Supporting Information:

A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions

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The structures of the Reactant, Transition State, and Product obtained using the different methods are here reported. Notice that at the semiempirical level two minima for the reactant state were found and are here reported: one “in-plane” and another “below” the flavin ring.

S1.1 Structures optimized with the standard AM1 in the SQUANTM module of CHARMM, no MOVB calculations performed here (cyan triangles in Figure 1 of main text).

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* ###############################################################################
* # SQUANTM - REACTANT IN-PLANE                                                 #
* ###############################################################################
*
   39
    1    1 FADN C1    -0.04966  -0.24362   0.22769 SOLU 1      0.00000
    2    1 FADN C2     0.03486  -0.32282   1.60294 SOLU 1      0.00000
    3    1 FADN C3     1.30025  -0.20761   2.24936 SOLU 1      0.00000
    4    1 FADN C4     2.48759  -0.04156   1.44595 SOLU 1      0.00000
    5    1 FADN C5     2.35501   0.06532   0.04282 SOLU 1      0.00000
    6    1 FADN C6     1.10407  -0.03890  -0.54567 SOLU 1      0.00000
    7    1 FADN C7     3.78659   0.07479   3.46762 SOLU 1      0.00000
    8    1 FADN C8     2.52020  -0.09408   4.22119 SOLU 1      0.00000
    9    1 FADN C9     2.57739  -0.10172   5.72658 SOLU 1      0.00000
   10    1 FADN C10    5.01295   0.27316   5.59538 SOLU 1      0.00000
   11    1 FADN H11   -1.03317  -0.33103  -0.26790 SOLU 1      0.00000
   12    1 FADN H12   -0.87872  -0.46472   2.21656 SOLU 1      0.00000
   13    1 FADN H13    3.22521   0.25185  -0.60712 SOLU 1      0.00000
   14    1 FADN H14    1.01459   0.04658  -1.64387 SOLU 1      0.00000
   15    1 FADN O15    1.58961  -0.26037   6.44413 SOLU 1      0.00000
   16    1 FADN O16    6.12450   0.44749   6.11039 SOLU 1      0.00000
   17    1 FADN N17    3.83629   0.08466   6.31085 SOLU 1      0.00000
   18    1 FADN H18    3.90718   0.08884   7.31364 SOLU 1      0.00000
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   19    1 FADN N19    4.95217   0.26897   4.15694 SOLU 1      0.00000
   20    1 FADN H20    5.83311   0.41603   3.69756 SOLU 1      0.00000
   21    1 FADN N21    3.74117   0.02259   2.09269 SOLU 1      0.00000
   22    1 FADN N22    1.35639  -0.24366   3.62694 SOLU 1      0.00000
   23    1 FADN C23    4.96482   0.03597   1.30895 SOLU 1      0.00000
   24    1 FADN H24    5.31296   1.09522   1.16715 SOLU 1      0.00000
   25    1 FADN H25    5.76605  -0.57225   1.81200 SOLU 1      0.00000
   26    1 FADN H26    4.78927  -0.43963   0.30585 SOLU 1      0.00000
   27    1 FADN H27   -1.59090   0.39473   4.04229 SOLU 1      0.00000
   28    1 FADN C28   -2.67811   0.62986   4.19321 SOLU 1      0.00000
   29    1 FADN H29   -2.83325   1.72825   4.03138 SOLU 1      0.00000
   30    1 FADN H30   -2.95757   0.38339   5.25322 SOLU 1      0.00000
   31    1 FADN N31   -3.42703  -0.12141   3.20801 SOLU 1      0.00000
   32    1 FADN C32   -4.76240   0.39420   2.99389 SOLU 1      0.00000
   33    1 FADN H33   -4.69180   1.46920   2.68270 SOLU 1      0.00000
   34    1 FADN H34   -5.24875  -0.18821   2.16808 SOLU 1      0.00000
   35    1 FADN H35   -5.41376   0.32851   3.90769 SOLU 1      0.00000
   36    1 FADN C36   -3.41486  -1.54417   3.47449 SOLU 1      0.00000
   37    1 FADN H37   -3.91830  -2.07814   2.62670 SOLU 1      0.00000
   38    1 FADN H38   -2.35036  -1.89131   3.54124 SOLU 1      0.00000
   39    1 FADN H39   -3.93709  -1.82214   4.43068 SOLU 1      0.00000

* ##############################################################################
* # SQUANTM - REACTANT BELOW                                                   #
* ##############################################################################
*
   39
    1    1 FADN C1     3.65154  -1.93744  10.98315 SOLU 1      0.00000
    2    1 FADN C2     2.48194  -1.28382  11.31139 SOLU 1      0.00000
    3    1 FADN C3     1.62090  -0.79831  10.28461 SOLU 1      0.00000
    4    1 FADN C4     2.00304  -0.97305   8.90525 SOLU 1      0.00000
    5    1 FADN C5     3.19394  -1.67625   8.60926 SOLU 1      0.00000
    6    1 FADN C6     3.99808  -2.14176   9.63718 SOLU 1      0.00000
    7    1 FADN C7    -0.05458   0.08594   8.24677 SOLU 1      0.00000
    8    1 FADN C8    -0.37542   0.22546   9.68931 SOLU 1      0.00000
    9    1 FADN C9    -1.68233   0.87009  10.07406 SOLU 1      0.00000
   10    1 FADN C10   -2.22854   1.09741   7.67816 SOLU 1      0.00000
   11    1 FADN H11    4.31836  -2.31139  11.78019 SOLU 1      0.00000
   12    1 FADN H12    2.19347  -1.13414  12.36887 SOLU 1      0.00000
   13    1 FADN H13    3.49754  -1.88609   7.57071 SOLU 1      0.00000
   14    1 FADN H14    4.92690  -2.68863   9.39252 SOLU 1      0.00000
   15    1 FADN O15   -2.02912   1.05972  11.23966 SOLU 1      0.00000
   16    1 FADN O16   -2.97447   1.43489   6.75067 SOLU 1      0.00000
   17    1 FADN N17   -2.52419   1.26228   9.02597 SOLU 1      0.00000
   18    1 FADN H18   -3.40608   1.69022   9.25001 SOLU 1      0.00000
   19    1 FADN N19   -0.97136   0.49301   7.31784 SOLU 1      0.00000
   20    1 FADN H20   -0.81837   0.39729   6.32963 SOLU 1      0.00000
   21    1 FADN N21    1.16614  -0.44670   7.89719 SOLU 1      0.00000
   22    1 FADN N22    0.43718  -0.18364  10.63818 SOLU 1      0.00000
   23    1 FADN C23    1.59389  -0.47234   6.50850 SOLU 1      0.00000
   24    1 FADN H24    1.15573  -1.37002   5.99313 SOLU 1      0.00000
   25    1 FADN H25    1.28258   0.47001   5.97922 SOLU 1      0.00000
   26    1 FADN H26    2.71538  -0.51373   6.44752 SOLU 1      0.00000
   27    1 FADN H27   -2.17099  -2.16262 -13.17438 SOLU 1      0.00000
   28    1 FADN C28   -2.29308  -2.25522 -14.28899 SOLU 1      0.00000
   29    1 FADN H29   -1.46470  -2.89931 -14.68448 SOLU 1      0.00000
   30    1 FADN H30   -2.20219  -1.23339 -14.74191 SOLU 1      0.00000
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   31    1 FADN N31   -3.56027  -2.82926 -14.67872 SOLU 1      0.00000
   32    1 FADN C32   -3.71310  -4.20291 -14.25784 SOLU 1      0.00000
   33    1 FADN H33   -2.85513  -4.80366 -14.65846 SOLU 1      0.00000
   34    1 FADN H34   -3.74168  -4.32463 -13.13975 SOLU 1      0.00000
   35    1 FADN H35   -4.66735  -4.60985 -14.68366 SOLU 1      0.00000
   36    1 FADN C36   -4.68968  -2.00003 -14.32618 SOLU 1      0.00000
   37    1 FADN H37   -4.82544  -1.88287 -13.21549 SOLU 1      0.00000
   38    1 FADN H38   -4.54825  -0.98250 -14.77575 SOLU 1      0.00000
   39    1 FADN H39   -5.62204  -2.45518 -14.75166 SOLU 1      0.00000

* ###############################################################################
* # SQUANTM - TS (RC = -0.020)                                                  #
* ###############################################################################
*
   39
    1    1 FADN C1     3.28653  -1.61239   1.92869 SOLU 1      0.00000
    2    1 FADN C2     2.32017  -0.75982   1.42849 SOLU 1      0.00000
    3    1 FADN C3     0.96032  -0.90577   1.80873 SOLU 1      0.00000
    4    1 FADN C4     0.59969  -1.96949   2.69960 SOLU 1      0.00000
    5    1 FADN C5     1.61328  -2.81368   3.20789 SOLU 1      0.00000
    6    1 FADN C6     2.93207  -2.63411   2.81912 SOLU 1      0.00000
    7    1 FADN C7    -1.65093  -1.12213   2.73885 SOLU 1      0.00000
    8    1 FADN C8    -1.24653  -0.10147   1.80364 SOLU 1      0.00000
    9    1 FADN C9    -2.26552   0.85670   1.29956 SOLU 1      0.00000
   10    1 FADN C10   -3.84897  -0.03780   2.95184 SOLU 1      0.00000
   11    1 FADN H11    4.34207  -1.48282   1.63611 SOLU 1      0.00000
   12    1 FADN H12    2.60226   0.05578   0.73953 SOLU 1      0.00000
   13    1 FADN H13    1.38405  -3.61300   3.93092 SOLU 1      0.00000
   14    1 FADN H14    3.71292  -3.30021   3.22547 SOLU 1      0.00000
   15    1 FADN O15   -2.09029   1.58902   0.31434 SOLU 1      0.00000
   16    1 FADN O16   -4.93689  -0.02557   3.54714 SOLU 1      0.00000
   17    1 FADN N17   -3.49880   0.87863   1.96188 SOLU 1      0.00000
   18    1 FADN H18   -4.17890   1.57268   1.71592 SOLU 1      0.00000
   19    1 FADN N19   -2.91281  -1.06451   3.29246 SOLU 1      0.00000
   20    1 FADN H20   -3.21261  -1.70034   4.00628 SOLU 1      0.00000
   21    1 FADN N21   -0.75305  -2.12236   3.07950 SOLU 1      0.00000
   22    1 FADN N22    0.03205   0.04012   1.34149 SOLU 1      0.00000
   23    1 FADN C23   -1.15510  -3.24554   3.89896 SOLU 1      0.00000
   24    1 FADN H24   -1.06595  -2.98554   4.98842 SOLU 1      0.00000
   25    1 FADN H25   -2.21023  -3.55268   3.66353 SOLU 1      0.00000
   26    1 FADN H26   -0.50474  -4.13347   3.67101 SOLU 1      0.00000
   27    1 FADN H27    0.01873  -0.00116  -0.00778 SOLU 1      0.00000
   28    1 FADN C28    0.00618  -0.03825  -1.33717 SOLU 1      0.00000
   29    1 FADN H29    1.08803  -0.24606  -1.52120 SOLU 1      0.00000
   30    1 FADN H30   -0.31857   1.01647  -1.52565 SOLU 1      0.00000
   31    1 FADN N31   -0.86703  -1.00506  -1.75403 SOLU 1      0.00000
   32    1 FADN C32   -0.43258  -2.34871  -2.01714 SOLU 1      0.00000
   33    1 FADN H33    0.68089  -2.43612  -1.91504 SOLU 1      0.00000
   34    1 FADN H34   -0.92283  -3.05579  -1.29366 SOLU 1      0.00000
   35    1 FADN H35   -0.72631  -2.64852  -3.06051 SOLU 1      0.00000
   36    1 FADN C36   -2.21993  -0.66991  -2.11082 SOLU 1      0.00000
   37    1 FADN H37   -2.89973  -1.52450  -1.85059 SOLU 1      0.00000
   38    1 FADN H38   -2.54941   0.25184  -1.55766 SOLU 1      0.00000
   39    1 FADN H39   -2.29321  -0.47683  -3.21643 SOLU 1      0.00000

* ###############################################################################
* # SQUANTM - PRODUCT                                                           #
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* ##########################################################################
*
   39
    1    1 FADN C1     3.10280  -2.50070   2.02178 SOLU 1      0.00000
    2    1 FADN C2     2.16254  -1.63101   1.47163 SOLU 1      0.00000
    3    1 FADN C3     0.94363  -1.39458   2.12414 SOLU 1      0.00000
    4    1 FADN C4     0.66792  -2.07132   3.35753 SOLU 1      0.00000
    5    1 FADN C5     1.62012  -2.96277   3.87549 SOLU 1      0.00000
    6    1 FADN C6     2.83040  -3.16494   3.21210 SOLU 1      0.00000
    7    1 FADN C7    -1.60172  -1.27778   3.28036 SOLU 1      0.00000
    8    1 FADN C8    -1.32606  -0.69427   2.03349 SOLU 1      0.00000
    9    1 FADN C9    -2.40869  -0.30424   1.13489 SOLU 1      0.00000
   10    1 FADN C10   -3.98545  -0.84357   2.93571 SOLU 1      0.00000
   11    1 FADN H11    4.06361  -2.65895   1.50807 SOLU 1      0.00000
   12    1 FADN H12    2.39482  -1.10911   0.53173 SOLU 1      0.00000
   13    1 FADN H13    1.42112  -3.51646   4.80731 SOLU 1      0.00000
   14    1 FADN H14    3.57024  -3.85902   3.64087 SOLU 1      0.00000
   15    1 FADN O15   -2.22362   0.05544  -0.05857 SOLU 1      0.00000
   16    1 FADN O16   -5.14689  -0.86463   3.38149 SOLU 1      0.00000
   17    1 FADN N17   -3.70428  -0.36778   1.64165 SOLU 1      0.00000
   18    1 FADN H18   -4.47912  -0.06107   1.09174 SOLU 1      0.00000
   19    1 FADN N19   -2.91983  -1.31738   3.73339 SOLU 1      0.00000
   20    1 FADN H20   -3.15781  -1.70659   4.62204 SOLU 1      0.00000
   21    1 FADN N21   -0.57563  -1.87394   4.02274 SOLU 1      0.00000
   22    1 FADN N22    0.01944  -0.42837   1.64232 SOLU 1      0.00000
   23    1 FADN C23   -0.63974  -1.90973   5.46088 SOLU 1      0.00000
   24    1 FADN H24   -1.18444  -1.01391   5.86507 SOLU 1      0.00000
   25    1 FADN H25   -1.17167  -2.84527   5.78531 SOLU 1      0.00000
   26    1 FADN H26    0.39617  -1.91016   5.89488 SOLU 1      0.00000
   27    1 FADN H27    0.01760  -0.28804   0.64668 SOLU 1      0.00000
   28    1 FADN C28   -0.00811   0.08065  -1.89586 SOLU 1      0.00000
   29    1 FADN H29    1.03119  -0.30633  -1.85982 SOLU 1      0.00000
   30    1 FADN H30   -0.33452   0.82618  -1.13074 SOLU 1      0.00000
   31    1 FADN N31   -0.84901  -0.33175  -2.79683 SOLU 1      0.00000
   32    1 FADN C32   -0.49318  -1.31532  -3.81026 SOLU 1      0.00000
   33    1 FADN H33    0.55005  -1.69753  -3.64974 SOLU 1      0.00000
   34    1 FADN H34   -1.21892  -2.17292  -3.75491 SOLU 1      0.00000
   35    1 FADN H35   -0.56393  -0.83577  -4.82539 SOLU 1      0.00000
   36    1 FADN C36   -2.22882   0.14160  -2.84824 SOLU 1      0.00000
   37    1 FADN H37   -2.89944  -0.67786  -2.46726 SOLU 1      0.00000
   38    1 FADN H38   -2.36353   1.03993  -2.18414 SOLU 1      0.00000
   39    1 FADN H39   -2.48898   0.39686  -3.90985 SOLU 1      0.00000
```

S1.2 AM1-MOVB optimized structures with the free energy perturbation method. A reference potential $V_{RP}(\lambda)$ was used to drive the reaction, with λ being a coupling parameter linearly connecting the reactant and product potentials (see Figure 5 in the main text).

```
* ##########################################################################
* # MOVB PERT (Emix Driven) - REACTANT IN-PLANE                             #
* ##########################################################################
*
   39
    1    1 FADN C1     0.06471  -0.26826   0.03909 SOLU 1      0.00000
    2    1 FADN C2     0.09297  -0.36171   1.41576 SOLU 1      0.00000
    3    1 FADN C3     1.32813  -0.23305   2.11609 SOLU 1      0.00000
    4    1 FADN C4     2.54477  -0.03830   1.36483 SOLU 1      0.00000
    5    1 FADN C5     2.46914   0.08288  -0.04148 SOLU 1      0.00000
```

```
     6    1 FADN C6     1.24600  -0.03532  -0.68305 SOLU 1      0.00000
     7    1 FADN C7     3.75706   0.07546   3.43983 SOLU 1      0.00000
     8    1 FADN C8     2.46344  -0.12283   4.13817 SOLU 1      0.00000
     9    1 FADN C9     2.45856  -0.14732   5.64454 SOLU 1      0.00000
    10    1 FADN C10    4.89084   0.26886   5.61880 SOLU 1      0.00000
    11    1 FADN H11   -0.89501  -0.36713  -0.49896 SOLU 1      0.00000
    12    1 FADN H12   -0.84149  -0.52692   1.98726 SOLU 1      0.00000
    13    1 FADN H13    3.36249   0.29148  -0.65217 SOLU 1      0.00000
    14    1 FADN H14    1.20087   0.06123  -1.78307 SOLU 1      0.00000
    15    1 FADN O15    1.44484  -0.33058   6.31869 SOLU 1      0.00000
    16    1 FADN O16    5.97707   0.45529   6.18129 SOLU 1      0.00000
    17    1 FADN N17    3.68892   0.05277   6.28258 SOLU 1      0.00000
    18    1 FADN H18    3.71820   0.04621   7.28745 SOLU 1      0.00000
    19    1 FADN N19    4.88962   0.28058   4.17902 SOLU 1      0.00000
    20    1 FADN H20    5.78627   0.44729   3.75834 SOLU 1      0.00000
    21    1 FADN N21    3.76933   0.03858   2.06371 SOLU 1      0.00000
    22    1 FADN N22    1.32790  -0.28428   3.49453 SOLU 1      0.00000
    23    1 FADN C23    5.02382   0.08079   1.33137 SOLU 1      0.00000
    24    1 FADN H24    5.35877   1.14725   1.21382 SOLU 1      0.00000
    25    1 FADN H25    5.81431  -0.51849   1.86137 SOLU 1      0.00000
    26    1 FADN H26    4.89806  -0.38789   0.31758 SOLU 1      0.00000
    27    1 FADN H27   -1.57410   0.38722   4.04868 SOLU 1      0.00000
    28    1 FADN C28   -2.64906   0.63550   4.25124 SOLU 1      0.00000
    29    1 FADN H29   -2.80471   1.73022   4.06641 SOLU 1      0.00000
    30    1 FADN H30   -2.87371   0.42222   5.33124 SOLU 1      0.00000
    31    1 FADN N31   -3.45184  -0.14008   3.32932 SOLU 1      0.00000
    32    1 FADN C32   -4.77566   0.40850   3.12567 SOLU 1      0.00000
    33    1 FADN H33   -4.67989   1.46123   2.75149 SOLU 1      0.00000
    34    1 FADN H34   -5.30646  -0.20222   2.34914 SOLU 1      0.00000
    35    1 FADN H35   -5.40037   0.41680   4.06020 SOLU 1      0.00000
    36    1 FADN C36   -3.48000  -1.54637   3.67166 SOLU 1      0.00000
    37    1 FADN H37   -4.00714  -2.10801   2.85677 SOLU 1      0.00000
    38    1 FADN H38   -2.42695  -1.92324   3.75035 SOLU 1      0.00000
    39    1 FADN H39   -4.00321  -1.75612   4.64466 SOLU 1      0.00000

* ##########################################################################
* # MOVB PERT (Emix Driven) - REACTANT BELOW                               #
* ##########################################################################
*
    39
     1    1 FADN C1     3.35499  -1.46294   2.63010 SOLU 1      0.00000
     2    1 FADN C2     2.44196  -0.47008   2.34117 SOLU 1      0.00000
     3    1 FADN C3     1.05990  -0.66186   2.63195 SOLU 1      0.00000
     4    1 FADN C4     0.62836  -1.91380   3.20256 SOLU 1      0.00000
     5    1 FADN C5     1.59900  -2.89442   3.51346 SOLU 1      0.00000
     6    1 FADN C6     2.93445  -2.66445   3.22425 SOLU 1      0.00000
     7    1 FADN C7    -1.62007  -1.05974   3.26533 SOLU 1      0.00000
     8    1 FADN C8    -1.09548   0.19837   2.67770 SOLU 1      0.00000
     9    1 FADN C9    -2.06135   1.32593   2.41840 SOLU 1      0.00000
    10    1 FADN C10   -3.86866  -0.05739   3.37260 SOLU 1      0.00000
    11    1 FADN H11    4.42527  -1.31320   2.40241 SOLU 1      0.00000
    12    1 FADN H12    2.76762   0.48572   1.88924 SOLU 1      0.00000
    13    1 FADN H13    1.32519  -3.84268   4.00401 SOLU 1      0.00000
    14    1 FADN H14    3.68292  -3.43940   3.47098 SOLU 1      0.00000
    15    1 FADN O15   -1.73449   2.39625   1.90605 SOLU 1      0.00000
    16    1 FADN O16   -5.04356  -0.24467   3.71177 SOLU 1      0.00000
    17    1 FADN N17   -3.39401   1.11252   2.79178 SOLU 1      0.00000
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   18    1 FADN H18   -4.06179   1.84839   2.63815 SOLU 1      0.00000
   19    1 FADN N19   -2.94261  -1.13661   3.60323 SOLU 1      0.00000
   20    1 FADN H20   -3.34507  -1.95270   4.02885 SOLU 1      0.00000
   21    1 FADN N21   -0.74883  -2.11107   3.44347 SOLU 1      0.00000
   22    1 FADN N22    0.17206   0.36143   2.36991 SOLU 1      0.00000
   23    1 FADN C23   -1.23363  -3.41067   3.87722 SOLU 1      0.00000
   24    1 FADN H24   -1.33599  -3.42318   4.99652 SOLU 1      0.00000
   25    1 FADN H25   -2.22117  -3.64809   3.39405 SOLU 1      0.00000
   26    1 FADN H26   -0.52179  -4.21871   3.55551 SOLU 1      0.00000
   27    1 FADN H27   -0.00546   0.00099  -1.67644 SOLU 1      0.00000
   28    1 FADN C28   -0.05465  -0.09889  -2.79684 SOLU 1      0.00000
   29    1 FADN H29    0.98076  -0.29437  -3.18103 SOLU 1      0.00000
   30    1 FADN H30   -0.41922   0.87208  -3.22364 SOLU 1      0.00000
   31    1 FADN N31   -0.92545  -1.16261  -3.23357 SOLU 1      0.00000
   32    1 FADN C32   -0.47046  -2.47578  -2.84938 SOLU 1      0.00000
   33    1 FADN H33    0.57791  -2.62250  -3.21982 SOLU 1      0.00000
   34    1 FADN H34   -0.47925  -2.64002  -1.73515 SOLU 1      0.00000
   35    1 FADN H35   -1.13179  -3.24640  -3.32548 SOLU 1      0.00000
   36    1 FADN C36   -2.31842  -0.92587  -2.94413 SOLU 1      0.00000
   37    1 FADN H37   -2.54598  -0.91457  -1.84136 SOLU 1      0.00000
   38    1 FADN H38   -2.61916   0.06378  -3.37778 SOLU 1      0.00000
   39    1 FADN H39   -2.93377  -1.73122  -3.42439 SOLU 1      0.00000

* ##############################################################################
* # MOVB PERT (Emix Driven) - TS (Ro = 0.44, Rc = -0.020)                      #
* ##############################################################################
*
   39
    1    1 FADN C1     3.26304  -1.63546   1.88011 SOLU 1      0.00000
    2    1 FADN C2     2.29997  -0.77370   1.38939 SOLU 1      0.00000
    3    1 FADN C3     0.94034  -0.91537   1.77372 SOLU 1      0.00000
    4    1 FADN C4     0.57937  -1.97825   2.66947 SOLU 1      0.00000
    5    1 FADN C5     1.59122  -2.82857   3.16985 SOLU 1      0.00000
    6    1 FADN C6     2.90814  -2.65696   2.77070 SOLU 1      0.00000
    7    1 FADN C7    -1.66656  -1.11811   2.71824 SOLU 1      0.00000
    8    1 FADN C8    -1.25870  -0.09604   1.78012 SOLU 1      0.00000
    9    1 FADN C9    -2.26357   0.90409   1.32245 SOLU 1      0.00000
   10    1 FADN C10   -3.85887  -0.02660   2.94864 SOLU 1      0.00000
   11    1 FADN H11    4.31742  -1.51323   1.57988 SOLU 1      0.00000
   12    1 FADN H12    2.58295   0.04587   0.70544 SOLU 1      0.00000
   13    1 FADN H13    1.36276  -3.62618   3.89496 SOLU 1      0.00000
   14    1 FADN H14    3.68748  -3.32932   3.16963 SOLU 1      0.00000
   15    1 FADN O15   -2.07977   1.69000   0.38298 SOLU 1      0.00000
   16    1 FADN O16   -4.95113  -0.02533   3.53635 SOLU 1      0.00000
   17    1 FADN N17   -3.49906   0.91061   1.98287 SOLU 1      0.00000
   18    1 FADN H18   -4.17202   1.61898   1.75771 SOLU 1      0.00000
   19    1 FADN N19   -2.92725  -1.06166   3.27403 SOLU 1      0.00000
   20    1 FADN H20   -3.23159  -1.70902   3.97557 SOLU 1      0.00000
   21    1 FADN N21   -0.77281  -2.12556   3.05012 SOLU 1      0.00000
   22    1 FADN N22    0.00968   0.01692   1.30221 SOLU 1      0.00000
   23    1 FADN C23   -1.18328  -3.25491   3.85680 SOLU 1      0.00000
   24    1 FADN H24   -1.11509  -2.99996   4.94914 SOLU 1      0.00000
   25    1 FADN H25   -2.23287  -3.56519   3.60044 SOLU 1      0.00000
   26    1 FADN H26   -0.52529  -4.13933   3.63730 SOLU 1      0.00000
   27    1 FADN H27    0.00478   0.00947  -0.01441 SOLU 1      0.00000
   28    1 FADN C28    0.00196   0.00784  -1.31146 SOLU 1      0.00000
   29    1 FADN H29    1.09853  -0.15500  -1.45133 SOLU 1      0.00000
```

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   30    1 FADN H30   -0.36267   1.05828  -1.44343 SOLU 1      0.00000
   31    1 FADN N31   -0.80922  -0.97211  -1.79117 SOLU 1      0.00000
   32    1 FADN C32   -0.33683  -2.31689  -1.97845 SOLU 1      0.00000
   33    1 FADN H33    0.78485  -2.34793  -1.97746 SOLU 1      0.00000
   34    1 FADN H34   -0.71972  -2.98341  -1.15629 SOLU 1      0.00000
   35    1 FADN H35   -0.71232  -2.71479  -2.96085 SOLU 1      0.00000
   36    1 FADN C36   -2.20311  -0.73422  -2.05835 SOLU 1      0.00000
   37    1 FADN H37   -2.83851  -1.41505  -1.42779 SOLU 1      0.00000
   38    1 FADN H38   -2.47429   0.33232  -1.83433 SOLU 1      0.00000
   39    1 FADN H39   -2.41968  -0.94862  -3.14115 SOLU 1      0.00000

* ###########################################################################
* # MOVB PERT (Emix Driven) - PRODUCT                                       #
* ###########################################################################
*
   39
    1    1 FADN C1     3.15746  -2.41090   2.06574 SOLU 1      0.00000
    2    1 FADN C2     2.19747  -1.57399   1.49914 SOLU 1      0.00000
    3    1 FADN C3     0.95894  -1.38077   2.12903 SOLU 1      0.00000
    4    1 FADN C4     0.68613  -2.06650   3.35784 SOLU 1      0.00000
    5    1 FADN C5     1.65894  -2.92569   3.89204 SOLU 1      0.00000
    6    1 FADN C6     2.88696  -3.08596   3.25033 SOLU 1      0.00000
    7    1 FADN C7    -1.60571  -1.34312   3.24600 SOLU 1      0.00000
    8    1 FADN C8    -1.33139  -0.75188   2.00310 SOLU 1      0.00000
    9    1 FADN C9    -2.41560  -0.38478   1.09534 SOLU 1      0.00000
   10    1 FADN C10   -3.99735  -0.97755   2.87578 SOLU 1      0.00000
   11    1 FADN H11    4.13244  -2.53453   1.56952 SOLU 1      0.00000
   12    1 FADN H12    2.43010  -1.04269   0.56485 SOLU 1      0.00000
   13    1 FADN H13    1.46219  -3.48651   4.82012 SOLU 1      0.00000
   14    1 FADN H14    3.64231  -3.75492   3.69171 SOLU 1      0.00000
   15    1 FADN O15   -2.22953  -0.01094  -0.09174 SOLU 1      0.00000
   16    1 FADN O16   -5.16310  -1.03703   3.30718 SOLU 1      0.00000
   17    1 FADN N17   -3.71482  -0.48733   1.58797 SOLU 1      0.00000
   18    1 FADN H18   -4.49145  -0.19960   1.03054 SOLU 1      0.00000
   19    1 FADN N19   -2.92729  -1.42042   3.68455 SOLU 1      0.00000
   20    1 FADN H20   -3.16331  -1.81913   4.56946 SOLU 1      0.00000
   21    1 FADN N21   -0.57376  -1.91274   4.00324 SOLU 1      0.00000
   22    1 FADN N22    0.01016  -0.44906   1.62764 SOLU 1      0.00000
   23    1 FADN C23   -0.65218  -1.93003   5.44151 SOLU 1      0.00000
   24    1 FADN H24   -1.22176  -1.04230   5.82883 SOLU 1      0.00000
   25    1 FADN H25   -1.16610  -2.87357   5.77172 SOLU 1      0.00000
   26    1 FADN H26    0.37847  -1.90155   5.88683 SOLU 1      0.00000
   27    1 FADN H27    0.02967  -0.31064   0.63257 SOLU 1      0.00000
   28    1 FADN C28    0.06277   0.05550  -1.93090 SOLU 1      0.00000
   29    1 FADN H29    0.98992  -0.54320  -1.81619 SOLU 1      0.00000
   30    1 FADN H30   -0.06911   0.96285  -1.29964 SOLU 1      0.00000
   31    1 FADN N31   -0.85930  -0.29262  -2.77739 SOLU 1      0.00000
   32    1 FADN C32   -0.74672  -1.48096  -3.61269 SOLU 1      0.00000
   33    1 FADN H33    0.22863  -2.00683  -3.43290 SOLU 1      0.00000
   34    1 FADN H34   -1.59709  -2.17643  -3.36955 SOLU 1      0.00000
   35    1 FADN H35   -0.81451  -1.17570  -4.69304 SOLU 1      0.00000
   36    1 FADN C36   -2.09775   0.46196  -2.94109 SOLU 1      0.00000
   37    1 FADN H37   -2.95721  -0.18974  -2.61983 SOLU 1      0.00000
   38    1 FADN H38   -2.08952   1.38081  -2.29423 SOLU 1      0.00000
   39    1 FADN H39   -2.20974   0.74609  -4.02171 SOLU 1      0.00000
```

S1.3 AM1-MOVB optimized structures using the geometric reaction coordinate Rc=R[C-H] – R[H-N]

(red points in Figure 1 of main text, and also Figures 2-4). The *optimized* parameters (α_{CH}, α_{HN}, $\Delta\varepsilon$, and γ_{rp}) are here emplyed.

```
* ##########################################################################
* # MOVB RXNC (Geometry Driven) - REACTANT IN-PLANE                        #
* ##########################################################################
*
   39
    1    1 FADN C1     0.03448  -0.25064   0.10805 SOLU 1      0.00000
    2    1 FADN C2     0.08655  -0.34689   1.48385 SOLU 1      0.00000
    3    1 FADN C3     1.33414  -0.22307   2.16259 SOLU 1      0.00000
    4    1 FADN C4     2.53799  -0.03005   1.39057 SOLU 1      0.00000
    5    1 FADN C5     2.43811   0.09449  -0.01386 SOLU 1      0.00000
    6    1 FADN C6     1.20354  -0.01919  -0.63412 SOLU 1      0.00000
    7    1 FADN C7     3.78638   0.07644   3.44435 SOLU 1      0.00000
    8    1 FADN C8     2.50459  -0.11950   4.16471 SOLU 1      0.00000
    9    1 FADN C9     2.52581  -0.14623   5.67082 SOLU 1      0.00000
   10    1 FADN C10    4.95855   0.26304   5.60344 SOLU 1      0.00000
   11    1 FADN H11   -0.93482  -0.34598  -0.41317 SOLU 1      0.00000
   12    1 FADN H12   -0.83791  -0.50983   2.07263 SOLU 1      0.00000
   13    1 FADN H13    3.32116   0.30237  -0.63955 SOLU 1      0.00000
   14    1 FADN H14    1.13954   0.08000  -1.73293 SOLU 1      0.00000
   15    1 FADN O15    1.52376  -0.32767   6.36258 SOLU 1      0.00000
   16    1 FADN O16    6.05504   0.44531   6.14724 SOLU 1      0.00000
   17    1 FADN N17    3.76776   0.04961   6.28767 SOLU 1      0.00000
   18    1 FADN H18    3.81446   0.04165   7.29184 SOLU 1      0.00000
   19    1 FADN N19    4.93231   0.27697   4.16400 SOLU 1      0.00000
   20    1 FADN H20    5.82196   0.44168   3.72799 SOLU 1      0.00000
   21    1 FADN N21    3.77474   0.04176   2.06816 SOLU 1      0.00000
   22    1 FADN N22    1.35749  -0.27707   3.54066 SOLU 1      0.00000
   23    1 FADN C23    5.01631   0.08075   1.31402 SOLU 1      0.00000
   24    1 FADN H24    5.35242   1.14624   1.19132 SOLU 1      0.00000
   25    1 FADN H25    5.81420  -0.52132   1.82955 SOLU 1      0.00000
   26    1 FADN H26    4.87117  -0.38676   0.30226 SOLU 1      0.00000
   27    1 FADN H27   -1.61600   0.38424   4.05691 SOLU 1      0.00000
   28    1 FADN C28   -2.68811   0.62222   4.24082 SOLU 1      0.00000
   29    1 FADN H29   -2.84593   1.71691   4.05708 SOLU 1      0.00000
   30    1 FADN H30   -2.92040   0.40074   5.31783 SOLU 1      0.00000
   31    1 FADN N31   -3.46522  -0.16010   3.30612 SOLU 1      0.00000
   32    1 FADN C32   -4.76633   0.40605   3.02278 SOLU 1      0.00000
   33    1 FADN H33   -4.63342   1.44804   2.63028 SOLU 1      0.00000
   34    1 FADN H34   -5.26798  -0.21396   2.23417 SOLU 1      0.00000
   35    1 FADN H35   -5.43706   0.44599   3.92401 SOLU 1      0.00000
   36    1 FADN C36   -3.53096  -1.55872   3.67247 SOLU 1      0.00000
   37    1 FADN H37   -4.02496  -2.12871   2.84274 SOLU 1      0.00000
   38    1 FADN H38   -2.48839  -1.94783   3.81086 SOLU 1      0.00000
   39    1 FADN H39   -4.10515  -1.74167   4.62181 SOLU 1      0.00000

* ##########################################################################
* # MOVB RXNC (Geometry Driven) - REACTANT BELOW                           #
* ##########################################################################
*
   39
    1    1 FADN C1     3.36211  -1.44157   2.65439 SOLU 1      0.00000
    2    1 FADN C2     2.44899  -0.44590   2.37569 SOLU 1      0.00000
    3    1 FADN C3     1.06571  -0.64428   2.65616 SOLU 1      0.00000
    4    1 FADN C4     0.63296  -1.90533   3.20561 SOLU 1      0.00000
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    5    1 FADN C5     1.60370  -2.88893   3.50668 SOLU 1      0.00000
    6    1 FADN C6     2.94024  -2.65262   3.22785 SOLU 1      0.00000
    7    1 FADN C7    -1.61725  -1.05565   3.26703 SOLU 1      0.00000
    8    1 FADN C8    -1.09124   0.21200   2.70199 SOLU 1      0.00000
    9    1 FADN C9    -2.05715   1.34212   2.45460 SOLU 1      0.00000
   10    1 FADN C10   -3.86891  -0.06005   3.37230 SOLU 1      0.00000
   11    1 FADN H11    4.43334  -1.28674   2.43481 SOLU 1      0.00000
   12    1 FADN H12    2.77534   0.51713   1.93982 SOLU 1      0.00000
   13    1 FADN H13    1.32942  -3.84496   3.98158 SOLU 1      0.00000
   14    1 FADN H14    3.68852  -3.43027   3.46643 SOLU 1      0.00000
   15    1 FADN O15   -1.72873   2.42170   1.96317 SOLU 1      0.00000
   16    1 FADN O16   -5.04644  -0.25553   3.69757 SOLU 1      0.00000
   17    1 FADN N17   -3.39216   1.12016   2.81462 SOLU 1      0.00000
   18    1 FADN H18   -4.06021   1.85713   2.66783 SOLU 1      0.00000
   19    1 FADN N19   -2.94207  -1.14036   3.59433 SOLU 1      0.00000
   20    1 FADN H20   -3.34559  -1.96370   4.00465 SOLU 1      0.00000
   21    1 FADN N21   -0.74520  -2.10788   3.43623 SOLU 1      0.00000
   22    1 FADN N22    0.17794   0.38161   2.40456 SOLU 1      0.00000
   23    1 FADN C23   -1.23232  -3.41324   3.84959 SOLU 1      0.00000
   24    1 FADN H24   -1.35412  -3.43639   4.96679 SOLU 1      0.00000
   25    1 FADN H25   -2.21070  -3.64889   3.34706 SOLU 1      0.00000
   26    1 FADN H26   -0.51276  -4.21639   3.53344 SOLU 1      0.00000
   27    1 FADN H27   -0.00784  -0.02111  -1.71651 SOLU 1      0.00000
   28    1 FADN C28   -0.05777  -0.12942  -2.82706 SOLU 1      0.00000
   29    1 FADN H29    0.97650  -0.34429  -3.20427 SOLU 1      0.00000
   30    1 FADN H30   -0.40856   0.84524  -3.25761 SOLU 1      0.00000
   31    1 FADN N31   -0.94450  -1.18220  -3.24938 SOLU 1      0.00000
   32    1 FADN C32   -0.50445  -2.50185  -2.87085 SOLU 1      0.00000
   33    1 FADN H33    0.53760  -2.66366  -3.25280 SOLU 1      0.00000
   34    1 FADN H34   -0.50351  -2.66534  -1.75639 SOLU 1      0.00000
   35    1 FADN H35   -1.18206  -3.26286  -3.33955 SOLU 1      0.00000
   36    1 FADN C36   -2.33352  -0.92696  -2.95786 SOLU 1      0.00000
   37    1 FADN H37   -2.55699  -0.90804  -1.85425 SOLU 1      0.00000
   38    1 FADN H38   -2.62297   0.06471  -3.39465 SOLU 1      0.00000
   39    1 FADN H39   -2.96029  -1.72673  -3.43271 SOLU 1      0.00000

* ##########################################################################
* # MOVB RXNC (Geometry Driven) - TS (Rc = -0.040 )                        #
* ##########################################################################
*
   39
    1    1 FADN C1     3.26083  -1.63244   1.87056 SOLU 1      0.00000
    2    1 FADN C2     2.29780  -0.76799   1.38508 SOLU 1      0.00000
    3    1 FADN C3     0.93833  -0.91005   1.77004 SOLU 1      0.00000
    4    1 FADN C4     0.57630  -1.97886   2.65724 SOLU 1      0.00000
    5    1 FADN C5     1.58866  -2.83070   3.15559 SOLU 1      0.00000
    6    1 FADN C6     2.90559  -2.65753   2.75729 SOLU 1      0.00000
    7    1 FADN C7    -1.66979  -1.12064   2.70808 SOLU 1      0.00000
    8    1 FADN C8    -1.25911  -0.08825   1.78212 SOLU 1      0.00000
    9    1 FADN C9    -2.26576   0.91175   1.32546 SOLU 1      0.00000
   10    1 FADN C10   -3.86192  -0.02827   2.94367 SOLU 1      0.00000
   11    1 FADN H11    4.31538  -1.50946   1.57025 SOLU 1      0.00000
   12    1 FADN H12    2.58128   0.05350   0.70352 SOLU 1      0.00000
   13    1 FADN H13    1.36112  -3.63092   3.87870 SOLU 1      0.00000
   14    1 FADN H14    3.68518  -3.33102   3.15440 SOLU 1      0.00000
   15    1 FADN O15   -2.08038   1.69792   0.38677 SOLU 1      0.00000
   16    1 FADN O16   -4.95364  -0.03120   3.53187 SOLU 1      0.00000
```

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   17    1 FADN N17   -3.50176   0.91522   1.98429 SOLU 1      0.00000
   18    1 FADN H18   -4.17559   1.62366   1.76011 SOLU 1      0.00000
   19    1 FADN N19   -2.93006  -1.06588   3.26375 SOLU 1      0.00000
   20    1 FADN H20   -3.23584  -1.71631   3.96235 SOLU 1      0.00000
   21    1 FADN N21   -0.77553  -2.12811   3.03805 SOLU 1      0.00000
   22    1 FADN N22    0.01140   0.03569   1.30885 SOLU 1      0.00000
   23    1 FADN C23   -1.18151  -3.25308   3.85400 SOLU 1      0.00000
   24    1 FADN H24   -1.10667  -2.99349   4.94512 SOLU 1      0.00000
   25    1 FADN H25   -2.23254  -3.56447   3.60475 SOLU 1      0.00000
   26    1 FADN H26   -0.52474  -4.13873   3.63520 SOLU 1      0.00000
   27    1 FADN H27    0.00689   0.01387  -0.00340 SOLU 1      0.00000
   28    1 FADN C28    0.00478  -0.00096  -1.27566 SOLU 1      0.00000
   29    1 FADN H29    1.09819  -0.16526  -1.44854 SOLU 1      0.00000
   30    1 FADN H30   -0.35203   1.04736  -1.45262 SOLU 1      0.00000
   31    1 FADN N31   -0.81179  -0.98426  -1.76192 SOLU 1      0.00000
   32    1 FADN C32   -0.33791  -2.32478  -1.95992 SOLU 1      0.00000
   33    1 FADN H33    0.78368  -2.35551  -1.95242 SOLU 1      0.00000
   34    1 FADN H34   -0.72533  -3.00214  -1.14855 SOLU 1      0.00000
   35    1 FADN H35   -0.70614  -2.71400  -2.94891 SOLU 1      0.00000
   36    1 FADN C36   -2.19806  -0.73716  -2.04914 SOLU 1      0.00000
   37    1 FADN H37   -2.84768  -1.41651  -1.43121 SOLU 1      0.00000
   38    1 FADN H38   -2.46635   0.33000  -1.82570 SOLU 1      0.00000
   39    1 FADN H39   -2.40243  -0.94598  -3.13573 SOLU 1      0.00000

* ##############################################################################
* # MOVB RXNC (Geometry Driven) - PRODUCT                                      #
* ##############################################################################
*
   39
    1    1 FADN C1     3.16009  -2.36854   2.02644 SOLU 1      0.00000
    2    1 FADN C2     2.19138  -1.54097   1.46262 SOLU 1      0.00000
    3    1 FADN C3     0.94502  -1.37139   2.08732 SOLU 1      0.00000
    4    1 FADN C4     0.68084  -2.06480   3.31433 SOLU 1      0.00000
    5    1 FADN C5     1.66429  -2.91354   3.84634 SOLU 1      0.00000
    6    1 FADN C6     2.89476  -3.05562   3.20581 SOLU 1      0.00000
    7    1 FADN C7    -1.61440  -1.34996   3.21450 SOLU 1      0.00000
    8    1 FADN C8    -1.34908  -0.75160   1.97057 SOLU 1      0.00000
    9    1 FADN C9    -2.44410  -0.35522   1.08653 SOLU 1      0.00000
   10    1 FADN C10   -4.00761  -0.95250   2.88130 SOLU 1      0.00000
   11    1 FADN H11    4.13884  -2.47621   1.53358 SOLU 1      0.00000
   12    1 FADN H12    2.41975  -0.99775   0.53395 SOLU 1      0.00000
   13    1 FADN H13    1.47390  -3.48143   4.77152 SOLU 1      0.00000
   14    1 FADN H14    3.65716  -3.71872   3.64411 SOLU 1      0.00000
   15    1 FADN O15   -2.27183   0.03628  -0.09598 SOLU 1      0.00000
   16    1 FADN O16   -5.16614  -1.00249   3.33202 SOLU 1      0.00000
   17    1 FADN N17   -3.73727  -0.44888   1.59693 SOLU 1      0.00000
   18    1 FADN H18   -4.51781  -0.14279   1.05442 SOLU 1      0.00000
   19    1 FADN N19   -2.93098  -1.42258   3.66662 SOLU 1      0.00000
   20    1 FADN H20   -3.15928  -1.82500   4.55206 SOLU 1      0.00000
   21    1 FADN N21   -0.57784  -1.92137   3.96188 SOLU 1      0.00000
   22    1 FADN N22   -0.01479  -0.46224   1.57498 SOLU 1      0.00000
   23    1 FADN C23   -0.65930  -1.97321   5.39942 SOLU 1      0.00000
   24    1 FADN H24   -1.23380  -1.09706   5.80581 SOLU 1      0.00000
   25    1 FADN H25   -1.16847  -2.92647   5.70820 SOLU 1      0.00000
   26    1 FADN H26    0.36997  -1.94809   5.84801 SOLU 1      0.00000
   27    1 FADN H27    0.01026  -0.32359   0.58230 SOLU 1      0.00000
   28    1 FADN C28    0.05986   0.02508  -1.83880 SOLU 1      0.00000
```

```
   29    1 FADN H29    0.96179  -0.60012  -1.67721 SOLU 1      0.00000
   30    1 FADN H30   -0.05782   0.96123  -1.24861 SOLU 1      0.00000
   31    1 FADN N31   -0.84588  -0.32030  -2.70582 SOLU 1      0.00000
   32    1 FADN C32   -0.74845  -1.54000  -3.49556 SOLU 1      0.00000
   33    1 FADN H33    0.20434  -2.08929  -3.27045 SOLU 1      0.00000
   34    1 FADN H34   -1.62684  -2.20033  -3.25434 SOLU 1      0.00000
   35    1 FADN H35   -0.77694  -1.27068  -4.58721 SOLU 1      0.00000
   36    1 FADN C36   -2.04903   0.47152  -2.93809 SOLU 1      0.00000
   37    1 FADN H37   -2.94417  -0.14436  -2.64505 SOLU 1      0.00000
   38    1 FADN H38   -2.03739   1.40190  -2.30796 SOLU 1      0.00000
   39    1 FADN H39   -2.10354   0.73862  -4.02760 SOLU 1      0.00000

* ##########################################################################
* # MOVB RXNC UNSCALED (Geom. Driv.) - REACTANT IN-PLANE                   #
* ##########################################################################
*
   39
    1    1 FADN C1     0.06975  -0.28545   0.08810 SOLU 1      0.00000
    2    1 FADN C2     0.11715  -0.38614   1.46371 SOLU 1      0.00000
    3    1 FADN C3     1.36004  -0.24914   2.14856 SOLU 1      0.00000
    4    1 FADN C4     2.56486  -0.03976   1.38239 SOLU 1      0.00000
    5    1 FADN C5     2.46956   0.08856  -0.02211 SOLU 1      0.00000
    6    1 FADN C6     1.23919  -0.03724  -0.64818 SOLU 1      0.00000
    7    1 FADN C7     3.80343   0.07460   3.44178 SOLU 1      0.00000
    8    1 FADN C8     2.52068  -0.13724   4.15613 SOLU 1      0.00000
    9    1 FADN C9     2.53554  -0.16710   5.66237 SOLU 1      0.00000
   10    1 FADN C10    4.96420   0.26713   5.60658 SOLU 1      0.00000
   11    1 FADN H11   -0.89611  -0.39042  -0.43777 SOLU 1      0.00000
   12    1 FADN H12   -0.80800  -0.56383   2.04609 SOLU 1      0.00000
   13    1 FADN H13    3.35288   0.30882  -0.64322 SOLU 1      0.00000
   14    1 FADN H14    1.17853   0.06532  -1.74691 SOLU 1      0.00000
   15    1 FADN O15    1.53196  -0.35971   6.34889 SOLU 1      0.00000
   16    1 FADN O16    6.05634   0.45912   6.15555 SOLU 1      0.00000
   17    1 FADN N17    3.77274   0.03924   6.28507 SOLU 1      0.00000
   18    1 FADN H18    3.81522   0.02881   7.28945 SOLU 1      0.00000
   19    1 FADN N19    4.94396   0.28525   4.16697 SOLU 1      0.00000
   20    1 FADN H20    5.83372   0.46072   3.73531 SOLU 1      0.00000
   21    1 FADN N21    3.79786   0.04393   2.06547 SOLU 1      0.00000
   22    1 FADN N22    1.37836  -0.30617   3.52667 SOLU 1      0.00000
   23    1 FADN C23    5.04227   0.09869   1.31693 SOLU 1      0.00000
   24    1 FADN H24    5.36828   1.16802   1.20051 SOLU 1      0.00000
   25    1 FADN H25    5.84375  -0.49776   1.83349 SOLU 1      0.00000
   26    1 FADN H26    4.90639  -0.36570   0.30246 SOLU 1      0.00000
   27    1 FADN H27   -1.65017   0.39811   4.05192 SOLU 1      0.00000
   28    1 FADN C28   -2.73093   0.64883   4.23651 SOLU 1      0.00000
   29    1 FADN H29   -2.88204   1.74214   4.04121 SOLU 1      0.00000
   30    1 FADN H30   -2.97182   0.44270   5.31417 SOLU 1      0.00000
   31    1 FADN N31   -3.51823  -0.13296   3.30671 SOLU 1      0.00000
   32    1 FADN C32   -4.84120   0.41005   3.08355 SOLU 1      0.00000
   33    1 FADN H33   -4.74437   1.46247   2.70883 SOLU 1      0.00000
   34    1 FADN H34   -5.35852  -0.20420   2.30075 SOLU 1      0.00000
   35    1 FADN H35   -5.47907   0.41752   4.00917 SOLU 1      0.00000
   36    1 FADN C36   -3.54609  -1.53807   3.65380 SOLU 1      0.00000
   37    1 FADN H37   -4.06023  -2.10444   2.83390 SOLU 1      0.00000
   38    1 FADN H38   -2.49296  -1.91104   3.74800 SOLU 1      0.00000
   39    1 FADN H39   -4.08167  -1.74622   4.62042 SOLU 1      0.00000
```

S1.4 AM1-MOVB optimized structures using the geometric reaction coordinate Rc=R[C-H] – R[H-N]. All the parameters (α_{CH}, α_{HN}, $\Delta\varepsilon$, and γ_{rp}) were set to zero.

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* ##########################################################################
* # MOVB RXNC UNSCALED (Geom. Driv.) - REACTANT BELOW                      #
* ##########################################################################
*
   39
    1    1 FADN C1     3.36235  -1.45475   2.66791 SOLU 1      0.00000
    2    1 FADN C2     2.45044  -0.45974   2.38292 SOLU 1      0.00000
    3    1 FADN C3     1.06707  -0.65420   2.66556 SOLU 1      0.00000
    4    1 FADN C4     0.63302  -1.91094   3.22361 SOLU 1      0.00000
    5    1 FADN C5     1.60234  -2.89427   3.53010 SOLU 1      0.00000
    6    1 FADN C6     2.93912  -2.66154   3.24932 SOLU 1      0.00000
    7    1 FADN C7    -1.61564  -1.05718   3.28370 SOLU 1      0.00000
    8    1 FADN C8    -1.08853   0.20558   2.70852 SOLU 1      0.00000
    9    1 FADN C9    -2.05318   1.33527   2.45405 SOLU 1      0.00000
   10    1 FADN C10   -3.86473  -0.05565   3.38881 SOLU 1      0.00000
   11    1 FADN H11    4.43372  -1.30273   2.44693 SOLU 1      0.00000
   12    1 FADN H12    2.77795   0.49991   1.94059 SOLU 1      0.00000
   13    1 FADN H13    1.32642  -3.84699   4.01072 SOLU 1      0.00000
   14    1 FADN H14    3.68655  -3.43859   3.49254 SOLU 1      0.00000
   15    1 FADN O15   -1.72386   2.40982   1.95224 SOLU 1      0.00000
   16    1 FADN O16   -5.04116  -0.24563   3.72105 SOLU 1      0.00000
   17    1 FADN N17   -3.38759   1.11879   2.81927 SOLU 1      0.00000
   18    1 FADN H18   -4.05472   1.85579   2.66818 SOLU 1      0.00000
   19    1 FADN N19   -2.93960  -1.13656   3.61539 SOLU 1      0.00000
   20    1 FADN H20   -3.34388  -1.95584   4.03309 SOLU 1      0.00000
   21    1 FADN N21   -0.74522  -2.11001   3.45703 SOLU 1      0.00000
   22    1 FADN N22    0.18039   0.37115   2.40785 SOLU 1      0.00000
   23    1 FADN C23   -1.23208  -3.41286   3.87854 SOLU 1      0.00000
   24    1 FADN H24   -1.33943  -3.43391   4.99725 SOLU 1      0.00000
   25    1 FADN H25   -2.21751  -3.64639   3.38917 SOLU 1      0.00000
   26    1 FADN H26   -0.51892  -4.21853   3.55392 SOLU 1      0.00000
   27    1 FADN H27   -0.00985  -0.00525  -1.71809 SOLU 1      0.00000
   28    1 FADN C28   -0.06157  -0.10769  -2.84161 SOLU 1      0.00000
   29    1 FADN H29    0.97338  -0.30543  -3.22532 SOLU 1      0.00000
   30    1 FADN H30   -0.42475   0.86394  -3.26757 SOLU 1      0.00000
   31    1 FADN N31   -0.93484  -1.16975  -3.27605 SOLU 1      0.00000
   32    1 FADN C32   -0.48180  -2.48392  -2.89315 SOLU 1      0.00000
   33    1 FADN H33    0.56706  -2.63112  -3.26209 SOLU 1      0.00000
   34    1 FADN H34   -0.49300  -2.65024  -1.77933 SOLU 1      0.00000
   35    1 FADN H35   -1.14305  -3.25283  -3.37209 SOLU 1      0.00000
   36    1 FADN C36   -2.32713  -0.93041  -2.98577 SOLU 1      0.00000
   37    1 FADN H37   -2.55456  -0.92154  -1.88302 SOLU 1      0.00000
   38    1 FADN H38   -2.62557   0.06104  -3.41698 SOLU 1      0.00000
   39    1 FADN H39   -2.94425  -1.73317  -3.46813 SOLU 1      0.00000

* ##########################################################################
* # MOVB RXNC UNSCALED (Geom. Driv.) - TS (Rc = 0.040 )                    #
* ##########################################################################
*
   39
    1    1 FADN C1     3.26925  -1.61674   1.93547 SOLU 1      0.00000
    2    1 FADN C2     2.32008  -0.71182   1.50415 SOLU 1      0.00000
    3    1 FADN C3     0.96010  -0.84916   1.89786 SOLU 1      0.00000
    4    1 FADN C4     0.58439  -1.96235   2.72433 SOLU 1      0.00000
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     5    1 FADN C5     1.58760  -2.85261   3.17499 SOLU 1      0.00000
     6    1 FADN C6     2.90293  -2.67839   2.77624 SOLU 1      0.00000
     7    1 FADN C7    -1.66395  -1.10993   2.77135 SOLU 1      0.00000
     8    1 FADN C8    -1.21767  -0.01611   1.91344 SOLU 1      0.00000
     9    1 FADN C9    -2.22263   0.99481   1.46133 SOLU 1      0.00000
    10    1 FADN C10   -3.88334  -0.05879   2.94484 SOLU 1      0.00000
    11    1 FADN H11    4.32272  -1.50317   1.62772 SOLU 1      0.00000
    12    1 FADN H12    2.60452   0.13446   0.85251 SOLU 1      0.00000
    13    1 FADN H13    1.35430  -3.68378   3.85962 SOLU 1      0.00000
    14    1 FADN H14    3.67505  -3.38306   3.13228 SOLU 1      0.00000
    15    1 FADN O15   -2.00911   1.84199   0.58850 SOLU 1      0.00000
    16    1 FADN O16   -5.00251  -0.11774   3.47428 SOLU 1      0.00000
    17    1 FADN N17   -3.49135   0.93752   2.05757 SOLU 1      0.00000
    18    1 FADN H18   -4.16947   1.64146   1.83121 SOLU 1      0.00000
    19    1 FADN N19   -2.94602  -1.09556   3.26689 SOLU 1      0.00000
    20    1 FADN H20   -3.27965  -1.78310   3.91619 SOLU 1      0.00000
    21    1 FADN N21   -0.76953  -2.11283   3.09546 SOLU 1      0.00000
    22    1 FADN N22    0.04785   0.12458   1.48634 SOLU 1      0.00000
    23    1 FADN C23   -1.18618  -3.26607   3.86956 SOLU 1      0.00000
    24    1 FADN H24   -1.13137  -3.03132   4.96729 SOLU 1      0.00000
    25    1 FADN H25   -2.23032  -3.57808   3.59399 SOLU 1      0.00000
    26    1 FADN H26   -0.52263  -4.14358   3.63985 SOLU 1      0.00000
    27    1 FADN H27    0.03126   0.05700  -0.00209 SOLU 1      0.00000
    28    1 FADN C28    0.01695  -0.00177  -1.53070 SOLU 1      0.00000
    29    1 FADN H29    1.10567  -0.18033  -1.64979 SOLU 1      0.00000
    30    1 FADN H30   -0.33899   1.04162  -1.67160 SOLU 1      0.00000
    31    1 FADN N31   -0.80991  -0.99235  -1.96750 SOLU 1      0.00000
    32    1 FADN C32   -0.35681  -2.35231  -2.05565 SOLU 1      0.00000
    33    1 FADN H33    0.75823  -2.38675  -2.17737 SOLU 1      0.00000
    34    1 FADN H34   -0.63817  -2.92821  -1.13096 SOLU 1      0.00000
    35    1 FADN H35   -0.83484  -2.84886  -2.94312 SOLU 1      0.00000
    36    1 FADN C36   -2.21908  -0.76497  -2.13842 SOLU 1      0.00000
    37    1 FADN H37   -2.80699  -1.33594  -1.36841 SOLU 1      0.00000
    38    1 FADN H38   -2.45754   0.32757  -2.04180 SOLU 1      0.00000
    39    1 FADN H39   -2.53251  -1.11947  -3.15823 SOLU 1      0.00000

* ###########################################################################
* # MOVB RXNC UNSCALED (Geom. Driv.) - PRODUCT                              #
* ###########################################################################
*
    39
     1    1 FADN C1     3.18547  -2.40942   2.16906 SOLU 1      0.00000
     2    1 FADN C2     2.23322  -1.57205   1.59036 SOLU 1      0.00000
     3    1 FADN C3     0.98450  -1.38370   2.20114 SOLU 1      0.00000
     4    1 FADN C4     0.69357  -2.07326   3.42349 SOLU 1      0.00000
     5    1 FADN C5     1.65965  -2.93224   3.97024 SOLU 1      0.00000
     6    1 FADN C6     2.89763  -3.08879   3.34714 SOLU 1      0.00000
     7    1 FADN C7    -1.59767  -1.35349   3.27782 SOLU 1      0.00000
     8    1 FADN C8    -1.30462  -0.76048   2.04110 SOLU 1      0.00000
     9    1 FADN C9    -2.37417  -0.40206   1.11198 SOLU 1      0.00000
    10    1 FADN C10   -3.98293  -0.98914   2.87076 SOLU 1      0.00000
    11    1 FADN H11    4.16812  -2.52999   1.68757 SOLU 1      0.00000
    12    1 FADN H12    2.47882  -1.03703   0.66145 SOLU 1      0.00000
    13    1 FADN H13    1.44936  -3.49621   4.89335 SOLU 1      0.00000
    14    1 FADN H14    3.64682  -3.75850   3.79770 SOLU 1      0.00000
    15    1 FADN O15   -2.17080  -0.03851  -0.07551 SOLU 1      0.00000
    16    1 FADN O16   -5.15556  -1.04527   3.28426 SOLU 1      0.00000
```

17	1	FADN	N17	-3.68088	-0.50252	1.58582	SOLU	1	0.00000
18	1	FADN	H18	-4.44918	-0.21710	1.01626	SOLU	1	0.00000
19	1	FADN	N19	-2.92606	-1.43176	3.69618	SOLU	1	0.00000
20	1	FADN	H20	-3.17533	-1.83289	4.57620	SOLU	1	0.00000
21	1	FADN	N21	-0.57727	-1.92620	4.04978	SOLU	1	0.00000
22	1	FADN	N22	0.04202	-0.45183	1.68679	SOLU	1	0.00000
23	1	FADN	C23	-0.67440	-1.92794	5.48727	SOLU	1	0.00000
24	1	FADN	H24	-1.23129	-1.02572	5.85936	SOLU	1	0.00000
25	1	FADN	H25	-1.21195	-2.85791	5.81838	SOLU	1	0.00000
26	1	FADN	H26	0.35035	-1.91702	5.94640	SOLU	1	0.00000
27	1	FADN	H27	0.06466	-0.32405	0.68972	SOLU	1	0.00000
28	1	FADN	C28	0.10528	0.04487	-2.11841	SOLU	1	0.00000
29	1	FADN	H29	1.04902	-0.53901	-2.11430	SOLU	1	0.00000
30	1	FADN	H30	0.01281	0.91249	-1.42718	SOLU	1	0.00000
31	1	FADN	N31	-0.88126	-0.28026	-2.89835	SOLU	1	0.00000
32	1	FADN	C32	-0.82181	-1.42525	-3.79763	SOLU	1	0.00000
33	1	FADN	H33	0.18089	-1.92710	-3.74218	SOLU	1	0.00000
34	1	FADN	H34	-1.62396	-2.15746	-3.50354	SOLU	1	0.00000
35	1	FADN	H35	-1.00762	-1.07422	-4.84983	SOLU	1	0.00000
36	1	FADN	C36	-2.14001	0.45785	-2.92117	SOLU	1	0.00000
37	1	FADN	H37	-2.95802	-0.22009	-2.54982	SOLU	1	0.00000
38	1	FADN	H38	-2.08683	1.35266	-2.24336	SOLU	1	0.00000
39	1	FADN	H39	-2.35287	0.77967	-3.97581	SOLU	1	0.00000

S2.1 B3LYP/6-31+G(d) optimized structures and absolute energies

```
39
B3LYP/6-31+G(d) REACTANT : E=-968.354103652; N.R.E.=1638.0099683553
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.379664
  C        1.233136    0.000000    2.083685
  C        2.468809   -0.015351    1.354797
  C        2.446706    0.002464   -0.047463
  C        1.221465    0.010400   -0.704658
  C        3.608399    0.058161    3.445817
  C        2.333761    0.067722    4.101718
  C        2.276474    0.115836    5.603772
  C        4.772448    0.208976    5.616866
  H       -0.939207    0.002805   -0.543685
  H       -0.928654    0.007699    1.944961
  H        3.354545    0.035337   -0.636026
  H        1.213695    0.030968   -1.790519
  O        1.250919    0.104814    6.238959
  O        5.831190    0.295378    6.188429
  N        3.534247    0.172759    6.220114
  H        3.538095    0.214534    7.237537
  N        4.736887    0.133398    4.193176
  H        5.660027    0.217521    3.781932
  N        3.657612   -0.041983    2.100716
  N        1.208781    0.025442    3.439258
  C        4.967212   -0.174552    1.424457
  H        5.413680    0.810358    1.255986
  H        5.626853   -0.799600    2.028654
  H        4.829834   -0.684316    0.474839
  H       -1.432761    0.442172    4.010650
  C       -2.489378    0.608864    4.239207
  H       -2.698820    1.678346    4.130443
```

```
  H       -2.683174    0.320093    5.288804
  N       -3.285209   -0.148678    3.272386
  C       -4.693587    0.243601    3.296718
  H       -4.783906    1.312473    3.077390
  H       -5.243902   -0.310797    2.529206
  H       -5.173548    0.047204    4.274723
  C       -3.139832   -1.585858    3.489685
  H       -3.681177   -2.136748    2.713014
  H       -2.081281   -1.868257    3.439332
  H       -3.526283   -1.908750    4.476015

39
B3LYP/6-31+G(d) TS : E=-968.354103652; N.R.E.=1638.0099683553
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.388200
  C        1.209395    0.000000    2.103708
  C        2.438484    0.011271    1.399256
  C        2.431357    0.034986   -0.002726
  C        1.219649    0.021208   -0.690982
  C        3.568266    0.268037    3.484621
  C        2.336429    0.238985    4.150936
  C        2.285380    0.444472    5.601363
  C        4.746703    0.836444    5.572987
  H       -0.937979    0.003330   -0.546148
  H       -0.928078    0.017596    1.952093
  H        3.354366    0.082275   -0.567842
  H        1.229834    0.042852   -1.776418
  O        1.270617    0.342172    6.274651
  O        5.785795    1.134547    6.119271
  N        3.523542    0.722636    6.200153
  H        3.516366    0.908391    7.199714
  N        4.705477    0.561488    4.188528
  H        5.584044    0.758090    3.724161
  N        3.642969    0.039947    2.144148
  N        1.150739    0.005396    3.504270
  C        4.937844   -0.082491    1.459590
  H        5.286128    0.884424    1.079103
  H        5.678125   -0.507169    2.139552
  H        4.835119   -0.780849    0.629284
  H        0.681884   -1.120891    3.912917
  C        0.190837   -2.300489    4.340908
  H       -0.049224   -2.754477    3.375729
  H       -0.657081   -1.873323    4.880580
  N        1.072134   -2.997360    5.109914
  C        1.912147   -4.047660    4.543775
  H        1.884148   -4.002397    3.453373
  H        2.946934   -3.932188    4.883721
  H        1.554138   -5.035034    4.867046
  C        1.048033   -2.872498    6.566071
  H        2.048253   -3.060027    6.966240
  H        0.734286   -1.863933    6.845987
  H        0.355509   -3.607633    6.999161

39
B3LYP/6-31+G(d) PRODUCT : E=-968.360772060; N.R.E.=1634.8734055169
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.399812
```

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  C        1.199629    0.000000    2.108637
  C        2.426049    0.009171    1.403333
  C        2.418079    0.039013    0.009981
  C        1.205694    0.023449   -0.694098
  C        3.606322    0.485729    3.429625
  C        2.410352    0.504627    4.104969
  C        2.289706    1.116889    5.377703
  C        4.735506    1.544448    5.333924
  H       -0.943457   -0.017193   -0.537453
  H       -0.939835   -0.026924    1.946816
  H        3.349938    0.075396   -0.543438
  H        1.218900    0.031058   -1.779364
  O        1.199099    1.238777    5.992772
  O        5.747857    1.978229    5.850058
  N        3.485305    1.567908    5.936192
  H        3.450721    1.994030    6.856246
  N        4.731035    0.982013    4.051369
  H        5.616337    1.055863    3.565734
  N        3.655275   -0.010678    2.153238
  N        1.262075   -0.070202    3.513229
  C        4.922024   -0.279535    1.479628
  H        5.313206    0.598201    0.946625
  H        5.659615   -0.625969    2.207965
  H        4.774393   -1.089562    0.762212
  H        0.479224    0.230890    4.081047
  C       -1.909700    1.149692    5.813781
  H       -2.660528    0.934282    5.058525
  H       -0.836882    1.088114    5.612091
  N       -2.285586    1.498252    6.990357
  C       -3.706695    1.620750    7.369388
  H       -4.342117    1.366830    6.520662
  H       -3.905243    0.943824    8.204566
  H       -3.896237    2.649427    7.687545
  C       -1.299991    1.801041    8.054750
  H       -1.466219    1.104994    8.881615
  H       -0.289590    1.695816    7.656089
  H       -1.476593    2.822483    8.402639
```

S2.1 M06-2X/6-31+G(d) optimized structures and absolute energies

```
39
M062X/6-31+G(d) REACTANT : E=-967.937640973; N.R.E.=1661.6194075564
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.376195
  C        1.236278    0.000000    2.069201
  C        2.459351   -0.020554    1.339521
  C        2.439202   -0.005439   -0.061040
  C        1.215969    0.005819   -0.709692
  C        3.620318    0.079933    3.403994
  C        2.350599    0.095761    4.070791
  C        2.305510    0.169998    5.571097
  C        4.793109    0.269615    5.557481
  H       -0.940822    0.005040   -0.540102
  H       -0.935049    0.007321    1.937711
  H        3.347990    0.026817   -0.648343
  H        1.202324    0.026770   -1.795066
  O        1.287028    0.173925    6.202003
```

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  O        5.849045    0.374352    6.113697
  N        3.564006    0.232635    6.173144
  H        3.581013    0.294369    7.189730
  N        4.749839    0.168358    4.137673
  H        5.669357    0.267970    3.719919
  N        3.651472   -0.044738    2.072489
  N        1.226887    0.038709    3.427036
  C        4.942056   -0.207633    1.379752
  H        5.363507    0.768553    1.124901
  H        5.623313   -0.774427    2.014480
  H        4.783940   -0.795124    0.479279
  H       -1.157127   -0.093906    3.984419
  C       -2.218821   -0.152965    4.232643
  H       -2.590315    0.860211    4.410420
  H       -2.352704   -0.747665    5.152626
  N       -2.897347   -0.731835    3.077358
  C       -4.344436   -0.606912    3.191491
  H       -4.619513    0.449203    3.257786
  H       -4.822889   -1.033635    2.305357
  H       -4.736306   -1.128138    4.083517
  C       -2.518864   -2.128186    2.925312
  H       -2.978052   -2.544427    2.023489
  H       -1.428957   -2.211791    2.830507
  H       -2.828947   -2.742247    3.790775

39
M062X/6-31+G(d) TS : E=-967.909967265; N.R.E.=1782.7586494036
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.384644
  C        1.210321    0.000000    2.088984
  C        2.431884   -0.012447    1.387578
  C        2.427432    0.005992   -0.011066
  C        1.216082    0.007788   -0.691335
  C        3.573303    0.237877    3.455173
  C        2.339314    0.273552    4.116845
  C        2.299838    0.397776    5.576380
  C        4.766198    0.703711    5.549597
  H       -0.936946    0.008074   -0.546428
  H       -0.921174    0.021298    1.959457
  H        3.350665    0.042080   -0.576935
  H        1.222347    0.028215   -1.776338
  O        1.291915    0.282370    6.238623
  O        5.809262    0.954996    6.093566
  N        3.547617    0.600222    6.179258
  H        3.551610    0.759849    7.183847
  N        4.717686    0.464139    4.159393
  H        5.602563    0.648842    3.700003
  N        3.634581   -0.008718    2.129432
  N        1.155916    0.017734    3.490790
  C        4.917864   -0.168190    1.441219
  H        5.283275    0.788431    1.054102
  H        5.647836   -0.607203    2.121865
  H        4.787618   -0.869356    0.617980
  H        0.968386   -1.188655    3.904712
  C        0.781090   -2.393541    4.318118
  H        0.615695   -2.904753    3.365575
  H       -0.094480   -2.268706    4.953395
```

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  N        1.948220   -2.680028    4.964439
  C        3.050816   -3.296820    4.245412
  H        2.980314   -3.052906    3.181873
  H        4.001489   -2.922567    4.637808
  H        3.032931   -4.388712    4.362182
  C        2.019681   -2.692850    6.419065
  H        2.990453   -2.304516    6.742816
  H        1.232742   -2.059813    6.831848
  H        1.907655   -3.718297    6.793674

39
M062X/6-31+G(d) PRODUCT : E=-967.947404275; N.R.E.=1668.1222007662
  C        0.000000    0.000000    0.000000
  C        0.000000    0.000000    1.396386
  C        1.193017    0.000000    2.104889
  C        2.416054    0.018115    1.406337
  C        2.412934    0.048631    0.017010
  C        1.205195    0.026828   -0.687585
  C        3.565817    0.560308    3.411007
  C        2.375347    0.563291    4.081357
  C        2.244153    1.214996    5.332461
  C        4.661816    1.731509    5.253393
  H       -0.941165   -0.018503   -0.539665
  H       -0.939311   -0.027464    1.944627
  H        3.346965    0.092081   -0.532548
  H        1.220905    0.036972   -1.772065
  O        1.163263    1.309594    5.947627
  O        5.650123    2.224877    5.741571
  N        3.416777    1.731875    5.860883
  H        3.366274    2.201026    6.760018
  N        4.674278    1.113147    4.002206
  H        5.551298    1.207233    3.503732
  N        3.634078    0.014072    2.159484
  N        1.243657   -0.074040    3.513810
  C        4.904753   -0.182589    1.481698
  H        5.242699    0.717045    0.950472
  H        5.660460   -0.493603    2.206198
  H        4.793793   -0.997672    0.764751
  H        0.436620    0.272152    4.023432
  C       -1.847478    1.251955    5.465775
  H       -2.591249    1.705443    4.815384
  H       -0.835753    1.654245    5.565156
  N       -2.161489    0.207311    6.129728
  C       -3.496146   -0.406684    6.057643
  H       -4.122613    0.145456    5.358264
  H       -3.382381   -1.442569    5.731420
  H       -3.937041   -0.388272    7.056742
  C       -1.203168   -0.457428    7.035593
  H       -1.101247   -1.495899    6.712457
  H       -0.242102    0.056586    6.987793
  H       -1.621562   -0.429400    8.044358
```