ZPE: 0.176870
H: -3388.977425
G: -3389.030168

10_O_TS_conf1

H 1.484220 2.760733 -2.295060
C 1.140379 2.474894 -1.311221
C 0.222768 1.730534 1.226051
C 0.015116 1.701273 -1.135946
C 1.782614 2.920707 -0.161740
C 1.321108 2.566175 1.101550
C -0.436114 1.270334 0.093063
H 2.651001 3.557882 -0.270716
H 1.828636 2.923759 1.987032
H -0.139475 1.402167 2.193379
O -1.491202 0.383200 0.204960
C -1.078691 -0.932130 0.178735
C -0.244246 -3.581329 0.127863
C -0.470493 -1.469079 -0.950015
C -1.279397 -1.736152 1.288906
C -0.869922 -3.061295 1.254506
C -0.035048 -2.783115 -0.988387
H -1.754045 -1.309528 2.163368
H -1.032693 -3.689857 2.120228
H 0.445610 -3.182780 -1.871554
H 0.082665 -4.612372 0.111198
I -0.330392 -0.219534 -2.610359
Br -1.812397 2.885510 -2.455842
SCF: -3409.026414
ZPE: 0.163742
H: -3408.849118
G: -3408.901436

10_SO2_TS_conf1

H 1.817752 2.257631 -2.292527
C 1.339111 2.377571 -1.331117
C 0.038955 2.678233 1.132424

C 0.766303 1.313411 -0.670526
C 1.204463 3.625929 -0.739694
C 0.540310 3.784384 0.474269
C 0.181187 1.406254 0.568709
H 1.615820 4.485439 -1.253936
H 0.432800 4.766387 0.913605
H -0.448699 2.771860 2.095331
C -0.582045 -1.351355 0.573308
C -1.150478 -3.667924 -0.836174
C 0.329848 -1.867659 -0.340327
C -1.798571 -1.989042 0.759784
C -2.078218 -3.151931 0.054119
C 0.060373 -3.018099 -1.053057
H -2.512472 -1.578335 1.461061
H -3.024986 -3.652721 0.205547
H 0.762474 -3.399266 -1.782305
H -1.367917 -4.573264 -1.387643
I 2.052691 -0.790874 -0.812748
Br -0.886036 0.402962 -2.388360
S -0.219423 0.035564 1.616377
O 0.981563 -0.288686 2.343504
O -1.403307 0.369730 2.356975
SCF: -3882.425917
ZPE: 0.170240
H: -3882.239816
G: -3882.296624

10_SO_TS_conf1

H 1.747655 2.413201 -2.345266
C 1.327996 2.264106 -1.360764
C 0.213855 1.881184 1.190531
C 0.079818 1.711751 -1.171174
C 1.997402 2.673433 -0.213830
C 1.442558 2.501970 1.053056
C -0.469811 1.456368 0.054474
H 2.967395 3.141436 -0.326179
H 1.979362 2.836376 1.930365
H -0.238094 1.702415 2.159886
C -1.189489 -1.069461 0.116203
C 0.056624 -3.541551 0.003726
C -0.533818 -1.482003 -1.034387
C -1.223420 -1.901382 1.223500
C -0.602194 -3.141178 1.159276
C 0.105233 -2.707999 -1.106474

H -1.735721 -1.569444 2.117828
H -0.631622 -3.797294 2.019336
H 0.627069 -3.011522 -2.004164
H 0.542611 -4.507310 -0.039257
I -0.511874 -0.162678 -2.651718
Br -1.498771 3.091690 -2.637279
S -2.006731 0.538876 0.227584
O -2.446134 0.679015 1.634429
SCF: -3807.198908
ZPE: 0.164599
H: -3807.019100
G: -3807.074858

11_TS_conf1

H 1.508532 2.757090 -2.290206
C 1.141308 2.457013 -1.318999
C 0.217161 1.739217 1.223089
C 0.008837 1.689671 -1.143259
C 1.758039 2.893918 -0.162248
C 1.318332 2.570788 1.109379
C -0.439682 1.271598 0.093747
H 1.842012 2.945045 1.977593
H -0.145321 1.420691 2.193261
O -1.494063 0.382697 0.210011
C -1.079568 -0.931361 0.181907
C -0.250673 -3.548567 0.123770
C -0.472524 -1.464613 -0.948414
C -1.274836 -1.739569 1.290687
C -0.867540 -3.063554 1.261520
C -0.032021 -2.775586 -0.999607
H -1.747945 -1.319763 2.168926
H -1.014359 -3.715438 2.112195
H 0.449898 -3.198475 -1.870916
I -0.334434 -0.206200 -2.599502
Br -1.793739 2.885992 -2.453452
F 0.155013 -4.827082 0.102369
F 2.838171 3.680087 -0.292451
SCF: -3607.526405
ZPE: 0.147209
H: -3607.363966
G: -3607.420268

Ph2I_TS_conf1

C -1.783865 -0.000683 0.494519

C -1.248655 0.010746 3.197741
C -1.649490 -1.211798 1.160714
C -1.650161 1.216004 1.150592
C -1.382232 1.212587 2.513546
C -1.381526 -1.196842 2.523593
H -1.752549 -2.148294 0.628660
H -1.753662 2.147945 0.610688
H -1.276678 2.153683 3.038043
H -1.275378 -2.133466 3.055919
H -1.039185 0.015270 4.259807
I -2.094730 -0.009588 -1.567726
C 0.284550 -0.008794 -2.131697
C 2.791523 0.001152 -1.043291
C 0.868093 -1.227230 -1.853715
C 0.863748 1.214413 -1.865850
C 2.144544 1.199009 -1.320950
C 2.148837 -1.201708 -1.308988
H 0.364679 -2.160003 -2.063517
H 0.356916 2.143195 -2.084829
H 2.628615 2.145840 -1.114199
H 2.636363 -2.144650 -1.092791
H 3.785656 0.005047 -0.616788
Br -0.583416 -0.021639 -4.483183
SCF: -3335.014254
ZPE: 0.180513
H: -3334.819461
G: -3334.875440

1_CF3_radical_conf1

H -3.468923 -0.059263 2.235840
C -2.391669 -0.032811 2.329229
C 0.413025 0.037710 2.545176
C -1.555116 -0.039104 1.235290
C -1.776502 0.011513 3.573336
C -0.389130 0.046182 3.674004
C -0.163960 -0.006842 1.275054
H -2.389608 0.019192 4.464593
H 0.074114 0.080985 4.651015
H 1.489459 0.067504 2.648423
C 0.558018 -0.011080 0.000820
C 1.735693 0.010557 -2.550116
C -0.190647 -0.043586 -1.171114
C 1.947995 0.022130 -0.145688
C 2.521460 0.027785 -1.402552

C 0.355329 -0.025260 -2.442228
H 2.578856 0.042426 0.732857
H 3.598277 0.051446 -1.498315
H 2.192494 0.027180 -3.530476
I -2.231419 -0.121637 -0.739106
C -0.502639 0.031691 -3.675405
F -1.598812 -0.742122 -3.549410
F -0.949575 1.273281 -3.900604
F 0.143180 -0.367876 -4.760721
SCF: -1096.685688
ZPE: 0.164601
H: -1096.507985
G: -1096.558401

1_CN_radical_conf1

H -3.665966 0.000000 -1.573809
C -2.600332 0.000000 -1.758044
C 0.178315 0.000000 -2.214745
C -1.673119 0.000000 -0.741237
C -2.091111 0.000000 -3.050778
C -0.717367 0.000000 -3.271078
C -0.289695 0.000000 -0.900841
H -2.778421 0.000000 -3.886291
H -0.339849 0.000000 -4.284860
H 1.243723 0.000000 -2.404321
C 0.538750 0.000000 0.304388
C 1.921281 0.000000 2.760642
C -0.112718 0.000000 1.528261
C 1.936405 0.000000 0.343111
C 2.608361 0.000000 1.552673
C 0.530287 0.000000 2.758139
H 2.495058 0.000000 -0.583395
H 3.689717 0.000000 1.560598
H 2.447788 0.000000 3.705083
I -2.179452 0.000000 1.294122
C -0.234555 0.000000 3.966332
N -0.907003 0.000000 4.895848
SCF: -851.851922
ZPE: 0.158447
H: -851.680326
G: -851.732593

1_F_radical_conf1

H -3.547054 0.000000 -1.704195

C -2.468358 0.000000 -1.782245
C 0.340776 0.000000 -1.961699
C -1.646442 0.000000 -0.678429
C -1.834594 0.000000 -3.018528
C -0.445656 0.000000 -3.101616
C -0.253586 0.000000 -0.699446
H -2.436103 0.000000 -3.917669
H 0.030360 0.000000 -4.073080
H 1.419910 0.000000 -2.042927
C 0.452479 0.000000 0.582369
C 1.536843 0.000000 3.186797
C -0.338164 0.000000 1.726842
C 1.833380 0.000000 0.776084
C 2.355140 0.000000 2.060583
C 0.171149 0.000000 3.004630
H 2.496136 0.000000 -0.078850
H 3.428251 0.000000 2.195989
H 1.939478 0.000000 4.190991
I -2.360467 0.000000 1.297108
F -0.673379 0.000000 4.037091
SCF: -858.850458
ZPE: 0.151744
H: -858.686566
G: -858.735893

1_H_radical_conf1

H 0.000000 0.051540 0.105931
C 0.000000 0.075444 1.186712
C 0.000000 0.109430 3.997489
C 0.000000 -1.072184 1.948142
C 0.000000 1.277843 1.880647
C 0.000000 1.288771 3.272071
C 0.000000 -1.121730 3.340220
H 0.000000 2.206252 1.325745
H 0.000000 2.233538 3.798923
H 0.000000 0.139202 5.079159
C 0.000000 -2.438047 3.980952
C 0.000000 -5.068188 4.966534
C 0.000000 -3.563575 3.160396
C 0.000000 -2.681185 5.355234
C 0.000000 -3.980273 5.834413
C 0.000000 -4.871388 3.592283
H 0.000000 -1.848677 6.046467
H 0.000000 -4.149825 6.902845

H 0.000000 -5.705862 2.904433
H 0.000000 -6.077787 5.354630
I 0.000000 -3.004099 1.145174
SCF: -759.600878
ZPE: 0.160044
H: -759.429680
G: -759.476042

1_NMe2_radical_conf1

H -1.601081 3.178720 -2.759835
C -1.035994 3.224628 -1.839230
C 0.434087 3.325458 0.554971
C -0.680520 2.092794 -1.139209
C -0.632074 4.441873 -1.305395
C 0.096729 4.486543 -0.121053
C 0.044969 2.083666 0.053100
H -0.889678 5.356245 -1.823251
H 0.406529 5.442626 0.279615
H 1.004225 3.374898 1.473691
C 0.329115 0.783817 0.664222
C 0.635245 -1.859113 1.586273
C -0.123240 -0.333188 -0.016914
C 0.967496 0.533223 1.880508
C 1.103358 -0.773218 2.324683
C 0.002863 -1.653717 0.362237
H 1.333875 1.355402 2.480945
H 1.590987 -0.957592 3.273104
H 0.766189 -2.866877 1.959076
I -1.172676 0.141034 -1.739526
N -0.507030 -2.650966 -0.503610
C 0.474893 -3.060680 -1.515960
C -1.064237 -3.814866 0.178985
H -0.028475 -3.673772 -2.262735
H 1.288686 -3.641169 -1.064678
H 0.905590 -2.188795 -2.008671
H -1.592880 -4.420453 -0.556514
H -0.287850 -4.435755 0.641452
H -1.768802 -3.490970 0.943615
SCF: -893.552663
ZPE: 0.232597
H: -893.305441
G: -893.358911

1_NMe2_radical_conf2

H 0.070597 3.775809 -2.100040
C 0.397560 3.913665 -1.078496
C 1.247961 4.254793 1.579936
C 0.667182 2.851281 -0.243947
C 0.565307 5.185181 -0.544432
C 0.987340 5.348886 0.771238
C 1.089650 2.961633 1.081945
H 0.364108 6.048573 -1.164605
H 1.114783 6.346263 1.170848
H 1.577330 4.397493 2.601209
C 1.324930 1.721673 1.824345
C 1.614858 -0.839328 2.959341
C 1.133390 0.539026 1.131176
C 1.680888 1.584053 3.167609
C 1.811779 0.316311 3.713958
C 1.271037 -0.746076 1.612820
H 1.833684 2.462466 3.780525
H 2.078219 0.219423 4.758394
H 1.733823 -1.814183 3.414734
I 0.484798 0.837317 -0.813521
N 1.058212 -1.822881 0.718062
C 0.437908 -2.995948 1.326577
C 2.284262 -2.194935 0.000063
H 1.121433 -3.521578 2.003732
H 0.150556 -3.681773 0.530214
H -0.453952 -2.697751 1.875835
H 3.002809 -2.681257 0.670983
H 2.023590 -2.883862 -0.802637
H 2.758459 -1.313873 -0.432664
SCF: -893.552556
ZPE: 0.232683
H: -893.305287
G: -893.358578

1_OMe_radical_conf1

H -2.634785 -0.627191 3.406991
C -1.589049 -0.439615 3.204642
C 1.126946 0.050107 2.657769
C -1.101013 -0.288257 1.925866
C -0.663741 -0.337975 4.235813
C 0.678580 -0.096291 3.960030
C 0.230656 -0.043122 1.593018
H -0.999937 -0.449570 5.258040
H 1.385745 -0.021159 4.775481

H 2.174453 0.236460 2.459037
C 0.567275 0.091820 0.174897
C 0.883587 0.291811 -2.619394
C -0.477959 -0.040201 -0.724077
C 1.827378 0.338781 -0.372521
C 1.962318 0.433410 -1.748035
C -0.384769 0.046822 -2.102402
H 2.686888 0.455692 0.273296
H 2.941046 0.624329 -2.168549
H 1.032616 0.371610 -3.687063
I -2.292383 -0.400268 0.201557
O -1.524071 -0.114683 -2.790402
C -1.456424 -0.033316 -4.214761
H -0.796733 -0.807741 -4.608193
H -1.106519 0.952853 -4.522364
H -2.470305 -0.194305 -4.568778
SCF: -874.125514
ZPE: 0.192674
H: -873.918915
G: -873.972757

1_OMe_radical_conf2

H -3.215283 -0.002624 2.932943
C -2.134412 -0.001684 2.904814
C 0.677078 0.000745 2.806024
C -1.429581 -0.001141 1.722058
C -1.382660 -0.000971 4.072972
C 0.007877 0.000238 4.018706
C -0.040079 0.000054 1.609592
H -1.892278 -0.001367 5.027218
H 0.577763 0.000781 4.938346
H 1.759160 0.001677 2.778152
C 0.537052 0.000459 0.264723
C 1.327598 0.000914 -2.440637
C -0.357905 -0.000393 -0.792490
C 1.891971 0.001607 -0.069816
C 2.260648 0.001799 -1.405277
C -0.030342 -0.000199 -2.137236
H 2.643107 0.002337 0.708377
H 3.312314 0.002679 -1.660402
H 1.655814 0.001104 -3.470608
I -2.332039 -0.002036 -0.172983
O -1.053446 -0.001089 -3.003714
C -0.740187 -0.000791 -4.397359

H -0.173116 -0.895089 -4.658968
H -0.174528 0.894421 -4.658901
H -1.694527 -0.001529 -4.915436
SCF: -874.125686
ZPE: 0.192810
H: -873.918979
G: -873.972682

2_CF3_radical_conf1

H 2.517177 0.123529 -3.750507
C 2.540385 0.072505 -2.671007
C 2.577320 -0.059385 0.139302
C 1.395379 0.060787 -1.907252
C 3.742690 0.014165 -1.977871
C 3.755382 -0.052061 -0.588223
C 1.346813 -0.001695 -0.516838
H 4.670769 0.020034 -2.533635
H 4.700794 -0.098512 -0.064504
H 2.608583 -0.111060 1.219671
C 0.031436 -0.003770 0.123317
C -2.585473 0.000274 1.105136
C -1.091472 0.050680 -0.697207
C -0.208549 -0.056008 1.498416
C -1.502956 -0.053352 1.979685
C -2.399824 0.054355 -0.266295
H 0.621468 -0.098250 2.190602
H -1.677826 -0.094183 3.047566
I -0.537660 0.129076 -2.708268
H -3.236222 0.096500 -0.950197
C -3.974822 0.001363 1.681296
F -4.919105 0.025865 0.738951
F -4.195625 -1.084146 2.434782
F -4.178464 1.063189 2.472974
SCF: -1096.693092
ZPE: 0.164706
H: -1096.514433
G: -1096.567828

2_CN_radical_conf1

H -2.254986 0.015507 -3.515578
C -1.278284 0.016657 -3.051907
C 1.255349 0.023493 -1.824095
C -1.108533 0.014770 -1.686501
C -0.117062 0.020554 -3.814659

C 1.132993 0.025504 -3.203325
C 0.114537 0.014925 -1.020728
H -0.197445 0.021349 -4.893491
H 2.025589 0.031296 -3.814461
H 2.234551 0.030413 -1.363249
C 0.099313 0.008792 0.440151
C -0.183577 0.009211 3.219808
C -1.140377 0.015005 1.078069
C 1.225190 -0.004301 1.263958
C 1.086426 -0.003211 2.637910
C -1.336916 0.016287 2.437575
H 2.212888 -0.016373 0.823509
H 1.962483 -0.011621 3.271907
I -2.692011 0.017757 -0.316621
H -2.318154 0.022345 2.891663
C -0.311758 0.013627 4.648628
N -0.410219 0.018012 5.791435
SCF: -851.854036
ZPE: 0.158268
H: -851.682642
G: -851.734463

2_F_radical_conf1

H -2.388206 0.000000 -3.153898
C -1.394734 0.000000 -2.727219
C 1.177906 0.000000 -1.589948
C -1.175961 0.000000 -1.367937
C -0.263003 0.000000 -3.532186
C 1.007448 0.000000 -2.964106
C 0.068476 0.000000 -0.744225
H -0.381413 0.000000 -4.607368
H 1.879001 0.000000 -3.605139
H 2.172554 0.000000 -1.164350
C 0.105238 0.000000 0.717503
C -0.078687 0.000000 3.485992
C -1.107516 0.000000 1.400352
C 1.257820 0.000000 1.506211
C 1.169500 0.000000 2.885475
C -1.259784 0.000000 2.768916
H 2.231452 0.000000 1.033925
H 2.056369 0.000000 3.504552
I -2.707981 0.000000 0.058806
H -2.215485 0.000000 3.274361
F -0.153096 0.000000 4.820384

SCF: -858.853342

ZPE: 0.151223

H: -858.689972

G: -858.739106

2_NMe2_radical_conf1

H -1.240891 3.482721 -3.750137

C -0.714882 3.481870 -2.808365

C 0.639592 3.381887 -0.355464

C -0.558894 2.333926 -2.076739

C -0.154002 4.667356 -2.275930

C 0.523111 4.573101 -1.032064

C 0.094650 2.193375 -0.858094

H 0.962580 5.456824 -0.594275

H 1.165997 3.364122 0.590715

C 0.151333 0.876039 -0.241228

C 0.123002 -1.763202 0.739522

C -0.457177 -0.187404 -0.906039

C 0.766009 0.558605 0.973446

C 0.748138 -0.741550 1.449295

C -0.500223 -1.493493 -0.471995

H 1.258007 1.338761 1.539906

H 1.230576 -0.965525 2.391773

I -1.317170 0.477860 -2.697134

H -0.990936 -2.274438 -1.036545

N -0.263773 5.842129 -2.935278

C -0.968587 5.900254 -4.201836

H -0.973807 6.926690 -4.555261

H -2.004577 5.568096 -4.092455

H -0.482992 5.274944 -4.956604

C 0.342284 7.042613 -2.388732

H 1.421235 6.919629 -2.263547

H -0.090853 7.300573 -1.418695

H 0.167361 7.865728 -3.074649

H 0.117093 -2.774288 1.123812

SCF: -893.562188

ZPE: 0.233150

H: -893.313304

G: -893.370956

2_OMe_radical_conf1

H -1.647076 0.000000 4.293971

C -0.710503 0.000000 3.753705

C 1.710066 0.000000 2.320869

C -0.653646 0.000000 2.377935

C 0.507727 0.000000 4.420436

C 1.702088 0.000000 3.705627

C 0.508306 0.000000 1.610252

H 0.517155 0.000000 5.502169

H 2.642927 0.000000 4.239849

H 2.648276 0.000000 1.781272

C 0.370093 0.000000 0.156884

C -0.154506 0.000000 -2.613545

C -0.906004 0.000000 -0.385671

C 1.417555 0.000000 -0.773726

C 1.160283 0.000000 -2.124250

C -1.230554 0.000000 -1.725770

H 2.441371 0.000000 -0.423020

H 1.972825 0.000000 -2.838882

I -2.341038 0.000000 1.138519

H -2.254714 0.000000 -2.066973

O -0.292437 0.000000 -3.946194

C -1.609214 0.000000 -4.485623

H -2.154700 0.893919 -4.176191

H -2.154700 -0.893919 -4.176191

H -1.489681 0.000000 -5.565349

SCF: -874.128684

ZPE: 0.192780

H: -873.922175

G: -873.974409

2_OMe_radical_conf2

H -2.167854 -0.000012 4.314777

C -1.218426 -0.000007 3.797513

C 1.237899 0.000005 2.427146

C -1.126286 -0.000004 2.423542

C -0.017576 -0.000004 4.495253

C 1.194650 0.000002 3.811220

C 0.054673 0.000002 1.685684

H -0.035935 -0.000006 5.576922

H 2.121536 0.000005 4.369409

H 2.189911 0.000009 1.911922

C -0.045253 0.000004 0.229013

C -0.497354 0.000007 -2.555708

C -1.314762 0.000001 -0.346174

C 1.016966 0.000009 -0.672701

C 0.802581 0.000011 -2.039848

C -1.594754 0.000002 -1.686906

H 2.032303 0.000012 -0.297799
H 1.655564 0.000014 -2.702543
I -2.785683 -0.000008 1.142372
H -2.598924 -0.000001 -2.087823
O -0.794613 0.000008 -3.862634
C 0.280394 0.000012 -4.796379
H 0.896090 -0.893624 -4.678241
H 0.896085 0.893651 -4.678240
H -0.181333 0.000012 -5.779777
SCF: -874.128241
ZPE: 0.192754
H: -873.921741
G: -873.974087

3_CF3_radical_conf1
H 2.168769 -0.020445 -4.028050
C 2.198041 -0.002079 -2.947586
C 2.249571 0.046048 -0.135146
C 1.056948 -0.009718 -2.177672
C 3.404107 0.031215 -2.259782
C 3.423794 0.055743 -0.868842
C 1.015318 0.011627 -0.785851
H 4.329279 0.038273 -2.820325
H 4.371905 0.082426 -0.348650
H 2.287744 0.065403 0.946130
C -0.297911 -0.004075 -0.140927
C -2.926606 -0.042357 0.854421
C -1.426388 -0.035572 -0.953794
C -0.529294 0.008308 1.235861
C -1.827145 -0.009515 1.708981
C -2.733551 -0.055881 -0.516241
H 0.304917 0.031185 1.923689
H -3.932846 -0.058066 1.253481
I -0.880576 -0.052228 -2.969888
H -3.572768 -0.080999 -1.197370
C -2.094939 -0.001000 3.190355
F -2.889309 1.019962 3.538915
F -2.718677 -1.120665 3.582686
F -0.980384 0.102206 3.915601
SCF: -1096.693039
ZPE: 0.164649
H: -1096.515334
G: -1096.565974

3_CN_radical_conf1
H -0.310797 0.000000 -4.196818
C 0.288679 0.000000 -3.296695
C 1.830273 0.000000 -0.941467
C -0.266851 0.000000 -2.037204
C 1.676438 0.000000 -3.355144
C 2.433625 0.000000 -2.187901
C 0.438875 0.000000 -0.836937
H 2.162252 0.000000 -4.321678
H 3.513506 0.000000 -2.252452
H 2.437760 0.000000 -0.046091
C -0.330157 0.000000 0.407724
C -2.033833 0.000000 2.651925
C -1.720919 0.000000 0.321131
C 0.206787 0.000000 1.692138
C -0.644484 0.000000 2.790094
C -2.595323 0.000000 1.386118
H 1.277918 0.000000 1.841265
H -2.669198 0.000000 3.526806
I -2.328469 0.000000 -1.676184
H -3.669093 0.000000 1.258902
C -0.074160 0.000000 4.109134
N 0.377474 0.000000 5.163234
SCF: -851.853602
ZPE: 0.158591
H: -851.682878
G: -851.731368

3_F_radical_conf1
H -0.658378 0.000000 3.899927
C 0.023966 0.000000 3.061044
C 1.774921 0.000000 0.860118
C -0.415829 0.000000 1.756215
C 1.399572 0.000000 3.248843
C 2.261551 0.000000 2.156361
C 0.399355 0.000000 0.627026
H 1.793578 0.000000 4.256157
H 3.330820 0.000000 2.320054
H 2.460815 0.000000 0.023111
C -0.250246 0.000000 -0.684570
C -1.730999 0.000000 -3.079481
C -1.643563 0.000000 -0.723354
C 0.408949 0.000000 -1.911869
C -0.345968 0.000000 -3.064714

C -2.407839 0.000000 -1.870881
H 1.488765 0.000000 -1.977153
H -2.264581 0.000000 -4.019812
I -2.433972 0.000000 1.207398
H -3.488506 0.000000 -1.845512
F 0.297489 0.000000 -4.238907
SCF: -858.853300
ZPE: 0.151723
H: -858.689539
G: -858.738357

3_NMe2_radical_conf1
H 0.180489 2.331645 -4.840929
C 0.248283 2.396229 -3.763516
C 0.420091 2.533042 -0.960974
C 0.090526 1.296549 -2.949256
C 0.501388 3.604497 -3.127495
C 0.585630 3.666241 -1.739660
C 0.163241 1.298452 -1.558947
H 0.632842 4.497660 -3.723627
H 0.784090 4.614922 -1.258615
H 0.489699 2.599583 0.116956
C -0.032468 0.026897 -0.856567
C -0.443958 -2.506413 0.261575
C -0.279582 -1.103402 -1.632645
C 0.008004 -0.134472 0.520273
C -0.192692 -1.400013 1.112221
C -0.487150 -2.363380 -1.110130
H 0.195213 0.732121 1.136389
H -0.605317 -3.490112 0.675942
I -0.296502 -0.632582 -3.662698
H -0.679117 -3.221902 -1.739610
N -0.146607 -1.554744 2.458111
C -0.396090 -2.854676 3.051646
C 0.109077 -0.411113 3.311825
H -1.391321 -3.227109 2.793185
H -0.334032 -2.764334 4.131928
H 0.342505 -3.591376 2.723939
H -0.674990 0.345859 3.214015
H 0.140422 -0.743376 4.345011
H 1.068326 0.055408 3.071554
SCF: -893.559988
ZPE: 0.233032
H: -893.312989

G: -893.365216

3_OMe_radical_conf1
H 0.256347 0.000000 -4.847887
C 0.776766 0.000000 -3.900145
C 2.110835 0.000000 -1.424351
C 0.113610 0.000000 -2.693203
C 2.164387 0.000000 -3.841462
C 2.819713 0.000000 -2.613858
C 0.715850 0.000000 -1.438007
H 2.730676 0.000000 -4.763159
H 3.901289 0.000000 -2.586087
H 2.635361 0.000000 -0.477924
C -0.151737 0.000000 -0.258839
C -2.015910 0.000000 1.843843
C -1.532095 0.000000 -0.468209
C 0.281408 0.000000 1.057307
C -0.642130 0.000000 2.103780
C -2.473326 0.000000 0.533487
H 1.337389 0.000000 1.294399
H -2.736836 0.000000 2.647925
I -1.972455 0.000000 -2.507689
H -3.534775 0.000000 0.326977
O -0.118406 0.000000 3.340117
C -1.009800 0.000000 4.448887
H -1.637271 -0.893589 4.444376
H -1.637271 0.893589 4.444376
H -0.381521 0.000000 5.335346
SCF: -874.127432
ZPE: 0.192879
H: -873.920808
G: -873.973630

3_OMe_radical_conf2
H -0.221819 -0.000142 -4.709067
C 0.314793 -0.000086 -3.770502
C 1.690410 0.000060 -1.317571
C -0.327756 -0.000087 -2.552479
C 1.703053 -0.000009 -3.735607
C 2.378723 0.000064 -2.519111
C 0.294977 -0.000017 -1.306849
H 2.253685 -0.000005 -4.666718
H 3.460624 0.000123 -2.509482
H 2.234190 0.000116 -0.382145

C -0.554525 -0.000030 -0.114485
C -2.375022 -0.000067 2.012073
C -1.931128 -0.000109 -0.300022
C -0.086425 0.000031 1.199820
C -0.993367 0.000012 2.254458
C -2.861626 -0.000129 0.722138
H 0.977756 0.000095 1.382817
H -3.054383 -0.000078 2.854146
I -2.408208 -0.000196 -2.330432
H -3.926451 -0.000191 0.533430
O -0.631789 0.000065 3.547187
C 0.756758 0.000132 3.854714
H 1.242652 0.893601 3.457280
H 1.242732 -0.893306 3.457306
H 0.822346 0.000150 4.939104
SCF: -874.127667
ZPE: 0.193016
H: -873.921859
G: -873.971418

4_CF3_radical_conf1

H 2.103189 0.081625 -3.707768
C 2.073082 0.048932 -2.627272
C 1.938575 -0.054418 0.166348
C 0.886470 0.042292 -1.930346
C 3.237399 0.006977 -1.875793
C 3.157836 -0.050120 -0.491698
C 0.730943 0.002847 -0.540361
H 4.196337 0.011504 -2.376029
H 4.064262 -0.094464 0.097032
H 1.957915 -0.110424 1.238838
C -0.653848 0.005783 -0.014427
C -3.439089 -0.038495 0.585595
C -1.677593 -0.000985 -0.966694
C -1.125880 0.017503 1.317652
C -2.485108 -0.010083 1.592351
C -3.035881 -0.023966 -0.734592
H -4.491503 -0.061234 0.831711
I -0.946601 0.055748 -2.912930
H -3.754897 -0.029238 -1.542845
H -2.815414 -0.003967 2.620237
C -0.207725 0.081374 2.516170
F -0.881552 0.188117 3.661009
F 0.555986 -1.015084 2.629970

F 0.613000 1.139777 2.463742
SCF: -1096.682727
ZPE: 0.165210
H: -1096.503909
G: -1096.555580

4_CN_radical_conf1

H -3.131536 0.000000 -2.594390
C -2.070018 0.000000 -2.387762
C 0.678681 0.000000 -1.815378
C -1.571798 0.000000 -1.105660
C -1.136127 0.000000 -3.415141
C 0.221831 0.000000 -3.123218
C -0.221953 0.000000 -0.746448
H -1.477914 0.000000 -4.441385
H 0.943083 0.000000 -3.929541
H 1.742089 0.000000 -1.636431
C 0.094217 0.000000 0.688059
C 0.373892 0.000000 3.514050
C -0.975938 0.000000 1.582518
C 1.360095 0.000000 1.303849
C 1.488177 0.000000 2.691624
C -0.895395 0.000000 2.957743
H 0.490174 0.000000 4.588772
I -2.801751 0.000000 0.579679
H -1.778034 0.000000 3.582869
H 2.480748 0.000000 3.121113
C 2.587159 0.000000 0.561459
N 3.600416 0.000000 0.023518
SCF: -851.849628
ZPE: 0.158587
H: -851.678991
G: -851.727046

4_F_radical_conf1

H 1.029793 0.000000 3.798765
C 1.306753 0.000000 2.753560
C 1.989594 0.000000 0.025539
C 0.368580 0.000000 1.747595
C 2.637831 0.000000 2.358060
C 2.966999 0.000000 1.007977
C 0.636620 0.000000 0.377809
H 3.413252 0.000000 3.112344
H 4.007534 0.000000 0.712147

H 2.277104 0.000000 -1.014133
C -0.513553 0.000000 -0.527384
C -2.887454 0.000000 -2.058281
C -1.796936 0.000000 0.022630
C -0.498844 0.000000 -1.921700
C -1.648552 0.000000 -2.682355
C -2.983632 0.000000 -0.672287
H -3.790250 0.000000 -2.653560
I -1.689209 0.000000 2.107216
H -3.944807 0.000000 -0.177914
H -1.558480 0.000000 -3.760370
F 0.677555 0.000000 -2.555561
SCF: -858.851420
ZPE: 0.151594
H: -858.688654
G: -858.734825

4_NMe2_radical_conf1

H 2.323657 0.715539 -4.108910
C 2.222868 0.472039 -3.060011
C 1.916854 -0.189784 -0.351979
C 0.995332 0.373169 -2.444972
C 3.336581 0.229244 -2.267994
C 3.172943 -0.115340 -0.932229
C 0.761738 0.073705 -1.099927
H 4.324152 0.296279 -2.704243
H 4.042468 -0.330378 -0.325077
H 1.823432 -0.472262 0.684851
C -0.635860 -0.006729 -0.647479
C -3.380380 -0.453795 -0.187011
C -1.624984 0.086517 -1.626850
C -1.106773 -0.243926 0.672621
C -2.469085 -0.507877 0.854539
C -2.975466 -0.114552 -1.470621
H -4.428072 -0.644082 0.006042
I -0.801121 0.564649 -3.488935
H -3.679123 -0.026237 -2.286008
H -2.831947 -0.728943 1.847704
N -0.219704 -0.225895 1.747434
C 0.408557 1.067464 2.018158
C -0.651029 -0.868265 2.977862
H 0.651496 1.587865 1.095143
H 1.327289 0.913678 2.585426
H -0.266128 1.702687 2.604700

H -1.029523 -1.867882 2.768891
H 0.215015 -0.953256 3.634017
H -1.423290 -0.293633 3.504861
SCF: -893.553444
ZPE: 0.233452
H: -893.305841
G: -893.357737

4_NMe2_radical_conf2

H 3.168245 1.710753 -3.556660
C 3.173261 1.442883 -2.509224
C 3.134623 0.719293 0.199596
C 2.017461 1.383272 -1.764414
C 4.354203 1.126971 -1.851958
C 4.321698 0.753148 -0.514436
C 1.918328 1.055167 -0.409597
H 5.289648 1.160851 -2.394037
H 5.241175 0.482885 -0.011922
H 3.141792 0.412812 1.233781
C 0.575776 1.022398 0.190982
C -2.120075 0.680758 0.938463
C -0.508065 1.188670 -0.671224
C 0.240495 0.765251 1.548056
C -1.104607 0.555231 1.872025
C -1.841412 1.041460 -0.372616
H -3.148384 0.530442 1.240280
I 0.130379 1.689375 -2.599657
H -2.624517 1.185769 -1.103065
H -1.367302 0.319484 2.893038
N 1.239882 0.711841 2.518027
C 0.918811 0.046244 3.769502
C 1.948656 1.969856 2.754040
H 0.468937 -0.926189 3.574510
H 0.240966 0.636671 4.398864
H 1.848133 -0.102983 4.319094
H 2.114448 2.508989 1.824594
H 1.368008 2.613056 3.426352
H 2.914837 1.761745 3.215307
SCF: -893.553566
ZPE: 0.233504
H: -893.305924
G: -893.357771

4_OMe_radical_conf1

H 2.087368 0.000000 -4.045643
C 2.071582 0.000000 -2.964496
C 1.985154 0.000000 -0.157760
C 0.896030 0.000000 -2.250325
C 3.247077 0.000000 -2.225667
C 3.193293 0.000000 -0.837929
C 0.772229 0.000000 -0.857938
H 4.197853 0.000000 -2.741334
H 4.112862 0.000000 -0.267777
H 1.978556 0.000000 0.919422
C -0.585440 0.000000 -0.302047
C -3.293395 0.000000 0.474114
C -1.656663 0.000000 -1.192842
C -0.944854 0.000000 1.064952
C -2.289432 0.000000 1.430720
C -2.995921 0.000000 -0.880600
H -4.328360 0.000000 0.789232
I -0.978508 0.000000 -3.168112
H -3.771346 0.000000 -1.633133
H -2.562257 0.000000 2.475279
O 0.059061 0.000000 1.951658
C -0.255416 0.000000 3.341748
H -0.820137 -0.894222 3.610276
H -0.820137 0.894222 3.610276
H 0.700405 0.000000 3.858031
SCF: -874.125939
ZPE: 0.193055
H: -873.920144
G: -873.969454

4_OMe_radical_conf2

H 1.552722 -0.157327 -4.278393
C 1.673605 -0.146340 -3.203824
C 1.945592 -0.118872 -0.408829
C 0.600667 -0.068177 -2.346416
C 2.931564 -0.212411 -2.619586
C 3.055172 -0.197718 -1.236430
C 0.655421 -0.050434 -0.949623
H 3.807426 -0.274194 -3.251386
H 4.038500 -0.248748 -0.787782
H 2.076162 -0.109598 0.660349
C -0.617718 0.036073 -0.225721
C -3.199240 0.208114 0.889010
C -1.792262 0.095701 -0.972705

C -0.798737 0.066134 1.175900
C -2.082987 0.153184 1.709925
C -3.078332 0.179414 -0.492569
H -4.183660 0.274195 1.333112
I -1.372780 0.041104 -3.018283
H -3.942879 0.220303 -1.139257
H -2.219537 0.178366 2.780684
O 0.307682 0.007393 1.928365
C 0.170766 0.028112 3.346792
H -0.296728 0.957260 3.676247
H 1.181808 -0.033757 3.739298
H -0.412231 -0.827580 3.691223
SCF: -874.125891
ZPE: 0.192864
H: -873.920220
G: -873.969771

5_CF3_radical_conf1

H 1.838353 1.358037 -3.505705
C 1.881989 1.078646 -2.461838
C 1.988640 0.152206 0.175078
C 0.792394 0.567792 -1.796203
C 3.054690 1.199883 -1.734456
C 3.109541 0.682085 -0.451613
C 0.727190 0.189738 -0.448798
H 3.937488 1.619170 -2.196498
H 4.060048 0.650686 0.066395
C -0.619903 -0.185443 0.053900
C -3.216586 -1.205451 0.607567
C -1.552492 -0.562568 -0.921115
C -1.162802 -0.152534 1.352301
C -2.417700 -0.688350 1.613342
C -2.810319 -1.077212 -0.710662
H -4.184206 -1.629215 0.837562
I -0.928866 0.005702 -2.824925
H -3.461674 -1.353495 -1.528797
H -2.795077 -0.662985 2.628118
C -0.584975 0.634450 2.508787
F -1.490630 1.534320 2.922036
F -0.295119 -0.116462 3.573918
F 0.507324 1.326931 2.185391
C 2.309205 -0.632095 1.429149
F 1.271956 -1.322246 1.903265
F 2.789276 0.122289 2.420832

F 3.262955 -1.533880 1.151168
SCF: -1433.757945
ZPE: 0.169061
H: -1433.571705
G: -1433.631423

5_CN_radical_conf1

H -3.238540 -0.225782 -2.358468
C -2.170091 -0.120138 -2.227131
C 0.571034 0.307052 -1.849833
C -1.584017 -0.082116 -0.982134
C -1.326018 0.000909 -3.321178
C 0.021402 0.256760 -3.129926
C -0.219657 0.041295 -0.714500
H -1.735022 -0.040368 -4.321056
H 0.661761 0.458087 -3.977891
C 0.194156 -0.036221 0.691506
C 0.671085 -0.004999 3.483921
C -0.808657 0.086775 1.654693
C 1.472718 -0.304312 1.219364
C 1.701300 -0.257479 2.593740
C -0.629708 0.118915 3.018924
H 0.867079 0.032277 4.546442
I -2.696959 0.005961 0.777564
H -1.459197 0.221887 3.705300
H 2.698489 -0.459664 2.960282
C 2.542897 -0.827216 0.420725
N 3.397607 -1.332217 -0.153649
C 1.903391 0.828370 -1.754000
N 2.933445 1.332224 -1.729294
SCF: -944.091750
ZPE: 0.156708
H: -943.921201
G: -943.973227

5_F_radical_conf1

H 0.987882 -0.049222 3.782045
C 1.295346 -0.024943 2.745889
C 2.037096 0.071980 0.067697
C 0.388630 -0.011694 1.713670
C 2.637397 -0.001300 2.391875
C 3.000272 0.054077 1.058189
C 0.665044 0.016978 0.339166
H 3.396299 -0.014307 3.162257

H 4.038516 0.093508 0.756621
C -0.486833 0.008613 -0.580379
C -2.924714 0.025289 -2.049566
C -1.766057 0.041934 -0.006377
C -0.525584 -0.051697 -1.978287
C -1.704545 -0.034245 -2.698556
C -2.973176 0.053814 -0.662531
H -3.843820 0.036692 -2.619087
I -1.660859 0.018282 2.072165
H -3.916492 0.078717 -0.135417
H -1.640450 -0.077115 -3.777685
F 0.598448 -0.147853 -2.683474
F 2.476704 0.162493 -1.184516
SCF: -958.096875
ZPE: 0.143185
H: -957.942575
G: -957.988289

5_NMe2_radical_conf1

H 1.857932 1.394327 -4.258255
C 1.759748 1.034404 -3.244445
C 1.486114 -0.164722 -0.671116
C 0.553736 0.725469 -2.672916
C 2.867715 0.840072 -2.418843
C 2.737010 0.239895 -1.183353
C 0.317465 0.258720 -1.375734
H 3.852742 1.097171 -2.786173
H 3.631740 0.011441 -0.622418
C -1.077658 0.228736 -0.920410
C -3.813965 -0.229330 -0.435273
C -2.069716 0.246864 -1.906012
C -1.569074 0.217974 0.421197
C -2.925965 -0.116687 0.614872
C -3.412629 0.028609 -1.746430
H -4.854440 -0.448687 -0.233703
I -1.241908 0.792072 -3.753016
H -4.116034 0.059145 -2.565817
H -3.301073 -0.221396 1.622769
N -0.760794 0.521863 1.478504
C 0.148222 1.653954 1.418019
C -1.165009 0.173388 2.824860
H 0.209025 2.053409 0.409745
H 1.149415 1.371804 1.749614
H -0.224218 2.448723 2.072815

H -1.567796 -0.838294 2.855655
H -0.282475 0.210029 3.464098
H -1.911776 0.868214 3.228099
N 1.401315 -0.933684 0.453361
C 0.490621 -2.064277 0.515965
H -0.095634 -2.044987 1.436672
H 1.070290 -2.992889 0.491955
H -0.185704 -2.071233 -0.334091
C 2.544075 -1.060959 1.334127
H 3.016441 -0.092512 1.493450
H 3.291415 -1.763757 0.946046
H 2.190846 -1.432768 2.296381
SCF: -1027.501897
ZPE: 0.306210
H: -1027.177241
G: -1027.238059

5_NMe2_radical_conf2

H 2.869670 2.156604 -3.209594
C 2.729953 1.886182 -2.173048
C 2.345100 0.919259 0.482290
C 1.499981 1.631629 -1.626025
C 3.802936 1.760002 -1.290525
C 3.618088 1.271210 -0.013507
C 1.207551 1.279426 -0.304266
H 4.803865 1.979188 -1.638989
H 4.487672 1.087600 0.600849
C -0.206559 1.289065 0.091892
C -2.965096 0.877722 0.492299
C -1.154815 1.223866 -0.934323
C -0.757095 1.391405 1.406822
C -2.123320 1.077891 1.567088
C -2.504643 1.021746 -0.816672
H -4.014649 0.678306 0.665529
I -0.247092 1.611438 -2.783589
H -3.171156 0.983533 -1.666010
H -2.543371 1.060735 2.562398
N 0.004590 1.777819 2.472082
C 0.918269 2.902564 2.363282
C -0.466368 1.543695 3.821604
H 1.048258 3.204068 1.328042
H 1.893713 2.655365 2.786229
H 0.506517 3.755694 2.912891
H -0.873178 0.537651 3.917241

H 0.383952 1.635200 4.497869
H -1.230112 2.268977 4.127838
N 2.212175 0.258167 1.669631
C 3.319769 0.213454 2.601891
H 4.083244 -0.516599 2.306537
H 2.929404 -0.075131 3.578244
H 3.783766 1.194625 2.694677
C 1.302486 -0.868014 1.795332
H 0.645156 -0.940200 0.933709
H 0.696015 -0.780780 2.698691
H 1.883017 -1.794862 1.853893
SCF: -1027.501999
ZPE: 0.306059
H: -1027.177447
G: -1027.238446

5_OMe_radical_conf1

H 3.079401 -0.583543 -3.107215
C 2.690669 -0.455799 -2.106533
C 1.648651 0.004518 0.465463
C 1.357752 -0.236756 -1.857770
C 3.522329 -0.494586 -0.995429
C 3.002867 -0.244396 0.261196
C 0.736356 -0.063323 -0.612993
H 4.580762 -0.677330 -1.123783
H 3.648643 -0.209229 1.128945
C -0.736356 0.063323 -0.612993
C -3.522329 0.494586 -0.995429
C -1.357752 0.236756 -1.857770
C -1.648651 -0.004518 0.465463
C -3.002867 0.244396 0.261196
C -2.690669 0.455799 -2.106533
H -4.580762 0.677330 -1.123783
I 0.000000 0.000000 -3.422792
H -3.079401 0.583543 -3.107215
H -3.648643 0.209230 1.128945
O -1.273544 -0.298061 1.730866
C -0.842348 -1.644833 1.932345
H -0.046791 -1.921691 1.239169
H -1.689233 -2.323577 1.805560
H -0.469503 -1.700778 2.951523
O 1.273544 0.298061 1.730866
C 0.842348 1.644833 1.932345
H 1.689233 2.323577 1.805560

H 0.469503 1.700778 2.951523
H 0.046791 1.921691 1.239169
SCF: -988.635872
ZPE: 0.224961
H: -988.395547
G: -988.449628

5_OMe_radical_conf2

H 2.998076 -0.081981 -3.167979
C 2.570405 -0.069647 -2.175653
C 1.442899 0.120312 0.403188
C 1.237467 0.174214 -1.946493
C 3.343691 -0.288594 -1.043973
C 2.794723 -0.177220 0.222090
C 0.579079 0.209297 -0.715083
H 4.398030 -0.505710 -1.153252
H 3.434981 -0.288512 1.084658
C -0.881959 0.415283 -0.724010
C -3.614215 1.110696 -1.105378
C -1.446156 0.826125 -1.941526
C -1.840486 0.219991 0.300613
C -3.163334 0.613248 0.102170
C -2.748348 1.181437 -2.189444
H -4.650907 1.394774 -1.226741
I -0.052722 0.711739 -3.492403
H -3.089284 1.490120 -3.167859
H -3.845735 0.478810 0.931229
O -1.571669 -0.339621 1.499651
C -1.088781 -1.681060 1.471797
H -0.224953 -1.797742 0.816802
H -1.885290 -2.350689 1.138183
H -0.804402 -1.927155 2.492157
O 0.910478 0.375521 1.598309
C 1.669683 0.095774 2.768281
H 2.004526 -0.943293 2.772590
H 0.995345 0.269428 3.602681
H 2.528956 0.764453 2.845396
SCF: -988.638269
ZPE: 0.225102
H: -988.397741
G: -988.452965

6_CF3_radical_conf1

H 2.191175 -0.094536 -4.000226

C 2.208005 -0.074804 -2.919759
C 2.230440 -0.024015 -0.103310
C 1.058510 -0.046026 -2.160127
C 3.406021 -0.078553 -2.225763
C 3.402839 -0.053570 -0.833385
C 1.004784 -0.018399 -0.770579
H 4.339470 -0.102120 -2.773764
H 2.259708 -0.005443 0.977584
C -0.312942 0.011826 -0.135816
C -2.952919 0.062015 0.833158
C -1.435567 0.007942 -0.962331
C -0.558990 0.043627 1.233167
C -1.865172 0.065963 1.695840
C -2.743563 0.032895 -0.539391
H 0.266662 0.050316 1.934162
H -3.964024 0.080627 1.215162
I -0.867322 -0.041916 -2.972301
H -3.576975 0.030274 -1.228347
C -2.076340 0.108563 3.186526
F -3.363551 0.018031 3.522978
F -1.434140 -0.891309 3.804726
F -1.609098 1.247699 3.716380
C 4.733477 -0.073707 -0.128479
F 4.615034 0.027649 1.196327
F 5.520375 0.931636 -0.533670
F 5.402505 -1.207464 -0.379064
SCF: -1433.784507
ZPE: 0.169400
H: -1433.599287
G: -1433.656504

6_CF3_radical_conf2

H 2.591790 0.934120 -3.038472
C 2.616349 0.953222 -1.958129
C 2.659807 1.005189 0.856548
C 1.473698 0.966606 -1.190579
C 3.821834 0.967677 -1.273914
C 3.828801 0.995980 0.116405
C 1.429685 0.992533 0.201060
H 4.749546 0.959042 -1.830147
H 2.699264 1.025265 1.937767
C 0.115679 1.006106 0.844455
C -2.515571 1.025081 1.827952
C -1.009556 0.992687 0.026767

C -0.119469 1.031017 2.220121
C -1.419607 1.039575 2.687233
C -2.318473 1.001938 0.457877
H 0.711659 1.043122 2.912070
H -3.523484 1.031424 2.223130
I -0.457727 0.954695 -1.987747
H -3.155466 0.992118 -0.226506
C -1.694976 1.061732 4.167401
F -2.382018 -0.021982 4.553554
F -0.580500 1.102640 4.898463
F -2.433805 2.124954 4.512082
C 5.150826 0.970016 0.837701
F 5.085097 1.562801 2.033170
F 6.111974 1.584934 0.142389
F 5.569648 -0.286491 1.049747
SCF: -1433.784548
ZPE: 0.169388
H: -1433.599336
G: -1433.656572

6_CF3_radical_conf3

H 1.598346 -0.006615 -4.030126
C 1.620756 -0.004923 -2.949580
C 1.657600 -0.000959 -0.132751
C 0.475144 0.001471 -2.183597
C 2.822327 -0.010243 -2.262124
C 2.826164 -0.008143 -0.869534
C 0.428026 0.004237 -0.793225
H 3.752897 -0.016901 -2.815391
H 1.693138 0.000114 0.948105
C -0.887120 0.009271 -0.152234
C -3.520376 0.012555 0.825930
C -2.010728 0.008429 -0.972478
C -1.125085 0.013469 1.223187
C -2.426172 0.014970 1.687597
C -3.320515 0.009799 -0.543876
H -0.295511 0.015548 1.917075
H -4.529035 0.012845 1.219244
I -1.453952 0.004468 -2.985579
H -4.156065 0.008587 -1.230089
C -2.705087 0.017312 3.167196
F -3.405010 -1.064600 3.534932
F -1.592245 0.034660 3.901604
F -3.432987 1.083395 3.526253

C 4.161019 -0.028093 -0.172636
F 4.937219 0.989600 -0.567456
F 4.837594 -1.152572 -0.444475
F 4.049660 0.052321 1.154028
SCF: -1433.784642
ZPE: 0.169346
H: -1433.599458
G: -1433.656755

6_CN_radical_conf1

H -0.287887 0.000000 -4.196067
C 0.307647 0.000000 -3.293504
C 1.841703 0.000000 -0.925242
C -0.249459 0.000000 -2.034029
C 1.690905 0.000000 -3.358332
C 2.439226 0.000000 -2.180000
C 0.453072 0.000000 -0.830916
H 2.187624 0.000000 -4.318637
H 2.456289 0.000000 -0.035230
C -0.318726 0.000000 0.412297
C -2.031423 0.000000 2.646178
C -1.708745 0.000000 0.318141
C 0.213750 0.000000 1.697958
C -0.643029 0.000000 2.791636
C -2.588327 0.000000 1.378143
H 1.284132 0.000000 1.852775
H -2.671182 0.000000 3.517908
I -2.307754 0.000000 -1.682374
H -3.661614 0.000000 1.246823
C -0.079915 0.000000 4.113816
N 0.366511 0.000000 5.169951
C 3.873613 0.000000 -2.268813
N 5.017889 0.000000 -2.342081
SCF: -944.105738
ZPE: 0.157206
H: -943.934544
G: -943.987611

6_F_radical_conf1

H -0.648349 0.000000 3.903118
C 0.029270 0.000000 3.060527
C 1.775461 0.000000 0.847285
C -0.416296 0.000000 1.756062
C 1.400928 0.000000 3.256298

C 2.232238 0.000000 2.147878
C 0.400121 0.000000 0.627050
H 1.823882 0.000000 4.251646
H 2.482849 0.000000 0.028418
C -0.248362 0.000000 -0.684558
C -1.728165 0.000000 -3.076690
C -1.641208 0.000000 -0.721817
C 0.412373 0.000000 -1.910764
C -0.342833 0.000000 -3.063837
C -2.406285 0.000000 -1.868506
H 1.492451 0.000000 -1.975572
H -2.262045 0.000000 -4.017152
I -2.430504 0.000000 1.210454
H -3.487005 0.000000 -1.844368
F 0.298862 0.000000 -4.237595
F 3.554415 0.000000 2.350823
SCF: -958.105597
ZPE: 0.143347
H: -957.949308
G: -958.001084

6_NMe2_radical_conf1

H -0.208690 2.497596 -4.633057
C -0.020257 2.483798 -3.568047
C 0.468938 2.442200 -0.808367
C -0.151508 1.333490 -2.817168
C 0.364439 3.638861 -2.918400
C 0.621512 3.648743 -1.524282
C 0.079980 1.272573 -1.444723
H 0.468417 4.541478 -3.501321
H 0.655851 2.414790 0.254325
C -0.106170 -0.026312 -0.784192
C -0.521229 -2.597194 0.249963
C -0.489219 -1.102456 -1.581736
C 0.067167 -0.263554 0.571610
C -0.133178 -1.548086 1.120901
C -0.700310 -2.378538 -1.100640
H 0.358065 0.558881 1.207701
H -0.685208 -3.593550 0.631615
I -0.709892 -0.526938 -3.573383
H -0.997417 -3.193208 -1.747312
N 0.040027 -1.774379 2.447073
C -0.207232 -3.092572 2.999414
C 0.408405 -0.683179 3.327515

H -1.243850 -3.404888 2.842758
H -0.013768 -3.067161 4.067627
H 0.448885 -3.841905 2.548794
H -0.348831 0.106786 3.325024
H 0.504187 -1.064757 4.339525
H 1.364928 -0.241990 3.034174
N 1.004496 4.788326 -0.896437
C 1.270313 4.778389 0.528631
H 2.073855 4.079766 0.778432
H 0.380562 4.496869 1.099641
H 1.574774 5.774192 0.836494
C 1.139247 6.022780 -1.645765
H 1.444518 6.813375 -0.967011
H 0.192559 6.313375 -2.109914
H 1.893539 5.932201 -2.432364
SCF: -1027.518935
ZPE: 0.306152
H: -1027.195078
G: -1027.255915

6_NMe2_radical_conf2

H 0.196041 2.453757 -3.544113
C 0.500034 2.451294 -2.506097
C 1.293381 2.437257 0.182729
C 0.335759 1.344574 -1.698496
C 1.074289 3.576194 -1.950538
C 1.483875 3.600270 -0.593645
C 0.717363 1.297402 -0.359257
H 1.208898 4.443852 -2.578455
H 1.595341 2.422142 1.219172
C 0.479430 0.042877 0.367606
C -0.063468 -2.445348 1.536768
C -0.110157 -1.004584 -0.337012
C 0.798540 -0.181112 1.698975
C 0.536755 -1.423588 2.314864
C -0.388440 -2.239829 0.211567
H 1.258401 0.616917 2.262106
H -0.280042 -3.409128 1.972100
I -0.505663 -0.461387 -2.309759
H -0.846613 -3.032589 -0.364544
N 0.851112 -1.636133 3.617071
C 0.589461 -2.925219 4.228261
C 1.443785 -0.572046 4.403343
H -0.478347 -3.161940 4.222594

H 0.929989 -2.900703 5.259009
H 1.121764 -3.727141 3.709438
H 0.791990 0.305594 4.439287
H 1.595944 -0.926344 5.418423
H 2.411156 -0.264429 3.995523
N 2.044841 4.712799 -0.057641
C 2.499881 4.705825 1.318802
H 3.255236 3.932098 1.484403
H 1.672421 4.531720 2.012667
H 2.942607 5.670581 1.547735
C 2.226119 5.900661 -0.869923
H 2.652243 6.685697 -0.252517
H 1.272946 6.257515 -1.268824
H 2.902132 5.714599 -1.709723
SCF: -1027.518860
ZPE: 0.306342
H: -1027.194903
G: -1027.255228

6_NMe2_radical_conf3

H 0.614856 2.316810 -3.637450
C 0.831163 2.302034 -2.577561
C 1.395460 2.255601 0.167740
C 0.633089 1.174547 -1.806948
C 1.322109 3.431551 -1.955084
C 1.614691 3.439727 -0.567904
C 0.902534 1.111249 -0.441629
H 1.479870 4.316376 -2.553118
H 1.610583 2.225411 1.225015
C 0.643282 -0.163325 0.241041
C 0.074810 -2.685408 1.320793
C 0.146352 -1.213408 -0.528050
C 0.855591 -0.402300 1.590894
C 0.578508 -1.662334 2.162928
C -0.142581 -2.465018 -0.023897
H 1.239954 0.399087 2.203789
H -0.150429 -3.662389 1.720812
I -0.102851 -0.641987 -2.517171
H -0.527956 -3.259649 -0.648423
N 0.787744 -1.889967 3.483503
C 0.489987 -3.189433 4.054888
C 1.282895 -0.825544 4.334016
H -0.569160 -3.440823 3.947957
H 0.733272 -3.171364 5.113012

H 1.079704 -3.977998 3.579732
H 0.600823 0.029807 4.340447
H 1.373354 -1.199597 5.349317
H 2.266322 -0.477315 4.005435
N 2.093018 4.556636 0.034833
C 2.306239 5.766395 -0.736088
H 1.375764 6.121108 -1.188093
H 3.037285 5.608784 -1.533922
H 2.682705 6.540890 -0.074700
C 2.388404 4.547015 1.454105
H 2.756216 5.526854 1.743270
H 3.154688 3.805216 1.696974
H 1.495805 4.324664 2.046135
SCF: -1027.518928
ZPE: 0.306284
H: -1027.194976
G: -1027.255632

6_NMe2_radical_conf4

H 0.830629 2.263306 -3.618444
C 1.033126 2.283276 -2.555969
C 1.548976 2.334156 0.199162
C 0.742002 1.212700 -1.735235
C 1.598203 3.402883 -1.980314
C 1.872278 3.458006 -0.590612
C 0.982431 1.199615 -0.362996
H 1.827900 4.243940 -2.616883
H 1.740858 2.344972 1.261570
C 0.616173 -0.015421 0.376681
C -0.158174 -2.429845 1.568680
C 0.058508 -1.065160 -0.349762
C 0.783587 -0.198654 1.741413
C 0.401439 -1.402925 2.370031
C -0.330925 -2.264922 0.209567
H 1.218501 0.601581 2.320930
H -0.464114 -3.365274 2.012155
I -0.104782 -0.583183 -2.370886
H -0.760539 -3.061229 -0.383189
N 0.564509 -1.574321 3.705538
C 0.178024 -2.824081 4.331943
C 1.109576 -0.501225 4.513787
H -0.894501 -3.011353 4.225785
H 0.414921 -2.774386 5.390470
H 0.718621 -3.669659 3.898429

H 0.497259 0.402106 4.440195
H 1.129155 -0.817311 5.552388
H 2.129843 -0.249573 4.209595
N 2.430552 4.562559 -0.035894
C 2.769538 5.702949 -0.865443
H 1.883875 6.121196 -1.351873
H 3.491459 5.431995 -1.640963
H 3.211854 6.472075 -0.239352
C 2.701208 4.602151 1.387647
H 3.140569 5.563657 1.635391
H 3.402062 3.815876 1.683223
H 1.784098 4.481218 1.971238
SCF: -1027.518861
ZPE: 0.306000
H: -1027.195138
G: -1027.255921

6_OMe_radical_conf1

H -0.052777 0.002893 -4.910674
C 0.499848 -0.011309 -3.981387
C 1.926516 -0.048204 -1.568884
C -0.123782 -0.014301 -2.756362
C 1.887732 -0.027485 -3.996223
C 2.598017 -0.046039 -2.792389
C 0.541715 -0.031975 -1.529303
H 2.398188 -0.024605 -4.947742
C -0.274678 -0.031682 -0.312213
C -2.044313 -0.027317 1.870235
C -1.662658 -0.014129 -0.461845
C 0.215319 -0.047254 0.983610
C -0.660808 -0.045158 2.069928
C -2.558690 -0.011424 0.581055
H 1.280626 -0.061285 1.174060
H -2.729193 -0.025388 2.705290
I -2.192714 0.007553 -2.481584
H -3.628807 0.002462 0.423833
O -0.083242 -0.061203 3.282154
C -0.925729 -0.058171 4.428313
H -1.563412 -0.944285 4.445579
H -1.541757 0.842803 4.456342
H -0.259951 -0.071389 5.286863
H 2.508623 -0.062271 -0.656707
O 3.938621 -0.062380 -2.718758
C 4.678470 -0.064674 -3.933601

H 5.725629 -0.080602 -3.644391
H 4.472908 0.835370 -4.516016
H 4.448896 -0.951551 -4.527185
SCF: -988.653896
ZPE: 0.225817
H: -988.412633
G: -988.468366

6_OMe_radical_conf2

H 0.351723 0.985729 -3.343248
C 0.914256 0.994025 -2.419827
C 2.366737 1.014650 -0.022451
C 0.303964 1.006687 -1.188172
C 2.301860 0.991527 -2.449541
C 3.024858 1.002271 -1.253246
C 0.981825 1.016488 0.032697
H 2.802101 0.981196 -3.406410
C 0.176153 1.026159 1.257019
C -1.565377 1.040326 3.448932
C -1.206227 1.025819 1.121375
C 0.691377 1.034204 2.553576
C -0.176086 1.041189 3.640895
C -2.098536 1.032573 2.177460
H 1.761373 1.034645 2.699365
H -2.213638 1.045535 4.315251
I -1.760476 1.013081 -0.890873
H -3.170031 1.031612 2.030000
O 0.232107 1.048768 4.919552
C 1.630765 1.049719 5.177924
H 2.102674 1.940980 4.759301
H 2.102382 0.154178 4.768211
H 1.734241 1.055106 6.259429
H 2.961740 1.022218 0.881487
O 4.366295 1.001148 -1.193901
C 5.093274 0.990589 -2.416682
H 6.143556 0.992381 -2.138431
H 4.869773 1.879445 -3.009658
H 4.868938 0.092255 -2.994838
SCF: -988.654212
ZPE: 0.225944
H: -988.412889
G: -988.468325

6_OMe_radical_conf3

H 0.338400 0.932768 -3.306841
C 0.894197 0.933870 -2.379399
C 2.330421 0.935398 0.042567
C 0.272055 0.985057 -1.146194
C 2.271572 0.881451 -2.384811
C 2.990987 0.883022 -1.180698
C 0.935831 0.986444 0.074245
H 2.814289 0.838894 -3.319723
C 0.120567 1.037079 1.291261
C -1.641283 1.127839 3.466332
C -1.260165 1.082307 1.142767
C 0.622649 1.038770 2.593229
C -0.254577 1.083750 3.671708
C -2.161897 1.127598 2.189764
H 1.690207 1.004549 2.751126
H -2.297245 1.161030 4.326167
I -1.792832 1.069073 -0.873262
H -3.231230 1.160692 2.030713
O 0.141542 1.087541 4.954261
C 1.536804 1.041981 5.226125
H 2.043281 1.912784 4.804839
H 1.980550 0.126984 4.828430
H 1.630362 1.053183 6.308458
H 2.884719 0.938051 0.969480
O 4.326518 0.830982 -1.305589
C 5.113877 0.820721 -0.121378
H 6.147987 0.772834 -0.451075
H 4.883646 -0.053574 0.490653
H 4.955867 1.732025 0.458745
SCF: -988.654404
ZPE: 0.225901
H: -988.413130
G: -988.468514

7_CF3_radical_conf1

H 2.535515 0.298610 -3.735986
C 2.552044 0.166226 -2.663453
C 2.582064 -0.173215 0.132224
C 1.405467 0.138477 -1.901372
C 3.741858 0.014988 -1.970787
C 3.759748 -0.153911 -0.588864
C 1.356309 -0.024908 -0.520210
H 4.704890 -0.272136 -0.073806
H 2.611977 -0.305139 1.205245

C 0.040230 -0.026861 0.119290
C -2.575106 0.006663 1.096940
C -1.076383 0.131480 -0.696152
C -0.204098 -0.173235 1.486244
C -1.499260 -0.154995 1.965948
C -2.384561 0.154457 -0.267225
H 0.620995 -0.299742 2.173778
H -1.678643 -0.267310 3.027925
I -0.514711 0.338375 -2.695641
H -3.216377 0.279161 -0.946452
C -3.965574 0.035873 1.672323
F -4.907179 0.083676 0.728831
F -4.209538 -1.045101 2.423465
F -4.144578 1.101970 2.464213
C 5.052744 0.027556 -2.709443
F 4.897566 0.207642 -4.021780
F 5.856330 1.003747 -2.267334
F 5.719074 -1.122450 -2.542825
SCF: -1433.784589
ZPE: 0.169425
H: -1433.598403
G: -1433.658702

7_CF3_radical_conf2

H 1.896330 0.076762 -3.417018
C 1.916147 0.048735 -2.336735
C 1.953629 -0.025610 0.478628
C 0.769961 0.050787 -1.573231
C 3.109648 0.005577 -1.634791
C 3.131022 -0.031432 -0.243125
C 0.724509 0.014931 -0.182718
H 4.078686 -0.066815 0.279447
H 1.986886 -0.055531 1.559246
C -0.591150 0.015279 0.457129
C -3.206888 0.006213 1.434249
C -1.712595 0.043763 -0.366489
C -0.830462 -0.014729 1.832464
C -2.125822 -0.018729 2.311497
C -3.021400 0.039070 0.061943
H -0.001292 -0.035202 2.526590
H -2.302071 -0.043040 3.379561
I -1.156377 0.094725 -2.378052
H -3.857994 0.058413 -0.622931
C -4.597601 -0.005748 2.009320

F -4.807877 1.048866 2.807727
F -5.540325 0.018634 1.065949
F -4.810205 -1.098391 2.754206
C 4.420096 -0.022332 -2.374385
F 4.265265 0.103816 -3.693313
F 5.233251 0.962845 -1.973609
F 5.076628 -1.170856 -2.161558
SCF: -1433.784606
ZPE: 0.169423
H: -1433.598427
G: -1433.658693

7_CN_radical_conf1

H -2.245536 0.000049 -3.535017
C -1.274872 0.007528 -3.058903
C 1.263781 0.032736 -1.831552
C -1.106773 0.009865 -1.696285
C -0.104579 0.015661 -3.815571
C 1.153141 0.031009 -3.208541
C 0.119703 0.017339 -1.033718
H 2.041864 0.041150 -3.824387
H 2.242476 0.047472 -1.370994
C 0.101978 0.010797 0.427054
C -0.187155 0.009340 3.202899
C -1.139629 0.013177 1.060972
C 1.226717 -0.000630 1.251224
C 1.084258 -0.000363 2.625100
C -1.339963 0.013664 2.419381
H 2.215321 -0.011542 0.812888
H 1.958563 -0.007525 3.261397
I -2.689934 0.009136 -0.335853
H -2.321903 0.016906 2.872002
C -0.318701 0.013140 4.631895
N -0.420172 0.017123 5.774221
C -0.207179 0.009807 -5.246907
N -0.287507 0.004160 -6.390904
SCF: -944.106132
ZPE: 0.156892
H: -943.934228
G: -943.991040

7_F_radical_conf1

H -2.383839 0.000000 -3.178565
C -1.401943 0.000000 -2.725734

C 1.176683 0.000000 -1.595094
C -1.178162 0.000000 -1.367061
C -0.259677 0.000000 -3.503044
C 1.017638 0.000000 -2.968031
C 0.068030 0.000000 -0.747315
H 1.872348 0.000000 -3.630752
H 2.172619 0.000000 -1.173473
C 0.106375 0.000000 0.714492
C -0.079977 0.000000 3.483157
C -1.106514 0.000000 1.397197
C 1.257920 0.000000 1.504287
C 1.168386 0.000000 2.883531
C -1.260215 0.000000 2.765608
H 2.232346 0.000000 1.033792
H 2.055037 0.000000 3.502722
I -2.706177 0.000000 0.054666
H -2.216667 0.000000 3.269613
F -0.155578 0.000000 4.817891
F -0.402535 0.000000 -4.832284
SCF: -958.105556
ZPE: 0.142832
H: -957.949670
G: -958.001226

7_NMe2_radical_conf1

H -1.228416 3.443578 -3.737134
C -0.717249 3.457093 -2.787024
C 0.595658 3.387929 -0.312569
C -0.597129 2.323458 -2.022624
C -0.141432 4.642463 -2.276845
C 0.513441 4.565148 -1.021818
C 0.034502 2.197853 -0.791793
H 0.964593 5.450461 -0.598976
H 1.106985 3.381913 0.642325
C 0.053468 0.895111 -0.144593
C -0.047430 -1.768713 0.907410
C -0.563073 -0.175547 -0.779698
C 0.638581 0.571044 1.085639
C 0.591588 -0.706844 1.595951
C -0.650336 -1.471448 -0.335844
H 1.141893 1.346850 1.649878
H 1.060754 -0.894759 2.550241
I -1.392075 0.466824 -2.599326
H -1.158157 -2.229927 -0.911559

N -0.082671 -3.025875 1.415999
C -0.777314 -4.076005 0.698632
C 0.493488 -3.297999 2.718968
H -1.841476 -3.847204 0.582888
H -0.682274 -5.004156 1.254086
H -0.348500 -4.225786 -0.296148
H 0.007853 -2.709415 3.502965
H 0.360401 -4.351450 2.946867
H 1.563396 -3.074616 2.734848
N -0.217999 5.806510 -2.968477
C -0.905851 5.845410 -4.243323
H -0.875168 6.859588 -4.629925
H -1.953527 5.547757 -4.139264
H -0.431203 5.182275 -4.972769
C 0.383963 7.011204 -2.430629
H 1.459736 6.885719 -2.280208
H -0.066485 7.290171 -1.473835
H 0.228862 7.823884 -3.133919
SCF: -1027.521561
ZPE: 0.305913
H: -1027.196990
G: -1027.261025

7_NMe2_radical_conf2

H 0.205794 2.920752 -2.229399
C 0.688096 2.940194 -1.264330
C 1.908764 2.888500 1.257515
C 0.744472 1.821863 -0.470669
C 1.286293 4.117817 -0.761848
C 1.891899 4.049936 0.518212
C 1.324853 1.706266 0.786079
H 2.357444 4.929932 0.936517
H 2.385868 2.889113 2.230041
C 1.270499 0.421408 1.466287
C 1.029427 -2.207928 2.580685
C 0.642166 -0.643657 0.833296
C 1.789445 0.110914 2.729259
C 1.675662 -1.150450 3.269215
C 0.489275 -1.923150 1.305902
H 2.292954 0.884316 3.296494
H 2.095670 -1.328174 4.248031
I -0.086441 -0.022195 -1.035937
H -0.021443 -2.678560 0.728557
N 0.929352 -3.449149 3.118419

C 0.239607 -4.497617 2.394055
C 1.469342 -3.714598 4.438056
H -0.808931 -4.238897 2.217058
H 0.273989 -5.411304 2.979659
H 0.713668 -4.690143 1.427277
H 0.989967 -3.092749 5.199612
H 1.293052 -4.757424 4.684524
H 2.546399 -3.529466 4.471638
N 1.276348 5.266339 -1.483836
C 1.834923 6.480988 -0.921574
H 1.721200 7.284975 -1.642706
H 2.899300 6.363790 -0.702272
H 1.323056 6.767845 0.001909
C 0.607255 5.304859 -2.768660
H -0.461411 5.087743 -2.672073
H 1.043231 4.580898 -3.462491
H 0.720062 6.296714 -3.195802
SCF: -1027.521587
ZPE: 0.305997
H: -1027.196968
G: -1027.260774

7_OMe_radical_conf1

H 3.178815 -0.000177 -1.863163
C 2.750675 -0.000097 -0.872100
C 1.567336 0.000110 1.680462
C 1.386889 -0.000067 -0.665384
C 3.540466 -0.000016 0.276716
C 2.935889 0.000086 1.542265
C 0.730470 0.000034 0.556105
H 3.574947 0.000143 2.415484
H 1.132124 0.000184 2.671303
C -0.728602 0.000050 0.558590
C -3.539524 0.000050 0.288502
C -1.389070 -0.000045 -0.660711
C -1.561739 0.000154 1.685759
C -2.930754 0.000154 1.552051
C -2.753524 -0.000051 -0.862891
H -1.123318 0.000233 2.675222
H -3.566929 0.000232 2.427376
I -0.003678 -0.000176 -2.229311
H -3.184955 -0.000131 -1.852517
O -4.880713 0.000056 0.272594
C -5.534928 -0.000035 -0.990471

H -5.276022 -0.894019 -1.561404
H -5.275996 0.893850 -1.561547
H -6.599837 -0.000002 -0.775480
O 4.881589 -0.000032 0.256436
C 5.531594 -0.000129 -1.008781
H 5.270735 -0.894098 -1.578865
H 6.597213 -0.000117 -0.797341
H 5.270741 0.893756 -1.578999
SCF: -988.655797
ZPE: 0.225553
H: -988.413855
G: -988.472462

7_OMe_radical_conf2

H 3.168848 0.000001 -2.280982
C 2.758525 0.000000 -1.282318
C 1.622351 0.000000 1.291092
C 1.398590 0.000001 -1.050505
C 3.569356 0.000000 -0.148031
C 2.988080 0.000000 1.128361
C 0.764752 0.000000 0.182506
H 3.643153 0.000000 1.989717
H 1.204427 0.000000 2.289310
C -0.694112 0.000000 0.214117
C -3.510585 0.000001 -0.002211
C -1.377581 0.000001 -1.000624
C -1.504697 0.000000 1.348224
C -2.885889 0.000000 1.248482
C -2.737347 0.000001 -1.167825
H -1.049315 0.000000 2.330398
H -3.475015 0.000000 2.153965
I -0.018885 0.000001 -2.593127
H -3.219623 0.000001 -2.135772
O -4.839447 0.000001 -0.188076
C -5.677340 0.000000 0.962235
H -5.507993 0.893639 1.565728
H -5.507993 -0.893638 1.565727
H -6.696777 0.000001 0.586479
O 4.909880 0.000000 -0.192323
C 5.536993 -0.000002 -1.469030
H 5.265630 -0.893942 -2.034409
H 6.606284 -0.000003 -1.276802
H 5.265632 0.893937 -2.034410
SCF: -988.655501

ZPE: 0.225472
H: -988.413622
G: -988.472338

7_OMe_radical_conf3

H 4.194495 0.963737 -1.149309
C 3.734616 0.951012 -0.170571
C 2.556731 0.914396 2.370570
C 2.378919 0.967556 0.026681
C 4.533157 0.916687 0.977480
C 3.935299 0.896650 2.241121
C 1.721654 0.954196 1.255386
H 4.542911 0.866928 3.133810
H 2.121802 0.895676 3.361704
C 0.262320 0.980044 1.257175
C -2.549735 1.022902 0.985678
C -0.397191 1.005429 0.029874
C -0.570753 0.983810 2.374602
C -1.949573 1.004293 2.248253
C -1.753268 1.026355 -0.164296
H -0.133941 0.972123 3.365044
H -2.555659 1.005605 3.142478
I 0.989362 1.011901 -1.539861
H -2.214994 1.043508 -1.142099
O -3.874786 1.039368 0.774139
C -4.734515 1.032804 1.908243
H -4.570049 1.918309 2.524990
H -4.582838 0.131265 2.504790
H -5.746638 1.044528 1.513394
O 5.857783 0.903436 0.763071
C 6.719625 0.879009 1.895337
H 6.569346 1.764285 2.516132
H 7.731009 0.877513 1.498426
H 6.556011 -0.022626 2.488464
SCF: -988.655049
ZPE: 0.225547
H: -988.413147
G: -988.471783

8_CF3_radical_conf1

C -2.400129 0.071080 2.345799
C 0.387153 -0.003036 2.532296
C -1.596936 0.045152 1.221180
C -1.778614 0.058599 3.586688

C -0.394025 0.023157 3.673101
C -0.204747 0.005777 1.268528
H -2.386109 0.077166 4.482992
H 0.078726 0.016274 4.645488
H 1.464221 -0.028364 2.624109
C 0.524218 -0.023350 -0.004007
C 1.726589 -0.076419 -2.535070
C -0.220961 -0.005710 -1.181438
C 1.913131 -0.070341 -0.132504
C 2.501358 -0.096184 -1.383971
C 0.342334 -0.030481 -2.443309
H 2.537399 -0.088441 0.750399
H 3.578740 -0.132757 -1.467818
H 2.191249 -0.096789 -3.513402
I -2.256682 0.063914 -0.752568
C -0.444542 -0.023474 -3.725635
F -0.256859 -1.142610 -4.423273
F -1.770544 0.081489 -3.506943
F -0.100567 0.994830 -4.510387
C -3.904621 0.091031 2.314575
F -4.383409 0.224013 1.061552
F -4.399669 1.099455 3.027253
F -4.421704 -1.034183 2.806364
SCF: -1433.741262
ZPE: 0.167160
H: -1433.557494
G: -1433.615909

8_CN_radical_conf1

C -2.624587 0.000000 -1.735988
C 0.127703 0.000000 -2.238336
C -1.685500 0.000000 -0.715291
C -2.152020 0.000000 -3.044524
C -0.782526 0.000000 -3.280668
C -0.313332 0.000000 -0.912256
H -2.861039 0.000000 -3.861221
H -0.423439 0.000000 -4.300477
H 1.189609 0.000000 -2.447245
C 0.534780 0.000000 0.278955
C 1.948641 0.000000 2.714047
C -0.099902 0.000000 1.511284
C 1.931983 0.000000 0.296143
C 2.619538 0.000000 1.497002
C 0.557510 0.000000 2.732646

H 2.476182 0.000000 -0.638934
H 3.700844 0.000000 1.490742
H 2.488435 0.000000 3.651022
I -2.174114 0.000000 1.310662
C -0.195307 0.000000 3.948201
N -0.865500 0.000000 4.879282
C -4.019908 0.000000 -1.423150
N -5.119252 0.000000 -1.095296
SCF: -944.102071
ZPE: 0.156950
H: -943.930960
G: -943.984090

8_F_radical_conf1

C -2.431310 0.000000 -1.777426
C 0.343134 0.000000 -1.975232
C -1.630202 0.000000 -0.660148
C -1.846335 0.000000 -3.025229
C -0.457041 0.000000 -3.107626
C -0.239425 0.000000 -0.709620
H -2.475279 0.000000 -3.905550
H 0.007474 0.000000 -4.084263
H 1.420702 0.000000 -2.067946
C 0.458614 0.000000 0.577050
C 1.523183 0.000000 3.186732
C -0.341705 0.000000 1.715659
C 1.837167 0.000000 0.778629
C 2.349908 0.000000 2.067153
C 0.158184 0.000000 2.996404
H 2.502720 0.000000 -0.074185
H 3.421849 0.000000 2.210516
H 1.917710 0.000000 4.194101
I -2.368515 0.000000 1.277281
F -0.693667 0.000000 4.022353
F -3.755870 0.000000 -1.623453
SCF: -958.099489
ZPE: 0.143380
H: -957.943833
G: -957.993075

8_NMe2_radical_conf1

C -0.707400 2.396701 -1.049518
C 1.234717 2.641614 0.996167
C -0.207370 1.326302 -0.335160

C -0.203895 3.644672 -0.687812
C 0.750733 3.752495 0.321947
C 0.747346 1.375291 0.670893
H -0.555868 4.531061 -1.199787
H 1.125734 4.733118 0.584725
H 1.969886 2.752746 1.782547
C 1.089041 0.099503 1.305023
C 1.435332 -2.484309 2.357396
C 0.416054 -1.019876 0.836393
C 1.979226 -0.114418 2.357925
C 2.134251 -1.393412 2.871147
C 0.547127 -2.314119 1.297447
H 2.529626 0.717162 2.778244
H 2.820173 -1.551515 3.693206
H 1.584297 -3.471138 2.776310
I -0.970870 -0.582753 -0.649334
N -0.213525 -3.331069 0.669794
C 0.477078 -3.899818 -0.494122
C -0.667457 -4.386213 1.570467
H -0.222250 -4.530593 -1.042111
H 1.339160 -4.504462 -0.186592
H 0.829621 -3.108867 -1.156292
H -1.390987 -5.002237 1.037143
H 0.153712 -5.032002 1.903652
H -1.152340 -3.944786 2.439985
N -1.667804 2.142730 -2.058270
C -1.047244 1.816141 -3.348078
H -0.578527 2.700741 -3.796616
H -1.816826 1.441332 -4.022166
H -0.283852 1.047761 -3.225106
C -2.668579 3.193080 -2.216153
H -3.100317 3.439451 -1.247116
H -3.456468 2.818586 -2.869117
H -2.251435 4.101198 -2.667261
SCF: -1027.503372
ZPE: 0.305427
H: -1027.179876
G: -1027.240353

8_NMe2_radical_conf2

C 0.381053 3.213571 -0.066416
C 2.071007 3.653550 2.161966
C 0.893661 2.200981 0.719227
C 0.734690 4.505578 0.317477

C 1.566216 4.709067 1.417509
C 1.730509 2.345212 1.816473
H 0.363770 5.351871 -0.246424
H 1.826679 5.722010 1.695766
H 2.709116 3.839072 3.016075
C 2.112423 1.111639 2.508535
C 2.563980 -1.417280 3.648811
C 1.593565 -0.068558 1.994420
C 2.897615 0.991112 3.655605
C 3.105485 -0.262505 4.210626
C 1.785068 -1.340758 2.495816
H 3.323867 1.873097 4.115574
H 3.707590 -0.349027 5.105749
H 2.751379 -2.381089 4.104247
I 0.335745 0.229896 0.365240
N 1.186044 -2.428950 1.816043
C 0.750314 -3.518416 2.684057
C 2.027444 -2.936999 0.725509
H 1.593591 -4.084163 3.098048
H 0.138791 -4.200631 2.094145
H 0.149197 -3.120964 3.500617
H 2.906710 -3.463392 1.116758
H 1.439133 -3.627433 0.121916
H 2.370110 -2.120155 0.090349
N -0.439063 2.859730 -1.165460
C 0.345200 2.584572 -2.375745
H 0.775584 3.506358 -2.786217
H -0.308938 2.134670 -3.121927
H 1.158535 1.892263 -2.157923
C -1.511644 3.808139 -1.447852
H -2.065825 4.020366 -0.534663
H -2.185985 3.354648 -2.173751
H -1.135615 4.748118 -1.868881
SCF: -1027.503392
ZPE: 0.305409
H: -1027.179920
G: -1027.240341

8_NMe2_radical_conf3

C 0.589425 3.473541 -0.048416
C 1.989964 3.776880 2.393243
C 1.028757 2.414503 0.720306
C 0.865075 4.739434 0.464383
C 1.554454 4.875714 1.668058

C 1.723848 2.491825 1.918887
H 0.544503 5.618357 -0.080138
H 1.756139 5.869764 2.045602
H 2.515651 3.910102 3.329790
C 2.046931 1.217370 2.565631
C 2.413227 -1.380825 3.574393
C 1.623425 0.069911 1.909864
C 2.687434 1.025466 3.790427
C 2.853804 -0.261645 4.278644
C 1.782818 -1.232302 2.340620
H 3.033269 1.878386 4.359783
H 3.342641 -0.403876 5.233723
H 2.564163 -2.372278 3.981723
I 0.566412 0.465587 0.163273
N 1.301526 -2.277017 1.515411
C 0.798762 -3.438379 2.242007
C 2.283094 -2.682511 0.501624
H 1.603967 -4.015502 2.712184
H 0.283281 -4.086745 1.534028
H 0.092796 -3.117526 3.006740
H 3.124357 -3.218190 0.958352
H 1.792957 -3.337532 -0.217997
H 2.674872 -1.812354 -0.025220
N -0.090034 3.189390 -1.258235
C -1.149024 4.137043 -1.590835
H -1.723668 3.728567 -2.421702
H -0.753716 5.113844 -1.894151
H -1.809186 4.266901 -0.734454
C 0.832679 3.021107 -2.387607
H 1.634208 2.329079 -2.129171
H 1.281880 3.978946 -2.677702
H 0.279008 2.616968 -3.234568
SCF: -1027.503423
ZPE: 0.305338
H: -1027.180000
G: -1027.240428

8_OMe_radical_conf1

C 2.794815 0.004940 -0.206675
C 1.499495 0.019170 2.302723
C 1.406231 0.003073 -0.089374
C 3.518019 0.012680 0.989757
C 2.883462 0.021306 2.213772
C 0.735331 0.007353 1.143578

H 4.597675 0.013365 0.913069
H 3.477544 0.029804 3.117976
H 1.022848 0.029186 3.271794
C -0.735332 0.001207 1.143575
C -3.518020 -0.003439 0.989758
C -1.406234 0.006770 -0.089370
C -1.499494 -0.011620 2.302710
C -2.883462 -0.013376 2.213763
C -2.794819 0.005280 -0.206669
H -1.022840 -0.022648 3.271767
H -3.477543 -0.022608 3.117961
H -4.597677 -0.003816 0.913073
I -0.000002 0.005713 -1.632094
O -3.552596 0.010593 -1.315339
C -2.992988 0.027220 -2.617103
H -2.420799 -0.883079 -2.815896
H -2.414818 0.938797 -2.790650
H -3.837426 0.039355 -3.301743
O 3.552587 0.001012 -1.315354
C 2.992991 -0.016755 -2.617110
H 2.415037 -0.928592 -2.789962
H 3.837433 -0.029152 -3.301738
H 2.420580 0.893258 -2.816603
SCF: -988.594974
ZPE: 0.222768
H: -988.356417
G: -988.412866

8_OMe_radical_conf2

C 3.013833 0.000000 -0.486969
C 1.881057 0.000000 2.104258
C 1.636489 0.000000 -0.285249
C 3.809940 0.000000 0.664888
C 3.257533 0.000000 1.927759
C 1.049449 0.000000 0.995406
H 4.882585 0.000000 0.519513
H 3.909776 0.000000 2.791069
H 1.453288 0.000000 3.096923
C -0.414626 0.000000 1.082403
C -3.230981 0.000000 0.921154
C -1.111179 0.000000 -0.110569
C -1.185019 0.000000 2.247842
C -2.566389 0.000000 2.147226
C -2.488454 0.000000 -0.253738

H -0.708460 0.000000 3.218527
H -3.158818 0.000000 3.052837
H -4.311394 0.000000 0.885288
I 0.130094 0.000000 -1.752689
O -2.956041 0.000000 -1.510986
C -4.373214 0.000000 -1.690084
H -4.811786 0.894697 -1.246569
H -4.811786 -0.894697 -1.246569
H -4.536065 0.000000 -2.763771
O 3.705199 0.000000 -1.638027
C 3.074529 0.000000 -2.907910
H 2.489516 -0.910434 -3.062661
H 3.881214 0.000000 -3.636742
H 2.489516 0.910434 -3.062661
SCF: -988.606618
ZPE: 0.222906
H: -988.366849
G: -988.427097

8_OMe_radical_conf3

C 2.711938 0.000000 -0.507148
C 1.576749 0.000000 2.078280
C 1.347209 0.000000 -0.277201
C 3.528487 0.000000 0.619705
C 2.949154 0.000000 1.887189
C 0.733713 0.000000 0.966738
H 4.604032 0.000000 0.512291
H 3.601085 0.000000 2.751032
H 1.159003 0.000000 3.075874
C -0.731030 0.000000 0.968848
C -3.526797 0.000000 0.629663
C -1.348036 0.000000 -0.273340
C -1.570947 0.000000 2.082778
C -2.943890 0.000000 1.895517
C -2.713396 0.000000 -0.499461
H -1.150425 0.000000 3.079222
H -3.593396 0.000000 2.761183
H -4.602646 0.000000 0.525218
I -0.002661 0.000000 -1.852185
O -3.109478 0.000000 -1.780748
C -4.514395 0.000000 -2.039031
H -4.977396 0.894665 -1.620857
H -4.977396 -0.894665 -1.620857
H -4.616406 0.000000 -3.120098

O 3.104528 0.000000 -1.789516
C 4.508757 0.000000 -2.051535
H 4.972868 0.894669 -1.634598
H 4.607905 0.000000 -3.132863
H 4.972868 -0.894669 -1.634598
SCF: -988.649359
ZPE: 0.225393
H: -988.408190
G: -988.464857

9_radical_conf1

H 0.000000 0.013323 0.108206
C 0.000000 0.054694 1.188455
C 0.000000 0.137713 4.002671
C 0.000000 -1.076017 1.970470
C 0.000000 1.269042 1.863246
C 0.000000 1.302594 3.252269
C 0.000000 -1.105586 3.365919
H 0.000000 2.187578 1.292135
H 0.000000 2.255838 3.763427
H 0.000000 0.193354 5.080478
C 0.000000 -2.422104 4.004151
C 0.000000 -5.079093 4.956343
C 0.000000 -3.536118 3.165166
C 0.000000 -2.701370 5.365973
C 0.000000 -4.004992 5.832165
C 0.000000 -4.840318 3.594639
I 0.000000 -3.016301 1.170513
F 0.000000 -5.843253 2.730881
F 0.000000 -6.313464 5.422841
F 0.000000 -4.234390 7.132785
F 0.000000 -1.730731 6.268666
SCF: -1156.580899
ZPE: 0.127360
H: -1156.439498
G: -1156.492233

10_CCF2_radical_conf1

H 2.766438 -0.878919 2.511299
C 1.875420 -0.338012 2.222123
C -0.420907 1.047303 1.433363
C 0.874752 -0.926092 1.475259
C 1.694188 0.987261 2.593582
C 0.551626 1.670615 2.199945

C -0.287940 -0.290597 1.058739
H 2.455849 1.480642 3.182261
H 0.419805 2.706644 2.482705
H -1.295311 1.596702 1.109234
I 1.066589 -2.944595 0.925654
C 0.166431 -2.642214 -0.947744
C -1.059247 -2.242413 -3.337059
C -0.880949 -1.730624 -0.979195
C 0.629870 -3.355104 -2.034944
C -0.010693 -3.148052 -3.248989
C -1.482720 -1.534072 -2.222994
H 1.455311 -4.049393 -1.952612
H 0.322646 -3.691555 -4.122854
H -2.284264 -0.811774 -2.308071
H -1.548179 -2.075696 -4.287792
C -1.301099 -0.978113 0.225345
C -2.586526 -0.905085 0.546911
F -3.064033 -0.273364 1.586813
F -3.557959 -1.476494 -0.115178
SCF: -1035.480225
ZPE: 0.177330
H: -1035.289394
G: -1035.341089

10_CH2_2_radical_conf1

C 3.002717 -1.969700 -0.337976
C 1.752570 -1.350867 -0.326598
C 1.767148 -0.003662 -0.010522
C 2.894685 0.739858 0.283929
C 4.117690 0.082851 0.250201
C 4.167063 -1.267788 -0.061425
C 0.493099 -2.117854 -0.599699
C -0.492360 -2.119031 0.597015
C -1.752026 -1.351641 0.325842
C -3.002169 -1.970510 0.338235
C -4.166923 -1.268412 0.063969
C -4.118036 0.082578 -0.246206
C -2.895117 0.739678 -0.280750
C -1.767108 -0.004075 0.011345
I -0.000072 1.179063 -0.000904
H 3.046334 -3.026681 -0.570941
H 2.845981 1.792118 0.535618
H 5.020399 0.635163 0.474589
H 5.118774 -1.782325 -0.083881

H 0.764020 -3.141550 -0.848460
H 0.004313 -1.701201 -1.485320
H -0.003492 -1.704057 1.483361
H -0.763175 -3.143226 0.843836
H -3.045418 -3.027732 0.570173
H -5.118564 -1.783045 0.087114
H -5.021059 0.635103 -0.468802
H -2.846881 1.792245 -0.531264
SCF: -838.171688
ZPE: 0.215157
H: -837.944115
G: -837.993108

10_CH2_2_radical_conf2

C 2.756689 -1.887606 0.639066
C 1.695560 -1.254163 -0.006982
C 1.600347 0.113902 0.206582
C 2.463361 0.866014 0.982438
C 3.513641 0.196274 1.594582
C 3.653021 -1.174739 1.422985
C 0.711371 -2.025244 -0.839693
C -0.575069 -2.395020 -0.099838
C -1.571600 -1.347416 0.364905
C -2.689126 -1.858772 1.041661
C -3.712375 -1.059995 1.514416
C -3.662280 0.317574 1.340941
C -2.573865 0.877149 0.698106
C -1.571035 0.034079 0.230942
I -0.005783 1.084169 -0.731015
H 2.875726 -2.956896 0.511604
H 2.330053 1.931321 1.114488
H 4.213362 0.750094 2.206133
H 4.470288 -1.695741 1.904750
H 1.178830 -2.965449 -1.130797
H 0.491673 -1.496657 -1.769249
H -0.300524 -2.972596 0.786380
H -1.134183 -3.079100 -0.741774
H -2.737057 -2.932352 1.184527
H -4.552602 -1.513871 2.023645
H -4.453079 0.956655 1.710192
H -2.508821 1.949794 0.572019
SCF: -838.187721
ZPE: 0.216312
H: -837.959184

G: -838.008046

10_CH2_2_radical_conf3

C 2.428270 -1.836479 1.111907
C 1.534797 -1.262090 0.207938
C 1.483624 0.127191 0.238345
C 2.237217 0.941930 1.060543
C 3.129182 0.323738 1.927563
C 3.213266 -1.060487 1.954751
C 0.772205 -2.115253 -0.772119
C -0.788938 -2.117115 -0.750254
C -1.527436 -1.262276 0.246971
C -2.397640 -1.835575 1.174040
C -3.163955 -1.058498 2.032919
C -3.084242 0.325823 1.998893
C -2.214399 0.943100 1.109002
C -1.478311 0.127249 0.272248
I -0.011098 1.032311 -0.942594
H 2.512924 -2.916019 1.136055
H 2.136549 2.018591 1.039817
H 3.741598 0.929474 2.582060
H 3.899707 -1.544938 2.637144
H 1.107500 -3.140056 -0.629640
H 1.096254 -1.824666 -1.774343
H -1.117807 -3.142216 -0.595385
H -1.141108 -1.830890 -1.744194
H -2.479578 -2.915185 1.203780
H -3.832696 -1.542270 2.733141
H -3.682645 0.932210 2.665624
H -2.116605 2.019976 1.081997
SCF: -838.189094
ZPE: 0.216440
H: -837.960284
G: -838.010230

10_CH2_3_radical_conf1

C -3.093686 -1.739981 -0.592767
C -1.826665 -1.148715 -0.601570
C -1.767688 0.110849 -0.028432
C -2.842086 0.787859 0.526405
C -4.080543 0.165314 0.496669
C -4.201768 -1.098955 -0.063883
C -0.648244 -1.921686 -1.116207
C -0.000503 -2.753850 -0.001585

C 0.647369 -1.924080 1.114750
C 1.826154 -1.150534 0.601838
C 3.092954 -1.742262 0.591997
C 4.201353 -1.100560 0.064609
C 4.080694 0.164941 -0.493289
C 2.842476 0.788016 -0.521916
C 1.767739 0.110230 0.031320
I 0.000221 1.290872 0.002477
H -3.191925 -2.730536 -1.021349
H -2.735054 1.768596 0.972642
H -4.938608 0.671757 0.917918
H -5.165650 -1.590468 -0.085849
H 0.085113 -1.259429 -1.582510
H -0.996298 -2.596879 -1.897577
H 0.760052 -3.399732 -0.445169
H -0.761197 -3.400469 0.440682
H 0.995062 -2.600929 1.894843
H -0.085802 -1.262439 1.582228
H 3.190737 -2.733756 1.018510
H 5.165044 -1.592484 0.085679
H 4.939022 0.671951 -0.913318
H 2.735902 1.769756 -0.966053
SCF: -877.483966
ZPE: 0.266496
H: -877.204034
G: -877.255227

10_CH2_3_radical_conf2

C -2.860335 -1.376359 1.196218
C -1.878985 -1.063307 0.251169
C -1.545412 0.284238 0.181063
C -2.116427 1.288786 0.946183
C -3.094491 0.929085 1.860354
C -3.455847 -0.405669 1.986585
C -1.292407 -2.160852 -0.597340
C 0.004340 -2.812789 -0.081344
C 1.334499 -2.159810 -0.502440
C 1.856084 -1.063375 0.388641
C 2.760990 -1.378243 1.406491
C 3.293282 -0.408890 2.242254
C 2.943685 0.926307 2.089742
C 2.039891 1.287871 1.102753
C 1.529490 0.284318 0.294590
I 0.040562 0.867257 -1.077010

H -3.162538 -2.412311 1.293748
H -1.809595 2.320783 0.842795
H -3.561979 1.691026 2.469616
H -4.215157 -0.693463 2.702270
H -1.143358 -1.812119 -1.622243
H -2.049358 -2.943005 -0.651509
H 0.019228 -3.823987 -0.489111
H -0.034565 -2.914603 1.005694
H 1.259323 -1.809603 -1.534819
H 2.094043 -2.941451 -0.502522
H 3.053973 -2.414517 1.526079
H 3.993718 -0.698056 3.015151
H 3.362788 1.687041 2.734691
H 1.742825 2.320281 0.976472
SCF: -877.495600
ZPE: 0.245076
H: -877.237135
G: -877.288455

10_CH2_3_radical_conf3

C -3.153534 -1.478998 -0.799486
C -2.061170 -1.111063 -0.013194
C -1.615487 0.192665 -0.202142
C -2.172267 1.107516 -1.081201
C -3.261882 0.697734 -1.834942
C -3.747577 -0.593974 -1.688565
C -1.435405 -2.103959 0.931892
C 0.072690 -2.409462 0.732962
C 0.656207 -2.118449 -0.665742
C 1.737290 -1.066588 -0.730340
C 2.921830 -1.350148 -1.416838
C 3.943385 -0.422834 -1.551801
C 3.816610 0.846622 -1.008226
C 2.656863 1.183233 -0.326905
C 1.667696 0.219793 -0.203556
I 0.008746 0.868739 0.943898
H -3.537379 -2.487347 -0.705074
H -1.776184 2.109232 -1.179180
H -3.720979 1.388328 -2.529542
H -4.596337 -0.920092 -2.275948
H -2.001106 -3.028497 0.830714
H -1.591402 -1.759727 1.958290
H 0.207660 -3.469745 0.940344
H 0.662073 -1.898050 1.493980

H -0.135844 -1.831454 -1.362146
H 1.085647 -3.031482 -1.072923
H 3.031318 -2.336065 -1.852270
H 4.843223 -0.695367 -2.088074
H 4.606076 1.579028 -1.111291
H 2.539075 2.174847 0.090791
SCF: -877.488122
ZPE: 0.244908
H: -877.229659
G: -877.282777

10_CH2_radical_conf1

H 2.880170 -0.710414 2.355887
C 1.895654 -0.301988 2.171092
C -0.646644 0.730675 1.641744
C 0.895016 -1.045583 1.577139
C 1.585462 1.005418 2.519839
C 0.321352 1.514894 2.252731
C -0.383635 -0.592515 1.292803
H 2.339959 1.621340 2.990624
H 0.086775 2.537012 2.519914
H -1.629082 1.136011 1.433583
I 1.296950 -3.029382 0.996704
C 0.179900 -2.821260 -0.776439
C -1.283805 -2.467221 -3.029080
C -0.976959 -2.066701 -0.661711
C 0.646004 -3.402557 -1.939247
C -0.118092 -3.220144 -3.083871
C -1.703829 -1.893223 -1.837668
H 1.565112 -3.972060 -1.967063
H 0.209945 -3.661394 -4.015482
H -2.611887 -1.304122 -1.803253
H -1.871858 -2.321642 -3.925837
C -1.426694 -1.470041 0.647942
H -2.336509 -0.896020 0.489792
H -1.672305 -2.286783 1.337655
SCF: -798.891870
ZPE: 0.187876
H: -798.692219
G: -798.740371

10_CMe2_radical_conf1

H 2.935267 -0.705020 2.303967
C 1.950817 -0.284142 2.146278

C -0.569422 0.774036 1.660849
C 0.946424 -0.999837 1.521023
C 1.659692 1.007072 2.556728
C 0.401335 1.529216 2.303609
C -0.338875 -0.543717 1.251961
H 2.419548 1.595421 3.053270
H 0.165223 2.541474 2.604998
H -1.531999 1.228034 1.480674
I 1.466662 -2.926639 0.865155
C 0.228371 -2.772004 -0.824845
C -1.246330 -2.534622 -3.077610
C -0.939257 -2.026266 -0.711601
C 0.689345 -3.395218 -1.969848
C -0.078949 -3.280022 -3.117556
C -1.660714 -1.918572 -1.905189
H 1.620125 -3.947001 -1.980732
H 0.247997 -3.757992 -4.031203
H -2.574018 -1.343928 -1.926075
H -1.847839 -2.423869 -3.970453
C -1.440290 -1.397644 0.600190
C -1.884012 -2.512443 1.576304
H -1.099658 -3.209671 1.860416
H -2.686747 -3.086282 1.112073
H -2.264527 -2.050796 2.488052
C -2.691744 -0.555472 0.346607
H -2.507039 0.274901 -0.335591
H -3.064063 -0.161061 1.290738
H -3.477322 -1.185235 -0.067690
SCF: -877.500075
ZPE: 0.244583
H: -877.241097
G: -877.294533

10_CO_radical_conf1

H 2.655947 -0.968885 2.782290
C 1.797845 -0.408978 2.433899
C -0.419339 1.024661 1.538495
C 0.899995 -0.936644 1.528310
C 1.567445 0.883696 2.886532
C 0.463944 1.596090 2.438039
C -0.222016 -0.271658 1.058480
H 2.261127 1.327110 3.588503
H 0.290739 2.603840 2.791048
H -1.281505 1.573670 1.183756

I 1.230977 -2.917910 0.930798
C 0.167394 -2.745088 -0.867638
C -1.262252 -2.656116 -3.187691
C -0.842250 -1.799534 -0.962371
C 0.485426 -3.648864 -1.861049
C -0.247034 -3.590806 -3.039682
C -1.556218 -1.774362 -2.162055
H 1.277107 -4.376859 -1.741663
H -0.011841 -4.280068 -3.839721
H -2.345046 -1.041817 -2.270580
H -1.828231 -2.613583 -4.108492
C -1.227855 -0.792555 0.077976
O -2.340861 -0.327640 0.068415
SCF: -872.911265
ZPE: 0.167093
H: -872.732559
G: -872.779528

10_NAc_radical_conf1

H 2.776917 -0.760497 2.530090
C 1.858122 -0.274001 2.231781
C -0.520201 0.966288 1.406516
C 0.828088 -0.970366 1.632120
C 1.661786 1.083867 2.440769
C 0.482047 1.693398 2.030286
C -0.361778 -0.399689 1.204778
H 2.441437 1.663187 2.916804
H 0.343944 2.754870 2.188328
H -1.432136 1.442795 1.073900
I 0.985692 -3.026381 1.252746
C 0.053307 -2.802743 -0.609806
C -1.214806 -2.341433 -2.968968
C -0.987648 -1.882921 -0.618316
C 0.494509 -3.491486 -1.720580
C -0.174093 -3.259557 -2.915420
C -1.610052 -1.642734 -1.837702
H 1.322516 -4.185609 -1.669059
H 0.135748 -3.789960 -3.805786
H -2.401387 -0.905612 -1.885498
H -1.716456 -2.151898 -3.908693
N -1.357434 -1.193581 0.568965
C -2.639274 -1.256109 1.126366
O -2.907431 -0.595344 2.102358
C -3.617426 -2.194310 0.481033

H -3.149938 -3.133886 0.189340
H -4.044217 -1.731595 -0.409760
H -4.414635 -2.378291 1.196107
SCF: -967.593143
ZPE: 0.213460
H: -967.365495
G: -967.418508

10_NH_radical_conf1

H 3.098419 -0.218967 1.996187
C 2.029467 -0.050917 1.991187
C -0.736616 0.346121 1.957928
C 1.161748 -0.953793 1.403366
C 1.480393 1.066094 2.599236
C 0.100561 1.248572 2.588271
C -0.216155 -0.793720 1.339238
H 2.128958 1.783916 3.082288
H -0.329946 2.119357 3.065405
H -1.807048 0.509962 1.925524
I 1.878354 -2.740500 0.591388
C 0.449314 -2.723180 -0.932222
C -1.538944 -2.826611 -2.780480
C -0.796437 -2.235375 -0.560184
C 0.754907 -3.217394 -2.187540
C -0.265699 -3.273218 -3.122416
C -1.802118 -2.301750 -1.528388
H 1.750588 -3.567284 -2.426598
H -0.065624 -3.669128 -4.108567
H -2.786662 -1.925734 -1.276992
H -2.337783 -2.872956 -3.509267
N -1.061566 -1.711407 0.708474
H -2.041907 -1.487887 0.838361
SCF: -814.940869
ZPE: 0.176367
H: -814.752818
G: -814.801088

10_O_radical_conf1

H 0.211812 0.493862 0.055599
C 0.062686 0.295147 1.108699
C -0.331993 -0.250063 3.834404
C -0.770099 -0.717351 1.543450
C 0.694699 1.059450 2.079633
C 0.492931 0.788307 3.427724

C -0.978801 -1.017410 2.879775
H 1.346508 1.866787 1.774733
H 0.991853 1.388944 4.176729
H -0.488271 -0.478122 4.880792
O -1.834572 -2.014495 3.285266
C -1.620752 -3.288983 2.815845
C -1.266462 -5.888400 1.881751
C -1.576551 -3.582329 1.462661
C -1.488411 -4.330972 3.718783
C -1.321635 -5.624156 3.245150
C -1.388158 -4.855742 0.962458
H -1.521094 -4.110816 4.777908
H -1.224584 -6.436162 3.953655
H -1.346494 -5.045082 -0.101948
H -1.127738 -6.899854 1.524865
I -1.827272 -1.929663 0.211267
SCF: -834.798175
ZPE: 0.163087
H: -834.623490
G: -834.672079

10_SO2_radical_conf1

H 3.080063 -0.381585 2.029763
C 2.031243 -0.117067 2.047693
C -0.679903 0.605935 2.027257
C 1.053500 -0.983728 1.613660
C 1.623033 1.134578 2.503676
C 0.285265 1.492906 2.489282
C -0.294681 -0.654620 1.601026
H 2.371941 1.831691 2.855079
H -0.016596 2.472292 2.834931
H -1.726771 0.878889 2.007087
I 1.637781 -2.868586 0.883742
C 0.276433 -2.839776 -0.720075
C -1.477725 -2.714132 -2.817000
C -0.994356 -2.325866 -0.503721
C 0.701268 -3.292949 -1.948740
C -0.208162 -3.235894 -3.002723
C -1.874824 -2.245877 -1.570037
H 1.703352 -3.670058 -2.104324
H 0.099759 -3.590594 -3.977275
H -2.862598 -1.831767 -1.415159
H -2.169224 -2.664407 -3.647233
S -1.535260 -1.820349 1.106432

O -2.786530 -1.137851 0.978816
O -1.422710 -2.960785 1.975044
SCF: -1308.200198
ZPE: 0.169707
H: -1308.016615
G: -1308.069624

10_SO_radical_conf1

H 3.085938 -0.437918 1.956085
C 2.029223 -0.208653 1.984885
C -0.717375 0.389780 2.010496
C 1.072822 -1.128226 1.608688
C 1.576541 1.039310 2.400968
C 0.220776 1.335715 2.405958
C -0.282500 -0.861848 1.610000
H 2.299184 1.782098 2.711171
H -0.114682 2.314465 2.722306
H -1.778181 0.606777 2.012886
I 1.657979 -3.018350 0.890933
C 0.331569 -2.909036 -0.739862
C -1.424151 -2.619238 -2.805086
C -0.940105 -2.441653 -0.470734
C 0.771071 -3.232834 -2.006324
C -0.141434 -3.090785 -3.046774
C -1.832423 -2.290282 -1.518119
H 1.779917 -3.576825 -2.191284
H 0.166700 -3.343395 -4.052505
H -2.831195 -1.924200 -1.315426
H -2.119109 -2.505243 -3.626434
S -1.503225 -2.124531 1.210321
O -2.815941 -1.457131 1.118849
SCF: -1232.964367
ZPE: 0.163954
H: -1232.787189
G: -1232.838789

11_radical_conf1

H 0.225629 0.509465 0.053985
C 0.057817 0.287711 1.099719
C -0.333268 -0.256214 3.831322
C -0.780066 -0.717230 1.540916
C 0.679734 1.025988 2.088078
C 0.499146 0.777275 3.436690
C -0.988584 -1.017235 2.875994

H 1.015685 1.387021 4.165837
H -0.487596 -0.482628 4.878154
O -1.853043 -2.008976 3.276498
C -1.629714 -3.283828 2.812209
C -1.261312 -5.852355 1.892618
C -1.584478 -3.576886 1.460226
C -1.488557 -4.324970 3.716245
C -1.312691 -5.618572 3.254961
C -1.386665 -4.846154 0.954125
H -1.521951 -4.107205 4.775617
H -1.206233 -6.446429 3.943112
H -1.338839 -5.065752 -0.104227
I -1.839142 -1.926180 0.209466
F -1.080356 -7.103949 1.457081
F 1.492584 2.021004 1.716375
SCF: -1033.300932
ZPE: 0.146411
H: -1033.141185
G: -1033.194231