From CO_2 to CS_2: a Theoretical Investigation of the Cycloaddition to Aziridines Mediated by Metal-free Porphyrin-based Catalytic Systems

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Supplementary Information

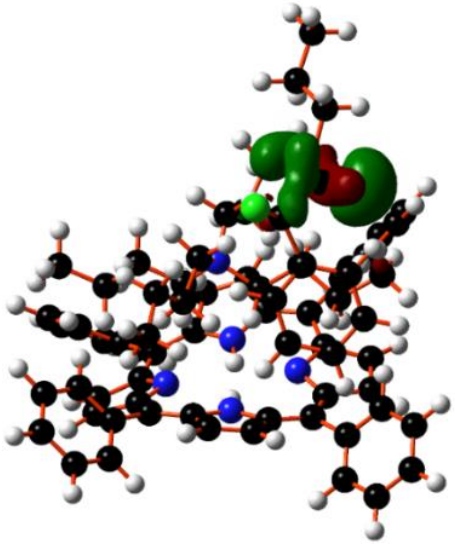

Figure S1. Plot of the HOMO-1 orbital at the aziridine nitrogen, N_{az} in the intermediate $\mathbf{3^{Bu}}$

Cartesian coordinates and free energies of all the structures optimized in the computational analysis (B97D level of theory).

Compound **$TPPH_2$**
Cartesian Coordinates

N 0.000337 -2.124710 -0.031618
N 2.050608 0.000307 0.017518
C 2.473703 2.453839 -0.010806
C -2.473683 -2.453831 -0.010690
C 2.877743 1.094046 -0.085174
H 1.350580 -5.114563 0.350969
C 0.690528 -4.263104 0.230041
C 4.266531 -0.682604 -0.295396
C 2.878088 -1.093164 -0.085158
C 1.137632 -2.906587 0.056010
H 5.108530 1.352601 -0.442758
C -0.689173 -4.263318 0.230085
C 2.474465 -2.453081 -0.010746
C 4.266318 0.683911 -0.295383
C -1.136715 -2.906942 0.056083
H 5.108958 -1.351023 -0.442774
H -1.348932 -5.114996 0.351056
C -2.877709 -1.094034 -0.085126
N -2.050594 -0.000304 0.017633
C 1.136731 2.906948 0.055899
N -0.000319 2.124723 -0.031831
C -1.137609 2.906595 0.055916
C -0.690502 4.263100 0.229944
C 0.689201 4.263322 0.229894
H 1.348963 5.115004 0.350819
H -1.350539 5.114559 0.350930
C -2.474437 2.453082 -0.010798
C -2.878052 1.093166 -0.085167
C -4.266464 0.682599 -0.295596
C -4.266250 -0.683907 -0.295584
H -5.108437 -1.352595 -0.443121
H 0.000183 -1.109489 -0.094656
H -0.000168 1.109495 -0.094740
C 3.538170 -3.504808 0.002707
C 4.504480 -3.531477 1.032982
C 3.596155 -4.487482 -1.010537
C 5.503951 -4.518043 1.050996
H 4.461445 -2.778083 1.820354
C 4.598047 -5.471878 -0.995881
H 2.857734 -4.467311 -1.812999
C 5.554544 -5.491040 0.035854
H 6.239378 -4.528246 1.857024
H 4.633508 -6.219264 -1.790104
H 6.331935 -6.256497 0.048385
C 3.537086 3.505877 0.002735
C 4.503348 3.532799 1.033048
C 3.594849 4.488574 -1.010491
C 5.502537 4.519643 1.051124
H 4.460499 2.779372 1.820397
C 4.596468 5.473251 -0.995783
H 2.856488 4.468201 -1.812999
C 5.552908 5.492671 0.035999
H 6.237929 4.530037 1.857182
H 4.631763 6.220647 -1.790003
H 6.330087 6.258342 0.048575
C -3.537079 -3.505856 0.002776
C -4.503540 -3.532620 1.032912
C -3.594709 -4.488664 -1.010353
C -5.502761 -4.519433 1.050934
H -4.460821 -2.779090 1.820170
C -4.596358 -5.473309 -0.995700
H -2.856228 -4.468392 -1.812756

C -5.552976 -5.492586 0.035921
H -6.238295 -4.529705 1.856864
H -4.631543 -6.220789 -1.789846
H -6.330176 -6.258237 0.048453
H -5.108852 1.351017 -0.443161
C -3.538149 3.504780 0.002703
C -3.596173 4.487517 -1.010467
C -4.504470 3.531347 1.032970
C -4.598108 5.471868 -0.995762
H -2.857781 4.467396 -1.812952
C -5.503968 4.517879 1.051057
H -4.461400 2.777908 1.820294
C -5.554602 5.490938 0.035977
H -4.633613 6.219285 -1.789955
H -6.239388 4.528011 1.857093
H -6.332017 6.256370 0.048556

Free Energy: -1911.893838

Compound **TBACl**
Cartesian Coordinates
Cl 2.167162 -7.610589 8.973934
N 0.669908 -3.646539 8.249511
C -0.197215 -2.395496 8.412300
H -0.696717 -2.249064 7.448050
H 0.501574 -1.563529 8.556483
C 3.467225 -4.072028 5.540629
H 2.811182 -3.857751 4.680162
H 4.002719 -3.136664 5.775607
C 2.603601 -4.483776 6.749489
H 2.064142 -5.411549 6.514764
H 3.256765 -4.702946 7.605311
C -0.997702 -4.841234 6.662600
H -1.672897 -3.972186 6.641722
H -0.331307 -4.769159 5.790111
C 1.628623 -3.359835 7.090026
H 0.992019 -3.122126 6.229998
H 2.169061 -2.447206 7.365748
C -2.009378 -1.109441 9.578142
H -1.305615 -0.270382 9.706918
H -2.509328 -0.962814 8.606291
C 1.443310 -3.962168 9.536259
H 0.680802 -4.189487 10.290153
H 1.984971 -4.892118 9.331223
C 4.110142 -4.447279 11.077865
H 4.649796 -4.688579 12.006230
H 4.851996 -4.148795 10.319132
H 3.615710 -5.364919 10.725395
C 3.101166 -3.307602 11.318611
H 3.626084 -2.433407 11.734188
H 2.354971 -3.616797 12.069975
C -1.836615 -6.130576 6.541266
H -2.508565 -6.208229 7.411990
H -1.164003 -7.002888 6.577305
C -3.052299 -1.094558 10.709379
H -3.608510 -0.145168 10.720558
H -2.565281 -1.219204 11.689614
H -3.775992 -1.915418 10.582657
C -0.188296 -4.885423 7.956837
H 0.504080 -5.736365 7.964226
H -0.849675 -4.994721 8.823415
C -2.659587 -6.156079 5.241627
H -3.253350 -7.079736 5.168877
H -1.999061 -6.102675 4.361444
H -3.350989 -5.299042 5.200411
C 4.477426 -5.170783 5.165700
H 5.088097 -4.868054 4.301556
H 3.956217 -6.106568 4.909251
H 5.153577 -5.381133 6.009366
C -1.219399 -2.434118 9.547342
H -0.718705 -2.574288 10.516568
H -1.925224 -3.266401 9.411414
C 2.370100 -2.853110 10.033501
H 1.795232 -1.940777 10.250186
H 3.123153 -2.603324 9.270886

Free Energy: -1145.537115

Adduct **1** between **$TPPH_2$** and TBACl
Cartesian Coordinates
Cl 5.747578 -0.615775 1.282222
N 8.025618 -0.042499 -2.345751
C 9.242083 0.275316 -3.226015
H 8.995191 1.191127 -3.773947
H 9.304337 -0.537167 -3.958786
C 4.325769 -0.661164 -3.419434
H 4.205151 0.385202 -3.741060
H 4.462437 -1.254933 -4.331713

C 5.574630 -0.780339 -2.531289
H 5.418802 -0.198778 -1.612614
H 5.696551 -1.827593 -2.216508
C 7.188892 2.393547 -2.092677
H 7.804288 2.668460 -2.962203
H 6.164682 2.227155 -2.456240
C 6.832972 -0.315744 -3.269916
H 6.659155 0.615534 -3.817304
H 7.171701 -1.060857 -3.996024
C 11.706328 0.813840 -3.408900
H 11.826595 0.034660 -4.172957
H 11.440370 1.743721 -3.932541
C 8.300133 -1.267380 -1.467478
H 9.104870 -0.976297 -0.783140
H 7.397939 -1.412431 -0.861902
C 9.220201 -5.007208 -2.033741
H 9.333457 -5.850769 -1.336209
H 10.169139 -4.884341 -2.579103
H 8.441538 -5.268727 -2.767812
C 8.848404 -3.716194 -1.283572
C 7.177576 3.574945 -1.102449
H 8.202869 3.746593 -0.734516
H 6.562082 3.310629 -0.227036
C 13.031882 0.996663 -2.651579
H 13.850137 1.249490 -3.343125
H 13.309463 0.069984 -2.124178
H 12.950158 1.802661 -1.905042
C 7.712945 1.131719 -1.403813
H 6.992237 0.753816 -0.668703
H 8.644745 1.337393 -0.867577
C 6.636301 4.855748 -1.762126
H 6.638327 5.697490 -1.053056
H 5.605901 4.706503 -2.119854
H 7.254116 5.132648 -2.631003
C 3.060580 -1.135975 -2.686636
H 2.173913 -1.043127 -3.332576
H 2.889492 -0.543038 -1.774253
H 3.158983 -2.192381 -2.389663
C 10.561197 0.421874 -2.460606
H 10.822845 -0.525974 -1.968571
H 10.479929 1.189333 -1.677979
C 8.674087 -2.527433 -2.248180
H 9.609747 -2.374054 -2.806538
H 7.895778 -2.778855 -2.983890
N 6.464771 0.521548 -6.444593
N 8.667131 2.450144 -6.298087
N 10.669978 0.322484 -6.543524
N 8.459244 -1.604523 -6.322033
C 5.623855 -0.560305 -6.621801
C 4.290187 -0.030879 -6.719553
C 4.358976 1.335599 -6.549529
C 5.736709 1.691889 -6.342120
C 6.253020 2.969522 -6.027599
C 7.634131 3.293046 -5.958857
C 8.139824 4.604490 -5.556380
C 9.497033 4.556660 -5.713592
C 9.807247 3.208262 -6.185097
C 11.130613 2.764250 -6.449497
C 11.508067 1.417468 -6.638880
C 12.840491 0.901227 -6.798616
C 12.778908 -0.474463 -6.715649
C 11.400736 -0.850433 -6.546827
C 10.887238 -2.150072 -6.346726
C 9.512109 -2.486713 -6.255251
C 9.037140 -3.868995 -6.217746
C 7.674994 -3.808788 -6.300468
C 7.329737 -2.389610 -6.370984
C 6.002495 -1.919244 -6.546236
H 3.400812 -0.634608 -6.857051
H 3.537223 2.042472 -6.548516
H 7.538266 5.432657 -5.196701
H 10.223367 5.336512 -5.507388
H 13.725499 1.513686 -6.926335
H 13.604617 -1.175326 -6.757187
H 9.666285 -4.752229 -6.173202
H 6.971228 -4.633995 -6.337508
H 7.474922 0.453803 -6.351387
H 9.662430 0.377667 -6.417150
C 5.252314 4.041546 -5.742960
C 5.233508 5.236198 -6.497104
C 4.306534 3.877697 -4.705878
C 4.295056 6.242867 -6.218189
H 5.953188 5.365227 -7.306051
C 3.370651 4.884735 -4.423683
H 4.317700 2.962414 -4.114192
C 3.362299 6.071542 -5.178753
H 4.290354 7.157272 -6.813342
H 2.655233 4.745111 -3.611920
H 2.635593 6.855187 -4.959858
C 12.219169 3.788594 -6.455210
C 12.191201 4.848886 -7.388101
C 13.275106 3.732544 -5.518620
C 13.201248 5.824897 -7.391077
H 11.377257 4.897979 -8.112499
C 14.282047 4.711169 -5.517250
H 13.294546 2.928059 -4.784253
C 14.249623 5.759395 -6.454981
H 13.169609 6.633580 -8.122796
H 15.086125 4.657726 -4.781695
H 15.032613 6.519062 -6.455055
C 11.887698 -3.257707 -6.235300
C 12.695857 -3.625923 -7.331611
C 12.029448 -3.953843 -5.015744
C 13.628546 -4.669781 -7.210090
H 12.582849 -3.097648 -8.279242
C 12.961105 -4.997446 -4.893038
H 11.406582 -3.670772 -4.166814
C 13.764403 -5.357969 -5.990445
H 14.243178 -4.948012 -8.067560
H 13.060480 -5.524805 -3.942995
H 14.488166 -6.168852 -5.896737
C 4.892184 -2.920874 -6.588241

C 4.089645 -3.068370 -7.739668
C 4.615560 -3.717344 -5.455071
C 3.032095 -3.993133 -7.757761
H 4.301800 -2.459695 -8.619664
C 3.557464 -4.640151 -5.471896
H 5.228084 -3.602584 -4.560472
C 2.761625 -4.780014 -6.623416
H 2.422728 -4.099909 -8.656460
H 3.352490 -5.243050 -4.586019
H 1.938256 -5.495535 -6.636703
H 7.911480 -3.865204 -0.722580
H 9.628924 -3.474094 -0.543173

Free Energy: -3057.442998

Compound *N*-butyl-2-phenylaziridine
Cartesian Coordinates
C -4.801987 -1.045784 -2.314332
C -6.208935 -0.822529 -2.804103
N -5.600635 0.104123 -1.845256
H -7.013146 -1.453483 -2.413637
H -6.333339 -0.481215 -3.839311
C -4.446929 -2.124184 -1.342121
C -5.263170 -2.405806 -0.225099
C -3.283795 -2.895033 -1.548427
C -4.923183 -3.438447 0.663719
H -6.156386 -1.802822 -0.056826
C -2.942598 -3.930506 -0.660240
H -2.645044 -2.680062 -2.408143
C -3.762007 -4.206225 0.449379
H -5.561956 -3.643830 1.524704
H -2.038103 -4.516510 -0.832742
H -3.498665 -5.008237 1.140881
H -4.014755 -0.818780 -3.043821
C -5.208681 1.413544 -2.400911
C -6.388478 2.392847 -2.372212
H -4.838880 1.313032 -3.443976
H -4.376841 1.799930 -1.789811
C -6.015153 3.774036 -2.939260
H -7.222425 1.967630 -2.956933
H -6.743837 2.500227 -1.333627
C -7.199189 4.757655 -2.912031
H -5.173894 4.189356 -2.358000
H -5.655049 3.655466 -3.975773
H -6.915045 5.739363 -3.322132
H -8.041488 4.368758 -3.507161
H -7.556507 4.907985 -1.880298

Free Energy -521.668765

Compound *N*-aryl-2-phenylaziridine
Cartesian Coordinates
N -0.244537 0.340537 0.921491
C 0.694239 0.907619 1.887792
C 0.806767 -0.545336 1.505333
C -1.605376 0.181446 1.223178
C -2.349009 1.244971 1.780219
C -2.255563 -1.029027 0.909595
C -3.721658 1.086726 2.008998
H -1.848169 2.178435 2.028390
C -3.628438 -1.169904 1.161675
H -1.680426 -1.853381 0.492630
C -4.380063 -0.120758 1.710276
H -5.443591 -0.235811 1.903020
C -4.270397 -2.499071 0.831562
C -4.539098 2.205003 2.616091
H 0.312190 1.137557 2.887647
H 1.412929 1.626491 1.485932
H 1.573965 -0.810317 0.772889
C 0.455635 -1.660176 2.439399
C -0.384861 -1.486201 3.561028
C 0.946787 -2.951632 2.152863
C -0.722068 -2.577770 4.375827
H -0.787105 -0.501428 3.796257
C 0.615322 -4.044788 2.971115
H 1.590217 -3.096708 1.282696
C -0.223702 -3.861277 4.084411
H -1.375429 -2.426110 5.236237
H 1.006535 -5.035737 2.736083
H -0.488286 -4.708792 4.718313
F -4.173616 -2.792154 -0.507142
F -3.657168 -3.535272 1.492251
F -5.594751 -2.555129 1.152406
F -5.041207 1.853835 3.846641
F -3.832054 3.357634 2.795168
F -5.625716 2.522227 1.839629

Free Energy -1269.206683

Compound **CS_2**
Cartesian Coordinates
C 0.000000 0.000000 0.000000
S 1.570543 0.000000 0.000000
S -1.570543 0.000000 0.000000

Free Energy -834.472909

Adduct between **$TPPH_2$** and **CS_2**
Cartesian Coordinates
N 0.031997 2.177116 -0.072691
N -2.012884 0.051740 -0.013112
C -2.433614 -2.401903 0.002026
C 2.505662 2.508767 -0.056189
C -2.839862 -1.043749 -0.083266
H -1.320091 5.168113 0.294547
C -0.659312 4.316767 0.176912
C -4.237153 0.728167 -0.277029
C -2.844497 1.142527 -0.102965
C -1.105470 2.958582 0.014104
H -5.078625 -1.309473 -0.383238
C 0.720353 4.318267 0.172284
C -2.442066 2.503035 -0.039705
C -4.234143 -0.638082 -0.263845
C 1.168495 2.961012 0.006969
H -5.084135 1.393865 -0.409515
H 1.379965 5.171046 0.286249
C 2.911599 1.149177 -0.118168
N 2.084603 0.055760 -0.013296
C -1.097007 -2.853892 0.057693
N 0.039015 -2.072856 -0.048921
C 1.176110 -2.852167 0.048652
C 0.731280 -4.206318 0.241224
C -0.647973 -4.207319 0.247908
H -1.305820 -5.058025 0.384555
H 1.392282 -5.055129 0.374009
C 2.512098 -2.396774 -0.010318
C 2.914148 -1.037450 -0.095544
C 4.304352 -0.627529 -0.295411
C 4.302592 0.738855 -0.310831
H 5.145418 1.407166 -0.456349
H 0.031961 1.161485 -0.130554
H 0.038150 -1.057708 -0.112198
C -3.506307 3.554273 -0.018300
C -4.454923 3.590585 1.027879
C -3.580221 4.528469 -1.038535
C -5.453521 4.577876 1.053921
H -4.398973 2.844513 1.821424
C -4.580992 5.513896 -1.015512
H -2.854538 4.501129 -1.852370
C -5.520382 5.542300 0.031598
H -6.175312 4.595618 1.872055
H -4.628838 6.254817 -1.815140
H -6.296910 6.308466 0.050568
C -3.495714 -3.454053 0.051872
C -4.439964 -3.468028 1.102510
C -3.572746 -4.451217 -0.945630
C -5.437042 -4.455631 1.155269
H -4.382065 -2.703418 1.877448
C -4.571844 -5.437355 -0.895908
H -2.850769 -4.441911 -1.763150
C -5.506632 -5.443438 0.155673
H -6.155541 -4.455362 1.976490
H -4.622127 -6.196208 -1.678362
H -6.282055 -6.209961 0.195348
C 3.567611 3.562199 -0.048980
C 4.528112 3.602432 0.986272
C 3.629719 4.533058 -1.073152
C 5.525818 4.590873 0.998501
H 4.482487 2.858559 1.782549
C 4.629913 5.519333 -1.064271
H 2.896197 4.502224 -1.879806
C 5.580619 5.552028 -0.027586
H 6.256582 4.611724 1.808533
H 4.668615 6.257381 -1.866994
H 6.356678 6.318852 -0.019676
H 5.149280 -1.296189 -0.426704
C 3.577151 -3.445538 0.036311
C 3.650657 -4.447502 -0.956667
C 4.526930 -3.452404 1.082133
C 4.651571 -5.431693 -0.907275
H 2.924038 -4.443629 -1.770062
C 5.525893 -4.438179 1.134494
H 4.472152 -2.683507 1.853473
C 5.591832 -5.430877 0.139433
H 4.698962 -6.194520 -1.686037
H 6.248575 -4.432827 1.951988
H 6.368607 -6.196023 0.179097
S -1.774080 -1.271952 3.514120
C -0.246781 -1.633392 3.525279
S 1.281747 -1.992065 3.531593

Free Energy -2746.361236

Compound **3**^{Bu}
Cartesian Coordinates

N 0.9462 -2.3087 1.7861
N 0.3468 0.3571 2.8339
C 0.7721 2.7886 2.4775
C 2.4863 -3.4283 0.1638
C 0.1368 1.6817 3.1294
H -1.6862 -4.2775 2.1808
C -0.7479 -3.8129 1.8939
C -1.2819 0.5525 4.5067
C -0.5662 -0.3484 3.6008
C -0.2658 -2.5632 2.4315
H -1.1896 2.7773 4.6186
C 0.1651 -4.2638 0.9399
C -0.9133 -1.7163 3.3777
C -0.8681 1.8312 4.1832
C 1.2645 -3.3293 0.8920
H -2.0115 0.2528 5.2558
H 0.0839 -5.1554 0.3225
C 3.5500 -2.4597 0.2290
N 3.4310 -1.1693 0.6817
C 1.9854 2.6851 1.7469
N 2.7390 1.5201 1.6075
C 3.9368 1.7781 0.9436
C 3.9301 3.1857 0.6292
C 2.7300 3.7312 1.0871
H 2.3853 4.7569 0.9738
H 4.7235 3.6934 0.0870
C 4.9207 0.8178 0.5749
C 4.6751 -0.5855 0.5002
C 5.6411 -1.5721 0.0204
C 4.9262 -2.7398 -0.1880
H 5.2926 -3.6992 -0.5539
H 1.5040 -1.4576 1.9009
H 2.4091 0.5940 1.8959
C -2.0962 -2.2905 4.0778
C -3.3578 -1.6547 4.0084
C -1.9834 -3.5077 4.7949
C -4.4765 -2.2159 4.6496
H -3.4627 -0.7356 3.4262
C -3.1020 -4.0668 5.4344
H -1.0121 -4.0037 4.8515
C -4.3525 -3.4223 5.3641
H -5.4452 -1.7202 4.5732
H -2.9973 -5.0017 5.9882
H -5.2219 -3.8594 5.8575
C 0.0863 4.1176 2.5353
C -1.2799 4.1962 2.1419
C 0.7452 5.3093 2.9403
C -1.9595 5.4320 2.1392
H -1.7935 3.2863 1.8244
C 0.0608 6.5409 2.9387
H 1.7861 5.2584 3.2696
C -1.2896 6.6071 2.5346
H -3.0024 5.4733 1.8207
H 0.5802 7.4464 3.2591
H -1.8134 7.5648 2.5298
C 2.6877 -4.6073 -0.7377
C 3.0247 -4.3851 -2.1041
C 2.5430 -5.9456 -0.2806
C 3.1940 -5.4718 -2.9872
H 3.1350 -3.3585 -2.4653
C 2.7149 -7.0268 -1.1663
H 2.3113 -6.1278 0.7721
C 3.0356 -6.7941 -2.5216
H 3.4395 -5.2834 -4.0349
H 2.6055 -8.0490 -0.7977
H 3.1645 -7.6351 -3.2061
H 6.7021 -1.3963 -0.1481
C 6.2335 1.3773 0.1466
C 6.7959 1.0712 -1.1159
C 6.9277 2.2677 1.0064
C 8.0264 1.6381 -1.5055
H 6.2561 0.4025 -1.7910
C 8.1562 2.8274 0.6183
H 6.4978 2.5066 1.9824
C 8.7094 2.5155 -0.6393
H 8.4435 1.4000 -2.4859
H 8.6807 3.5033 1.2969
H 9.6621 2.9536 -0.9419
C -4.8906 -0.5008 -2.6604
C -5.8080 0.7131 -2.8014
N -5.0501 1.7080 -1.9358
H -6.8046 0.5151 -2.4026
H -5.9097 1.0030 -3.8534
C -4.7873 -1.2322 -1.3706
C -5.7074 -1.0930 -0.3344
C -3.7415 -2.1549 -1.2158
C -5.5843 -1.8426 0.8327
H -6.5065 -0.3714 -0.4223
C -3.6036 -2.9125 -0.0567
H -3.0426 -2.2823 -2.0395
C -4.5316 -2.7591 0.9866
H -6.3025 -1.7025 1.6411

H -2.7704 -3.6098 0.0399
H -4.4258 -3.3233 1.9122
Cl -5.6767 -1.8463 -3.7743
N -0.0961 0.5023 -1.6425
C 1.4003 0.2871 -1.4982
C 2.1348 0.1426 -2.8324
H 1.5428 -0.5980 -0.8649
H 1.7789 1.1478 -0.9255
C 3.6497 -0.0098 -2.6186
H 1.7673 -0.7396 -3.3776
H 1.9546 1.0220 -3.4693
C 4.3976 -0.1535 -3.9566
H 4.0286 0.8655 -2.0635
H 3.8348 -0.8968 -1.9873
H 5.4812 -0.2735 -3.7982
H 4.0360 -1.0363 -4.5090
H 4.2414 0.7340 -4.5914
C -0.7311 0.4307 -0.2439
C -2.1453 1.0122 -0.1586
H -0.0556 0.9664 0.4380
H -0.7017 -0.6266 0.0440
C -2.8196 0.6270 1.1674
H -2.0882 2.1056 -0.2283
H -2.7827 0.6794 -0.9730
C -4.1132 1.4357 1.3934
H -3.0426 -0.4470 1.1429
H -2.1241 0.8011 1.9992
H -4.6523 1.0749 2.2832
H -3.8777 2.5008 1.5496
H -4.7598 1.3561 0.5121
C -0.3679 1.8733 -2.2740
C 0.1902 3.0571 -1.4723
H -1.4488 1.9448 -2.3816
H 0.0649 1.8407 -3.2790
C -0.4594 4.3745 -1.9418
H -0.0043 2.9307 -0.3955
H 1.2830 3.1245 -1.5910
C 0.1087 5.5896 -1.1921
H -0.3071 4.4933 -3.0266
H -1.5454 4.3123 -1.7794
H -0.3720 6.5200 -1.5295
H -0.0619 5.4878 -0.1096
H 1.1936 5.6821 -1.3635
C -0.7092 -0.5752 -2.5542
C -0.4103 -2.0282 -2.1651
H -0.3368 -0.3624 -3.5620
H -1.7815 -0.3944 -2.5425
C -0.8002 -2.9799 -3.3197
H 0.6574 -2.1772 -1.9436
H -0.9669 -2.3019 -1.2583
C -0.7402 -4.4498 -2.8762
H -1.8111 -2.7423 -3.6867
H -0.1141 -2.8106 -4.1661
H -0.9893 -5.1232 -3.7100
H 0.2687 -4.7014 -2.5156
H -1.4554 -4.6365 -2.0599
H -3.9417 -0.3542 -3.1550
C -4.1291 2.4020 -2.7559
C -4.7691 3.6542 -3.4195
H -3.6218 1.8481 -3.5680
H -3.3391 2.7748 -2.0928
C -3.7374 4.4840 -4.1940
H -5.5700 3.3368 -4.0964
H -5.2359 4.2726 -2.6444
C -4.3597 5.7234 -4.8587
H -2.9346 4.7973 -3.5098
H -3.2629 3.8511 -4.9602
H -3.6053 6.3106 -5.4040
H -5.1442 5.4307 -5.5729
H -4.8218 6.3789 -4.1051

Free Energy -3579.0514820

Adduct **4**
Cartesian Coordinates
N -2.187300 -1.974600 -1.599000
N -0.335000 0.212300 -1.944100
C -0.100600 2.653600 -2.243400
C -4.647600 -2.402700 -1.511400
C 0.342400 1.315500 -2.409300
H -0.709800 -4.825600 -0.840900
C -1.400700 -4.028900 -1.086500
C 1.814100 -0.393800 -2.632100
C 0.551300 -0.829000 -2.039000
C -1.013600 -2.686500 -1.425400
H 2.386800 1.602600 -3.370100
C -2.779800 -4.101800 -1.134400
C 0.286700 -2.171300 -1.640800
C 1.665100 0.938700 -2.905900
C -3.286500 -2.795200 -1.451500
H 2.683900 -1.017600 -2.819300
H -3.402500 -4.966500 -0.933600
C -5.091100 -1.061700 -1.382800
N -4.262200 0.003700 -1.115400
C -1.312800 3.014700 -1.602700
N -2.386600 2.185800 -1.351900
C -3.376900 2.857800 -0.656300

C -2.864700 4.175700 -0.393400
C -1.627000 4.281200 -0.998800
H -0.964600 5.139700 -1.002200
H -3.382100 4.935500 0.180100
C -4.661900 2.338700 -0.379600
C -5.090600 1.037300 -0.771600
C -6.492900 0.645400 -0.883000
C -6.493000 -0.656900 -1.307500
H -7.350100 -1.283700 -1.531500
H -2.213700 -0.973400 -1.776400
H -2.446300 1.204300 -1.611800
C 1.442100 -3.091700 -1.462400
C 2.518700 -2.708200 -0.629100
C 1.496400 -4.351200 -2.103200
C 3.609900 -3.564500 -0.431400
H 2.495500 -1.734800 -0.139300
C 2.584100 -5.213000 -1.895500
H 0.690800 -4.641000 -2.778000
C 3.642000 -4.823000 -1.054900
H 4.451200 -3.244800 0.179900
H 2.613100 -6.178300 -2.403400
H 4.498300 -5.481700 -0.904900
C 0.780000 3.789000 -2.646200
C 2.107000 3.905400 -2.175300
C 0.272000 4.800600 -3.494800
C 2.904400 5.000100 -2.542800
H 2.503300 3.140700 -1.511700
C 1.071900 5.891400 -3.870200
H -0.750700 4.718100 -3.864700
C 2.391100 5.996200 -3.392700
H 3.922700 5.073900 -2.162700
H 0.666400 6.656200 -4.534400
H 3.013100 6.845300 -3.679800
C -5.641700 -3.510800 -1.605900
C -6.671500 -3.667500 -0.650500
C -5.544800 -4.453800 -2.656100
C -7.583700 -4.730100 -0.746700
H -6.742700 -2.962700 0.175400
C -6.459700 -5.513800 -2.756100
H -4.753400 -4.342200 -3.398200
C -7.482800 -5.656200 -1.800800
H -8.366500 -4.838400 0.005700
H -6.374700 -6.225400 -3.578700
H -8.192100 -6.481700 -1.875600
H -7.345700 1.291400 -0.696600
C -5.633300 3.199200 0.350700
C -6.257500 2.697000 1.517400
C -5.950600 4.508900 -0.075600
C -7.159100 3.486800 2.246600
H -6.018300 1.688200 1.854300
C -6.853500 5.299300 0.653200
H -5.498600 4.896300 -0.988700
C -7.457400 4.793200 1.819100
H -7.621200 3.085800 3.150000
H -7.091300 6.306000 0.306400
H -8.156600 5.409800 2.385700
C 6.888200 0.361900 2.108900
C 7.447300 -0.282500 0.827700
N 6.477700 -0.367100 -0.277800
H 7.782700 -1.301600 1.044600
H 8.323700 0.305000 0.507500
C 5.623500 -0.217900 2.685200
C 4.896400 0.548300 3.621600
C 5.147600 -1.493100 2.318200
C 3.716800 0.050700 4.191200
H 5.261100 1.539400 3.897900
C 3.954700 -1.985500 2.875900
H 5.701300 -2.092400 1.594000
C 3.244000 -1.219500 3.816200
H 3.161900 0.653200 4.911800
H 3.582100 -2.965000 2.574700
H 2.327000 -1.608900 4.259300
H 6.792400 1.449400 2.010800
Cl 8.283000 0.218700 3.381600
N -1.413900 -0.142400 2.377600
C -2.714800 -0.602800 1.702100
C -3.810200 -1.058600 2.666800
H -2.432900 -1.397100 1.005900
H -3.059400 0.235500 1.091400
C -5.028700 -1.598900 1.898500
H -3.441200 -1.844500 3.342600
H -4.142300 -0.215400 3.289900
C -6.146200 -2.034700 2.860500
H -5.405700 -0.820000 1.221800
H -4.716500 -2.444000 1.266600
H -7.024900 -2.403500 2.310000
H -5.799900 -2.839100 3.528900
H -6.470500 -1.187500 3.486000
C -0.517100 0.441200 1.280300
C 0.841700 0.936500 1.772200
H -1.090400 1.250500 0.818600
H -0.411100 -0.340200 0.523300
C 1.600200 1.664600 0.648500
H 0.718400 1.640400 2.608300
H 1.454500 0.099800 2.137100
C 2.914200 2.263500 1.172300
H 1.803300 0.964900 -0.174200
H 0.959700 2.459900 0.238800
H 3.471000 2.775900 0.375600
H 2.716500 2.992300 1.975000
H 3.558300 1.475900 1.584800
C -1.718400 0.911100 3.447400
C -2.378600 2.184100 2.913700
H -0.765900 1.141700 3.935100

H -2.353100 0.414600 4.188900
C -2.800400 3.103900 4.075200
H -1.680900 2.728200 2.260700
H -3.268400 1.947100 2.313100
C -3.420200 4.414100 3.556100
H -3.526600 2.571400 4.711900
H -1.922700 3.326100 4.704700
H -3.724400 5.063600 4.390900
H -2.695400 4.966200 2.937100
H -4.307300 4.206600 2.938600
C -0.710500 -1.316300 3.070800
C -0.241800 -2.436600 2.139600
H -1.417900 -1.695100 3.816400
H 0.140000 -0.879300 3.606100
C 0.313800 -3.621400 2.955400
H -1.067700 -2.806000 1.517000
H 0.540700 -2.071600 1.460100
C 0.745300 -4.782900 2.042200
H 1.170800 -3.285200 3.559300
H -0.457500 -3.967600 3.663400
H 1.171600 -5.607400 2.633200
H -0.119000 -5.172500 1.482700
H 1.499200 -4.451100 1.313100
C 6.495100 -1.440800 -1.163400
S 7.320200 -2.906500 -0.714500
S 5.673400 -1.301600 -2.682500
C 5.794600 0.899800 -0.600600
C 6.690200 1.909200 -1.335800
H 5.428500 1.336900 0.337700
H 4.918400 0.664000 -1.214700
C 5.897900 3.166600 -1.731000
H 7.544000 2.194300 -0.697800
H 7.094800 1.424600 -2.237800
C 6.764200 4.201600 -2.469300
H 5.050700 2.866400 -2.370000
H 5.462800 3.623500 -0.824700
H 6.179700 5.090900 -2.753300
H 7.601900 4.532400 -1.834200
H 7.188000 3.765600 -3.388200

Free Energy -4413.551626

Transition State $\mathbf{4}_{\mathbf{TS}}$
Imaginary frequency at -217 cm^{-1}
Cartesian Coordinates
N -1.924465 -2.143861 -1.586126
N -0.143445 0.094001 -1.973130
C -0.000747 2.525637 -2.408162
C -4.370944 -2.644753 -1.507684
C 0.494169 1.198004 -2.493832
H -0.371533 -4.942900 -0.779207
C -1.081631 -4.166252 -1.035068
C 2.011169 -0.474319 -2.671984
C 0.771079 -0.924147 -2.044702
C -0.730906 -2.818620 -1.394368
H 2.514839 1.505491 -3.495914
C -2.457475 -4.279243 -1.086901
C 0.553542 -2.266442 -1.614662
C 1.821116 0.841501 -2.991933
C -2.999842 -2.993239 -1.429387
H 2.889827 -1.084960 -2.854913
H -3.055841 -5.158702 -0.876521
C -4.862123 -1.316566 -1.442200
N -4.076590 -0.207810 -1.224130
C -1.234597 2.874233 -1.801267
N -2.287925 2.025074 -1.535470
C -3.302812 2.690660 -0.869252
C -2.830684 4.029924 -0.646012
C -1.590528 4.150283 -1.244657
H -0.950774 5.025455 -1.268017
H -3.371383 4.792593 -0.098825
C -4.571067 2.136936 -0.580999
C -4.946976 0.806529 -0.927365
C -6.331976 0.354392 -1.023208
C -6.279251 -0.964999 -1.386271
H -7.110142 -1.636181 -1.578455
H -1.979041 -1.146462 -1.779203
H -2.318027 1.031654 -1.752595
C 1.745533 -3.129647 -1.398302
C 2.809188 -2.647320 -0.601476
C 1.857514 -4.422339 -1.963803
C 3.938656 -3.436302 -0.352841
H 2.766993 -1.643877 -0.180117
C 2.986478 -5.216428 -1.709863
H 1.068702 -4.789662 -2.620615
C 4.027211 -4.728739 -0.895906
H 4.748576 -3.002170 0.230490
H 3.061000 -6.207269 -2.161316
H 4.909914 -5.342969 -0.709530
C 0.833456 3.669073 -2.878101
C 2.171261 3.844104 -2.457576
C 0.271290 4.627124 -3.755542
C 2.927129 4.937224 -2.906568

H 2.612049 3.125358 -1.771332
C 1.027475 5.719754 -4.207165
H -0.759182 4.499586 -4.089170
C 2.359331 5.879328 -3.782977
H 3.956958 5.052392 -2.568847
H 0.579106 6.441991 -4.891073
H 2.948845 6.728414 -4.131856
C -5.332519 -3.785495 -1.547407
C -6.325985 -3.943380 -0.555241
C -5.239835 -4.752916 -2.574442
C -7.210430 -5.032983 -0.593358
H -6.389145 -3.214953 0.251012
C -6.127030 -5.840390 -2.616417
H -4.474600 -4.640061 -3.343466
C -7.115577 -5.984320 -1.625561
H -7.966352 -5.142333 0.185818
H -6.047543 -6.572359 -3.421581
H -7.802972 -6.830930 -1.655951
H -7.210712 0.973276 -0.867951
C -5.575080 2.981827 0.121923
C -6.200940 2.480621 1.288864
C -5.922196 4.276772 -0.326079
C -7.132102 3.255907 1.995667
H -5.941014 1.483106 1.643049
C -6.853189 5.053580 0.381605
H -5.471725 4.663309 -1.240171
C -7.458138 4.548444 1.547190
H -7.593894 2.855154 2.899240
H -7.112099 6.049099 0.018091
H -8.178354 5.155111 2.097835
C 5.779989 0.493830 2.315162
C 6.408324 -0.279944 1.158198
N 5.376104 -0.475229 0.171288
H 6.768524 -1.258957 1.516078
H 7.303987 0.279929 0.819933
C 4.675186 -0.142912 3.104323
C 3.827536 0.679083 3.879141
C 4.492208 -1.541661 3.151862
C 2.831341 0.122009 4.695947
H 3.963987 1.761213 3.849839
C 3.494562 -2.100979 3.963850
H 5.120509 -2.186655 2.540667
H -2.203795 3.687532 4.485700
H -4.107717 5.273270 3.971645
H -2.943190 5.212504 2.622260
H -4.490650 4.335718 2.503535
C -0.452865 -0.850449 3.091139
C 0.251168 -1.899449 2.214300
H -1.171294 -1.318515 3.772500
H 0.281993 -0.310106 3.696875
C 0.326106 -3.255132 2.944841
H -0.269882 -2.054085 1.259257
C 2.666940 -1.272947 4.745392
H 2.188244 0.773150 5.290684
H 3.358405 -3.182530 3.984274
H 1.897288 -1.711390 5.381989
H 5.509821 1.509546 2.005764
Cl 7.233007 0.936234 3.625845
N -1.245557 0.218185 2.330020
C -2.474463 -0.413360 1.651718
C -3.581612 -0.843199 2.618723
H -2.100829 -1.262690 1.072806
H -2.849401 0.319767 0.932782
C -4.700121 -1.609011 1.890379
H -3.179878 -1.483800 3.417732
H -4.026483 0.039700 3.100622
C -5.791084 -2.059132 2.876721
H -5.140358 -0.961653 1.121572
H -4.272586 -2.479004 1.368725
H -6.598414 -2.601029 2.361728
H -5.372156 -2.724207 3.648871
H -6.238019 -1.188716 3.383515
C -0.374085 0.844899 1.235759
C 0.874162 1.555221 1.758513
H -1.024569 1.537411 0.693220
H -0.119562 0.039564 0.540925
C 1.613923 2.273721 0.615542
H 0.598940 2.314194 2.504678
H 1.554577 0.845013 2.248367
C 2.781192 3.117489 1.152025
H 1.976566 1.535751 -0.115952
H 0.904618 2.924215 0.083583
H 3.301576 3.641866 0.337956
H 2.416314 3.871013 1.868603
H 3.514882 2.483720 1.669231
C -1.688015 1.280741 3.340928
C -2.457385 2.446421 2.719321
H -0.779784 1.631795 3.841023
H -2.288776 0.755675 4.090976
C -3.018330 3.380527 3.808443
H -1.797531 3.025000 2.056795
H -3.290345 2.080291 2.103681
C -3.681885 4.625352 3.190653
H -3.751012 2.825648 4.417950
H 1.264261 -1.551456 1.967654
C 1.147198 -4.289572 2.159399
H 0.768390 -3.109674 3.942256
H -0.701319 -3.624591 3.102616
H 1.190177 -5.248175 2.698706
H 0.703692 -4.467453 1.169526
H 2.173905 -3.931678 1.998366
C 6.616710 -1.835966 -1.519676
S 7.712233 -2.675126 -0.675781
S 5.919449 -1.489980 -2.935653

C 5.036396 0.705210 -0.606578
C 6.155232 1.696024 -0.999905
H 4.239394 1.284563 -0.094956
H 4.564231 0.351149 -1.540815
C 5.621380 2.816780 -1.904957
H 6.608712 2.152960 -0.103399
H 6.956020 1.141916 -1.517623
C 6.717262 3.791648 -2.370479
H 5.121573 2.371070 -2.782193
H 4.845053 3.374070 -1.354742
H 6.306947 4.588730 -3.011749
H 7.208060 4.267710 -1.505730
H 7.491599 3.258157 -2.945164

Free Energy -4413.510956

Transition State $\mathbf{5}_{\mathbf{TS}}$
Imaginary frequency at -60.3 cm^{-1}
Cartesian Coordinates
N 2.478500 2.527300 -1.077900
N 0.510000 0.868000 -2.426000
C 0.127800 -1.299500 -3.563600
C 4.868400 2.476300 -0.357500
C -0.120600 0.083700 -3.366200
H 1.202800 5.345600 0.073500
C 1.835300 4.514400 -0.214400
C -1.212400 2.065200 -3.455100
C -0.154400 2.066800 -2.447300
C 1.397500 3.386700 -0.991500
H -1.778000 0.476700 -4.875000
C 3.173100 4.336800 0.080400
C 0.161600 3.205800 -1.652500
C -1.168200 0.837200 -4.053500
C 3.588900 3.074100 -0.468400
H -1.864200 2.901000 -3.688000
H 3.818400 4.996700 0.649600
C 5.132000 1.100100 -0.579600
N 4.171100 0.160100 -0.870600
C 1.131400 -2.031900 -2.878000
N 2.221200 -1.509900 -2.213000
C 2.939000 -2.510900 -1.580500
C 2.230100 -3.736500 -1.828600
C 1.152600 -3.448700 -2.644700
H 0.405000 -4.139200 -3.018500
H 2.508800 -4.704000 -1.428600
C 4.165600 -2.322500 -0.902200
C 4.791800 -1.053800 -0.735900
C 6.204800 -0.887000 -0.407100
C 6.426500 0.462700 -0.347700
H 7.363100 0.975200 -0.152800
H 2.441900 1.614800 -1.525300
H 2.435900 -0.520600 -2.116100
C -0.851600 4.294900 -1.568000
C -2.173800 3.982900 -1.174200
C -0.533800 5.634500 -1.890600
C -3.148900 4.988700 -1.093200
H -2.431900 2.956100 -0.909500
C -1.511400 6.639100 -1.810700
H 0.475200 5.879000 -2.223800
C -2.822100 6.320000 -1.408300
H -4.161300 4.727800 -0.780600
H -1.253000 7.666600 -2.072000
H -3.581400 7.101400 -1.347200
C -0.754500 -2.091000 -4.467400
C -2.164700 -2.036400 -4.369800
C -0.179300 -2.942100 -5.441900
C -2.972700 -2.805000 -5.221200
H -2.624300 -1.400400 -3.616400
C -0.987200 -3.708300 -6.296000
H 0.906700 -2.986700 -5.531200
C -2.388500 -3.643800 -6.187800
H -4.058000 -2.753300 -5.122400
H -0.523600 -4.350700 -7.046300
H -3.018300 -4.241200 -6.848700
C 5.965600 3.369100 0.119600
C 6.697200 3.072900 1.291400
C 6.272800 4.553600 -0.589000
C 7.712600 3.932200 1.740000
H 6.455900 2.172400 1.852800
C 7.291900 5.411100 -0.144700
H 5.713000 4.790900 -1.494500
C 8.015300 5.103700 1.022300
H 8.260900 3.690100 2.651800
H 7.521300 6.316100 -0.709400
H 8.804800 5.771600 1.370000
H 6.922500 -1.691900 -0.279200
C 4.845100 -3.518100 -0.329600
C 5.242800 -3.510100 1.028900
C 5.104800 -4.674200 -1.100800
C 5.865900 -4.628600 1.602600
H 5.051600 -2.623900 1.634000
C 5.728700 -5.793500 -0.527600
H 4.830300 -4.682700 -2.155700
C 6.107800 -5.776800 0.827300
H 6.154100 -4.605700 2.654600
H 5.926200 -6.674200 -1.140600
H 6.589400 -6.648300 1.272800

C -4.886800 -1.104500 2.386000
C -5.952900 -0.067300 2.002300
N -6.051100 0.069600 0.544900
H -5.696600 0.906200 2.441300
H -6.936500 -0.360200 2.386500
C -4.074600 -0.920600 3.626400
C -2.951100 -1.755000 3.825700
C -4.403500 0.020800 4.624300
C -2.159900 -1.635700 4.975400
H -2.714100 -2.506900 3.071800
C -3.605900 0.148800 5.773600
H -5.274400 0.664200 4.505900
C -2.480300 -0.674800 5.952900
H -1.294000 -2.285300 5.110500
H -3.866600 0.890600 6.529900
H -1.863200 -0.574500 6.846800
H -4.299300 -1.456500 1.543300
Cl -5.928900 -2.846800 2.675400
N 0.610000 -0.919400 1.724600
C 2.033300 -0.395800 1.491800
C 2.798000 -0.108400 2.784300
H 1.936600 0.495800 0.866100
H 2.543100 -1.149100 0.887000
C 4.184100 0.504200 2.517300
H 2.229300 0.583000 3.422800
H 2.939600 -1.039500 3.352800
C 4.973300 0.653900 3.829600
H 4.743400 -0.127000 1.812400
H 4.063000 1.483400 2.032900
H 5.972100 1.080300 3.654300
H 4.440900 1.313200 4.534000
H 5.105600 -0.326300 4.315400
C -0.024100 -1.173300 0.347800
C -1.373500 -1.891400 0.391100
H 0.708300 -1.769100 -0.203500
H -0.094100 -0.198700 -0.147600
C -1.976300 -2.009700 -1.019000
H -1.257800 -2.904900 0.803800
H -2.083300 -1.339500 1.019800
C -3.358400 -2.681200 -0.988000
H -2.060600 -1.005600 -1.459400
H -1.294200 -2.587800 -1.657000
H -3.728700 -2.863000 -2.007400
H -3.314300 -3.648400 -0.460900
H -4.088600 -2.038200 -0.476900
C 0.643700 -2.219600 2.532000
C 1.396800 -3.365600 1.857000
H -0.401900 -2.487400 2.711500
H 1.089300 -1.971800 3.500700
C 1.378700 -4.626500 2.741600
H 0.942200 -3.605900 0.885500
H 2.443100 -3.088100 1.667400
C 2.096500 -5.798600 2.047300
H 1.866700 -4.402400 3.704700
H 0.335000 -4.902900 2.965800
H 2.101500 -6.694600 2.686300
H 1.591300 -6.053600 1.102100
H 3.139100 -5.532900 1.813800
C -0.216200 0.098100 2.523200
C -0.191200 1.532100 1.997200
H 0.168300 0.058500 3.548800
H -1.240200 -0.284100 2.543600
C -1.010400 2.434200 2.943100
H 0.836400 1.919700 1.952800
H -0.619400 1.583400 0.986400
C -1.041800 3.889900 2.448200
H -2.035700 2.041100 3.021100
H -0.567900 2.388900 3.952900
H -1.614200 4.528600 3.138600
H -0.020800 4.296300 2.368000
H -1.508300 3.951400 1.454100
C -5.007600 0.646700 -0.139800
S -3.575200 0.975900 0.793300
S -5.134400 1.004200 -1.824900
C -7.340400 -0.306400 -0.061800
C -8.399300 0.799700 0.081700
H -7.680400 -1.227400 0.436100
H -7.166000 -0.525500 -1.122000
C -9.745600 0.384800 -0.535400
H -8.540400 1.038500 1.149900
H -8.023600 1.710200 -0.412300
C -10.817800 1.480000 -0.389900
H -9.595400 0.150500 -1.603200
H -10.095200 -0.544700 -0.053100
H -11.774200 1.168300 -0.838400
H -10.996600 1.709900 0.673200
H -10.493400 2.409200 -0.886000

Free Energy -4413.545782

Compound **5**
Cartesian Coordinates
C -0.015829 -0.619475 0.459383
C 1.114048 -0.150851 -0.482231
C -0.814544 1.601647 0.007294
N -1.135798 0.327141 0.331460
H 0.334359 -0.630072 1.503999
H -0.365504 -1.624591 0.187944

S -1.824794 2.947674 0.008667
S 0.901883 1.717831 -0.454324
C -2.452738 -0.077732 0.844840
C -2.524611 -0.022948 2.381217
H -2.641011 -1.100254 0.484587
H -3.201056 0.594371 0.405406
C -3.916240 -0.433330 2.893052
H -1.760750 -0.690249 2.813018
H -2.291854 1.003089 2.708002
C -4.007175 -0.381793 4.428906
H -4.674327 0.235872 2.452060
H -4.147343 -1.453040 2.540120
H -5.008683 -0.675171 4.779496
H -3.270873 -1.062862 4.885432
H -3.799675 0.636245 4.796010
C 1.059914 -0.703187 -1.889770
C 2.257681 -1.070938 -2.535631
C -0.162843 -0.844873 -2.582007
C 2.238879 -1.572574 -3.848837
H 3.206576 -0.965403 -2.005566
C -0.183307 -1.348614 -3.891957
H -1.096739 -0.560463 -2.096399
C 1.017464 -1.712166 -4.531011
H 3.174173 -1.855290 -4.334348
H -1.135213 -1.455926 -4.414259
H 0.999550 -2.102272 -5.549664
H 2.089184 -0.366494 -0.029890

Free Energy -1356.167802

Compound **3**^{Ar}
Cartesian Coordinates
N -2.240800 -1.365700 -2.076500
N -0.566200 1.050100 -1.882300
C -0.388600 3.361900 -0.992700
C -4.473500 -2.186500 -1.344400
C 0.086400 2.247900 -1.739300
H -0.286500 -4.009600 -2.354500
C -1.105000 -3.314900 -2.206700
C 1.518800 0.970400 -2.935500
C 0.316800 0.234900 -2.553400
C -1.003300 -1.894000 -2.391400
H 2.076700 3.055000 -2.477200
C -2.383800 -3.601300 -1.771400
C 0.160400 -1.164400 -2.731600
C 1.381900 2.225600 -2.412000
C -3.117500 -2.367900 -1.700000
H 2.348900 0.576400 -3.510200
H -2.786300 -4.570900 -1.503000
C -5.108800 -0.921900 -1.204600
N -4.463900 0.282600 -1.083500
C -1.725000 3.522000 -0.562100
N -2.770400 2.662000 -0.850900
C -3.964200 3.165500 -0.371000
C -3.649300 4.403400 0.289400
C -2.288000 4.609000 0.191900
H -1.716800 5.430900 0.606200
H -4.376700 5.029000 0.794300
C -5.237100 2.555600 -0.477000
C -5.456500 1.208400 -0.868200
C -6.776600 0.586000 -0.948600
C -6.557900 -0.752000 -1.132800
H -7.292200 -1.545400 -1.234500
H -2.447600 -0.372600 -2.006200
H -2.662100 1.766700 -1.321300
C 1.322200 -1.963200 -3.216400
C 2.570400 -1.893800 -2.558800
C 1.185300 -2.830300 -4.325400
C 3.658400 -2.663800 -2.995400
H 2.683100 -1.243800 -1.691500
C 2.273400 -3.598300 -4.768800
H 0.225400 -2.887800 -4.840400
C 3.511700 -3.517100 -4.103700
H 4.596800 -2.599700 -2.438300
H 2.155100 -4.255300 -5.632100
H 4.355500 -4.119300 -4.445400
C 0.602300 4.410200 -0.615600
C 1.784000 4.032300 0.065500
C 0.398100 5.776200 -0.913400
C 2.730600 4.994100 0.447200
H 1.947600 2.981200 0.300100
C 1.347000 6.739100 -0.533600
H -0.497400 6.075600 -1.458600
C 2.514200 6.351800 0.151000
H 3.633800 4.681800 0.973400
H 1.179400 7.788700 -0.779700
H 3.250600 7.101200 0.444900
C -5.276100 -3.411500 -1.062000
C -5.929200 -3.549700 0.185100
C -5.386600 -4.457800 -2.005300
C -6.663800 -4.707100 0.485200
H -5.845900 -2.749500 0.920900
C -6.124600 -5.614500 -1.707100
H -4.900200 -4.352900 -2.975500
C -6.762600 -5.744800 -0.459700
H -7.152300 -4.801000 1.456200

H -6.205700 -6.409800 -2.449500
H -7.333000 -6.645200 -0.227400
H -7.728000 1.101600 -0.866100
C -6.405600 3.392600 -0.071700
C -7.279300 2.974500 0.957700
C -6.647800 4.633800 -0.704000
C -8.368200 3.772900 1.341700
H -7.093400 2.026800 1.460200
C -7.739700 5.430700 -0.323900
H -5.980500 4.963200 -1.501400
C -8.603500 5.003100 0.701200
H -9.028100 3.436500 2.143000
H -7.916900 6.381400 -0.829000
H -9.450700 5.622900 0.998200
C 5.292200 -2.896700 1.713500
C 6.319800 -2.912400 0.561900
N 5.904500 -2.061200 -0.535400
H 6.412300 -3.951400 0.203000
H 7.304100 -2.632400 0.991000
C 3.943600 -3.538200 1.472400
C 2.997800 -3.588300 2.522100
C 3.583800 -4.072800 0.218400
C 1.744200 -4.185900 2.335300
H 3.260300 -3.174200 3.496500
C 2.312500 -4.641100 0.020700
H 4.278400 -4.005100 -0.614900
C 1.390300 -4.710200 1.078300
H 1.045500 -4.239100 3.171300
H 2.048300 -5.027600 -0.964600
H 0.410100 -5.164200 0.926600
C 6.066000 -0.734300 -0.381500
C 5.678000 0.122500 -1.480600
C 6.575700 -0.043800 0.783900
C 5.726200 1.509700 -1.385800
H 5.316400 -0.353900 -2.390100
C 6.602600 1.355300 0.848100
H 6.910700 -0.612600 1.648400
C 6.170600 2.169900 -0.214100
H 6.187400 3.254200 -0.145900
C 6.990700 2.018400 2.145100
C 5.369700 2.364900 -2.573300
F 4.717200 1.693400 -3.571600
F 7.871700 1.283300 2.895400
F 5.892000 2.232600 2.961500
F 7.566900 3.253100 1.972700
F 6.488200 2.925200 -3.161100
F 4.565300 3.430700 -2.233800
H 5.160200 -1.879000 2.097200
Cl 6.120500 -3.768600 3.233700
N -1.421500 -0.860000 2.013100
C -2.845300 -0.474700 1.605000
C -3.857200 -0.498000 2.749000
H -3.133900 -1.161800 0.805300
H -2.774700 0.517600 1.152100
C -5.201600 0.095900 2.291600
H -4.017200 -1.530900 3.093700
H -3.488300 0.081100 3.608900
C -6.265300 0.009300 3.398200
H -5.045600 1.143400 1.993100
H -5.553800 -0.432900 1.395000
H -7.224300 0.432200 3.062300
H -6.440700 -1.039800 3.686300
H -5.944200 0.560100 4.296700
C -0.589800 -0.905900 0.722000
C 0.924500 -1.078800 0.907200
H -0.814600 0.014900 0.174000
H -1.017600 -1.731200 0.152100
C 1.725700 0.230900 0.802100
H 1.160200 -1.585800 1.852900
H 1.273000 -1.772300 0.129300
C 3.216400 0.008100 1.082300
H 1.591000 0.643200 -0.207500
H 1.328500 0.979600 1.501800
H 3.804800 0.914700 0.885500
H 3.374500 -0.285500 2.132500
H 3.618700 -0.796300 0.452500
C -0.848500 0.160600 2.997600
C -0.989400 1.623500 2.568700
H 0.203500 -0.113200 3.133000
H -1.360700 -0.006100 3.951700
C -0.109600 2.515400 3.466500
H -0.696000 1.758000 1.518000
H -2.037500 1.944000 2.657400
C -0.306300 4.010600 3.166300
H -0.346800 2.311200 4.524000
H 0.948100 2.239900 3.319500
H 0.328400 4.627600 3.820200
H -0.042800 4.234300 2.123000
H -1.356000 4.304200 3.324900
C -1.407700 -2.229500 2.701400
C -2.042200 -3.365700 1.896600
H -1.934500 -2.094800 3.653100
H -0.357800 -2.447100 2.922300
C -2.081800 -4.664300 2.724600
H -3.071600 -3.111200 1.609800
H -1.481500 -3.552100 0.970800
C -2.731300 -5.808800 1.925600
H -1.059900 -4.948100 3.022000
H -2.647700 -4.485900 3.653900
H -2.769500 -6.734000 2.519700
H -3.758600 -5.542300 1.630800
H -2.159600 -6.014600 1.006600

Free Energy -4326.612910

Compound **6**
Cartesian Coordinates

N -3.280900 -2.006200 -1.559900
N -1.067900 -0.264200 -2.294500
C -0.363600 2.062800 -2.765500
C -5.726100 -1.904900 -1.073300
C -0.248200 0.655200 -2.909100
H -2.308400 -5.096800 -0.921100
C -2.855200 -4.174600 -1.081700
C 0.734500 -1.342400 -3.316300
C -0.471300 -1.481100 -2.503000
C -2.269900 -2.950700 -1.558300
H 1.615100 0.471700 -4.202100
C -4.202600 -3.949900 -0.872400
C -0.954900 -2.733500 -2.028700
C 0.854300 -0.010200 -3.599100
C -4.479900 -2.572100 -1.177900
H 1.375800 -2.154000 -3.642300
H -4.943000 -4.656400 -0.513500
C -5.873900 -0.493900 -1.039200
N -4.825400 0.395600 -0.990300
C -1.392900 2.702800 -2.030300
N -2.587000 2.135500 -1.633700
C -3.336000 3.032400 -0.890800
C -2.534000 4.218700 -0.760000
C -1.369500 4.030000 -1.479700
H -0.544800 4.724500 -1.595000
H -2.818500 5.095900 -0.191300
C -4.662500 2.813000 -0.453300
C -5.385200 1.605800 -0.679200
C -6.840100 1.505900 -0.597700
C -7.148400 0.197900 -0.860600
H -8.132000 -0.257500 -0.915100
H -3.140400 -1.025400 -1.789500
H -2.863600 1.172900 -1.810600
C -0.021200 -3.893300 -2.050800
C 1.235100 -3.780700 -1.414400
C -0.352500 -5.109000 -2.692600
C 2.134900 -4.855800 -1.407800
H 1.497900 -2.850600 -0.910600
C 0.549600 -6.184500 -2.690700
H -1.310200 -5.199000 -3.206100
C 1.794800 -6.062600 -2.045800
H 3.089100 -4.744500 -0.891700
H 0.283500 -7.113700 -3.197700
H 2.492800 -6.901100 -2.041900
C 0.693700 2.953900 -3.326100
C 2.064700 2.748600 -3.046200
C 0.327900 4.050000 -4.144400
C 3.039800 3.612000 -3.568400
H 2.360100 1.917700 -2.409300
C 1.303500 4.910100 -4.672900
H -0.726500 4.213200 -4.372200
C 2.664000 4.695200 -4.384300
H 4.090400 3.445600 -3.331000
H 1.002000 5.743500 -5.310100
H 3.423900 5.365000 -4.789700
C -6.927100 -2.775200 -0.909400
C -7.807500 -2.620000 0.185400
C -7.193200 -3.796100 -1.851700
C -8.926700 -3.455000 0.329600
H -7.601300 -1.850600 0.926600
C -8.314200 -4.629000 -1.710500
H -6.520000 -3.922800 -2.700100
C -9.185700 -4.461200 -0.618900
H -9.591000 -3.323700 1.185000
H -8.508500 -5.404400 -2.452800
H -10.056600 -5.108800 -0.507600
H -7.519600 2.329800 -0.399700
C -5.351800 3.904700 0.289700
C -5.942600 3.622100 1.544700
C -5.429600 5.224000 -0.211400
C -6.577700 4.631600 2.283800
H -5.888400 2.607900 1.940400
C -6.063700 6.234800 0.528300
H -5.003700 5.447800 -1.189600
C -6.636300 5.943700 1.780200
H -7.016900 4.395900 3.254300
H -6.117900 7.246400 0.123400
H -7.125900 6.730900 2.355300
C 5.617800 0.419500 3.284400
C 6.506700 -0.546500 2.470600
N 5.750600 -1.115100 1.345800
H 6.863900 -1.369000 3.097900
H 7.388300 -0.014000 2.093500
C 4.478300 -0.197800 4.045800
C 3.250100 0.490800 4.108100
C 4.611200 -1.431500 4.714100
C 2.167100 -0.049200 4.816400
H 3.146600 1.447100 3.592600
C 3.523800 -1.978000 5.411800
H 5.553500 -1.980700 4.674100
C 2.297600 -1.289600 5.465300
H 1.227000 0.494800 4.869500
H 3.633100 -2.942800 5.908800
H 1.452000 -1.715400 6.008500
C 5.720700 -0.432800 0.129400
C 5.294900 -1.081700 -1.060900
C 6.156100 0.910100 0.019600
C 5.253700 -0.387900 -2.272900
H 4.996400 -2.128300 -1.028500
C 6.124300 1.580000 -1.214700
H 6.492000 1.459000 0.890400
C 5.658600 0.955900 -2.376700
H 5.618500 1.482000 -3.326300
C 6.499400 3.043100 -1.239200

C 4.851200 -1.118300 -3.534400
F 5.951100 -1.580500 -4.225600
F 7.637400 3.312000 -0.520500
F 5.508300 3.827100 -0.685600
F 6.703600 3.519400 -2.505100
F 4.168100 -0.310300 -4.407500
F 4.058900 -2.205000 -3.298300
H 5.244300 1.229700 2.649100
Cl 6.772200 1.320100 4.490900
N -1.656300 0.204800 2.204400
C -3.091100 -0.055100 1.724600
C -4.123600 -0.203700 2.845500
H -3.044000 -0.952100 1.098500
H -3.354500 0.776100 1.063800
C -5.499700 -0.588800 2.274100
H -3.813200 -0.970700 3.571700
H -4.229800 0.746000 3.391900
C -6.557900 -0.697900 3.383300
H -5.812200 0.165400 1.540300
H -5.413900 -1.541400 1.729900
H -7.545400 -0.953700 2.968800
H -6.282000 -1.473500 4.115600
H -6.654800 0.259600 3.920300
C -0.815600 0.542000 0.967200
C 0.662000 0.770900 1.266100
H -1.274300 1.431500 0.526400
H -0.962700 -0.273300 0.252800
C 1.440300 1.121100 -0.010400
H 0.785700 1.596700 1.981500
H 1.118900 -0.125400 1.707000
C 2.908200 1.417700 0.320300
H 1.376200 0.281000 -0.717800
H 0.975300 1.987900 -0.501200
H 3.502900 1.564600 -0.589700
H 2.998600 2.326200 0.935500
H 3.341200 0.574400 0.873100
C -1.627900 1.369500 3.200100
C -2.130000 2.697300 2.629700
H -0.591400 1.458900 3.539900
H -2.229200 1.049300 4.058200
C -2.269800 3.754800 3.742600
H -1.431900 3.070800 1.865800
H -3.105900 2.567300 2.141200
C -2.705800 5.114800 3.166000
H -3.008700 3.404500 4.484300
H -1.307700 3.862500 4.272100
H -2.815700 5.865500 3.964800
H -1.957600 5.486200 2.445700
H -3.669400 5.023000 2.640900
C -1.089900 -1.027400 2.924400
C -0.924100 -2.277000 2.058400
H -1.761400 -1.221100 3.767700
H -0.121900 -0.718400 3.333300
C -0.291000 -3.413500 2.886900
H -1.893200 -2.618000 1.666500
H -0.272700 -2.070400 1.198500
C -0.157000 -4.701500 2.056200
H 0.702300 -3.092500 3.238600
H -0.908000 -3.603500 3.781500
H 0.306900 -5.505300 2.647900
H -1.145300 -5.048700 1.716300
H 0.465200 -4.525500 1.166600
C 5.054400 -2.383000 1.551800
S 6.007500 -3.686900 2.099100
S 3.376400 -2.419200 1.249500

Free Energy -5161.087322

Transition State **6**$_{TS}$
Imaginary Frequency at -182 cm^{-1}
Cartesian Coordinates
N -3.265704 -2.048217 -1.486864
N -1.039647 -0.363154 -2.297909
C -0.313904 1.933328 -2.873273
C -5.713939 -1.905335 -1.027194
C -0.221940 0.519662 -2.966757
H -2.329010 -5.118498 -0.717649
C -2.864746 -4.198097 -0.917683
C 0.724224 -1.506241 -3.316080
C -0.463075 -1.594778 -2.469982
C -2.264477 -3.001884 -1.443084
H 1.603553 0.259259 -4.297406
C -4.211274 -3.952789 -0.728137
C -0.950525 -2.820237 -1.931731
C 0.853927 -0.188361 -3.655498
C -4.473389 -2.586920 -1.092771
H 1.347527 -2.338937 -3.622325
H -4.960641 -4.637936 -0.347549
C -5.849059 -0.492888 -1.054206
N -4.791891 0.386918 -1.041406
C -1.332640 2.611784 -2.156575
N -2.540002 2.078865 -1.753534
C -3.271333 3.005421 -1.029709
C -2.445965 4.177441 -0.922795
C -1.282774 3.948769 -1.633551
H -0.442164 4.621969 -1.759004
H -2.713114 5.071448 -0.372453

C -4.599967 2.817371 -0.583453
C -5.338338 1.613425 -0.773567
C -6.793994 1.531834 -0.687116
C -7.116251 0.218120 -0.900916
H -8.104495 -0.229100 -0.935188
H -3.113738 -1.078728 -1.754064
H -2.835215 1.117571 -1.905398
C -0.024850 -3.987027 -1.910524
C 1.250096 -3.846722 -1.317051
C -0.377607 -5.236447 -2.471256
C 2.142079 -4.927085 -1.264435
H 1.532763 -2.886499 -0.888943
C 0.516861 -6.317376 -2.424638
H -1.346313 -5.348654 -2.958812
C 1.777550 -6.168116 -1.816136
H 3.115376 -4.796772 -0.790031
H 0.233267 -7.272474 -2.869483
H 2.470395 -7.010010 -1.778082
C 0.757306 2.788242 -3.461529
C 2.127150 2.552153 -3.198512
C 0.409580 3.883401 -4.288352
C 3.117138 3.381788 -3.745479
H 2.412683 1.725166 -2.553677
C 1.399884 4.710915 -4.840333
H -0.642841 4.071639 -4.504009
C 2.758269 4.463949 -4.569121
H 4.165339 3.188055 -3.519704
H 1.111274 5.544309 -5.482638
H 3.529088 5.108714 -4.993736
C -6.923212 -2.757275 -0.829959
C -7.793945 -2.555337 0.264850
C -7.205329 -3.807085 -1.734868
C -8.918457 -3.375323 0.447657
H -7.574997 -1.760603 0.974981
C -8.332562 -4.624491 -1.555897
H -6.539922 -3.968651 -2.583723
C -9.193037 -4.412048 -0.463025
H -9.574430 -3.208728 1.303531
H -8.539852 -5.423370 -2.269484
H -10.067676 -5.048702 -0.321907
H -7.464290 2.369366 -0.517785
C -5.268822 3.934393 0.139392
C -5.863050 3.684508 1.399887
C -5.321761 5.246633 -0.383089
C -6.476344 4.718107 2.123404
H -5.828802 2.676204 1.812609
C -5.935585 6.281246 0.340402
H -4.893350 5.446363 -1.365316
C -6.511125 6.022292 1.597887
H -6.917150 4.507047 3.098818
H -5.971351 7.286730 -0.081380
H -6.984070 6.828243 2.160611
C 5.611564 0.588927 3.137134
C 6.557250 -0.485326 2.550715
N 5.976518 -1.167497 1.418476
H 6.796295 -1.230677 3.324935
H 7.510142 0.008373 2.278611
C 4.428314 0.124830 3.942934
C 3.219432 0.844863 3.852275
C 4.498818 -0.977722 4.818305
C 2.102933 0.468169 4.613201
H 3.158961 1.700877 3.179415
C 3.376175 -1.370441 5.562991
H 5.425919 -1.540857 4.910907
C 2.172476 -0.649182 5.463703
H 1.182042 1.048085 4.549753
H 3.441023 -2.238479 6.220598
H 1.300425 -0.951463 6.045675
C 5.879012 -0.529678 0.233016
C 5.319559 -1.242333 -0.885628
C 6.342186 0.805334 -0.043683
C 5.222594 -0.658805 -2.146960
H 4.988236 -2.265648 -0.729306
C 6.235042 1.360143 -1.325656
H 6.788538 1.401629 0.749008
C 5.667233 0.658073 -2.402002
H 5.588054 1.097592 -3.391761
C 6.654420 2.797341 -1.510631
C 4.741654 -1.488295 -3.310520
F 5.795576 -2.053967 -4.004241
F 7.826599 3.099915 -0.864746
F 5.712960 3.675170 -1.007939
F 6.830694 3.149868 -2.823612
F 4.043296 -0.753237 -4.236291
F 3.932561 -2.527884 -2.944106
H 5.278666 1.269735 2.347335
Cl 6.656880 1.755094 4.258729
N -1.608197 0.367794 2.151865
C -3.039011 0.082477 1.673407
C -4.070328 -0.036470 2.797224
H -2.985546 -0.831753 1.075353
H -3.302462 0.891292 0.987417
C -5.443559 -0.462248 2.249893
H -3.752050 -0.772373 3.549851
H -4.184748 0.929741 3.310614
C -6.480363 -0.574816 3.379932
H -5.783755 0.269695 1.505951
H -5.343332 -1.423642 1.723989
H -7.468530 -0.861122 2.989614
H -6.173553 -1.330218 4.120846
H -6.590270 0.389452 3.902005
C -0.754574 0.643830 0.909212
C 0.716454 0.921214 1.210068
H -1.222842 1.493030 0.403709

H -0.875394 -0.221212 0.250503
C 1.514540 1.119859 -0.088407
H 0.819674 1.829107 1.822735
H 1.167099 0.093297 1.773110
C 2.994803 1.395767 0.209862
H 1.413981 0.223648 -0.720144
H 1.079083 1.955181 -0.654064
H 3.580518 1.493510 -0.712629
H 3.108788 2.329247 0.784873
H 3.429413 0.573890 0.793570
C -1.591593 1.576754 3.091159
C -2.120505 2.870801 2.472754
H -0.552732 1.699608 3.411566
H -2.177047 1.286541 3.970462
C -2.187243 3.988616 3.530600
H -1.470232 3.196245 1.648394
H -3.124313 2.722700 2.052793
C -2.653799 5.318263 2.910145
H -2.878776 3.684658 4.334124
H -1.194123 4.116940 3.992348
H -2.713876 6.109462 3.672650
H -1.949577 5.647316 2.129487
H -3.646440 5.206108 2.448966
C -1.047782 -0.828641 2.932383
C -0.862347 -2.110997 2.120693
H -1.732213 -0.991269 3.771333
H -0.089550 -0.499078 3.347034
C -0.345485 -3.240918 3.033620
H -1.808040 -2.432229 1.661629
H -0.139284 -1.952283 1.308740
C -0.165941 -4.552797 2.250066
H 0.616078 -2.936286 3.476824
H -1.055691 -3.389617 3.864201
H 0.208072 -5.354531 2.904722
H -1.123877 -4.879621 1.815047
H 0.551369 -4.415893 1.427150
C 4.461197 -2.782531 2.039165
S 5.392811 -3.851453 2.796181
S 3.036243 -2.268133 1.511810

Free Energy -5161.064789

Transition State $\mathbf{7}_{TS}$
Imaginary Frequency at -40 cm^{-1}
Cartesian Coordinates
N 3.079900 1.791300 -1.865200
N 0.985800 -0.114900 -2.485300
C 0.380300 -2.495000 -2.753600
C 5.533500 1.854600 -1.420400
C 0.215400 -1.113400 -3.036000
H 1.935600 4.845100 -1.356900
C 2.533600 3.950800 -1.485800
C -0.900700 0.797400 -3.515300
C 0.304800 1.048600 -2.731300
C 2.011700 2.670100 -1.878400
H -1.667700 -1.107900 -4.314300
C 3.898800 3.820600 -1.313300
C 0.702100 2.344700 -2.297400
C -0.931500 -0.550800 -3.745700
C 4.251200 2.446900 -1.549300
H -1.612600 1.544300 -3.849700
H 4.603900 4.589700 -1.017900
C 5.745700 0.460600 -1.258000
N 4.734700 -0.461600 -1.112500
C 1.423500 -3.015300 -1.946600
C -2.290100 5.454100 -2.194300
H -3.402500 4.088900 -0.925700
H -0.944700 6.585300 -3.470000
N 2.588600 -2.362000 -1.600000
C 3.358800 -3.139800 -0.753100
C 2.601600 -4.337200 -0.504400
C 1.442000 -4.274100 -1.253500
H 0.645300 -5.008200 -1.299900
H 2.906900 -5.133200 0.163700
C 4.665500 -2.812800 -0.322800
C 5.341000 -1.607500 -0.675200
C 6.790700 -1.441400 -0.611700
C 7.047100 -0.158500 -1.017100
H 8.012700 0.324100 -1.128000
H 2.991200 0.791600 -2.030900
H 2.830000 -1.413100 -1.874800
C -0.324800 3.423100 -2.290900
C -1.525900 3.231200 -1.571400
C -0.128200 4.644800 -2.974300
C -2.496800 4.241300 -1.513800
H -1.688400 2.294900 -1.038600
C -1.105900 5.651300 -2.929300
H 0.785500 4.792800 -3.550700
H -3.046500 6.239300 -2.152000
C -0.655000 -3.473100 -3.198000
C -2.024800 -3.274900 -2.908700

C -0.274500 -4.646500 -3.890600
C -2.987400 -4.216500 -3.302300
H -2.328300 -2.384900 -2.364100
C -1.237300 -5.586800 -4.290600
H 0.779100 -4.808900 -4.121200
C -2.597300 -5.376100 -3.996600
H -4.037000 -4.046600 -3.058100
H -0.926400 -6.480800 -4.833200
H -3.344200 -6.109600 -4.303800
C 6.687400 2.796500 -1.359400
C 7.602800 2.779400 -0.281600
C 6.869000 3.756000 -2.383600
C 8.671200 3.688200 -0.232700
H 7.463400 2.061500 0.524000
C 7.939800 4.662500 -2.337500
H 6.170100 3.777100 -3.220500
H 7.214600 -6.196300 3.045900
C -4.400100 0.240200 3.186400
C -5.704800 0.983300 2.796600
N -5.686800 1.511800 1.424800
H -5.850300 1.843100 3.459100
H -6.581900 0.340100 2.921700
C -3.625900 0.670200 4.394500
C -2.249000 0.363600 4.458300
C -4.231500 1.306500 5.496500
C -1.486100 0.711200 5.579900
H -1.794400 -0.161600 3.618200
C -3.468400 1.659200 6.623000
H -5.298400 1.529300 5.486000
C -2.093700 1.368700 6.667900
H -0.422100 0.472200 5.615300
H -3.950500 2.159300 7.464200
H -1.501300 1.643800 7.541500
C -5.815000 0.668900 0.321600
C -5.386200 1.081800 -0.971600
C -6.330900 -0.646100 0.452600
C -5.471800 0.211600 -2.061600
H -4.963700 2.070300 -1.111500
C -6.405900 -1.495400 -0.659300
H -6.635500 -1.030900 1.419700
C -5.981400 -1.091200 -1.933000
H -6.030400 -1.764800 -2.784300
C -6.845700 -2.926200 -0.450700
C -5.033200 0.677700 -3.431400
F -6.108300 1.017800 -4.221700
F -7.763000 -3.062600 0.555400
F -5.781700 -3.734600 -0.112300
F -7.402500 -3.479200 -1.571800
F -4.356500 -0.299700 -4.116100
F -4.217900 1.771900 -3.396300
H -3.772200 0.037100 2.323800
Cl -4.932500 -1.655100 3.618100
N 1.603300 0.133600 1.999300
C 8.845200 4.632400 -1.261000
H 9.361500 3.663900 0.611900
H 8.067900 5.388600 -3.141700
H 9.675900 5.338400 -1.222900
H 7.502200 -2.211100 -0.327200
C 5.381400 -3.765800 0.569400
C 5.933500 -3.285300 1.781400
C 5.521400 -5.138500 0.261500
C 6.588600 -4.152700 2.667900
H 5.831600 -2.228100 2.026600
C 6.177100 -6.007100 1.148400
H 5.128800 -5.515800 -0.682600
C 6.708600 -5.519000 2.356500
H 6.996200 -3.764200 3.602300
H 6.280600 -7.062500 0.892500

C 3.040600 0.373900 1.520700
C 4.060100 0.605000 2.636300
H 2.995900 1.225400 0.835700
H 3.314800 -0.497100 0.919900
C 5.437500 0.954500 2.045400
H 3.742800 1.421500 3.302100
H 4.162700 -0.300900 3.251400
C 6.480900 1.189000 3.149800
H 5.772500 0.137200 1.391000
H 5.342500 1.850100 1.413000
H 7.466000 1.427500 2.720900
H 6.181600 2.023100 3.804200
H 6.592400 0.288200 3.774600
C 0.783000 -0.278500 0.772200
C -0.703100 -0.485500 1.057400
H 1.250200 -1.187700 0.383600
H 0.939800 0.502600 0.023100
C -1.426600 -1.075300 -0.164100
H -0.843100 -1.182700 1.896200
H -1.179600 0.467000 1.333500
C -2.923000 -1.243100 0.124500
H -1.287600 -0.415300 -1.030500
H -0.969200 -2.043200 -0.418700
H -3.462800 -1.685400 -0.722800
H -3.092200 -1.884200 1.003200
H -3.374000 -0.261800 0.316400
C 1.576900 -0.965200 3.067400
C 2.111200 -2.320000 2.601100
H 0.537500 -1.052800 3.396400
H 2.156500 -0.577900 3.912200
C 2.197500 -3.303600 3.783900
H 1.454200 -2.743500 1.828200
H 3.109800 -2.215300 2.156000
C 2.660800 -4.698000 3.324800
H 2.898900 -2.903300 4.534800
H 1.211500 -3.377300 4.272200

H 2.734700 -5.387600 4.179200
H 1.948000 -5.123200 2.601000
H 3.647000 -4.641100 2.840300
C 1.015600 1.403300 2.626100
C 0.851200 2.586200 1.671300
H 1.671100 1.661300 3.464700
H 0.043100 1.113800 3.039300
C 0.298900 3.807000 2.434300
H 1.808200 2.860400 1.204800
H 0.152100 2.332900 0.862600
C 0.132500 5.020500 1.503000
H -0.673300 3.545200 2.881200
H 0.982400 4.058100 3.262800
H -0.283600 5.880000 2.049900
H 1.104300 5.318900 1.078800
H -0.544600 4.782000 0.668900
C -4.953500 2.771200 1.313500
S -5.765400 4.090000 0.628200
S -3.380600 2.707800 1.955600

Free Energy -5161.074789

Compound **7**
Cartesian Coordinates

C -1.820819 -0.012020 -0.059220
C -3.026683 -0.912515 -0.374244
C -1.027921 -2.075479 0.918107
N -0.687136 -0.907428 0.271670
H -2.038749 0.640049 0.800892
C 0.643009 -0.418246 0.144764
C 0.928874 0.916398 0.471853
C 1.657100 -1.254621 -0.360642
C 2.234867 1.408311 0.299267
H 0.149026 1.567733 0.860456
C 2.953270 -0.747486 -0.514675
H 1.424522 -2.276978 -0.642588
C 3.259438 0.584628 -0.182616
H 4.267607 0.969468 -0.310939
H -1.555497 0.604979 -0.926250
C 4.054750 -1.667220 -0.998616
C 2.492338 2.860865 0.638150
F 2.123244 3.153679 1.926145
F 1.762741 3.698878 -0.168801
F 3.799106 3.220809 0.506008
F 5.036411 -0.997808 -1.673441
F 4.667988 -2.305471 0.052001
F 3.591886 -2.645608 -1.832182
C -4.366599 -0.227534 -0.233416
C -4.744346 0.416489 0.964668
C -5.254696 -0.219069 -1.327626
C -5.984726 1.065758 1.060146
H -4.073852 0.399353 1.825047
C -6.498012 0.430545 -1.232712
H -4.967909 -0.719909 -2.254245
C -6.864998 1.075368 -0.038922
H -6.265997 1.560024 1.991000
H -7.175385 0.430835 -2.087735
H -7.829621 1.579029 0.037558
H -2.922623 -1.329961 -1.384520
S -0.023250 -3.127560 1.741990
S -2.778056 -2.342187 0.814867
Free Energy -2103.681983

Compound **$TPPH_4Cl_2$**
Cartesian Coordinates

N 2.047543 0.700725 -0.159686
N -0.693596 2.041678 0.163236
C -3.132133 1.542526 0.029747
C 3.130513 -1.541077 -0.093997
C -1.991085 2.352001 -0.194499
H 4.129397 2.796936 1.331126
C 3.649108 1.943923 0.864257
C -0.657914 4.083857 -0.830628
C 0.145391 3.077626 -0.191633
C 2.358885 1.986802 0.231208
H -2.827170 4.115066 -1.286173
C 4.092350 0.638403 0.826950
C 1.545093 3.131028 0.034670
C -1.962808 3.638425 -0.836775
C 3.084247 -0.148175 0.169281
H -0.261115 4.990924 -1.273770
H 5.000017 0.231346 1.258989
C 1.979632 -2.338887 -0.320164
N 0.696586 -2.028215 0.083592
C -3.075002 0.148939 0.288124
N -2.029534 -0.686686 -0.044861
C -2.347853 -1.986273 0.298267
C -3.640572 -1.959502 0.928140
C -4.087672 -0.654103 0.916188

H -5.004288 -0.258577 1.340610
H -4.126090 -2.824384 1.366974
C -1.544244 -3.123726 0.038299
C -0.156144 -3.061115 -0.250782
C 0.620897 -4.056004 -0.937102
C 1.927701 -3.614570 -0.979715
H 2.775758 -4.088163 -1.462391
H -1.300072 -0.435457 -0.745818
C 2.190856 4.464150 0.064292
C 1.598356 5.532893 0.781512
C 3.407889 4.694751 -0.622834
C 2.207908 6.795407 0.811326
H 0.674178 5.355791 1.331678
C 4.011235 5.960231 -0.597376
H 3.858425 3.883853 -1.195157
C 3.414283 7.013983 0.119812
H 1.747697 7.604877 1.379349
H 4.940766 6.126301 -1.143090
H 3.885557 7.997580 0.138782
C -4.470141 2.177698 -0.038287
C -4.727898 3.406751 0.616217
C -5.512187 1.565508 -0.777669
C -5.993650 4.005235 0.532730
H -3.937885 3.872485 1.205334
C -6.774131 2.170292 -0.866222
H -5.313609 0.629826 -1.300815
C -7.019273 3.391192 -0.210245
H -6.181920 4.946186 1.051289
H -7.561252 1.695422 -1.453443
H -8.001605 3.860872 -0.277115
C 4.454842 -2.203867 -0.107668
C 4.645237 -3.443693 0.551431
C 5.558025 -1.602621 -0.762598
C 5.905094 -4.058474 0.562821
H 3.806660 -3.901237 1.076426
C 6.816184 -2.221577 -0.752546
H 5.412457 -0.660942 -1.291969
C 6.994694 -3.449012 -0.087053
H 6.039253 -5.004855 1.088211
H 7.654927 -1.750832 -1.267131
H 7.975574 -3.925942 -0.072920
H 0.206057 -4.954797 -1.380519
C -2.186115 -4.460149 0.064668
C -3.427918 -4.685200 -0.578780
C -1.566356 -5.536327 0.746561
C -4.033789 -5.949412 -0.535146
H -3.899365 -3.870243 -1.127980
C -2.176030 -6.798364 0.791219
H -0.621023 -5.365023 1.261605
C -3.411943 -7.008846 0.151610
H -4.986973 -6.109402 -1.040766
H -1.693051 -7.612898 1.332555
H -3.887152 -7.990117 0.188564
H 1.296465 0.467083 -0.844279
H 0.479442 -1.297766 0.794133
Cl 0.132525 0.005338 2.477932
H -0.433095 1.296502 0.842576
Cl -0.076957 0.057204 -2.431256

Free Energy -2833.599918

Adduct **8**
Cartesian Coordinates
N -2.037975 0.555093 -1.072726
N 0.117283 -1.558232 -1.233859
C 2.588228 -1.775554 -1.352162
C -2.450402 2.979792 -0.651328
C 1.265836 -2.174666 -1.682239
H -4.603829 -1.066441 0.252996
C -3.904437 -0.326257 -0.118226
C -0.519410 -3.286839 -2.550496
C -0.994181 -2.222728 -1.711714
C -2.728586 -0.630329 -0.882680
H 1.548778 -3.894683 -3.077401
C -3.921825 1.035560 0.106400
C -2.335307 -1.901013 -1.384204
C 0.862032 -3.263848 -2.523714
C -2.766279 1.601600 -0.528778
H -1.161325 -3.940546 -3.130458
H -4.639125 1.602635 0.689295
C -1.154962 3.457338 -0.974362
N 0.017373 2.765640 -0.757271
C 2.930797 -0.450274 -0.980759
N 2.184160 0.683548 -1.261668
C 2.875508 1.805028 -0.837566
C 4.085570 1.355255 -0.212269
C 4.114961 -0.021914 -0.291375
H 4.850408 -0.693559 0.133736
H 4.796285 2.007991 0.282603
C 2.454148 3.151955 -1.000104
C 1.096655 3.529972 -1.151422
C 0.573457 4.752719 -1.692515
C -0.803182 4.710764 -1.579279
H -1.522771 5.442295 -1.930550
H 1.418036 0.717407 -1.971636

C -3.374132 -2.937431 -1.565238
C -3.121910 -4.286209 -1.209503
C -4.645527 -2.600033 -2.093880
C -4.109233 -5.264798 -1.377460
H -2.162115 -4.550030 -0.767057
C -5.632098 -3.581485 -2.259062
H -4.841544 -1.571282 -2.394875
C -5.367643 -4.916808 -1.901554
H -3.904639 -6.293782 -1.080831
H -6.602285 -3.307225 -2.674767
H -6.137187 -5.679367 -2.027649
C 3.651386 -2.802301 -1.398078
C 3.401663 -4.107721 -0.903867
C 4.937075 -2.507337 -1.916181
C 4.409256 -5.080914 -0.912708
H 2.423208 -4.339355 -0.484453
C 5.943474 -3.483132 -1.924631
H 5.130875 -1.518666 -2.331324
C 5.685176 -4.771234 -1.419754
H 4.203959 -6.074610 -0.512942
H 6.925159 -3.242339 -2.334218
H 6.470606 -5.527966 -1.424030
C -3.527685 3.975623 -0.456475
C -3.286204 5.149526 0.300149
C -4.812110 3.780155 -1.022467
C -4.302735 6.095805 0.490473
H -2.307373 5.297240 0.756558
C -5.824697 4.731145 -0.834425
H -4.998742 2.893635 -1.628348
C -5.574549 5.890250 -0.076049
H -4.106074 6.987163 1.087337
H -6.804887 4.572557 -1.285560
H -6.364516 6.627579 0.071988
H 1.179688 5.525972 -2.151495
C 3.485586 4.212488 -0.991857
C 4.704853 4.035202 -1.692883
C 3.274637 5.422611 -0.284558
C 5.681382 5.040828 -1.688961
H 4.865215 3.117264 -2.258345
C 4.254886 6.424711 -0.279986
H 2.350893 5.556078 0.278246
C 5.460212 6.237976 -0.982566
H 6.609204 4.895257 -2.243480
H 4.083360 7.345647 0.278524
H 6.221310 7.019277 -0.979388
H -1.325609 0.677734 -1.827801
H 0.095164 1.983946 -0.093240
H 0.103784 -0.929139 -0.420389
Cl -0.037492 0.870092 -3.526476
C -0.217646 0.228486 2.928268
Cl -3.712239 -2.298489 5.824622
N -0.596197 -1.219920 3.299983
C -0.342367 -1.718515 4.678857
C 0.496312 -2.284738 3.582667
H 0.092804 -0.962916 5.332287
H -1.170152 -2.290175 5.106780
H 0.188299 -3.251497 3.187071
C -1.914594 -1.619505 2.641887
C -2.204681 -3.119338 2.605708
H -1.874883 -1.206889 1.629021
H -2.679670 -1.099863 3.232983
C -3.654430 -3.367772 2.146705
H -1.511133 -3.628141 1.917068
H -2.090198 -3.551247 3.610306
C -4.008857 -4.862836 2.203133
H -4.331354 -2.800768 2.803752
H -3.785884 -2.995791 1.120144
H -5.035978 -5.037899 1.849456
H -3.327799 -5.452067 1.569666
H -3.928529 -5.236005 3.236337
C 1.939808 -1.981943 3.372045
C 2.618128 -0.962716 4.071375
C 2.652604 -2.782399 2.454151
C 3.986302 -0.745574 3.848562
H 2.082623 -0.331019 4.779128
C 4.021901 -2.570449 2.237059
H 2.128725 -3.568714 1.908663
C 4.691265 -1.549539 2.934171
H 4.501155 0.049031 4.389790
H 4.557119 -3.193388 1.520310
H 5.755532 -1.379146 2.765115
S 0.569463 0.344524 1.437345
S -0.661493 1.404205 4.017451

Free Energy -4189.694328

Transition State $\mathbf{8}_{\mathbf{TS}}$
Imaginary Frequency at –144 cm^{-1}
Cartesian Coordinates
N -0.980899 1.783871 -1.311256
N -0.463171 -1.170419 -1.640180
C 1.396939 -2.814729 -1.526067
C -0.000278 3.933920 -0.507247
C 0.181775 -2.313442 -2.062334
H -4.206521 1.899751 -0.560869
C -3.155787 2.110369 -0.723554
C -1.710501 -2.058524 -3.302698

C -1.635833 -0.991620 -2.346430
C -2.251900 1.237899 -1.414195
H -0.322082 -3.743354 -3.698842
C -2.428869 3.187334 -0.256177
C -2.576425 0.040915 -2.108695
C -0.607233 -2.870762 -3.121801
C -1.065106 3.008777 -0.662658
H -2.486046 -2.151052 -4.054501
H -2.783604 4.013928 0.349499
C 1.366723 3.571685 -0.610192
N 1.860406 2.300120 -0.412523
C 2.356548 -1.992662 -0.881254
N 2.467757 -0.617173 -1.033429
C 3.587124 -0.171434 -0.347771
C 4.165240 -1.302640 0.316507
C 3.408015 -2.412712 -0.000532
H 3.520108 -3.421298 0.379047
H 5.010320 -1.246254 0.993804
C 4.063397 1.166842 -0.316286
C 3.234509 2.294134 -0.540491
C 3.625789 3.630151 -0.890124
C 2.485917 4.411619 -0.927194
H 2.404913 5.457693 -1.201656
H 2.032297 -0.082256 -1.820932
C -3.959861 -0.136238 -2.597582
C -4.614018 -1.389195 -2.488573
C -4.660780 0.949301 -3.180690
C -5.925339 -1.550918 -2.951293
H -4.101551 -2.217957 -2.001896
C -5.974363 0.784416 -3.640273
H -4.158769 1.910034 -3.291806
C -6.610590 -0.465788 -3.527787
H -6.420460 -2.516041 -2.842400
H -6.497440 1.626911 -4.093920
H -7.634000 -0.592322 -3.882982
C 1.664790 -4.262563 -1.656379
C 0.620386 -5.201480 -1.460740
C 2.961459 -4.743905 -1.965983
C 0.867717 -6.576610 -1.557533
H -0.374013 -4.843445 -1.197431
C 3.206408 -6.120713 -2.061767
H 3.764392 -4.031664 -2.153959
C 2.162486 -7.041657 -1.854582
H 0.056016 -7.284559 -1.386607
H 4.207994 -6.474689 -2.308500
H 2.355928 -8.112617 -1.926370
C -0.323799 5.353333 -0.242191
C 0.402478 6.081134 0.733408
C -1.356373 6.010306 -0.956677
C 0.098958 7.425176 0.990680
H 1.183334 5.576976 1.302947
C -1.653238 7.356082 -0.700456
H -1.901942 5.465856 -1.727182
C -0.928764 8.066972 0.274726
H 0.656488 7.968192 1.754654
H -2.442909 7.851925 -1.266048
H -1.163366 9.113085 0.475134
H 4.641684 3.925561 -1.127987
C 5.493047 1.391155 -0.009010
C 6.490501 0.574758 -0.598918
C 5.890780 2.421811 0.879027
C 7.845867 0.787303 -0.311685
H 6.194193 -0.205189 -1.300316
C 7.246952 2.628889 1.166828
H 5.128295 3.036358 1.357317
C 8.228389 1.813934 0.571904
H 8.603025 0.159577 -0.782965
H 7.537459 3.417853 1.861481
H 9.283316 1.977375 0.795661
H -0.212186 1.539985 -1.979026
H 1.336619 1.563622 0.059617
H -0.237165 -0.676444 -0.780596
Cl 1.249801 1.039982 -3.446163
C -0.213882 0.223213 2.878891
Cl -5.323965 0.436421 4.649913
N -1.938665 -1.140078 2.797643
C -2.344878 -1.748042 4.052748
C -1.772857 -2.606989 2.955420
H -1.715136 -1.480151 4.906630
H -3.416234 -1.782691 4.265088
H -2.494430 -3.201539 2.388535
C -2.951861 -0.553101 1.887886
C -4.161195 -1.438383 1.544533
H -2.419473 -0.265213 0.969768
H -3.307360 0.355635 2.394164
C -5.271604 -0.623360 0.859795
H -3.853112 -2.269419 0.888228
H -4.575184 -1.870785 2.468113
C -6.517759 -1.477972 0.575600
H -5.539679 0.217456 1.518859
H -4.891423 -0.202497 -0.082643
H -7.294484 -0.890380 0.062395
H -6.266893 -2.338356 -0.064824
H -6.941125 -1.863744 1.516892
C -0.397993 -3.204393 2.976689
C 0.565400 -2.861101 3.946774
C -0.057701 -4.146006 1.983097
C 1.844237 -3.439921 3.917001
H 0.324149 -2.132969 4.720587
C 1.220280 -4.727431 1.950364
H -0.799564 -4.418140 1.229805
C 2.176602 -4.373837 2.918340
H 2.580518 -3.161300 4.672635
H 1.467079 -5.445120 1.167557
H 3.171426 -4.821871 2.895871
S 0.665286 -0.204234 1.591236
S -0.461545 1.105023 4.186265

Free Energy -4189.68476

Transition State $\mathbf{9}_{TS}$
Imaginary Frequency at –73 cm^{-1}
Cartesian Coordinates

N 0.666922 2.299609 -0.934761
N -1.092083 -0.055950 -1.641287
C -0.971020 -2.519831 -1.909751
C 2.879162 2.944591 0.021066
C -1.442170 -1.229754 -2.272492
H -1.492429 4.593031 0.086528
C -0.612645 3.999774 -0.134686
C -2.534438 0.478374 -3.303847
C -1.757512 1.006767 -2.218820
C -0.603989 2.847291 -0.989411
H -2.745055 -1.602691 -4.046737
C 0.656529 4.148715 0.387349
C -1.679603 2.351026 -1.774718
C -2.348741 -0.891002 -3.330687
C 1.477758 3.099802 -0.146044
H -3.110291 1.084305 -3.994609
H 0.996354 4.888167 1.104046
C 3.565751 1.730212 -0.231463
N 2.991855 0.477110 -0.207614
C 0.271111 -2.738545 -1.260760
N 1.342257 -1.858173 -1.250293
C 2.416793 -2.451408 -0.610905
C 1.986877 -3.739328 -0.148210
C 0.674400 -3.910628 -0.536483
H 0.016340 -4.736633 -0.298788
H 2.594511 -4.404952 0.454872
C 3.708950 -1.881481 -0.453330
C 3.947157 -0.484631 -0.466811
C 5.183793 0.202261 -0.712538
C 4.951693 1.556382 -0.564328
H 5.647332 2.372695 -0.725781
H 1.437670 -1.044429 -1.898851
C -2.768962 3.279049 -2.146162
C -4.121296 2.854680 -2.121773
C -2.482064 4.613423 -2.529800
C -5.152302 3.736428 -2.468827
H -4.355708 1.842226 -1.794975
C -3.516452 5.493889 -2.874723
H -1.444257 4.942123 -2.578275
C -4.854759 5.058822 -2.845093
H -6.187909 3.398131 -2.427239
H -3.278696 6.514713 -3.175986
H -5.659120 5.745583 -3.111462
C -1.832577 -3.679901 -2.220225
C -3.234970 -3.594460 -2.025803
C -1.285778 -4.899271 -2.692518
C -4.060069 -4.698338 -2.276375
H -3.664240 -2.669480 -1.642374
C -2.113771 -6.002199 -2.942700
H -0.214553 -4.966781 -2.880323
C -3.502063 -5.907672 -2.731360
H -5.133623 -4.620416 -2.101603
H -1.678030 -6.931619 -3.311000
H -4.143945 -6.768665 -2.921659
C 3.676704 4.117152 0.445314
C 4.696308 3.975743 1.419566
C 3.445981 5.395701 -0.120912
C 5.458169 5.082865 1.818627
H 4.866450 2.999809 1.874258
C 4.212379 6.499761 0.277393
H 2.683061 5.507098 -0.891132
C 5.219402 6.347533 1.248997
H 6.230996 4.961343 2.578492
H 4.031523 7.474934 -0.176256
H 5.814071 7.207724 1.559035
H 6.103836 -0.285127 -1.016055
C 4.855510 -2.792592 -0.245518
C 4.973928 -3.984914 -1.003165
C 5.853903 -2.493211 0.715357
C 6.059845 -4.849138 -0.807056
H 4.222348 -4.211614 -1.759325
C 6.937468 -3.360861 0.910305
H 5.755993 -1.593344 1.322328
C 7.044865 -4.540425 0.149843
H 6.142899 -5.756889 -1.405868
H 7.691435 -3.123023 1.661635
H 7.889051 -5.214062 0.302529
H 1.035520 1.653536 -1.669659
H 2.104283 0.270382 0.270574
H -0.680252 -0.036255 -0.697431
Cl 1.754675 0.515305 -3.327445
C -0.358637 0.225293 2.800772
Cl -5.537606 -1.587087 3.800501
N -1.867165 0.414493 2.802105
C -2.662394 0.017843 3.997663
C -2.899088 -0.845469 2.822493
H -2.050262 -0.355049 4.818123
H -3.439043 0.722550 4.292154
H -3.745516 -0.601340 2.190959
C -2.259075 1.702312 2.105727
C -3.743452 1.842797 1.754230
H -1.646306 1.754731 1.200336
H -1.942659 2.499242 2.794720
C -4.072134 3.296416 1.361364
H -3.995408 1.170958 0.919429
H -4.380697 1.560095 2.605483
C -5.574946 3.481039 1.092571
H -3.751358 3.971487 2.171870
H -3.500834 3.573158 0.463247
H -5.794745 4.512592 0.779579

H -5.913093 2.804879 0.293014
H -6.160686 3.258863 1.998461
C -2.348005 -2.211032 2.646366
C -1.466360 -2.804208 3.572422
C -2.751634 -2.945373 1.511080
C -0.998509 -4.111102 3.365331
H -1.139449 -2.253478 4.453613
C -2.294299 -4.254206 1.309274
H -3.435405 -2.488105 0.795536
C -1.414423 -4.840402 2.237211
H -0.315103 -4.560183 4.087041
H -2.620369 -4.809933 0.430015
H -1.054223 -5.858495 2.081536
S 0.230468 -0.455570 1.366927
S 0.460170 0.723015 4.168012

Free Energy -4189.684837

Compound **9**
Cartesian Coordinates
N -3.190274 -0.593101 -0.362319
N -0.538113 -1.756455 -1.209863
C 1.735636 -1.096730 -1.926891
C -4.306251 1.539583 0.295659
C 0.614418 -1.962174 -1.938720
H -4.521677 -2.967703 1.521459
C -4.272498 -2.042152 1.014207
C -0.755034 -3.748345 -2.272971
C -1.381357 -2.839314 -1.352201
C -3.305483 -1.935002 -0.041041
H 1.191094 -3.613822 -3.330024
C -4.745308 -0.773473 1.284916
C -2.604792 -3.004051 -0.659834
C 0.468009 -3.213569 -2.627652
C -4.079615 0.141150 0.402094
H -1.210444 -4.663311 -2.635640
H -5.450472 -0.475733 2.053241
C -3.360181 2.444496 -0.245180
N -2.003241 2.212868 -0.339605
C 1.672963 0.262375 -1.527149
N 0.544717 1.061992 -1.511657
C 0.897767 2.338894 -1.116543
C 2.301719 2.329241 -0.823993
C 2.773748 1.058100 -1.067075
H 3.769483 0.673072 -0.892420
H 2.846832 3.171482 -0.415847
C 0.023561 3.453440 -1.027580
C -1.376353 3.326256 -0.857066
C -2.393595 4.297623 -1.149312
C -3.607936 3.757754 -0.775818
H -4.594636 4.190809 -0.899039
H -0.344971 0.830120 -2.001619
C -3.164282 -4.370311 -0.535939
C -2.328283 -5.461664 -0.195071
C -4.544894 -4.608066 -0.745370
C -2.857917 -6.753248 -0.067667
H -1.271888 -5.282544 -0.002850
C -5.071511 -5.901892 -0.621930
H -5.191459 -3.776297 -1.025264
C -4.230630 -6.978299 -0.282026
H -2.202732 -7.580155 0.209380
H -6.134504 -6.071587 -0.797600
H -4.642187 -7.983631 -0.183446

C 3.061443 -1.653304 -2.282797
C 3.474883 -2.907511 -1.770942
C 3.952373 -0.928511 -3.110925
C 4.746042 -3.416588 -2.071005
H 2.805068 -3.461594 -1.114755
C 5.220529 -1.442290 -3.414449
H 3.635979 0.030327 -3.521149
C 5.623453 -2.685466 -2.893058
H 5.055598 -4.375990 -1.654451
H 5.893248 -0.874437 -4.058300
H 6.613784 -3.080342 -3.123765
C -5.596726 2.079040 0.781192
C -5.639059 3.273383 1.543301
C -6.813433 1.411903 0.492648
C -6.861718 3.783186 2.002411
H -4.706505 3.779667 1.792288
C -8.034603 1.925022 0.951810
H -6.792428 0.505713 -0.112498
C -8.063153 3.111823 1.708018
H -6.876340 4.696896 2.597819
H -8.963263 1.405661 0.711980
H -9.013724 3.509796 2.065589
H -2.208407 5.251520 -1.631146
C 0.609710 4.810440 -1.088341
C 1.623356 5.118249 -2.029722
C 0.175714 5.823276 -0.197086
C 2.184425 6.402004 -2.078459
H 1.947521 4.350370 -2.732053
C 0.740562 7.105475 -0.246797
H -0.582456 5.585933 0.549067
C 1.745646 7.399363 -1.187278
H 2.956390 6.626874 -2.815501
H 0.405885 7.870719 0.454626
H 2.184366 8.397376 -1.224833
H -2.771676 -0.243058 -1.252322
H -1.501352 1.489068 0.213706
H -0.585480 -1.104292 -0.400152
Cl -2.109919 0.426284 -3.184154

C 0.926291 0.375983 2.305441
N 1.970674 -0.526068 2.241593
C 3.050188 -0.509834 3.249173
C 4.440791 -0.826520 2.668929
H 3.055688 0.476485 3.721363
H 2.820106 -1.262993 4.019846
H 4.508610 -1.863404 2.322987
C 1.881904 -1.774994 1.461278
C 1.369249 -2.987589 2.252353
H 2.874149 -1.982490 1.038063
H 1.217239 -1.590538 0.619466
C 1.190646 -4.201673 1.323491
H 2.068753 -3.241712 3.065415
H 0.404043 -2.723254 2.711082
C 0.615580 -5.425984 2.055692
H 0.524658 -3.917239 0.491282
H 2.163663 -4.463874 0.873585
H 0.501465 -6.283573 1.374412
H 1.277814 -5.731975 2.881319
H -0.373308 -5.193916 2.481912
C 4.976553 0.110211 1.621419
C 4.787479 1.504674 1.711765
C 5.730565 -0.417535 0.552874
C 5.364291 2.356717 0.758416
H 4.180870 1.920007 2.516696
C 6.302395 0.434864 -0.405586
H 5.864445 -1.497496 0.470556
C 6.126632 1.826275 -0.298958
H 5.212809 3.434313 0.835174
H 6.870900 0.013508 -1.234525
H 6.568864 2.491870 -1.041598
S 1.078689 1.869689 3.142664
S -0.608251 -0.051281 1.560469
Cl 5.605435 -0.831701 4.154942

Free Energy -4189.724362

Transition State **10$_{TS}$**
Imaginary Frequency at –57 cm^{-1}
Cartesian Coordinates

N -2.485243 2.085506 -0.813244
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C -0.907094 -2.882558 -1.297702
C -1.015357 4.096440 -1.011302
C -2.164626 -2.240485 -1.194406
H -4.865758 2.888337 1.342014
C -4.029923 2.880730 0.651086
C -4.406934 -1.848109 -1.220578
C -3.732860 -0.694719 -0.692279
C -3.644519 1.745213 -0.139802
H -3.593819 -3.759066 -1.997046
C -3.116094 3.888224 0.417566
C -4.328554 0.505139 -0.231082
C -3.448415 -2.790061 -1.532765
C -2.141957 3.389793 -0.511648
H -5.477139 -1.906382 -1.385791
H -3.069848 4.866626 0.883056
C 0.161342 3.466653 -1.484977
N 0.527564 2.162936 -1.210670
C 0.336279 -2.202025 -1.273739
N 0.536796 -0.855713 -1.521184
C 1.887127 -0.564377 -1.406196
C 2.553497 -1.777221 -1.023663
C 1.608484 -2.775802 -0.942734
H 1.757047 -3.797667 -0.615581
H 3.607004 -1.855038 -0.785506
C 2.492088 0.694074 -1.633748
C 1.775758 1.915007 -1.736740
C 2.202634 3.103653 -2.422019
C 1.208342 4.050300 -2.278957
H 1.169170 5.044056 -2.711289
H -0.136176 -0.272988 -2.063681
C -5.748748 0.453208 0.187824
C -6.215890 -0.608329 1.002275
C -6.662249 1.458745 -0.213320
C -7.558475 -0.661053 1.402925
H -5.514222 -1.373115 1.335391
C -8.005210 1.401188 0.185913
H -6.314886 2.267202 -0.856700
C -8.457541 0.342143 0.995410
H -7.900453 -1.478070 2.039508
H -8.699695 2.176131 -0.140944
H -9.502169 0.299473 1.306431
C -0.884376 -4.362441 -1.391759
C -1.679550 -5.150457 -0.524780
C -0.057672 -5.012034 -2.340057
C -1.646672 -6.550099 -0.603481
H -2.298325 -4.657512 0.224018
C -0.030679 -6.411867 -2.420516
H 0.544603 -4.410653 -3.021170
C -0.823431 -7.185149 -1.551965
H -2.255000 -7.143844 0.080031
H 0.602853 -6.898291 -3.163257
H -0.799043 -8.273938 -1.613244
C -1.066864 5.576887 -0.992845
C 0.035111 6.337157 -0.529324
C -2.228480 6.257746 -1.434301
C -0.022967 7.738062 -0.512643
H 0.921059 5.820516 -0.160564
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C -1.179784 8.403255 -0.960163

H 0.828876 8.309468 -0.141951
H -3.178197 8.169060 -1.775429
H -1.222769 9.493163 -0.948263
H 3.121871 3.182525 -2.992561
C 3.968615 0.755199 -1.754255
C 4.683870 -0.162640 -2.560467
C 4.689552 1.730418 -1.022529
C 6.083874 -0.112091 -2.623769
H 4.134096 -0.900460 -3.144623
C 6.089584 1.775142 -1.083886
H 4.143553 2.420574 -0.379961
C 6.790932 0.852936 -1.882029
H 6.622181 -0.821216 -3.253808
H 6.632270 2.517728 -0.497728
H 7.880418 0.885272 -1.926037
H -2.109476 1.566221 -1.637378
H 0.122703 1.626116 -0.407740
H -1.691349 -0.431516 -0.145497
Cl -1.463626 0.681961 -3.473170
C 0.844993 0.152670 2.069233
N 0.919930 -1.160308 2.439095
C 2.099721 -1.609103 3.194313
C 3.380246 -1.541737 2.334810
H 2.227371 -0.966139 4.076854
H 1.905091 -2.629666 3.540737
H 3.196375 -1.156967 1.335139
C -0.144146 -2.146108 2.166403
C -1.239602 -2.207333 3.242942
H 0.340039 -3.125468 2.047274
H -0.601068 -1.884784 1.207303
C -2.419546 -3.071175 2.761010
H -0.827476 -2.612925 4.181846
H -1.590767 -1.183911 3.443918
C -3.577016 -3.112072 3.773638
H -2.784208 -2.665151 1.801928
H -2.063452 -4.095444 2.557122
H -4.407402 -3.735724 3.407022
H -3.238327 -3.524013 4.737930
H -3.965670 -2.097247 3.956741
C 4.639443 -1.012705 2.942248
C 4.945551 -1.210334 4.304199
C 5.564074 -0.334835 2.119221
C 6.149537 -0.721852 4.838326
H 4.247130 -1.748782 4.946171
C 6.765951 0.153037 2.650825
H 5.325011 -0.169901 1.067890
C 7.062861 -0.038201 4.014664
H 6.375090 -0.876288 5.894661
H 7.466449 0.685454 2.005417
H 7.996969 0.342061 4.431014
Cl 3.809824 -3.448736 1.834681
S -0.648557 0.800248 1.430486
S 2.244224 1.125787 2.276234

Free Energy -4189.717493