

## Supporting Information for:

# Standard Redox Potentials, pKas, and Hydricities of Inorganic Complexes Under Electrochemical Conditions and Implications for Electrocatalysis

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## Construction of Pourbaix diagrams:

Pourbaix diagrams for each inorganic complex were obtained by calculating the absolute Gibbs free energy of all possible intermediate states that could be obtained by adding up to two protons and two electrons. Intermediate states,  $\text{bpy}_{mn}$ , having the minimum  $\Delta G_{\text{rxn}}$  according to Eq. S1 at any given pH and applied potential were represented in the Pourbaix diagram.

$$(S1) \Delta G_{\text{rxn}} = \min\{G(\text{bpy}_{mn}) - G(\text{bpy}) - m \times G(\text{H}^+) - n \times G(\text{e}^-)\}$$

$$(S2) G = E_{\text{SCF}} + (H - TS) + G_{\text{solv}}$$

$$(S3) G(\text{H}^+) = -272.3 - k_B T \ln(10) \times \text{pH} \times 23.061 + 1.89 \text{ (kcal/mol)}$$

$$(S4) G(\text{e}^-) = -(U + 4.480) \times 23.061 \text{ (kcal/mol)}$$

In Eq. S1,  $G(\text{bpy}_{mn})$  and  $G(\text{bpy})$  are the calculated  $G_{298}$  values obtained using Turbomole using Eq. S2 and basis sets and the level of theory mentioned in the computational methods section of the main text.  $G(\text{H}^+)$  is the solvation energy of proton, -272.3 kcal/mol,<sup>1</sup> a pH correction and the standard state free energy correction for species at 1 M (Eq. S3).  $G(\text{e}^-)$  is the free energy of an electron referenced to Ag/AgCl electrode, 4.480 V (Eq. S4).<sup>2</sup>

For example, the energy of reaction involving transfer of two protons and two electrons to bipyridine (bpy) at pH 5 and  $E = -1.0$  V is given as:  $\text{bpy} + 2\text{H}^+ + 2\text{e}^- \rightarrow \text{bpy}_{22}$

$$\begin{aligned} \Delta G_{\text{rxn}} &= G(\text{bpy}_{22}) - G(\text{bpy}) - 2 G(\text{H}^+) - 2 G(\text{e}^-) \\ &= -311435.29 \text{ kcal/mol} - (-310711.32 \text{ kcal/mol}) - 2 (-272.3 - 0.592 \times (\ln 10) \times 5 \times 23.061 + 1.89) \text{ kcal/mol} \\ &\quad - 2 [(-1.0 + 4.480) \times 23.061] \text{ kcal/mol} \\ &= -29.3 \text{ kcal/mol} \end{aligned}$$

### Fukui functions:

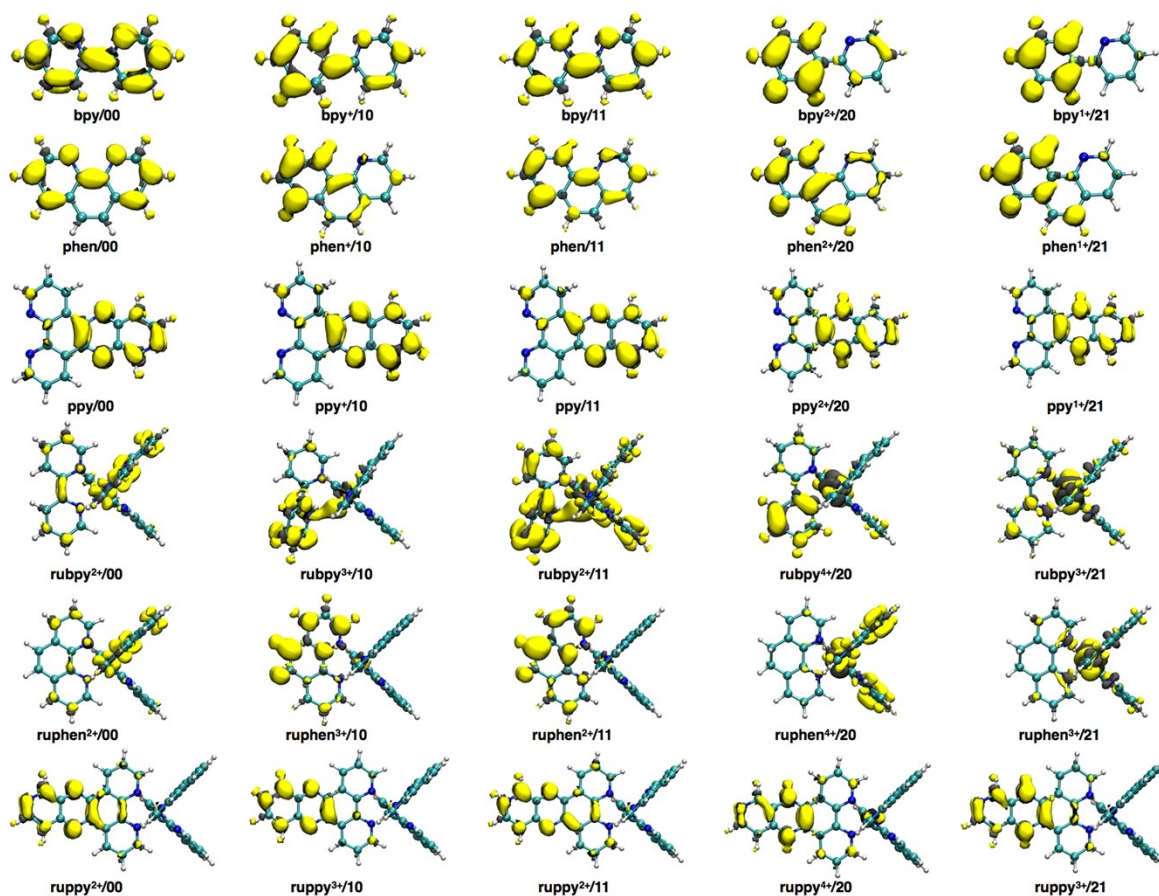


Figure S1: Electron density difference plots of all the molecules considered in our study.

Isosurfaces in yellow indicate an increase in electron density and isosurfaces in blue indicate decrease in electron density upon the subtraction of an electron. These plots show the location of the LUMO orbital for each lowest energy structure.

### Reference:

1. M. D. Tissandier, K. A. Cowen, W. Y. Feng, E. Gundlach, M. H. Cohen, A. D. Earhart, J. V. Coe and T. R. Tuttle, *The Journal of Physical Chemistry A*, 1998, **102**, 7787-7794.
2. A. A. Isse and A. Gennaro, *J. Phys. Chem. B*, 2010, **114**, 7894-7899.

Below, we provide the calculated energies and xyz coordinate for all structures calculated for this study.

bpy\_00

G(bpy\_00) = -310711.32 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.1609957  | 2.6884403  | -0.3028837 |
| C | 0.0542841  | 3.5021363  | -0.0277359 |
| C | -1.1533442 | 2.8755865  | 0.2854841  |
| C | -1.2020065 | 1.4804984  | 0.3035176  |
| C | -0.0361631 | 0.7490477  | 0.0043867  |
| N | 1.1221333  | 1.3587195  | -0.2880026 |
| H | 0.1430391  | 4.5924071  | -0.0557872 |
| H | -2.0464989 | 3.4633890  | 0.5215808  |
| H | -2.1300588 | 0.9683902  | 0.5700755  |
| H | 2.1304915  | 3.1421575  | -0.5510208 |
| C | -0.0359144 | -0.7492893 | 0.0034851  |
| C | -1.2010570 | -1.4804891 | -0.2987439 |
| C | -1.1516088 | -2.8755861 | -0.2853207 |
| C | 0.0561619  | -3.5024319 | 0.0268412  |
| C | 1.1619734  | -2.6889225 | 0.3063172  |
| N | 1.1223827  | -1.3591030 | 0.2957537  |
| H | -2.1289212 | -0.9679236 | -0.5649993 |
| H | 2.1314943  | -3.1430105 | 0.5538469  |
| H | -2.0441214 | -3.4631054 | -0.5246085 |
| H | 0.1457476  | -4.5927142 | 0.0505660  |

bpy\_10

G(bpy\_10) = -310982.83 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | -1.0767542 | 0.0968737  | 0.0337482  |
| C | -2.1976418 | 0.9129178  | -0.0003749 |
| C | -3.4640775 | 0.3078598  | -0.0311230 |
| C | -3.5856127 | -1.0837051 | -0.0269353 |
| C | -2.4322555 | -1.8741607 | 0.0085241  |
| N | -1.2339842 | -1.2394675 | 0.0368969  |
| H | -2.0822970 | 1.9992119  | -0.0029585 |
| H | -4.3644808 | 0.9287982  | -0.0583819 |
| H | -4.5709097 | -1.5518839 | -0.0508993 |
| H | -0.0506896 | 0.4728762  | 0.0591614  |
| C | -2.3433570 | -3.3541473 | 0.0208985  |
| C | -3.4622637 | -4.1958140 | -0.0021605 |
| C | -3.2451142 | -5.5781939 | 0.0152307  |
| C | -1.9354408 | -6.0581939 | 0.0540655  |
| C | -0.8793059 | -5.1326481 | 0.0740210  |
| N | -1.0834509 | -3.8192692 | 0.0578720  |
| H | -4.4795874 | -3.7989096 | -0.0325567 |
| H | 0.1629326  | -5.4697126 | 0.1043080  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -4.0937668 | -6.2680798 | -0.0012185 |
|---|------------|------------|------------|

|   |            |            |           |
|---|------------|------------|-----------|
| H | -1.7254500 | -7.1312061 | 0.0690707 |
|---|------------|------------|-----------|

|   |            |            |           |
|---|------------|------------|-----------|
| H | -0.4355991 | -1.8998010 | 0.0622315 |
|---|------------|------------|-----------|

bpy\_22

G(bpy\_22) = -311433.97 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | -1.0521773 | 0.1726779  | 0.0346052  |
| C | -2.1358783 | 0.9694862  | -0.0257436 |
| C | -3.5434444 | 0.4125120  | -0.0876636 |
| C | -3.5217802 | -1.1019673 | -0.0692486 |
| C | -2.3788391 | -1.8297586 | -0.0063398 |
| N | -1.1403916 | -1.2070556 | 0.0459298  |
| H | -1.9954468 | 2.0547760  | -0.0307406 |
| H | -4.1592845 | 0.7982684  | 0.7567983  |
| H | -4.4838458 | -1.6183285 | -0.1102124 |
| H | -0.0353345 | 0.5752385  | 0.0789634  |
| C | -2.3107853 | -3.3161693 | 0.0136255  |
| C | -3.4507356 | -4.1428826 | -0.0253868 |
| C | -3.2858246 | -5.5253927 | -0.0035267 |
| C | -1.9926416 | -6.0585719 | 0.0571234  |
| C | -0.9214923 | -5.1636431 | 0.0934599  |
| N | -1.0736093 | -3.8386968 | 0.0726232  |
| H | -4.4516905 | -3.7102681 | -0.0718300 |
| H | 0.1113270  | -5.5331704 | 0.1419342  |
| H | -4.1602374 | -6.1835354 | -0.0331716 |
| H | -1.8182029 | -7.1382218 | 0.0760359  |
| H | -0.3295961 | -1.8138269 | 0.0888499  |
| H | -4.0741940 | 0.7782846  | -0.9963850 |

phen\_00

G(phen\_00) = -358526.89 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | -0.6810132 | -2.1271141 | 0.0000003  |
| C | 0.6835851  | -2.1262937 | 0.0000003  |
| C | 1.4215945  | -0.8930300 | 0.0000003  |
| C | 0.7309760  | 0.3577513  | -0.0000002 |
| C | -0.7314034 | 0.3568693  | -0.0000010 |
| C | -1.4205087 | -0.8947415 | -0.0000001 |
| C | 2.8368797  | -0.8608463 | 0.0000002  |
| C | 3.4883668  | 0.3581190  | 0.0000001  |
| C | 2.7039593  | 1.5347330  | 0.0000000  |
| N | 1.3847399  | 1.5383122  | -0.0000001 |
| C | -2.8358315 | -0.8642662 | -0.0000001 |
| C | -3.4887953 | 0.3539099  | -0.0000014 |

|   |            |            |            |
|---|------------|------------|------------|
| C | -2.7058081 | 1.5314708  | -0.0000027 |
| N | -1.3865942 | 1.5366407  | -0.0000024 |
| H | -1.2372397 | -3.0704703 | 0.0000005  |
| H | 1.2409398  | -3.0689828 | 0.0000002  |
| H | 3.3972990  | -1.8021925 | 0.0000001  |
| H | 4.5806356  | 0.4222260  | -0.0000001 |
| H | 3.1971317  | 2.5171023  | 0.0000000  |
| H | -3.2001645 | 2.5132445  | -0.0000038 |
| H | -4.5811398 | 0.4166879  | -0.0000014 |
| H | -3.3951191 | -1.8062882 | 0.0000012  |

phen\_10

G(phen\_10) = -358801.80 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | -0.6714141 | -2.1659518 | -0.0000004 |
| C | 0.6976146  | -2.1537025 | -0.0000013 |
| C | 1.4413169  | -0.9211784 | -0.0000015 |
| C | 0.7450039  | 0.3164431  | 0.0000006  |
| C | -0.6920428 | 0.2832420  | 0.0000007  |
| C | -1.4153418 | -0.9358833 | 0.0000001  |
| C | 2.8571502  | -0.8466579 | -0.0000033 |
| C | 3.4650374  | 0.3963412  | -0.0000019 |
| C | 2.6608785  | 1.5642460  | 0.0000009  |
| N | 1.3398619  | 1.5262237  | 0.0000020  |
| C | -2.8281990 | -0.8526842 | 0.0000001  |
| C | -3.4705696 | 0.3833035  | 0.0000002  |
| C | -2.7042282 | 1.5522189  | 0.0000005  |
| N | -1.3687114 | 1.4638411  | 0.0000008  |
| H | -1.2202774 | -3.1115115 | 0.0000001  |
| H | 1.2519226  | -3.0969958 | -0.0000018 |
| H | 3.4527539  | -1.7647221 | -0.0000061 |
| H | 4.5542108  | 0.4907429  | -0.0000032 |
| H | 3.1290702  | 2.5556066  | 0.0000024  |
| H | -3.1373233 | 2.5556471  | 0.0000002  |
| H | -4.5603245 | 0.4572121  | 0.0000000  |
| H | -3.4195067 | -1.7739509 | -0.0000002 |
| H | -0.7632120 | 2.2967406  | 0.0000012  |

phen\_22

G(phen\_22) = -359257.65 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | -0.6245036 | -2.1327600 | 0.0100977  |
| C | 0.7573854  | -2.1491635 | -0.0033181 |
| C | 1.4747288  | -0.9225953 | -0.0039960 |
| C | 0.7497636  | 0.3115487  | 0.0042206  |
| C | -0.6867343 | 0.2862915  | 0.0183160  |
| C | -1.3737773 | -0.9292509 | 0.0259628  |
| C | 2.8923815  | -0.8285392 | -0.0157465 |
| C | 3.4960542  | 0.4122981  | -0.0188020 |
| C | 2.6752684  | 1.5702129  | -0.0122326 |

|   |            |            |            |
|---|------------|------------|------------|
| N | 1.3598925  | 1.5247090  | -0.0025307 |
| C | -2.8975341 | -0.9635224 | 0.0668711  |
| C | -3.4948798 | 0.4184730  | -0.0784746 |
| C | -2.7383029 | 1.5308055  | -0.0865912 |
| N | -1.3567129 | 1.4895161  | 0.0131664  |
| H | -1.1731333 | -3.0813270 | 0.0122686  |
| H | 1.3079990  | -3.0952114 | -0.0139460 |
| H | 3.4901253  | -1.7468294 | -0.0223005 |
| H | 4.5855352  | 0.5153266  | -0.0271399 |
| H | 3.1383324  | 2.5665128  | -0.0165966 |
| H | -0.7815408 | 2.3231714  | -0.0308612 |
| H | -3.1698721 | 2.5322061  | -0.1751444 |
| H | -3.2376118 | -1.4359121 | 1.0158811  |
| H | -4.5809324 | 0.5157439  | -0.1642647 |
| H | -3.2778800 | -1.6371836 | -0.7296795 |

ppy\_00

G(ppy\_00) = -581468.78 kcal/mol

|   |            |            |            |
|---|------------|------------|------------|
| C | 0.0233857  | -0.0067139 | 0.0000467  |
| C | 2.3193662  | -0.0053450 | 0.0026728  |
| C | -0.0465348 | 1.3997032  | -0.0019072 |
| H | -0.8996151 | -0.6029633 | 0.0000066  |
| C | 2.3629422  | 1.4120936  | -0.0002855 |
| C | 1.1418052  | 2.1142871  | -0.0024751 |
| H | -1.0158882 | 1.9072205  | -0.0029194 |
| H | 1.1623019  | 3.2066021  | -0.0041567 |
| C | 4.6210525  | -2.8259931 | 0.0156415  |
| C | 3.5805546  | -0.7790005 | 0.0076437  |
| C | 5.9067824  | -2.2518441 | 0.0223207  |
| C | 4.8252360  | -0.0988809 | 0.0120091  |
| C | 6.0046664  | -0.8689278 | 0.0200725  |
| H | 6.7979676  | -2.8861994 | 0.0287939  |
| H | 6.9678663  | -0.3535581 | 0.0242549  |
| N | 1.1604857  | -0.6848928 | 0.0022391  |
| C | 4.8794941  | 1.3649007  | 0.0075264  |
| C | 3.6451846  | 2.1212663  | -0.0003814 |
| N | 3.6575736  | 3.4452131  | -0.0074144 |
| N | 3.5009683  | -2.1199755 | 0.0089092  |
| H | 4.5072179  | -3.9189257 | 0.0159334  |
| N | 6.0583076  | 1.9679605  | 0.0102164  |
| C | 6.0767087  | 3.3179440  | 0.0037746  |
| C | 4.8547447  | 4.0635415  | -0.0061436 |
| C | 4.9404175  | 5.4911902  | -0.0146204 |
| N | 6.0773385  | 6.1441149  | -0.0128730 |
| C | 7.2369576  | 5.4287243  | -0.0023170 |
| C | 7.2949080  | 4.0510849  | 0.0060300  |
| H | 4.0037564  | 6.0643803  | -0.0231053 |
| H | 8.1590346  | 6.0225262  | -0.0008707 |

H 8.2447384 3.5097508 0.0140940

#### ppy\_10

G(ppy\_10) = -581745.62 kcal/mol

C 0.0210287 -0.0033481 -0.0006019  
C 2.3147370 -0.0048630 0.0030535  
C -0.0497064 1.4041049 -0.0011891  
H -0.8997697 -0.6010013 -0.0007934  
C 2.3586899 1.4134189 0.0017006  
C 1.1372804 2.1193107 -0.0010641  
H -1.0193402 1.9095672 -0.0011718  
H 1.1503086 3.2113957 -0.0016060  
C 4.5996043 -2.8363597 0.0159211  
C 3.5741065 -0.7843412 0.0098794  
C 5.8931898 -2.2756920 0.0364943  
C 4.8288936 -0.1135245 0.0247100  
C 6.0063505 -0.8958592 0.0399425  
H 6.7756979 -2.9209504 0.0482598  
H 6.9777210 -0.3969156 0.0538968  
N 1.1606393 -0.6815539 0.0008645  
C 4.8878146 1.3350234 0.0222958  
C 3.6380183 2.1102198 0.0053029  
N 3.6644790 3.4295050 -0.0057315  
N 3.4841019 -2.1181899 0.0042374  
H 4.4729665 -3.9269156 0.0089435  
N 6.0693455 1.9411228 0.0339750  
C 6.0953466 3.2825052 0.0246956  
C 4.8710251 4.0354814 0.0019146  
C 4.9417014 5.4391786 -0.0126884  
N 6.1363849 6.0430941 -0.0032688  
C 7.3298250 5.3627904 0.0210194  
C 7.3314937 3.9921152 0.0354812  
H 4.0423048 6.0590533 -0.0319810  
H 8.2343178 5.9739173 0.0270377  
H 8.2693695 3.4325229 0.0543288  
H 6.1646074 7.0635347 -0.0146860

#### ppy\_22

G(ppy\_22) = -582213.72 kcal/mol

C 0.0055294 -0.0131456 -0.0178299  
C 2.3062260 -0.0191992 0.0061605  
C -0.0550225 1.3981226 -0.0224630  
H -0.9218028 -0.6029256 -0.0233360  
C 2.3679407 1.4100002 -0.0258595  
C 1.1315068 2.1065519 -0.0254442  
H -1.0203202 1.9129709 -0.0159569  
H 1.1002141 3.1998694 -0.0046673  
C 4.5918334 -2.8312976 0.1092225

C 3.5474293 -0.7818110 0.0534002  
C 5.8778760 -2.2470008 0.1159515  
C 4.7948796 -0.0785058 0.0750048  
C 5.9742752 -0.8686405 0.0975007  
H 6.7734480 -2.8749318 0.1295187  
H 6.9659578 -0.4064780 0.0839111  
N 1.1372558 -0.6892886 0.0024920  
C 4.8161941 1.3583810 0.0495418  
C 3.6401705 2.0826213 -0.0341844  
N 3.7000118 3.4793863 -0.0950934  
N 3.4778109 -2.1263746 0.0746150  
H 4.4842636 -3.9247015 0.1279792  
N 6.0394972 2.0505513 0.0863059  
C 6.1141447 3.4360385 0.0563402  
C 4.9133482 4.1754151 -0.0581542  
C 4.9986649 5.5654644 -0.1168989  
N 6.1524934 6.2497079 -0.0648854  
C 7.2740714 5.5526663 0.0596951  
C 7.3119230 4.1481329 0.1231181  
H 4.0766572 6.1561634 -0.2095591  
H 8.2109191 6.1226381 0.1109074  
H 8.2670872 3.6208745 0.2137626  
H 2.8844826 3.9862107 -0.4116443  
H 6.8815740 1.5414805 0.3137048

#### ppy\_32

G(ppy\_32) = -582495.91 kcal/mol

C 0.0101607 -0.0224916 -0.0001774  
C 2.3093541 -0.0205084 0.0021230  
C -0.0575697 1.3898795 -0.0022313  
H -0.9131754 -0.6163364 0.0001445  
C 2.3612874 1.4082944 -0.0046351  
C 1.1249606 2.1029602 -0.0051370  
H -1.0249087 1.8993675 -0.0009599  
H 1.0791916 3.1967671 -0.0049088  
C 4.5731504 -2.8490288 0.0307318  
C 3.5505644 -0.7903652 0.0118530  
C 5.8657595 -2.2771860 0.0447805  
C 4.8040640 -0.1030928 0.0186701  
C 5.9771891 -0.8998413 0.0381887  
H 6.7535394 -2.9149119 0.0604003  
H 6.9774767 -0.4543961 0.0496875  
N 1.1447590 -0.6931404 0.0025088  
C 4.8072863 1.3335518 0.0040715  
C 3.6408424 2.0638939 -0.0093340  
N 3.7213748 3.4696200 -0.0274506  
N 3.4671548 -2.1320708 0.0163347  
H 4.4540580 -3.9403809 0.0321491

|   |           |           |            |
|---|-----------|-----------|------------|
| N | 6.0359133 | 2.0478198 | 0.0005379  |
| C | 6.1291684 | 3.3917113 | -0.0217896 |
| C | 4.9127151 | 4.1585323 | -0.0384520 |
| C | 5.0018147 | 5.5384500 | -0.0647827 |
| N | 6.2311063 | 6.1557714 | -0.0726728 |
| C | 7.3830711 | 5.4644833 | -0.0559442 |
| C | 7.3631875 | 4.0817535 | -0.0305671 |
| H | 4.1267764 | 6.1892954 | -0.0801760 |
| H | 8.3108252 | 6.0405327 | -0.0637877 |
| H | 8.3066185 | 3.5314315 | -0.0182046 |
| H | 2.8604376 | 4.0003976 | -0.0489386 |
| H | 6.8964122 | 1.5114042 | 0.0095062  |
| H | 6.2593366 | 7.1729089 | -0.0922355 |

rubpy\_00

G(rubpy\_00) = -991556.54 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.4428199 | -0.0881260 | -0.0182816 |
| C  | 1.0473783  | -0.2864975 | 2.5353608  |
| C  | -1.2110790 | 0.1206026  | 2.9668673  |
| C  | 1.3259532  | -0.2794404 | 3.9093824  |
| C  | 0.2963839  | -0.0639910 | 4.8256874  |
| C  | 0.7779835  | 2.7465332  | 0.0931475  |
| C  | -1.5542437 | 2.6586891  | 0.0138641  |
| C  | 0.7773024  | 4.1392049  | 0.1432358  |
| H  | 1.7152183  | 2.1856337  | 0.1012208  |
| C  | -1.6224685 | 4.0583163  | 0.0618137  |
| C  | -0.4486177 | 4.8091854  | 0.1273445  |
| H  | 1.7249890  | 4.6813295  | 0.1942878  |
| H  | -2.5879948 | 4.5664147  | 0.0503970  |
| H  | -0.4927730 | 5.9012990  | 0.1659351  |
| C  | -3.5116442 | -0.4228700 | -0.1256797 |
| C  | -2.7424427 | 1.7810852  | -0.0578496 |
| C  | -4.8423590 | -0.0128784 | -0.1840949 |
| H  | -3.2514032 | -1.4835824 | -0.1253212 |
| C  | -4.0598691 | 2.2576680  | -0.1148127 |
| C  | -5.1223494 | 1.3559870  | -0.1792816 |
| H  | -5.6389524 | -0.7596440 | -0.2330587 |
| H  | -4.2610074 | 3.3298901  | -0.1116157 |
| H  | -6.1530904 | 1.7187576  | -0.2254455 |
| C  | -0.7982805 | -3.0578808 | 0.7554320  |
| C  | -0.7886412 | -2.6092306 | -1.5361719 |
| C  | -0.9580067 | -4.4257448 | 0.5411575  |
| H  | -0.7364474 | -2.6523396 | 1.7675867  |
| C  | -0.9474752 | -3.9733639 | -1.8182901 |
| C  | -1.0330246 | -4.8935010 | -0.7732407 |
| H  | -1.0207316 | -5.1052680 | 1.3948602  |
| H  | -1.0035568 | -4.3221691 | -2.8504775 |
| H  | -1.1567235 | -5.9595687 | -0.9842901 |

|   |            |            |            |
|---|------------|------------|------------|
| C | 2.4957298  | -0.6303278 | -0.8011033 |
| C | 2.0719505  | -0.5067126 | 1.4918284  |
| C | 3.8488700  | -0.8894862 | -0.5911278 |
| H | 2.0872613  | -0.5664547 | -1.8119242 |
| C | 3.4216629  | -0.7647067 | 1.7696625  |
| C | 4.3217569  | -0.9587022 | 0.7216796  |
| H | 4.5131124  | -1.0341781 | -1.4469685 |
| H | 3.7741986  | -0.8180134 | 2.8007129  |
| H | 5.3762938  | -1.1616173 | 0.9293102  |
| C | -0.4228455 | 0.7180120  | -3.0006649 |
| C | -0.6958283 | -1.5620247 | -2.5765086 |
| C | -0.5053240 | 0.5260755  | -4.3785398 |
| H | -0.2757280 | 1.7155287  | -2.5813176 |
| C | -0.7857447 | -1.8214942 | -3.9513941 |
| C | -0.6906646 | -0.7707767 | -4.8642594 |
| H | -0.4259618 | 1.3834081  | -5.0517516 |
| H | -0.9332221 | -2.8397659 | -4.3141018 |
| H | -0.7617384 | -0.9638624 | -5.9384845 |
| N | -0.3517660 | 2.0169336  | 0.0287381  |
| N | -2.4823535 | 0.4427669  | -0.0634946 |
| N | -0.5137634 | -0.2921529 | -2.1153659 |
| N | -0.7156227 | -2.1654837 | -0.2491936 |
| N | 1.6228863  | -0.4418616 | 0.2063420  |
| H | 2.3436178  | -0.4389089 | 4.2686223  |
| N | -0.2212670 | -0.0866949 | 2.0782687  |
| C | -0.9993200 | 0.1397174  | 4.3442186  |
| H | -2.2090689 | 0.2733924  | 2.5507118  |
| H | 0.5048992  | -0.0552818 | 5.8993567  |
| H | -1.8404599 | 0.3123339  | 5.0204694  |

rubpy\_22

G(rubpy\_22) = -992279.15 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.4158060 | -0.1018399 | -0.0582560 |
| C  | 1.0797519  | -0.2870365 | 2.4942626  |
| C  | -1.1886442 | 0.0462961  | 2.9306935  |
| C  | 1.3595268  | -0.2870665 | 3.8678655  |
| C  | 0.3247284  | -0.1142061 | 4.7871327  |
| C  | 0.7680548  | 2.7604277  | 0.0801771  |
| C  | -1.5622153 | 2.6391725  | 0.0245230  |
| C  | 0.7476054  | 4.1523385  | 0.1500872  |
| H  | 1.7140837  | 2.2143099  | 0.0697034  |
| C  | -1.6512711 | 4.0367181  | 0.0944611  |
| C  | -0.4880876 | 4.8040470  | 0.1585903  |
| H  | 1.6874400  | 4.7082839  | 0.1974656  |
| H  | -2.6242716 | 4.5305421  | 0.1001952  |
| H  | -0.5484655 | 5.8946394  | 0.2139424  |
| C  | -3.4799289 | -0.4646423 | -0.1719468 |
| C  | -2.7386472 | 1.7465844  | -0.0543291 |

|   |            |            |            |
|---|------------|------------|------------|
| C | -4.8160886 | -0.0707296 | -0.2122664 |
| H | -3.2028481 | -1.5203790 | -0.2045552 |
| C | -4.0625348 | 2.2071674  | -0.0912444 |
| C | -5.1137443 | 1.2938099  | -0.1705721 |
| H | -5.6037997 | -0.8257200 | -0.2763421 |
| H | -4.2771752 | 3.2762928  | -0.0611197 |
| H | -6.1492136 | 1.6444927  | -0.2008096 |
| C | -0.6067856 | -3.1473606 | 0.7604088  |
| C | -0.6932872 | -2.5992842 | -1.5597246 |
| C | -1.4013457 | -4.4235673 | 0.4726373  |
| C | -0.7818147 | -4.0262274 | -1.8799532 |
| C | -1.1305567 | -4.9079150 | -0.9219689 |
| H | -1.1381586 | -5.1909813 | 1.2205469  |
| H | -0.6083425 | -4.3560514 | -2.9053385 |
| H | -1.2632285 | -5.9680118 | -1.1636307 |
| C | 2.5309345  | -0.5805515 | -0.8457452 |
| C | 2.1091665  | -0.4704838 | 1.4489508  |
| C | 3.8912169  | -0.8036803 | -0.6388859 |
| H | 2.1184491  | -0.5269611 | -1.8554329 |
| C | 3.4657854  | -0.6923922 | 1.7232057  |
| C | 4.3684871  | -0.8611080 | 0.6728268  |
| H | 4.5574635  | -0.9300272 | -1.4959972 |
| H | 3.8217331  | -0.7380527 | 2.7534667  |
| H | 5.4284061  | -1.0361216 | 0.8782951  |
| C | -0.4348652 | 0.7193518  | -3.0445542 |
| C | -0.6485818 | -1.5647346 | -2.6136300 |
| C | -0.5334386 | 0.5178477  | -4.4224151 |
| H | -0.3046331 | 1.7227171  | -2.6327502 |
| C | -0.7593729 | -1.8334439 | -3.9840783 |
| C | -0.7020105 | -0.7824752 | -4.9022600 |
| H | -0.4810704 | 1.3738922  | -5.0999722 |
| H | -0.8981196 | -2.8562435 | -4.3366581 |
| H | -0.7895679 | -0.9792463 | -5.9745534 |
| N | -0.3511404 | 2.0149333  | 0.0184293  |
| N | -2.4614403 | 0.4123979  | -0.0921080 |
| N | -0.4910821 | -0.2875439 | -2.1559138 |
| N | -0.6513003 | -2.1549058 | -0.3279916 |
| N | 1.6560957  | -0.4157233 | 0.1641907  |
| H | 2.3819452  | -0.4200214 | 4.2244946  |
| N | -0.1940627 | -0.1202912 | 2.0394957  |
| C | -0.9767468 | 0.0551430  | 4.3083424  |
| H | -2.1912602 | 0.1751552  | 2.5174497  |
| H | 0.5338188  | -0.1121136 | 5.8606638  |
| H | -1.8221335 | 0.1935314  | 4.9871279  |
| H | -2.4932628 | -4.2556003 | 0.5908183  |
| H | -0.9639686 | -2.6655377 | 1.6811965  |
| H | 0.4621941  | -3.3981704 | 0.9183772  |

ruphen\_00  
G(ruphen\_00) = -1133807.06 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.3730479 | -0.0493294 | 0.0162660  |
| C  | 1.1787551  | -0.2596535 | 2.5034790  |
| C  | -1.0564346 | 0.0227575  | 3.0623098  |
| C  | 1.5732226  | -0.3131251 | 3.8652256  |
| C  | 0.5582773  | -0.1826885 | 4.8437697  |
| C  | 0.7126939  | 2.8764286  | 0.1275261  |
| C  | -1.5937352 | 2.6203585  | 0.1733800  |
| C  | 0.5963589  | 4.2765245  | 0.2198272  |
| H  | 1.6948946  | 2.4005537  | 0.0697072  |
| C  | -1.8059220 | 4.0198424  | 0.2680594  |
| C  | -0.6613643 | 4.8530930  | 0.2915870  |
| H  | 1.5020690  | 4.8880245  | 0.2343792  |
| H  | -0.7782609 | 5.9385942  | 0.3650376  |
| C  | -3.4676564 | -0.4668858 | 0.0159971  |
| C  | -2.7136984 | 1.7249319  | 0.1413911  |
| C  | -4.8106367 | -0.0460838 | 0.0616872  |
| H  | -3.2176217 | -1.5285078 | -0.0521408 |
| C  | -4.0348870 | 2.2383021  | 0.1992228  |
| C  | -5.0993176 | 1.3057310  | 0.1566629  |
| H  | -5.6064090 | -0.7943195 | 0.0241002  |
| H  | -6.1347339 | 1.6570789  | 0.1984539  |
| C  | -0.6323150 | -3.0826392 | 0.7072018  |
| C  | -0.6474346 | -2.5240544 | -1.5457492 |
| C  | -0.7559420 | -4.4525263 | 0.4060644  |
| H  | -0.5764351 | -2.7420539 | 1.7440222  |
| C  | -0.7743353 | -3.8804467 | -1.9417645 |
| C  | -0.8273562 | -4.8565476 | -0.9173821 |
| H  | -0.7940507 | -5.1776176 | 1.2229859  |
| H  | -0.9245395 | -5.9152204 | -1.1765090 |
| C  | 2.6151411  | -0.4259638 | -0.8098803 |
| C  | 2.1616905  | -0.3825822 | 1.4661408  |
| C  | 3.9898079  | -0.6137771 | -0.5698720 |
| H  | 2.2303691  | -0.3642925 | -1.8307820 |
| C  | 3.5279565  | -0.5656326 | 1.8015989  |
| C  | 4.4513034  | -0.6832854 | 0.7346300  |
| H  | 4.6731417  | -0.7010813 | -1.4183540 |
| H  | 5.5151516  | -0.8272431 | 0.9467843  |
| C  | -0.4145251 | 0.7797615  | -2.9944618 |
| C  | -0.5910209 | -1.4891228 | -2.5372365 |
| C  | -0.4871210 | 0.5433233  | -4.3806702 |
| H  | -0.3124559 | 1.7961041  | -2.6060932 |
| C  | -0.6669841 | -1.8211065 | -3.9145271 |
| C  | -0.6113407 | -0.7559193 | -4.8458128 |
| H  | -0.4434490 | 1.3903073  | -5.0699830 |
| H  | -0.6673496 | -0.9652280 | -5.9184688 |
| N  | -0.3462390 | 2.0638017  | 0.1035756  |

|   |            |            |            |
|---|------------|------------|------------|
| N | -2.4419763 | 0.3864819  | 0.0585820  |
| N | -0.4607829 | -0.2021477 | -2.0913845 |
| N | -0.5805908 | -2.1383183 | -0.2348336 |
| N | 1.7197980  | -0.3104689 | 0.1733364  |
| N | -0.1232001 | -0.0981396 | 2.1157130  |
| C | -0.7553806 | -0.0136215 | 4.4373032  |
| H | -2.0862587 | 0.1498634  | 2.7200354  |
| H | 0.8169388  | -0.2167828 | 5.9065204  |
| H | -1.5649651 | 0.0904214  | 5.1641997  |
| C | 3.9015633  | -0.6200841 | 3.1898110  |
| C | 2.9650595  | -0.4971168 | 4.1787320  |
| H | 4.9564778  | -0.7614047 | 3.4415252  |
| H | 3.2622692  | -0.5386080 | 5.2304466  |
| C | -4.2232296 | 3.6610251  | 0.2987486  |
| C | -3.1551368 | 4.5147174  | 0.3328834  |
| H | -5.2440030 | 4.0508762  | 0.3474339  |
| H | -3.3126851 | 5.5943458  | 0.4092062  |
| C | -0.7942658 | -3.2040006 | -4.2901338 |
| C | -0.8446165 | -4.1911758 | -3.3446101 |
| H | -0.8504229 | -3.4533498 | -5.3534444 |
| H | -0.9412896 | -5.2387260 | -3.6432569 |

ruphen\_22

G(ruphen\_22) = -1134539.42 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.3879942 | -0.0217830 | 0.0501110  |
| C  | 1.2161254  | -0.2316907 | 2.5027668  |
| C  | -1.0053459 | 0.0653056  | 3.1086730  |
| C  | 1.6386181  | -0.2895663 | 3.8559235  |
| C  | 0.6455981  | -0.1519176 | 4.8555532  |
| C  | 0.7035282  | 2.8929415  | 0.1783514  |
| C  | -1.6083407 | 2.6540480  | 0.2097243  |
| C  | 0.5949483  | 4.2763289  | 0.3260628  |
| H  | 1.6787207  | 2.4066819  | 0.1022021  |
| C  | -1.8070280 | 4.0327799  | 0.4034676  |
| C  | -0.6720266 | 4.8509486  | 0.4518548  |
| H  | 1.4991598  | 4.8896135  | 0.3557982  |
| H  | -0.7792484 | 5.9308573  | 0.5937296  |
| C  | -3.4710116 | -0.4711424 | 0.0433273  |
| C  | -2.7499441 | 1.7375210  | 0.1168109  |
| C  | -4.8053000 | -0.0669691 | -0.0191700 |
| H  | -3.1997705 | -1.5291527 | 0.0425648  |
| C  | -4.0628788 | 2.2314798  | 0.0158315  |
| C  | -5.1038735 | 1.2974443  | -0.0453955 |
| H  | -5.5970833 | -0.8194518 | -0.0600423 |
| H  | -6.1419493 | 1.6360194  | -0.1196778 |
| C  | -0.6137611 | -3.0564698 | 0.7644391  |
| C  | -0.6892338 | -2.5062335 | -1.4894763 |
| C  | -0.7400280 | -4.4279643 | 0.4716541  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -0.5327194 | -2.7132481 | 1.7987798  |
| C | -0.8222929 | -3.8647112 | -1.8766046 |
| C | -0.8450308 | -4.8370660 | -0.8477182 |
| H | -0.7541877 | -5.1505123 | 1.2915424  |
| H | -0.9452779 | -5.8970367 | -1.1002788 |
| C | 2.5830661  | -0.4059804 | -0.8396542 |
| C | 2.1763700  | -0.3612918 | 1.4450557  |
| C | 3.9607058  | -0.6050487 | -0.6279951 |
| H | 2.1788779  | -0.3405092 | -1.8528523 |
| C | 3.5476533  | -0.5563835 | 1.7521235  |
| C | 4.4479890  | -0.6806314 | 0.6665450  |
| H | 4.6260709  | -0.6966690 | -1.4901386 |
| H | 5.5145545  | -0.8345624 | 0.8567276  |
| C | -0.4909063 | 0.7905431  | -2.9621010 |
| C | -0.6593759 | -1.4760130 | -2.4875642 |
| C | -0.5954238 | 0.5461426  | -4.3448131 |
| H | -0.3767648 | 1.8089518  | -2.5823024 |
| C | -0.7676855 | -1.8151776 | -3.8610071 |
| C | -0.7329945 | -0.7553831 | -4.7992949 |
| H | -0.5649093 | 1.3886748  | -5.0402530 |
| H | -0.8141022 | -0.9708200 | -5.8691008 |
| N | -0.3743497 | 2.0907856  | 0.1244475  |
| N | -2.4571902 | 0.4100238  | 0.1052689  |
| N | -0.5189852 | -0.1863895 | -2.0525645 |
| N | -0.5901191 | -2.1151924 | -0.1819195 |
| N | 1.7085988  | -0.2847638 | 0.1616001  |
| N | -0.0927794 | -0.0610562 | 2.1425309  |
| C | -0.6751408 | 0.0267269  | 4.4768855  |
| H | -2.0416145 | 0.1977472  | 2.7878321  |
| H | 0.9263417  | -0.1888028 | 5.9124949  |
| H | -1.4679887 | 0.1356447  | 5.2212971  |
| C | 3.9495797  | -0.6164429 | 3.1321340  |
| C | 3.0349200  | -0.4863807 | 4.1404748  |
| H | 5.0080756  | -0.7680464 | 3.3619677  |
| H | 3.3540174  | -0.5325840 | 5.1856038  |
| C | -4.2774298 | 3.7246359  | -0.1077520 |
| C | -3.2123095 | 4.5455428  | 0.6332422  |
| H | -5.2828120 | 3.9967035  | 0.2525225  |
| H | -3.4107858 | 4.5112277  | 1.7235338  |
| C | -0.9031888 | -3.1997989 | -4.2267983 |
| C | -0.9280787 | -4.1822032 | -3.2756619 |
| H | -0.9854466 | -3.4545266 | -5.2871961 |
| H | -1.0303619 | -5.2313849 | -3.5669670 |
| H | -4.2590465 | 3.9809199  | -1.1861893 |
| H | -3.2836242 | 5.6068368  | 0.3446517  |

ruppy\_00

G(ruppy\_00) = -1357946.96 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.5180748 | 0.0847683  | 0.0681221  |
| C  | 1.0739690  | -0.1400226 | 2.5276844  |
| C  | -1.1585324 | 0.0746749  | 3.1263332  |
| C  | 1.4908647  | -0.2079557 | 3.8821966  |
| C  | 0.4885245  | -0.1237392 | 4.8784628  |
| C  | 0.5438354  | 3.0129792  | 0.2043553  |
| C  | -1.7599133 | 2.7409890  | 0.3277635  |
| C  | 0.4243485  | 4.4038566  | 0.3392853  |
| H  | 1.5235852  | 2.5413324  | 0.0969283  |
| C  | -1.9652986 | 4.1278238  | 0.4742472  |
| C  | -0.8368703 | 4.9698673  | 0.4787945  |
| H  | 1.3250531  | 5.0230400  | 0.3349929  |
| H  | -0.9806939 | 6.0471129  | 0.5906752  |
| C  | -3.6013486 | -0.3799599 | 0.1210401  |
| C  | -2.8834868 | 1.8223248  | 0.3022407  |
| C  | -4.9442285 | 0.0093223  | 0.2250970  |
| C  | -4.2066073 | 2.2944476  | 0.4201021  |
| C  | -5.2540223 | 1.3554231  | 0.3803518  |
| H  | -5.7281859 | -0.7513798 | 0.1869161  |
| H  | -6.2839002 | 1.7078292  | 0.4735144  |
| C  | -0.7242047 | -2.9641177 | 0.7082906  |
| C  | -0.7768883 | -2.3652201 | -1.5338112 |
| C  | -0.8311956 | -4.3300002 | 0.3839271  |
| H  | -0.6592064 | -2.6423798 | 1.7506065  |
| C  | -0.8875936 | -3.7163218 | -1.9524282 |
| C  | -0.9135354 | -4.7112370 | -0.9454746 |
| H  | -0.8483461 | -5.0701735 | 1.1879012  |
| H  | -0.9981481 | -5.7663686 | -1.2226853 |
| C  | 2.4626512  | -0.2360106 | -0.8094548 |
| C  | 2.0431542  | -0.2263103 | 1.4736139  |
| C  | 3.8443846  | -0.3971286 | -0.5924098 |
| H  | 2.0620874  | -0.1723290 | -1.8241683 |
| C  | 3.4181075  | -0.3841394 | 1.7859542  |
| C  | 4.3272186  | -0.4700499 | 0.7040253  |
| H  | 4.5161745  | -0.4609370 | -1.4519878 |
| H  | 5.3969007  | -0.5935160 | 0.8986745  |
| C  | -0.6010543 | 0.9658872  | -2.9285650 |
| C  | -0.7458290 | -1.3123329 | -2.5074803 |
| C  | -0.6784212 | 0.7510443  | -4.3180232 |
| H  | -0.5091859 | 1.9775132  | -2.5252614 |
| C  | -0.8281077 | -1.6223022 | -3.8896417 |
| C  | -0.7908442 | -0.5416327 | -4.8036054 |
| H  | -0.6477333 | 1.6092867  | -4.9939437 |
| H  | -0.8505131 | -0.7343403 | -5.8791242 |
| N  | -0.5172551 | 2.1949123  | 0.1980031  |
| N  | -0.6295104 | -0.0311374 | -2.0410585 |
| N  | -0.6996113 | -2.0021208 | -0.2169812 |
| N  | 1.5802115  | -0.1487467 | 0.1884539  |

|   |            |            |            |
|---|------------|------------|------------|
| N | -0.2374282 | -0.0019087 | 2.1629919  |
| C | -0.8353811 | 0.0168396  | 4.4955107  |
| H | -2.1969810 | 0.1820800  | 2.8036467  |
| H | 0.7648120  | -0.1721586 | 5.9361738  |
| H | -1.6359948 | 0.0825585  | 5.2366991  |
| C | 3.8150646  | -0.4479564 | 3.1672198  |
| C | 2.8913792  | -0.3619520 | 4.1719951  |
| H | 4.8767727  | -0.5678179 | 3.4009451  |
| H | 3.2060812  | -0.4118471 | 5.2182511  |
| C | -4.4476728 | 3.7335324  | 0.5879642  |
| C | -3.3305614 | 4.6416778  | 0.6182447  |
| C | -0.9404200 | -3.0001477 | -4.2880720 |
| C | -0.9682639 | -4.0038480 | -3.3595381 |
| H | -1.0025550 | -3.2322107 | -5.3550934 |
| H | -1.0531270 | -5.0475012 | -3.6754086 |
| N | -3.5105529 | 5.9442327  | 0.7792772  |
| N | -2.5894081 | 0.4974712  | 0.1635220  |
| H | -3.3297351 | -1.4319564 | 0.0061408  |
| N | -5.6933405 | 4.1600788  | 0.7140350  |
| C | -5.8904794 | 5.4854936  | 0.8791191  |
| C | -4.7700933 | 6.3892128  | 0.9138078  |
| C | -5.0374927 | 7.7858339  | 1.1003146  |
| N | -6.2472994 | 8.2612804  | 1.2356863  |
| C | -7.3067234 | 7.4020961  | 1.1988584  |
| C | -7.1902768 | 6.0379153  | 1.0276646  |
| H | -4.1888648 | 8.4813945  | 1.1314314  |
| H | -8.2929265 | 7.8651736  | 1.3179370  |
| H | -8.0629601 | 5.3807993  | 1.0063117  |

ruppy\_01

G(ruppy\_01) = -1358043.77 kcal/mol

|    |            |            |           |
|----|------------|------------|-----------|
| Ru | -0.4993974 | 0.0623586  | 0.0737390 |
| C  | 1.0804369  | -0.1370960 | 2.5369632 |
| C  | -1.1636487 | 0.0538883  | 3.1197330 |
| C  | 1.4835404  | -0.1910013 | 3.9006447 |
| C  | 0.4772029  | -0.1116942 | 4.8846291 |
| C  | 0.5644820  | 2.9875161  | 0.1955130 |
| C  | -1.7480103 | 2.7054599  | 0.3217300 |
| C  | 0.4443162  | 4.3788816  | 0.3136499 |
| H  | 1.5460092  | 2.5163719  | 0.0962528 |
| C  | -1.9510407 | 4.1084434  | 0.4518676 |
| C  | -0.8266821 | 4.9429298  | 0.4437190 |
| H  | 1.3432803  | 4.9996337  | 0.3078241 |
| H  | -0.9732572 | 6.0211018  | 0.5421613 |
| C  | -3.5785988 | -0.4061754 | 0.1240686 |
| C  | -2.8502940 | 1.8024850  | 0.3096447 |
| C  | -4.9222688 | -0.0170409 | 0.2272073 |
| C  | -4.1885643 | 2.2739347  | 0.4364258 |

|   |            |            |            |
|---|------------|------------|------------|
| C | -5.2270052 | 1.3351196  | 0.3935870  |
| H | -5.7075848 | -0.7751079 | 0.1786963  |
| H | -6.2561519 | 1.6889027  | 0.4895427  |
| C | -0.7387341 | -2.9881989 | 0.6932423  |
| C | -0.8029966 | -2.3651684 | -1.5468279 |
| C | -0.8778136 | -4.3442695 | 0.3598253  |
| H | -0.6555122 | -2.6744820 | 1.7369736  |
| C | -0.9461185 | -3.7145913 | -1.9724216 |
| C | -0.9837569 | -4.7144814 | -0.9783289 |
| H | -0.8998460 | -5.0909752 | 1.1574487  |
| H | -1.0928858 | -5.7650391 | -1.2636378 |
| C | 2.4875853  | -0.2272943 | -0.7912148 |
| C | 2.0520626  | -0.2092483 | 1.4947247  |
| C | 3.8656468  | -0.3563598 | -0.5672450 |
| H | 2.0884663  | -0.1789066 | -1.8076475 |
| C | 3.4330534  | -0.3383473 | 1.8106979  |
| C | 4.3467979  | -0.4103722 | 0.7394388  |
| H | 4.5434456  | -0.4122068 | -1.4225798 |
| H | 5.4176912  | -0.5090966 | 0.9403899  |
| C | -0.5799271 | 0.9758579  | -2.9031529 |
| C | -0.7558866 | -1.3092504 | -2.5061144 |
| C | -0.6733518 | 0.7802977  | -4.2905972 |
| H | -0.4751811 | 1.9800357  | -2.4846039 |
| C | -0.8522386 | -1.5970113 | -3.8956922 |
| C | -0.8059220 | -0.5104410 | -4.7938985 |
| H | -0.6423579 | 1.6473334  | -4.9547818 |
| H | -0.8779835 | -0.6888061 | -5.8709950 |
| N | -0.4894750 | 2.1641387  | 0.1953503  |
| N | -0.6113350 | -0.0316469 | -2.0245082 |
| N | -0.7042884 | -2.0137800 | -0.2231562 |
| N | 1.5921594  | -0.1497141 | 0.2017719  |
| N | -0.2356828 | -0.0229120 | 2.1605597  |
| C | -0.8513011 | 0.0136145  | 4.4883891  |
| H | -2.1994487 | 0.1509530  | 2.7849302  |
| H | 0.7461155  | -0.1470204 | 5.9447340  |
| H | -1.6577263 | 0.0833230  | 5.2224366  |
| C | 3.8174968  | -0.3908398 | 3.1978878  |
| C | 2.8863513  | -0.3208022 | 4.1959823  |
| H | 4.8800094  | -0.4894634 | 3.4392670  |
| H | 3.1956352  | -0.3627980 | 5.2445589  |
| C | -4.4334207 | 3.7084904  | 0.6012954  |
| C | -3.3139022 | 4.6261607  | 0.5988438  |
| C | -0.9935139 | -2.9707114 | -4.3029736 |
| C | -1.0395717 | -3.9819815 | -3.3843338 |
| H | -1.0650092 | -3.1921888 | -5.3720041 |
| H | -1.1479553 | -5.0204188 | -3.7110425 |
| N | -3.4960658 | 5.9313401  | 0.7336588  |
| N | -2.5643447 | 0.4629204  | 0.1702375  |

|   |            |            |           |
|---|------------|------------|-----------|
| H | -3.3087783 | -1.4589903 | 0.0052465 |
| N | -5.6795830 | 4.1360142  | 0.7474498 |
| C | -5.8738495 | 5.4683422  | 0.8947807 |
| C | -4.7636176 | 6.3758127  | 0.8820397 |
| C | -5.0352136 | 7.7683799  | 1.0336719 |
| N | -6.2466253 | 8.2538840  | 1.1904178 |
| C | -7.2935253 | 7.3891647  | 1.2095407 |
| C | -7.1691176 | 6.0192085  | 1.0679022 |
| H | -4.1884030 | 8.4669787  | 1.0183857 |
| H | -8.2821611 | 7.8429625  | 1.3485386 |
| H | -8.0365574 | 5.3545808  | 1.0876258 |

ruppy\_02

G(ruppy\_02) = -1358116.88 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.4821456 | 0.0578862  | 0.0962777  |
| C  | 1.1149319  | -0.1705770 | 2.5421099  |
| C  | -1.1320548 | 0.0072783  | 3.1461036  |
| C  | 1.5202206  | -0.2447548 | 3.9107712  |
| C  | 0.5242012  | -0.1877322 | 4.8972518  |
| C  | 0.5728270  | 2.9824340  | 0.2485153  |
| C  | -1.7428717 | 2.6941469  | 0.3339542  |
| C  | 0.4466677  | 4.3760555  | 0.3591184  |
| H  | 1.5569597  | 2.5116302  | 0.1717627  |
| C  | -1.9541343 | 4.1043299  | 0.4498515  |
| C  | -0.8299140 | 4.9367736  | 0.4578593  |
| H  | 1.3449302  | 4.9979744  | 0.3752183  |
| H  | -0.9827381 | 6.0149636  | 0.5489698  |
| C  | -3.5557726 | -0.4186781 | 0.1686318  |
| C  | -2.8336486 | 1.7958085  | 0.3242960  |
| C  | -4.9043127 | -0.0303056 | 0.2683994  |
| C  | -4.1800794 | 2.2702795  | 0.4439815  |
| C  | -5.2117809 | 1.3229743  | 0.4135345  |
| H  | -5.6869752 | -0.7918955 | 0.2294459  |
| H  | -6.2420261 | 1.6764303  | 0.5014931  |
| C  | -0.7499493 | -2.9891515 | 0.7020130  |
| C  | -0.8262086 | -2.3452467 | -1.5412710 |
| C  | -0.9156879 | -4.3353530 | 0.3658705  |
| H  | -0.6470811 | -2.6807254 | 1.7460628  |
| C  | -1.0014789 | -3.6977623 | -1.9661610 |
| C  | -1.0478643 | -4.6981922 | -0.9839065 |
| H  | -0.9350878 | -5.0865906 | 1.1592722  |
| H  | -1.1808973 | -5.7448004 | -1.2746503 |
| C  | 2.4954374  | -0.1891562 | -0.7970338 |
| C  | 2.0725880  | -0.2115265 | 1.4997193  |
| C  | 3.8716003  | -0.3067638 | -0.5884468 |
| H  | 2.0846375  | -0.1337007 | -1.8088496 |
| C  | 3.4651159  | -0.3267720 | 1.7963561  |
| C  | 4.3679333  | -0.3711830 | 0.7234448  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.5416630  | -0.3511011 | -1.4505671 |
| H | 5.4417254  | -0.4599538 | 0.9151508  |
| C | -0.5666867 | 0.9986243  | -2.8762629 |
| C | -0.7664027 | -1.2939109 | -2.4881738 |
| C | -0.6716938 | 0.8176333  | -4.2610129 |
| H | -0.4488414 | 1.9985159  | -2.4494267 |
| C | -0.8764616 | -1.5635239 | -3.8872536 |
| C | -0.8223552 | -0.4775555 | -4.7742482 |
| H | -0.6398945 | 1.6896322  | -4.9184854 |
| H | -0.9050038 | -0.6486107 | -5.8522055 |
| N | -0.4754363 | 2.1567519  | 0.2296325  |
| N | -0.5993343 | -0.0123335 | -1.9994774 |
| N | -0.7080336 | -2.0026417 | -0.2070547 |
| N | 1.6003763  | -0.1349973 | 0.2027039  |
| N | -0.2126879 | -0.0567297 | 2.1757418  |
| C | -0.8155867 | -0.0555472 | 4.5092569  |
| H | -2.1696271 | 0.1109797  | 2.8171255  |
| H | 0.7998970  | -0.2402500 | 5.9552110  |
| H | -1.6183905 | 0.0042951  | 5.2479569  |
| C | 3.8538725  | -0.3973826 | 3.1839230  |
| C | 2.9290392  | -0.3613568 | 4.1890820  |
| H | 4.9198614  | -0.4829620 | 3.4179799  |
| H | 3.2480571  | -0.4169396 | 5.2348719  |
| C | -4.4343117 | 3.6997888  | 0.5832567  |
| C | -3.3169727 | 4.6240759  | 0.5741264  |
| C | -1.0488831 | -2.9346945 | -4.2959033 |
| C | -1.1120810 | -3.9487304 | -3.3822889 |
| H | -1.1342060 | -3.1497351 | -5.3660053 |
| H | -1.2477396 | -4.9829076 | -3.7149336 |
| N | -3.5028819 | 5.9334468  | 0.6882797  |
| N | -2.5465427 | 0.4507803  | 0.2009131  |
| H | -3.2814972 | -1.4720330 | 0.0634393  |
| N | -5.6890863 | 4.1281222  | 0.7108499  |
| C | -5.8849104 | 5.4639840  | 0.8343625  |
| C | -4.7790684 | 6.3764774  | 0.8219546  |
| C | -5.0582388 | 7.7629793  | 0.9580283  |
| N | -6.2768794 | 8.2591023  | 1.0979200  |
| C | -7.3142076 | 7.3928353  | 1.1100739  |
| C | -7.1805278 | 6.0177834  | 0.9838927  |
| H | -4.2109366 | 8.4614701  | 0.9478626  |
| H | -8.3100033 | 7.8396637  | 1.2294130  |
| H | -8.0461270 | 5.3497479  | 0.9984102  |

ruppy\_12

G(ruppy\_12) = -1358405.61 kcal/mol

|    |            |            |           |
|----|------------|------------|-----------|
| Ru | -0.4774652 | 0.0242679  | 0.0884119 |
| C  | 1.0945238  | -0.1154501 | 2.5566532 |
| C  | -1.1496991 | 0.0816081  | 3.1238486 |

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.4981122  | -0.1107339 | 3.9184512  |
| C | 0.4867159  | 0.0063232  | 4.8981487  |
| C | 0.6236214  | 2.9171731  | 0.2310349  |
| C | -1.6964102 | 2.6688520  | 0.3411674  |
| C | 0.5042012  | 4.3306377  | 0.3475237  |
| H | 1.6001428  | 2.4375722  | 0.1386141  |
| C | -1.9231224 | 4.0968630  | 0.4746286  |
| C | -0.7382040 | 4.9061280  | 0.4673278  |
| H | 1.4093148  | 4.9432425  | 0.3420284  |
| H | -0.8059258 | 5.9945427  | 0.5553072  |
| C | -3.5629027 | -0.4187891 | 0.1462371  |
| C | -2.7969407 | 1.7818824  | 0.3181381  |
| C | -4.9005320 | -0.0051697 | 0.2428891  |
| C | -4.1272989 | 2.2806421  | 0.4315744  |
| C | -5.1786767 | 1.3524553  | 0.3903778  |
| H | -5.6991554 | -0.7498615 | 0.2035055  |
| H | -6.1994244 | 1.7331366  | 0.4765853  |
| C | -0.7012591 | -3.0425916 | 0.6489778  |
| C | -0.8102149 | -2.3724127 | -1.5712352 |
| C | -0.8405766 | -4.3934007 | 0.2851661  |
| H | -0.6022125 | -2.7516558 | 1.6979469  |
| C | -0.9619327 | -3.7073555 | -2.0283880 |
| C | -0.9734102 | -4.7324892 | -1.0540384 |
| H | -0.8443145 | -5.1586560 | 1.0655177  |
| H | -1.0870754 | -5.7763808 | -1.3612168 |
| C | 2.5091926  | -0.3408103 | -0.7623731 |
| C | 2.0721325  | -0.2273422 | 1.5158754  |
| C | 3.8875739  | -0.4820684 | -0.5297720 |
| H | 2.1129976  | -0.3222979 | -1.7809712 |
| C | 3.4486664  | -0.3543102 | 1.8428940  |
| C | 4.3642697  | -0.4842596 | 0.7751585  |
| H | 4.5656982  | -0.5830437 | -1.3807738 |
| H | 5.4337757  | -0.5859870 | 0.9826623  |
| C | -0.6132603 | 1.0006550  | -2.8506513 |
| C | -0.7866593 | -1.2904340 | -2.5109558 |
| C | -0.7541923 | 0.8381746  | -4.2428974 |
| H | -0.4896779 | 1.9917893  | -2.4075715 |
| C | -0.9273400 | -1.5469440 | -3.8999132 |
| C | -0.9076488 | -0.4333123 | -4.7723753 |
| H | -0.7412380 | 1.7219184  | -4.8854942 |
| H | -1.0163918 | -0.5838496 | -5.8507271 |
| N | -0.4471530 | 2.1277467  | 0.2275035  |
| N | -0.6214510 | -0.0308969 | -2.0036631 |
| N | -0.6869525 | -2.0502662 | -0.2466771 |
| N | 1.6167778  | -0.2117295 | 0.2242035  |
| N | -0.2176983 | -0.0304249 | 2.1750125  |
| C | -0.8375814 | 0.1050517  | 4.4961255  |
| H | -2.1845050 | 0.1584945  | 2.7819585  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 0.7541863  | 0.0197956  | 5.9591098  |
| H | -1.6462195 | 0.2030560  | 5.2245896  |
| C | 3.8324852  | -0.3455637 | 3.2306511  |
| C | 2.8997516  | -0.2254171 | 4.2227653  |
| H | 4.8941509  | -0.4372822 | 3.4775993  |
| H | 3.2069812  | -0.2183033 | 5.2726364  |
| C | -4.3816422 | 3.7188746  | 0.5894174  |
| C | -3.2349844 | 4.5921088  | 0.6018193  |
| C | -1.0824444 | -2.9078143 | -4.3371403 |
| C | -1.0968626 | -3.9422543 | -3.4417402 |
| H | -1.1905311 | -3.1027051 | -5.4081508 |
| H | -1.2154847 | -4.9725281 | -3.7896631 |
| N | -3.5156698 | 5.9454977  | 0.7497759  |
| N | -2.5379963 | 0.4358640  | 0.1868242  |
| H | -3.3099911 | -1.4773376 | 0.0378501  |
| N | -5.6323376 | 4.1253224  | 0.7085644  |
| C | -5.8751847 | 5.4749940  | 0.8589889  |
| C | -4.8189908 | 6.4250799  | 0.8856964  |
| C | -5.1183224 | 7.7787986  | 1.0455098  |
| N | -6.3669147 | 8.2452959  | 1.1772165  |
| C | -7.3648061 | 7.3630379  | 1.1524169  |
| C | -7.1746434 | 5.9822145  | 0.9971635  |
| H | -4.3056894 | 8.5201942  | 1.0679663  |
| H | -8.3794192 | 7.7673190  | 1.2623411  |
| H | -8.0181175 | 5.2870915  | 0.9824609  |
| H | -2.7618607 | 6.6192064  | 0.7837456  |

ruppy\_22

G(ruppy\_22) = -1358692.58 kcal/mol

|    |            |            |           |
|----|------------|------------|-----------|
| Ru | -0.5001409 | 0.0658849  | 0.0717070 |
| C  | 1.0923756  | -0.1506233 | 2.5317330 |
| C  | -1.1382780 | 0.0945608  | 3.1261305 |
| C  | 1.5087375  | -0.2020394 | 3.8868766 |
| C  | 0.5075090  | -0.0894413 | 4.8815156 |
| C  | 0.5636082  | 2.9797137  | 0.2370321 |
| C  | -1.7473566 | 2.7112324  | 0.3361571 |
| C  | 0.4404925  | 4.3760592  | 0.3842010 |
| H  | 1.5451880  | 2.5110094  | 0.1351591 |
| C  | -1.9698277 | 4.1118421  | 0.4929602 |
| C  | -0.8149271 | 4.9392252  | 0.5128522 |
| H  | 1.3392662  | 4.9971061  | 0.3956451 |
| H  | -0.8932190 | 6.0235257  | 0.6249846 |
| C  | -3.5724918 | -0.3917388 | 0.0927171 |
| C  | -2.8500951 | 1.8128939  | 0.2946467 |
| C  | -4.9218919 | 0.0117964  | 0.1711152 |
| C  | -4.1835181 | 2.3143859  | 0.3987325 |
| C  | -5.2272000 | 1.3496849  | 0.3270720 |
| H  | -5.7112999 | -0.7414548 | 0.1113107 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -6.2779115 | 1.6426655  | 0.3902960  |
| C | -0.6933368 | -2.9892665 | 0.6994553  |
| C | -0.7637128 | -2.3797747 | -1.5389025 |
| C | -0.7941396 | -4.3543526 | 0.3688015  |
| H | -0.6252418 | -2.6717339 | 1.7428918  |
| C | -0.8724146 | -3.7290494 | -1.9637965 |
| C | -0.8843380 | -4.7292462 | -0.9618680 |
| H | -0.8011994 | -5.0990148 | 1.1688507  |
| H | -0.9658050 | -5.7834236 | -1.2438212 |
| C | 2.4821204  | -0.2749247 | -0.8036532 |
| C | 2.0614859  | -0.2516978 | 1.4787480  |
| C | 3.8628408  | -0.4440481 | -0.5849614 |
| H | 2.0821071  | -0.2121958 | -1.8187693 |
| C | 3.4353916  | -0.4145009 | 1.7929985  |
| C | 4.3446112  | -0.5121996 | 0.7120956  |
| H | 4.5352290  | -0.5166748 | -1.4435184 |
| H | 5.4136775  | -0.6394452 | 0.9081556  |
| C | -0.6287263 | 0.9605507  | -2.9153573 |
| C | -0.7478830 | -1.3215702 | -2.5072339 |
| C | -0.7343390 | 0.7543006  | -4.3043587 |
| H | -0.5376555 | 1.9694720  | -2.5054323 |
| C | -0.8515399 | -1.6233147 | -3.8896002 |
| C | -0.8426195 | -0.5361392 | -4.7966059 |
| H | -0.7277635 | 1.6174165  | -4.9747514 |
| H | -0.9222502 | -0.7221677 | -5.8720492 |
| N | -0.4945981 | 2.1716447  | 0.2131215  |
| N | -0.6299435 | -0.0429379 | -2.0349257 |
| N | -0.6792155 | -2.0225525 | -0.2210002 |
| N | 1.5995544  | -0.1773966 | 0.1931400  |
| N | -0.2178889 | -0.0092461 | 2.1648763  |
| C | -0.8146814 | 0.0602594  | 4.4961024  |
| H | -2.1750074 | 0.2067285  | 2.7998009  |
| H | 0.7836626  | -0.1217232 | 5.9398323  |
| H | -1.6137561 | 0.1506287  | 5.2363984  |
| C | 3.8311429  | -0.4685007 | 3.1750311  |
| C | 2.9079427  | -0.3641385 | 4.1786422  |
| H | 4.8918841  | -0.5936626 | 3.4101662  |
| H | 3.2219638  | -0.4040324 | 5.2255307  |
| C | -4.4018496 | 3.7216460  | 0.5687684  |
| C | -3.3143456 | 4.6090061  | 0.6204054  |
| C | -0.9600583 | -2.9995851 | -4.2945020 |
| C | -0.9678720 | -4.0089564 | -3.3716130 |
| H | -1.0368389 | -3.2256478 | -5.3618303 |
| H | -1.0500874 | -5.0512910 | -3.6925915 |
| N | -3.5601457 | 5.9545595  | 0.7888584  |
| N | -2.5678838 | 0.4799403  | 0.1562838  |
| H | -3.3076855 | -1.4455777 | -0.0193762 |
| N | -5.6865818 | 4.2343282  | 0.6861108  |

|   |            |           |           |
|---|------------|-----------|-----------|
| C | -5.9485555 | 5.5957200 | 0.8874721 |
| C | -4.8573675 | 6.4820494 | 0.9403699 |
| C | -5.1084578 | 7.8368827 | 1.1406786 |
| N | -6.3397627 | 8.3410987 | 1.2851509 |
| C | -7.3682355 | 7.5050780 | 1.2352874 |
| C | -7.2286396 | 6.1176779 | 1.0385270 |
| H | -4.2722242 | 8.5483921 | 1.1860399 |
| H | -8.3680885 | 7.9392742 | 1.3561451 |
| H | -8.1099791 | 5.4699291 | 1.0057664 |
| H | -2.7903577 | 6.6071081 | 0.8512244 |
| H | -6.4811628 | 3.6102368 | 0.6643213 |

ruppy\_32

G(ruppy\_32) = -1358967.40 kcal/mol

|    |            |            |            |
|----|------------|------------|------------|
| Ru | -0.5105399 | 0.1023851  | 0.0933180  |
| C  | 1.1237376  | -0.1972893 | 2.5221105  |
| C  | -1.0926990 | 0.0489881  | 3.1689416  |
| C  | 1.5628577  | -0.3160170 | 3.8666695  |
| C  | 0.5801070  | -0.2385801 | 4.8830892  |
| C  | 0.5507575  | 3.0181837  | 0.2686093  |
| C  | -1.7584141 | 2.7587425  | 0.3591943  |
| C  | 0.4353460  | 4.4126295  | 0.4133869  |
| H  | 1.5311468  | 2.5459704  | 0.1704542  |
| C  | -1.9697542 | 4.1573006  | 0.5097898  |
| C  | -0.8190439 | 4.9848462  | 0.5346042  |
| H  | 1.3379072  | 5.0285406  | 0.4284436  |
| H  | -0.8890046 | 6.0702575  | 0.6441913  |
| C  | -3.5853275 | -0.3472084 | 0.1227555  |
| C  | -2.8677441 | 1.8556778  | 0.3165825  |
| C  | -4.9332027 | 0.0525106  | 0.1895850  |
| C  | -4.1991797 | 2.3494898  | 0.4076970  |
| C  | -5.2448122 | 1.3927914  | 0.3357332  |
| H  | -5.7208061 | -0.7027935 | 0.1285264  |
| H  | -6.2980227 | 1.6802265  | 0.3903298  |
| C  | -0.7228805 | -2.9455856 | 0.7461588  |
| C  | -0.7722744 | -2.3564655 | -1.4994543 |
| C  | -0.8291127 | -4.3130619 | 0.4278323  |
| H  | -0.6584802 | -2.6211466 | 1.7875900  |
| C  | -0.8809346 | -3.7097953 | -1.9119487 |
| C  | -0.9084513 | -4.7002610 | -0.8999741 |
| H  | -0.8462833 | -5.0500570 | 1.2348230  |
| H  | -0.9911260 | -5.7571000 | -1.1717832 |
| C  | 2.4549091  | -0.2246904 | -0.8402769 |
| C  | 2.0726899  | -0.2748542 | 1.4493914  |
| C  | 3.8365643  | -0.4199017 | -0.6516205 |
| H  | 2.0405374  | -0.1242397 | -1.8463077 |
| C  | 3.4488815  | -0.4720979 | 1.7332679  |

|   |            |            |            |
|---|------------|------------|------------|
| C | 4.3384624  | -0.5440859 | 0.6336115  |
| H | 4.4931955  | -0.4716997 | -1.5237337 |
| H | 5.4083281  | -0.6972149 | 0.8054371  |
| C | -0.5918509 | 0.9668837  | -2.9148655 |
| C | -0.7400218 | -1.3087412 | -2.4783996 |
| C | -0.6597291 | 0.7435892  | -4.3031478 |
| H | -0.4980171 | 1.9814378  | -2.5189784 |
| C | -0.8143699 | -1.6276599 | -3.8596482 |
| C | -0.7708649 | -0.5526629 | -4.7802698 |
| H | -0.6205397 | 1.5961340  | -4.9858138 |
| H | -0.8228679 | -0.7520036 | -5.8551043 |
| N | -0.5102260 | 2.2090523  | 0.2407348  |
| N | -0.6283198 | -0.0237571 | -2.0203961 |
| N | -0.6970987 | -1.9876610 | -0.1838932 |
| N | 1.5905643  | -0.1504473 | 0.1749899  |
| N | -0.1910094 | -0.0181052 | 2.1864897  |
| C | -0.7472270 | -0.0564096 | 4.5294436  |
| H | -2.1349985 | 0.1839349  | 2.8689755  |
| H | 0.8733941  | -0.3264460 | 5.9336173  |
| H | -1.5319334 | 0.0016830  | 5.2880669  |
| C | 3.8680104  | -0.5879245 | 3.1046040  |
| C | 2.9636078  | -0.5122939 | 4.1278698  |
| H | 4.9303674  | -0.7398354 | 3.3159258  |
| H | 3.2948978  | -0.6037372 | 5.1662087  |
| C | -4.3940378 | 3.7653125  | 0.5683084  |
| C | -3.3241985 | 4.6425679  | 0.6249077  |
| C | -0.9243677 | -3.0073878 | -4.2519164 |
| C | -0.9567166 | -4.0058633 | -3.3176259 |
| H | -0.9806580 | -3.2455945 | -5.3178208 |
| H | -1.0401626 | -5.0512547 | -3.6282627 |
| N | -3.5757072 | 6.0069426  | 0.7927325  |
| N | -2.5771367 | 0.5243765  | 0.1869414  |
| H | -3.3191780 | -1.4015017 | 0.0188544  |
| N | -5.6987925 | 4.2983234  | 0.6794379  |
| C | -5.9606771 | 5.6226825  | 0.8575152  |
| C | -4.8563975 | 6.5297318  | 0.9211171  |
| C | -5.1122152 | 7.8751019  | 1.1057326  |
| N | -6.4015218 | 8.3204589  | 1.2212192  |
| C | -7.4592691 | 7.4953195  | 1.1633903  |
| C | -7.2655188 | 6.1340770  | 0.9815551  |
| H | -4.3263271 | 8.6303722  | 1.1662687  |
| H | -8.4512659 | 7.9426634  | 1.2647002  |
| H | -8.1343651 | 5.4730503  | 0.9370309  |
| H | -2.7955793 | 6.6493424  | 0.8476581  |
| H | -6.4900472 | 3.6660574  | 0.6354594  |
| H | -6.5572623 | 9.3205422  | 1.3571271  |