**Electronic Supplementary Information (ESI)**

# Computational exploration of ligand effects in copper-catalyzed boracarboxylation of styrene with $CO_2$

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**Formation of LCu–Bpin**

In the experimental condition, the active catalyst LCu–Bpin can be generated from the reaction of LCu–O*t*Bu with $B_2pin_2$. This process has low barrier (**S1-TS**, $\Delta G^{\ddagger}$ = 14.2 kcal/mol) and is irreversible (Fig. S1). Thus, we chose the LCu–Bpin as the energy reference in the manuscript.

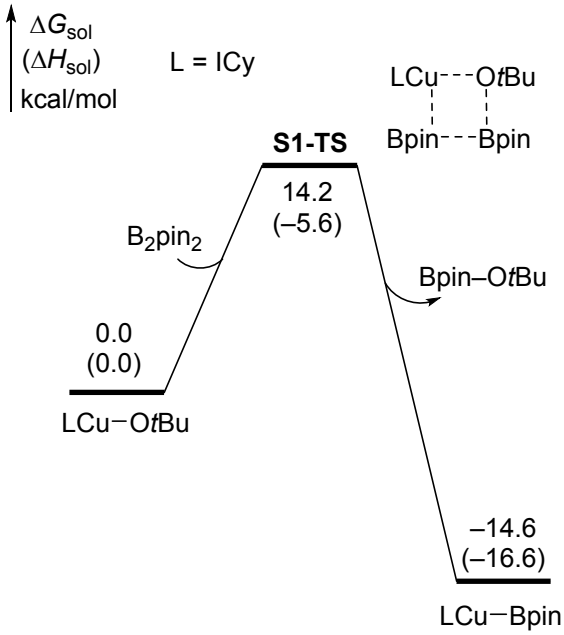


**Fig. S1** Generation of LCu–Bpin from the reaction of LCu–OtBu with $B_2pin_2$.

**Correlation between the $\Delta G^{\ddagger}$ and the $\nu_{co}$ of NHC ligands**

As shown in Fig. S2, the poor correlation between the barrier of $CO_2$ insertion and the TEP of NHC ligands indicates the electronic property of NHC ligands is not the major factor that dominates the reactivity. Instead, as discussed in the manuscript, the steric repulsion between the N-bound substituents of NHC and $CO_2$ is critical for the reactivity of $CO_2$ insertion.

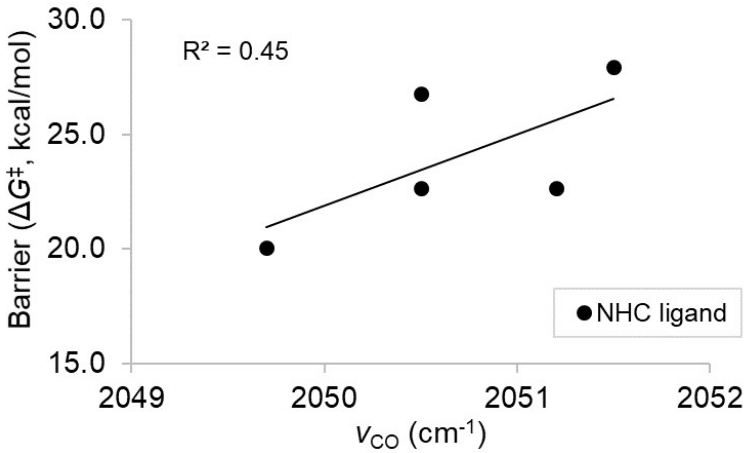


**Fig. S2** Correlation between the barrier of $CO_2$ insertion ($\Delta G^{\ddagger}$) and the $\nu_{co}$ of NHC ligands.

**Correlation between the $\Delta G^{\ddagger}$ and the $\%V_{bur}$ of monophosphine ligands**

In the manuscript, we have concluded that the reactivity with monophosphine ligands is controlled by the ligand's electron donation ability (Fig. 3). Here, the poor correlation between the $\Delta G^{\ddagger}$ and the $\%V_{bur}$ of monophosphine ligands further confirms the importance of the electronic property of monophosphine ligands.

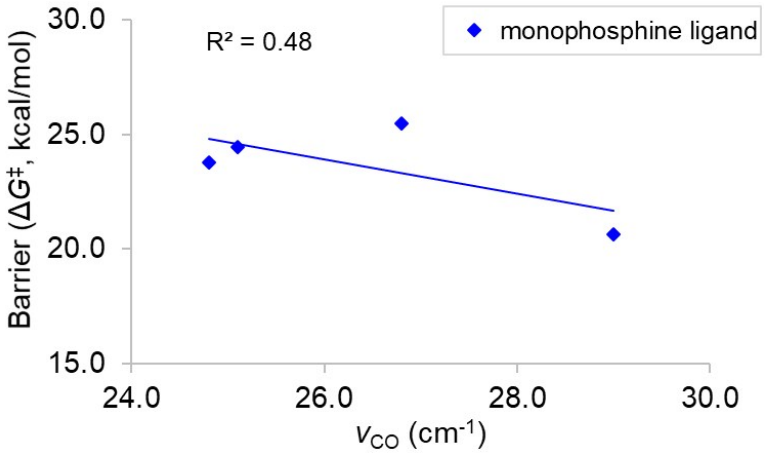


**Fig. S3** Correlation between the barrier of $CO_2$ insertion ($\Delta G^{\ddagger}$) and the $\%V_{bur}$ of monophosphine ligands.

**Hammett study**

We performed Hammett study to investigate the effect of electronic variation of the styrene on the reactivity of $CO_2$ insertion. The result shown in Fig. S4 indicates that the electronic variation of styrene has a significant impact on the rate of $CO_2$ insertion. Although a moderate linear correlation was observed, the difference between the effects of $NMe_2$ and $CF_3$ substituents suggests more electron-rich styrene leads to increased reaction rate. This is consistent with the nature of nucleophilic attacking of $CO_2$ with benzylic copper intermediates.

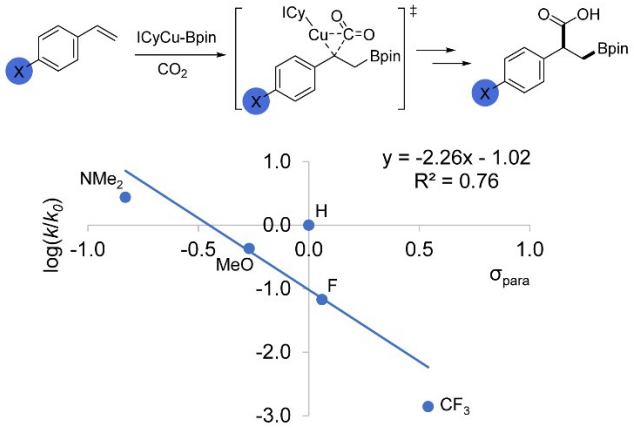


**Fig. S4** Hammett study with *para*-substituted styrenes.

**Energy profiles with bulkier styrenes**

To investigate the effect of bulkiness of styrenes on the reactivity of $CO_2$ insertion, we calculated the energy profiles of boracarboxylation of α-methylstyrene (**1a**), *trans*-β-methylstyrene (**1b**), and mesitylethylene (**1c**). Similar to the energy profile with styrene (Fig. 1 in the manuscript), the energetics shown in Fig. S5 indicate the $CO_2$ insertion steps with these substrates have higher barriers than the borocupration steps. As expected, the barriers of $CO_2$ insertion (22.4, 24.7, and 23.8 kcal/mol for **9-TSa**, **9-TSb**, and **9-TSc**, respectively) are higher than that with styrene (20.1 kcal/mol of **9-TS** in the manuscript). This is due to the greater bulkiness of alkyl copper intermediates (**6a**, **6b**, **6c**) derived from the borocupration of substrates **1a**, **1b**, **1c**. In addition, although the borocupration steps with **1a**, **1b**, **1c** have slightly higher barriers than that with styrene, these steps are irreversible and have high-level regioselectivity (**5-TSa** vs **7-TSa**, **5-TSb** vs **7-TSb**, **5-TSc** vs **7-TSc**).

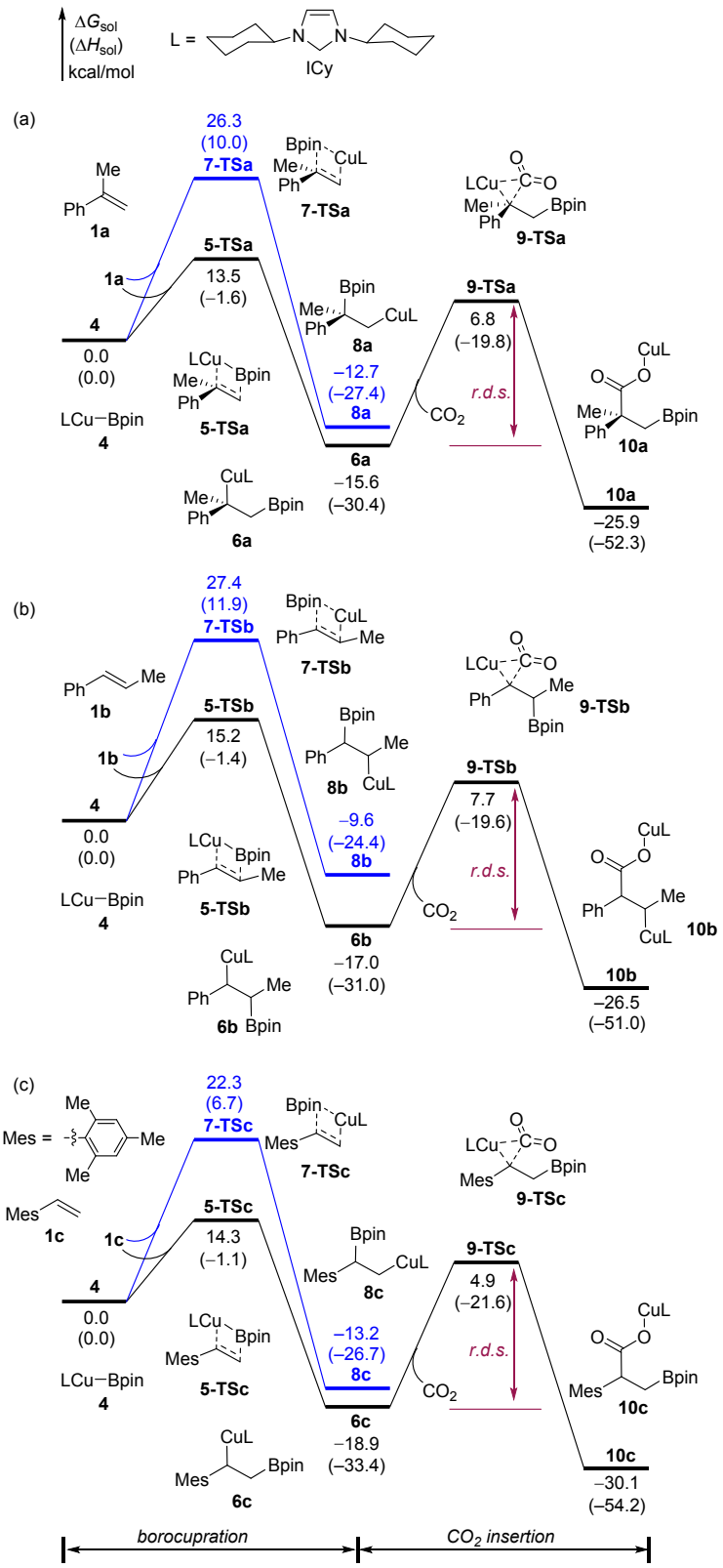


**Fig. S5** Energy profiles with α-methylstyrene **1a** (a), *trans*-β-methylstyrene **1b** (b), and mesitylethylene **1c** (c).

## Cartesian coordinates (Å) and energies of the optimized structures

```
 1
B3LYP SCF energy:                          -309.64179873 a.u.
B3LYP enthalpy:                            -309.500317 a.u.
B3LYP free energy:                         -309.539492 a.u.
M06 SCF energy in solution:                -309.47719102 a.u.
M06 enthalpy in solution:                  -309.335709 a.u.
M06 free energy in solution:               -309.374884 a.u.
Three lowest frequencies (cm-1):       43.9669    208.1723    237.1039

Cartesian coordinates
ATOM       X           Y           Z
C       -2.977841    0.335152    0.000003
C       -1.955066   -0.529561   -0.000001
H       -2.840576    1.413179    0.000008
H       -2.186623   -1.594945   -0.000008
C       -0.515382   -0.220585   -0.000001
C        0.406585   -1.281707    0.000000
C       -0.009001    1.092630   -0.000003
C        1.781276   -1.046367    0.000001
H        0.035116   -2.304164   -0.000001
C        1.362381    1.329944    0.000000
H       -0.694180    1.935446   -0.000005
C        2.265772    0.261994    0.000001
H        2.472503   -1.885090    0.000001
H        1.730465    2.352684    0.000000
H        3.335878    0.450702    0.000001
H       -4.004933   -0.016808   -0.000001



 10
B3LYP SCF energy:                        -1802.49160441 a.u.
B3LYP enthalpy:                          -1801.741287 a.u.
B3LYP free energy:                       -1801.856766 a.u.
M06 SCF energy in solution:              -1801.88195174 a.u.
M06 enthalpy in solution:                -1801.131634 a.u.
M06 free energy in solution:             -1801.247113 a.u.
Three lowest frequencies (cm-1):       8.6523     14.0852     17.0440

Cartesian coordinates
ATOM       X           Y           Z
Cu       0.901832   -0.043091    0.871286
N        3.200060    1.571745    0.019308
N        1.322136    2.594489   -0.280244
C        1.855402    1.430050    0.187243
C        3.499544    2.801882   -0.544953
C        2.317480    3.444876   -0.734247
C       -0.124766    2.884715   -0.306060
C       -0.644102    3.036362   -1.744721
C       -2.161717    3.286612   -1.746357
C       -2.531461    4.504145   -0.884893
C       -1.991856    4.357805    0.546062
C       -0.474049    4.108213    0.556381
C        4.188864    0.547596    0.405409
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| | | | |
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| C | 4.987135 | 0.042729 | -0.807356 |
| C | 5.988165 | -1.044877 | -0.382062 |
| C | 6.912386 | -0.559415 | 0.744743 |
| C | 6.106198 | -0.040506 | 1.945302 |
| C | 5.110310 | 1.053785 | 1.526689 |
| H | 4.508287 | 3.115675 | -0.761475 |
| H | 2.109772 | 4.419308 | -1.146931 |
| H | -0.592988 | 2.001035 | 0.140608 |
| H | -0.399400 | 2.133655 | -2.317534 |
| H | -0.130122 | 3.877102 | -2.233709 |
| H | -2.671950 | 2.395185 | -1.357353 |
| H | -2.508169 | 3.428063 | -2.777482 |
| H | -3.620368 | 4.634040 | -0.864077 |
| H | -2.115479 | 5.415814 | -1.339893 |
| H | -2.496001 | 3.514774 | 1.038703 |
| H | -2.221121 | 5.252162 | 1.138051 |
| H | 0.045186 | 4.995672 | 0.165402 |
| H | -0.113220 | 3.949805 | 1.579820 |
| H | 3.586600 | -0.280595 | 0.794218 |
| H | 5.531031 | 0.882426 | -1.264317 |
| H | 4.294010 | -0.347379 | -1.561218 |
| H | 6.577465 | -1.360635 | -1.251504 |
| H | 5.429629 | -1.929875 | -0.046273 |
| H | 7.558037 | 0.246666 | 0.365071 |
| H | 7.579848 | -1.370309 | 1.061032 |
| H | 6.777247 | 0.348379 | 2.720554 |
| H | 5.552580 | -0.874233 | 2.400345 |
| H | 4.503542 | 1.375347 | 2.381721 |
| H | 5.663901 | 1.936657 | 1.175177 |
| B | -3.119028 | -1.053023 | -0.572764 |
| O | -3.419718 | 0.142104 | 0.043502 |
| C | -4.710724 | -0.016604 | 0.706209 |
| C | -5.344258 | -1.247417 | -0.067905 |
| O | -4.180813 | -1.912830 | -0.628359 |
| C | -5.483652 | 1.295587 | 0.570848 |
| H | -4.943619 | 2.091654 | 1.094623 |
| H | -6.478015 | 1.212086 | 1.024682 |
| H | -5.603273 | 1.596901 | -0.472914 |
| C | -4.410453 | -0.300953 | 2.184381 |
| H | -3.858435 | 0.549002 | 2.600044 |
| H | -3.784923 | -1.190071 | 2.304688 |
| H | -5.332678 | -0.422554 | 2.763307 |
| C | -6.227515 | -0.844561 | -1.256717 |
| H | -5.707677 | -0.147541 | -1.922062 |
| H | -6.471854 | -1.741285 | -1.834855 |
| C | -6.078124 | -2.252516 | 0.819600 |
| H | -5.408180 | -2.674998 | 1.571141 |
| H | -6.458355 | -3.074529 | 0.204029 |
| H | -6.930700 | -1.784024 | 1.325107 |
| C | -0.981593 | -2.511009 | -0.358509 |
| C | -1.692086 | -1.386473 | -1.157857 |
| H | -7.164061 | -0.380496 | -0.929025 |
| C | 0.411785 | -2.873750 | -0.857166 |
| C | 2.981842 | -3.675328 | -1.727298 |
| C | 1.022346 | -2.267635 | -1.962670 |
| C | 1.118435 | -3.895830 | -0.198162 |
| C | 2.384911 | -4.291239 | -0.621642 |

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| H | 0.662852 | -4.382773 | 0.661209 |
| H | 2.905352 | -5.086668 | -0.093727 |
| H | 2.735634 | -2.186580 | -3.267804 |
| H | 3.964780 | -3.990850 | -2.068111 |
| H | -1.608442 | -3.406240 | -0.439224 |
| H | -1.786394 | -1.703768 | -2.205862 |
| H | -1.073605 | -0.478752 | -1.152266 |
| C | -1.018174 | -2.165142 | 1.162989 |
| O | -1.932504 | -2.636008 | 1.836873 |
| O | -0.097473 | -1.376074 | 1.638133 |

11-TS

B3LYP SCF energy: -1613.82808946 a.u.
B3LYP enthalpy: -1613.102710 a.u.
B3LYP free energy: -1613.209986 a.u.
M06 SCF energy in solution: -1613.24113212 a.u.
M06 enthalpy in solution: -1612.515753 a.u.
M06 free energy in solution: -1612.623029 a.u.
Three lowest frequencies (cm-1): -837.3020 8.5250 14.1113
Imaginary frequency: -837.3020 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.223767 | -0.047962 | -0.401015 |
| N | 2.306209 | 2.005014 | -0.031758 |
| N | 0.324282 | 2.860221 | 0.016900 |
| C | 0.985286 | 1.671299 | -0.116315 |
| C | 2.462844 | 3.372753 | 0.140444 |
| C | 1.217253 | 3.910340 | 0.176072 |
| C | -1.140562 | 2.986648 | 0.014612 |
| C | -1.631195 | 3.910578 | -1.112263 |
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| C | -3.705423 | 4.450695 | 0.256147 |
| C | -3.200873 | 3.535432 | 1.382457 |
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| C | 3.410360 | 1.028752 | -0.081335 |
| C | 4.267434 | 1.208678 | -1.345887 |
| C | 5.404303 | 0.173826 | -1.384859 |
| C | 6.265216 | 0.233133 | -0.113949 |
| C | 5.404571 | 0.062148 | 1.147385 |
| C | 4.264272 | 1.092145 | 1.196323 |
| H | 3.429466 | 3.843337 | 0.223787 |
| H | 0.900678 | 4.933591 | 0.301555 |
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| H | -1.264040 | 3.535951 | -2.075037 |
| H | -1.208931 | 4.916672 | -0.975086 |
| H | -3.584389 | 3.015362 | -1.360404 |
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| H | -3.379313 | 5.482884 | 0.453112 |
| H | -3.623347 | 2.528948 | 1.251439 |
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| H | -1.238431 | 4.419654 | 1.636597 |

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| H | 6.023013 | 0.159593 | 2.048540 |
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| H | 3.623774 | 0.919239 | 2.069377 |
| H | 4.690700 | 2.100485 | 1.303742 |
| B | -2.204143 | -1.936825 | -0.396040 |
| O | -3.103517 | -2.668284 | -1.132597 |
| C | -4.439626 | -2.309539 | -0.686337 |
| C | -4.166142 | -1.728496 | 0.756517 |
| O | -2.796324 | -1.251391 | 0.642903 |
| C | -5.315028 | -3.560965 | -0.729724 |
| H | -5.410050 | -3.905251 | -1.764662 |
| H | -6.321105 | -3.348998 | -0.349360 |
| H | -4.884087 | -4.375803 | -0.143525 |
| C | -4.967378 | -1.262332 | -1.677080 |
| H | -4.936173 | -1.683754 | -2.686629 |
| H | -4.346466 | -0.360599 | -1.670939 |
| H | -6.001142 | -0.976934 | -1.454178 |
| C | -4.170529 | -2.800162 | 1.855841 |
| H | -3.527283 | -3.644944 | 1.590436 |
| H | -3.784011 | -2.360792 | 2.780877 |
| C | -5.057115 | -0.557052 | 1.165462 |
| H | -4.971933 | 0.278702 | 0.466658 |
| H | -4.761744 | -0.200825 | 2.157972 |
| H | -6.108545 | -0.863098 | 1.215665 |
| C | 0.251536 | -1.987186 | 0.419013 |
| C | -0.676305 | -1.908394 | -0.704798 |
| H | -5.179993 | -3.178818 | 2.049174 |
| C | 1.576667 | -2.581595 | 0.324102 |
| C | 4.162966 | -3.795218 | 0.224941 |
| C | 2.221489 | -2.868549 | -0.906982 |
| C | 2.290978 | -2.923646 | 1.501713 |
| C | 3.547283 | -3.516533 | 1.453135 |
| C | 3.483031 | -3.462831 | -0.949740 |
| H | 1.721851 | -2.632234 | -1.843139 |
| H | 1.829000 | -2.721874 | 2.466471 |
| H | 4.051474 | -3.773577 | 2.382762 |
| H | 3.934588 | -3.676970 | -1.916696 |
| H | 5.141249 | -4.266456 | 0.187624 |
| H | -0.173873 | -1.912831 | 1.416726 |
| H | -0.409298 | -2.496842 | -1.582931 |
| H | -0.752007 | -0.625870 | -1.586844 |

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| | |
|---|---|
| B3LYP SCF energy: | -1071.87663944 a.u. |
| B3LYP enthalpy: | -1071.520263 a.u. |
| B3LYP free energy: | -1071.592117 a.u. |
| M06 SCF energy in solution: | -1071.54953195 a.u. |

M06 enthalpy in solution: -1071.193156 a.u.
M06 free energy in solution: -1071.265010 a.u.
Three lowest frequencies (cm-1): 20.4902 31.9206 43.0987

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | -0.955356 | -0.588059 | -0.417088 |
| O | -1.759710 | 0.523805 | -0.704079 |
| C | -3.101491 | 0.263785 | -0.168675 |
| C | -3.101039 | -1.308300 | 0.002681 |
| O | -1.689781 | -1.619402 | 0.097861 |
| C | -4.126604 | 0.800818 | -1.167143 |
| H | -4.032012 | 1.889814 | -1.254566 |
| H | -5.146401 | 0.586115 | -0.828576 |
| H | -3.992099 | 0.371632 | -2.162117 |
| C | -3.210795 | 1.021028 | 1.162859 |
| H | -3.178760 | 2.104867 | 0.977788 |
| H | -2.387605 | 0.770204 | 1.837285 |
| H | -4.164901 | 0.824399 | 1.661151 |
| C | -3.631903 | -2.061239 | -1.225974 |
| H | -3.133573 | -1.733446 | -2.143812 |
| H | -3.427043 | -3.128348 | -1.098047 |
| C | -3.789842 | -1.821965 | 1.267240 |
| H | -3.331565 | -1.412382 | 2.170127 |
| H | -3.698979 | -2.911758 | 1.309357 |
| H | -4.856891 | -1.571399 | 1.266074 |
| C | 1.495041 | -0.129223 | 0.459861 |
| C | 0.593508 | -0.698931 | -0.693864 |
| H | -4.712186 | -1.930440 | -1.349038 |
| C | 2.973598 | -0.317417 | 0.171752 |
| C | 5.708213 | -0.776097 | -0.344072 |
| C | 3.645735 | 0.405081 | -0.826811 |
| C | 3.697241 | -1.269210 | 0.903882 |
| C | 5.051070 | -1.500052 | 0.651214 |
| C | 4.999121 | 0.178100 | -1.078248 |
| H | 3.102416 | 1.164850 | -1.377162 |
| H | 3.192777 | -1.836153 | 1.683869 |
| H | 5.590244 | -2.242656 | 1.234494 |
| H | 5.504102 | 0.753381 | -1.850812 |
| H | 6.762587 | -0.950258 | -0.543821 |
| H | 1.250755 | -0.669453 | 1.379340 |
| H | 0.847986 | -1.754581 | -0.847752 |
| H | 0.855327 | -0.162670 | -1.613872 |
| C | 1.000169 | 1.317149 | 0.647358 |
| O | 0.145857 | 1.506638 | 1.566993 |
| O | 1.287860 | 2.171361 | -0.247018 |
| Na | -0.850304 | 2.681655 | -0.058807 |

13-TS
B3LYP SCF energy: -2268.12221369 a.u.
B3LYP enthalpy: -2267.138311 a.u.
B3LYP free energy: -2267.283178 a.u.
M06 SCF energy in solution: -2267.28497510 a.u.
M06 enthalpy in solution: -2266.301072 a.u.
M06 free energy in solution: -2266.445939 a.u.

Three lowest frequencies (cm-1):  -192.3260  10.8749  16.1777
Imaginary frequency:  -192.3260 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.306902 | -0.541718 | 0.065911 |
| N | 2.813663 | 0.996921 | 0.380244 |
| N | 1.081425 | 2.267918 | -0.012524 |
| C | 1.491617 | 0.987456 | 0.108546 |
| C | 3.357733 | 2.363331 | 0.550825 |
| C | 2.191134 | 3.241915 | 0.080978 |
| H | 4.263408 | 2.493717 | -0.047183 |
| H | 1.945870 | 4.039522 | 0.785745 |
| B | -3.672886 | -1.388415 | -0.591196 |
| O | -4.546812 | -0.415140 | -1.015297 |
| C | -5.731828 | -0.486952 | -0.178065 |
| C | -5.658639 | -1.962085 | 0.395013 |
| O | -4.247549 | -2.275940 | 0.290222 |
| C | -6.952426 | -0.191103 | -1.050816 |
| H | -6.887755 | 0.833890 | -1.431065 |
| H | -7.879655 | -0.278488 | -0.472247 |
| H | -7.013027 | -0.863912 | -1.909745 |
| C | -5.583557 | 0.597210 | 0.898741 |
| H | -5.472344 | 1.567766 | 0.403796 |
| H | -4.691354 | 0.428900 | 1.505973 |
| H | -6.463998 | 0.641050 | 1.549780 |
| C | -6.400976 | -2.993557 | -0.467536 |
| H | -6.101872 | -2.922409 | -1.518227 |
| H | -6.147204 | -3.997994 | -0.113720 |
| C | -6.075714 | -2.108682 | 1.858603 |
| H | -5.456485 | -1.490590 | 2.512011 |
| H | -5.956704 | -3.152084 | 2.169344 |
| H | -7.126952 | -1.830664 | 1.999772 |
| C | -1.198181 | -2.074209 | -0.171679 |
| C | -2.236195 | -1.611762 | -1.200220 |
| H | -7.487945 | -2.870968 | -0.406363 |
| C | 0.037891 | -2.772891 | -0.674277 |
| C | 2.284196 | -4.256738 | -1.573831 |
| C | 0.418264 | -2.776902 | -2.034916 |
| C | 0.831649 | -3.529101 | 0.224300 |
| C | 1.935533 | -4.250545 | -0.218768 |
| C | 1.517354 | -3.518106 | -2.475277 |
| H | -0.178365 | -2.229348 | -2.757999 |
| H | 0.554029 | -3.544679 | 1.274548 |
| H | 2.520030 | -4.825463 | 0.495206 |
| H | 1.765631 | -3.524974 | -3.534206 |
| H | 3.135647 | -4.836020 | -1.920412 |
| H | -1.670475 | -2.757926 | 0.536797 |
| H | -2.351041 | -2.398355 | -1.967862 |
| H | -1.924758 | -0.710080 | -1.740674 |
| C | 3.676722 | -0.144048 | 0.550100 |
| C | 5.438084 | -2.274514 | 0.861148 |
| C | 4.448590 | -0.566839 | -0.556236 |
| C | 3.803206 | -0.746548 | 1.822057 |
| C | 4.693115 | -1.821498 | 1.945453 |
| C | 5.319374 | -1.647323 | -0.375281 |
| H | 4.807558 | -2.306373 | 2.910055 |

| | | | |
|---|---|---|---|
| H | 5.916186 | -1.997327 | -1.212790 |
| H | 6.120382 | -3.111833 | 0.982846 |
| C | -0.236659 | 2.708956 | -0.393865 |
| C | -2.758877 | 3.615920 | -1.131763 |
| C | -0.592950 | 2.709198 | -1.761412 |
| C | -1.109067 | 3.194445 | 0.605639 |
| C | -2.372949 | 3.642354 | 0.204796 |
| C | -1.873572 | 3.159944 | -2.103429 |
| H | -3.068087 | 4.009699 | 0.953493 |
| H | -2.178960 | 3.158420 | -3.145921 |
| H | -3.749910 | 3.957463 | -1.418057 |
| C | 4.402820 | 0.137449 | -1.910277 |
| H | 3.628717 | 0.910049 | -1.863050 |
| C | 3.071898 | -0.231624 | 3.059463 |
| H | 2.280771 | 0.448786 | 2.729682 |
| C | -0.704991 | 3.292437 | 2.074573 |
| H | 0.220537 | 2.721263 | 2.204944 |
| C | 0.374054 | 2.299434 | -2.870177 |
| H | 1.284864 | 1.909938 | -2.404906 |
| C | -1.750018 | 2.685560 | 3.029818 |
| H | -1.995169 | 1.657999 | 2.750681 |
| H | -2.677381 | 3.271320 | 3.033881 |
| H | -1.359370 | 2.689690 | 4.054583 |
| C | -0.419694 | 4.760432 | 2.461999 |
| H | -1.328664 | 5.367877 | 2.376872 |
| H | 0.340690 | 5.221651 | 1.820342 |
| H | -0.072398 | 4.822505 | 3.500281 |
| C | -0.187239 | 1.175800 | -3.761027 |
| H | -1.096929 | 1.489904 | -4.285023 |
| H | -0.431416 | 0.288139 | -3.169726 |
| H | 0.551173 | 0.889098 | -4.519323 |
| C | 0.775735 | 3.520059 | -3.724943 |
| H | -0.090842 | 3.938241 | -4.249949 |
| H | 1.518021 | 3.233707 | -4.479745 |
| H | 1.205175 | 4.319821 | -3.110232 |
| C | 5.743618 | 0.837877 | -2.215356 |
| H | 5.680400 | 1.394370 | -3.158140 |
| H | 6.557746 | 0.110214 | -2.312128 |
| H | 6.025940 | 1.540919 | -1.422818 |
| C | 4.013741 | -0.812892 | -3.056779 |
| H | 3.939789 | -0.256320 | -3.999151 |
| H | 3.052460 | -1.295149 | -2.860227 |
| H | 4.761222 | -1.602417 | -3.197993 |
| C | 4.039437 | 0.565154 | 3.962456 |
| H | 4.528714 | 1.384707 | 3.422590 |
| H | 4.830063 | -0.083659 | 4.358390 |
| H | 3.499456 | 0.993177 | 4.815251 |
| C | 2.387649 | -1.351404 | 3.863904 |
| H | 1.668477 | -1.894306 | 3.248095 |
| H | 1.837035 | -0.916264 | 4.705384 |
| H | 3.115589 | -2.059370 | 4.278056 |
| C | -1.311894 | -0.889741 | 1.500053 |
| O | -2.312564 | -0.205862 | 1.372798 |
| O | -0.526763 | -1.260616 | 2.365326 |
| H | 2.369461 | 3.695995 | -0.901736 |
| H | 3.614258 | 2.530449 | 1.603173 |

14-TS

B3LYP SCF energy: -2266.92137323 a.u.
B3LYP enthalpy: -2265.961540 a.u.
B3LYP free energy: -2266.106307 a.u.
M06 SCF energy in solution: -2266.08239057 a.u.
M06 enthalpy in solution: -2265.122557 a.u.
M06 free energy in solution: -2265.267324 a.u.
Three lowest frequencies (cm-1): -192.7842 7.4079 13.1175
Imaginary frequency: -192.7842 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.295065 | -0.578980 | 0.028847 |
| N | 2.809125 | 0.969209 | 0.441375 |
| N | 1.146832 | 2.244866 | -0.060866 |
| C | 1.484496 | 0.929995 | 0.102853 |
| C | 3.278735 | 2.276509 | 0.487217 |
| C | 2.233904 | 3.078572 | 0.166546 |
| H | 4.302132 | 2.504812 | 0.737756 |
| H | 2.157850 | 4.150530 | 0.080613 |
| B | -3.680195 | -1.288164 | -0.617471 |
| O | -4.533265 | -0.249873 | -0.909268 |
| C | -5.707468 | -0.391317 | -0.065445 |
| C | -5.667935 | -1.925843 | 0.323161 |
| O | -4.266490 | -2.259083 | 0.162676 |
| C | -6.931818 | 0.040564 | -0.873454 |
| H | -6.843845 | 1.101945 | -1.128453 |
| H | -7.852208 | -0.092088 | -0.292629 |
| H | -7.023504 | -0.522287 | -1.805526 |
| C | -5.511293 | 0.549598 | 1.131708 |
| H | -5.372469 | 1.568597 | 0.755131 |
| H | -4.619311 | 0.281312 | 1.702463 |
| H | -6.382672 | 0.544247 | 1.796422 |
| C | -6.445433 | -2.824922 | -0.649727 |
| H | -6.156541 | -2.630345 | -1.687614 |
| H | -6.212781 | -3.871161 | -0.426754 |
| C | -6.075844 | -2.239196 | 1.762965 |
| H | -5.432494 | -1.724031 | 2.479342 |
| H | -5.986438 | -3.315871 | 1.942349 |
| H | -7.116822 | -1.949543 | 1.949095 |
| C | -1.222338 | -2.069360 | -0.305050 |
| C | -2.257145 | -1.477684 | -1.268931 |
| H | -7.528287 | -2.685490 | -0.558405 |
| C | 0.001660 | -2.727878 | -0.887069 |
| C | 2.231999 | -4.130142 | -1.942758 |
| C | 0.369832 | -2.604928 | -2.245539 |
| C | 0.800710 | -3.566777 | -0.069909 |
| C | 1.896291 | -4.248686 | -0.589315 |
| C | 1.462266 | -3.304930 | -2.763587 |
| H | -0.228958 | -1.987417 | -2.908091 |
| H | 0.536411 | -3.672258 | 0.978366 |
| H | 2.485005 | -4.889456 | 0.062477 |
| H | 1.701171 | -3.212975 | -3.820799 |
| H | 3.076719 | -4.678734 | -2.350520 |
| H | -1.704222 | -2.816925 | 0.328412 |

| | | | |
|---|---|---|---|
| H | -2.398560 | -2.177738 | -2.112073 |
| H | -1.927549 | -0.531737 | -1.716274 |
| C | 3.661646 | -0.177554 | 0.677243 |
| C | 5.365861 | -2.310950 | 1.129621 |
| C | 4.506776 | -0.601482 | -0.368753 |
| C | 3.656102 | -0.784123 | 1.951613 |
| C | 4.525151 | -1.864624 | 2.146057 |
| C | 5.359145 | -1.682378 | -0.111180 |
| H | 4.545456 | -2.361292 | 3.109970 |
| H | 6.024156 | -2.034254 | -0.894078 |
| H | 6.032478 | -3.150575 | 1.308558 |
| C | -0.164415 | 2.737834 | -0.426383 |
| C | -2.647543 | 3.734945 | -1.131018 |
| C | -0.504819 | 2.796874 | -1.793480 |
| C | -1.027182 | 3.180376 | 0.597167 |
| C | -2.276159 | 3.679971 | 0.208938 |
| C | -1.769047 | 3.302034 | -2.119935 |
| H | -2.969982 | 4.023699 | 0.969439 |
| H | -2.068577 | 3.358340 | -3.162128 |
| H | -3.626170 | 4.118247 | -1.406689 |
| C | 4.558011 | 0.096816 | -1.726270 |
| H | 3.706584 | 0.781643 | -1.790188 |
| C | 2.806871 | -0.255889 | 3.106624 |
| H | 1.921388 | 0.227022 | 2.683356 |
| C | -0.627363 | 3.180194 | 2.070914 |
| H | 0.245169 | 2.528498 | 2.184540 |
| C | 0.463468 | 2.394222 | -2.903031 |
| H | 1.299647 | 1.854908 | -2.447957 |
| C | -1.726480 | 2.620453 | 2.992500 |
| H | -2.036976 | 1.621510 | 2.674887 |
| H | -2.609056 | 3.271114 | 3.014683 |
| H | -1.345955 | 2.557896 | 4.019033 |
| C | -0.213661 | 4.598906 | 2.517821 |
| H | -1.054553 | 5.297035 | 2.428189 |
| H | 0.612176 | 4.995913 | 1.916149 |
| H | 0.106278 | 4.590411 | 3.566437 |
| C | -0.173597 | 1.442810 | -3.932116 |
| H | -0.980002 | 1.926784 | -4.494710 |
| H | -0.589413 | 0.554545 | -3.446090 |
| H | 0.581003 | 1.115223 | -4.656702 |
| C | 1.042427 | 3.644161 | -3.597996 |
| H | 0.250256 | 4.229988 | -4.078831 |
| H | 1.764479 | 3.354833 | -4.370993 |
| H | 1.554175 | 4.299485 | -2.883989 |
| C | 5.843667 | 0.940065 | -1.859752 |
| H | 5.859673 | 1.465464 | -2.822011 |
| H | 6.736409 | 0.305696 | -1.808144 |
| H | 5.924233 | 1.689201 | -1.064086 |
| C | 4.432956 | -0.885830 | -2.904710 |
| H | 4.392990 | -0.330858 | -3.849731 |
| H | 3.527606 | -1.493404 | -2.820883 |
| H | 5.291998 | -1.564394 | -2.961510 |
| C | 3.594361 | 0.806684 | 3.904551 |
| H | 3.905832 | 1.646982 | 3.273997 |
| H | 4.496364 | 0.369985 | 4.350604 |
| H | 2.975833 | 1.206554 | 4.716629 |
| C | 2.293456 | -1.360632 | 4.044837 |

| | | | |
|---|---|---|---|
| H | 1.743508 | -2.123903 | 3.490026 |
| H | 1.603117 | -0.924547 | 4.774501 |
| H | 3.106400 | -1.836079 | 4.607241 |
| C | -1.267272 | -1.075328 | 1.475779 |
| O | -2.260957 | -0.366989 | 1.459833 |
| O | -0.459870 | -1.543944 | 2.271284 |

15-TS

B3LYP SCF energy: -2032.27170701 a.u.
B3LYP enthalpy: -2031.468411 a.u.
B3LYP free energy: -2031.599804 a.u.
M06 SCF energy in solution: -2031.54886950 a.u.
M06 enthalpy in solution: -2030.745573 a.u.
M06 free energy in solution: -2030.876966 a.u.
Three lowest frequencies (cm-1): -181.5742 14.4287 20.0849
Imaginary frequency: -181.5742 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.711131 | -0.225853 | 0.205864 |
| N | -2.959734 | 1.347899 | -0.857197 |
| N | -1.150029 | 2.528891 | -0.540305 |
| C | -1.688030 | 1.300474 | -0.422957 |
| B | 3.296836 | -1.104479 | 0.483367 |
| O | 4.260969 | -0.191678 | 0.112047 |
| C | 5.217349 | -0.880250 | -0.740176 |
| C | 4.996094 | -2.397668 | -0.346929 |
| O | 3.642174 | -2.398687 | 0.170221 |
| C | 6.611945 | -0.331107 | -0.437109 |
| H | 6.655644 | 0.728622 | -0.710829 |
| H | 7.376852 | -0.859656 | -1.018053 |
| H | 6.860545 | -0.415546 | 0.623494 |
| C | 4.832212 | -0.562614 | -2.192065 |
| H | 4.859291 | 0.523422 | -2.332398 |
| H | 3.818913 | -0.905118 | -2.414286 |
| H | 5.532602 | -1.015771 | -2.902608 |
| C | 5.901497 | -2.873192 | 0.799067 |
| H | 5.852038 | -2.191429 | 1.654271 |
| H | 5.558694 | -3.857137 | 1.134786 |
| C | 5.065933 | -3.385313 | -1.511783 |
| H | 4.321009 | -3.152699 | -2.275556 |
| H | 4.866960 | -4.397475 | -1.144085 |
| H | 6.060389 | -3.381716 | -1.973675 |
| C | 0.784713 | -1.556388 | 0.996117 |
| C | 2.034726 | -0.750698 | 1.357383 |
| H | 6.947102 | -2.961492 | 0.484304 |
| C | -0.358348 | -1.564004 | 1.968890 |
| C | -2.547565 | -1.641119 | 3.781242 |
| C | -0.488895 | -0.613201 | 3.011854 |
| C | -1.372223 | -2.553093 | 1.865148 |
| C | -2.442705 | -2.585869 | 2.752538 |
| C | -1.564972 | -0.657922 | 3.902462 |
| H | 0.279484 | 0.143180 | 3.140121 |
| H | -1.299525 | -3.289716 | 1.069909 |
| H | -3.197266 | -3.361809 | 2.649225 |

| | | | |
|---|---|---|---|
| H | -1.623543 | 0.074940 | 4.704142 |
| H | -3.378146 | -1.679208 | 4.480875 |
| H | 1.040602 | -2.591845 | 0.767798 |
| H | 2.312591 | -0.974533 | 2.404257 |
| H | 1.859223 | 0.331028 | 1.321137 |
| C | -3.876548 | 0.241712 | -0.912846 |
| C | -5.744958 | -1.842412 | -1.046631 |
| C | -4.776368 | 0.053813 | 0.152781 |
| C | -3.883910 | -0.600616 | -2.039012 |
| C | -4.827413 | -1.633260 | -2.079539 |
| C | -5.700063 | -0.990886 | 0.062327 |
| H | -4.837519 | -2.294823 | -2.943075 |
| H | -6.397158 | -1.146368 | 0.883106 |
| C | 0.198896 | 2.858555 | -0.167387 |
| C | 2.839111 | 3.405542 | 0.591787 |
| C | 0.462261 | 3.279925 | 1.148757 |
| C | 1.225596 | 2.740633 | -1.121986 |
| C | 2.532749 | 3.023463 | -0.717308 |
| C | 1.788628 | 3.546280 | 1.504185 |
| H | 3.337972 | 2.908333 | -1.439032 |
| H | 2.006696 | 3.855248 | 2.524330 |
| C | -4.727016 | 0.918471 | 1.391198 |
| H | -3.823422 | 0.713236 | 1.977955 |
| C | -2.880148 | -0.454100 | -3.157588 |
| H | -1.934319 | -0.936372 | -2.880816 |
| C | 0.963161 | 2.255535 | -2.527561 |
| H | 0.947327 | 1.159162 | -2.549832 |
| C | -0.643085 | 3.410131 | 2.171732 |
| H | -1.413459 | 4.126471 | 1.859584 |
| H | -4.725343 | 1.989119 | 1.155955 |
| H | -5.591321 | 0.720106 | 2.032175 |
| H | -2.662920 | 0.593191 | -3.392751 |
| H | -3.247091 | -0.936158 | -4.069184 |
| H | 0.009028 | 2.614626 | -2.926822 |
| H | 1.758417 | 2.588303 | -3.202046 |
| H | -0.241690 | 3.757459 | 3.128577 |
| H | -1.144546 | 2.450917 | 2.345099 |
| C | -6.774560 | -2.945027 | -1.136376 |
| H | -6.393078 | -3.803247 | -1.699458 |
| H | -7.683622 | -2.598811 | -1.646644 |
| H | -7.073251 | -3.296340 | -0.143074 |
| C | 4.276167 | 3.605483 | 1.009437 |
| H | 4.350178 | 4.052097 | 2.006170 |
| H | 4.814831 | 4.251841 | 0.306269 |
| H | 4.794365 | 2.638470 | 1.029091 |
| C | 0.527920 | -1.514379 | -1.073195 |
| O | -0.430401 | -2.202103 | -1.406015 |
| O | 1.527569 | -1.000818 | -1.546097 |
| C | -2.096458 | 3.532996 | -1.071088 |
| H | -2.287200 | 4.310077 | -0.322322 |
| H | -1.681677 | 4.015853 | -1.961532 |
| C | -3.344538 | 2.680579 | -1.375774 |
| H | -4.244414 | 3.043794 | -0.869869 |
| H | -3.562730 | 2.615796 | -2.447865 |

16-TS

B3LYP SCF energy: -2031.06924660 a.u.
B3LYP enthalpy: -2030.290152 a.u.
B3LYP free energy: -2030.419995 a.u.
M06 SCF energy in solution: -2030.34564078 a.u.
M06 enthalpy in solution: -2029.566546 a.u.
M06 free energy in solution: -2029.696389 a.u.
Three lowest frequencies (cm-1): -183.7899 15.2363 21.1754
Imaginary frequency: -183.7899 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.717738 | -0.243603 | 0.202829 |
| N | -2.958516 | 1.387709 | -0.888325 |
| N | -1.170001 | 2.541359 | -0.556569 |
| C | -1.681385 | 1.283590 | -0.423938 |
| C | -3.235780 | 2.686226 | -1.305385 |
| C | -2.108725 | 3.413134 | -1.094917 |
| H | -4.197249 | 2.960503 | -1.710493 |
| H | -1.884458 | 4.452202 | -1.279010 |
| B | 3.286290 | -1.098999 | 0.490820 |
| O | 4.240344 | -0.176786 | 0.115624 |
| C | 5.203965 | -0.857908 | -0.734533 |
| C | 4.998677 | -2.376659 | -0.337180 |
| O | 3.646121 | -2.390420 | 0.182888 |
| C | 6.592819 | -0.293471 | -0.432555 |
| H | 6.625601 | 0.765880 | -0.709278 |
| H | 7.363309 | -0.815571 | -1.011947 |
| H | 6.842198 | -0.372418 | 0.628321 |
| C | 4.816352 | -0.548276 | -2.187516 |
| H | 4.834252 | 0.537514 | -2.331635 |
| H | 3.806096 | -0.900147 | -2.408738 |
| H | 5.520891 | -0.997542 | -2.896408 |
| C | 5.911248 | -2.840622 | 0.807801 |
| H | 5.856441 | -2.157725 | 1.661753 |
| H | 5.579119 | -3.827318 | 1.146152 |
| C | 5.075853 | -3.366200 | -1.500035 |
| H | 4.327374 | -3.142341 | -2.262947 |
| H | 4.887011 | -4.379317 | -1.129638 |
| H | 6.069410 | -3.354366 | -1.963726 |
| C | 0.777366 | -1.569413 | 1.002652 |
| C | 2.022249 | -0.757057 | 1.367080 |
| H | 6.957081 | -2.918917 | 0.491146 |
| C | -0.370400 | -1.578802 | 1.970392 |
| C | -2.574236 | -1.652608 | 3.765400 |
| C | -0.509654 | -0.626030 | 3.010407 |
| C | -1.381212 | -2.570439 | 1.862871 |
| C | -2.459209 | -2.601184 | 2.741539 |
| C | -1.592950 | -0.668672 | 3.892047 |
| H | 0.256785 | 0.131689 | 3.142573 |
| H | -1.301000 | -3.309931 | 1.071022 |
| H | -3.211716 | -3.378770 | 2.635033 |
| H | -1.658670 | 0.066570 | 4.691017 |
| H | -3.410932 | -1.688760 | 4.457828 |
| H | 1.039519 | -2.604386 | 0.778898 |
| H | 2.301569 | -0.983001 | 2.413073 |
| H | 1.839112 | 0.323665 | 1.335044 |

| | | | |
|---|---|---|---|
| C | -3.912737 | 0.304771 | -0.943101 |
| C | -5.803008 | -1.747058 | -1.060209 |
| C | -4.817348 | 0.152369 | 0.121499 |
| C | -3.916353 | -0.548340 | -2.058442 |
| C | -4.875535 | -1.566811 | -2.089899 |
| C | -5.755447 | -0.879976 | 0.036701 |
| H | -4.890137 | -2.239547 | -2.944391 |
| H | -6.461864 | -1.012416 | 0.853290 |
| C | 0.182684 | 2.890630 | -0.191341 |
| C | 2.813903 | 3.425655 | 0.569410 |
| C | 0.434017 | 3.327689 | 1.119607 |
| C | 1.205192 | 2.744698 | -1.143653 |
| C | 2.511832 | 3.024819 | -0.735288 |
| C | 1.760861 | 3.591401 | 1.474955 |
| H | 3.319502 | 2.892581 | -1.450984 |
| H | 1.976414 | 3.917894 | 2.489944 |
| C | -4.764537 | 1.039989 | 1.343152 |
| H | -3.868064 | 0.830850 | 1.939828 |
| C | -2.905899 | -0.421566 | -3.172853 |
| H | -1.960977 | -0.898090 | -2.882906 |
| C | 0.939918 | 2.243969 | -2.542841 |
| H | 0.923063 | 1.147339 | -2.551611 |
| C | -0.679532 | 3.479523 | 2.129972 |
| H | -1.482137 | 4.129933 | 1.762685 |
| H | -4.741752 | 2.104278 | 1.083512 |
| H | -5.636675 | 0.866351 | 1.980218 |
| H | -2.692881 | 0.622972 | -3.422933 |
| H | -3.268394 | -0.921080 | -4.076568 |
| H | -0.013941 | 2.602759 | -2.942223 |
| H | 1.736051 | 2.567547 | -3.220524 |
| H | -0.297712 | 3.909920 | 3.060433 |
| H | -1.135394 | 2.510743 | 2.367848 |
| C | -6.847613 | -2.836025 | -1.141484 |
| H | -6.478953 | -3.702200 | -1.700701 |
| H | -7.752758 | -2.479665 | -1.651583 |
| H | -7.148842 | -3.177606 | -0.145607 |
| C | 4.250590 | 3.621670 | 0.989974 |
| H | 4.323874 | 4.076363 | 1.983014 |
| H | 4.794684 | 4.259043 | 0.282850 |
| H | 4.762980 | 2.651880 | 1.019088 |
| C | 0.525611 | -1.528243 | -1.062348 |
| O | -0.433027 | -2.214030 | -1.400347 |
| O | 1.527223 | -1.016264 | -1.534443 |

3

B3LYP SCF energy: -720.33002871 a.u.
B3LYP enthalpy: -720.005246 a.u.
B3LYP free energy: -720.067674 a.u.
M06 SCF energy in solution: -720.02267060 a.u.
M06 enthalpy in solution: -719.697888 a.u.
M06 free energy in solution: -719.760316 a.u.
Three lowest frequencies (cm-1): 20.2066 36.2691 52.0413

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| B | -0.916567 | -0.367758 | 0.057266 |
| O | -1.897493 | -1.323875 | 0.190508 |
| C | -3.169758 | -0.696067 | -0.126466 |
| C | -2.859469 | 0.834061 | 0.113887 |
| O | -1.427187 | 0.899883 | -0.123684 |
| C | -4.243913 | -1.294004 | 0.781055 |
| H | -4.357083 | -2.360674 | 0.561537 |
| H | -5.212564 | -0.809102 | 0.613066 |
| H | -3.982041 | -1.194186 | 1.836898 |
| C | -3.472814 | -1.032777 | -1.593297 |
| H | -3.472257 | -2.120525 | -1.714498 |
| H | -2.710912 | -0.618384 | -2.261098 |
| H | -4.451671 | -0.651354 | -1.902866 |
| C | -3.089819 | 1.279579 | 1.564972 |
| H | -2.594386 | 0.605600 | 2.271086 |
| H | -2.667196 | 2.280042 | 1.700996 |
| C | -3.553431 | 1.798612 | -0.846999 |
| H | -3.294233 | 1.589074 | -1.887362 |
| H | -3.243974 | 2.824737 | -0.623144 |
| H | -4.642907 | 1.742883 | -0.739331 |
| C | 1.537525 | 0.267107 | -0.015741 |
| C | 0.594009 | -0.690895 | 0.100883 |
| H | -4.156141 | 1.318717 | 1.812072 |
| C | 2.998187 | 0.109178 | -0.008278 |
| C | 5.812675 | -0.085239 | -0.014400 |
| C | 3.637579 | -1.133468 | 0.165363 |
| C | 3.805267 | 1.248177 | -0.182501 |
| C | 5.196295 | 1.154974 | -0.186853 |
| C | 5.025767 | -1.228460 | 0.162302 |
| H | 3.041898 | -2.030606 | 0.305363 |
| H | 3.328134 | 2.216254 | -0.317415 |
| H | 5.797863 | 2.049586 | -0.324500 |
| H | 5.499028 | -2.197410 | 0.298641 |
| H | 6.896557 | -0.163265 | -0.016588 |
| H | 1.197027 | 1.296371 | -0.136178 |
| H | 0.896542 | -1.731694 | 0.218841 |

4

B3LYP SCF energy: -1304.19639419 a.u.
B3LYP enthalpy: -1303.608974 a.u.
B3LYP free energy: -1303.699960 a.u.
M06 SCF energy in solution: -1303.75376121 a.u.
M06 enthalpy in solution: -1303.166341 a.u.
M06 free energy in solution: -1303.257327 a.u.
Three lowest frequencies (cm-1): 12.0442 12.2053 22.2723

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.000000 | 0.000000 | 0.296181 |
| N | 0.898118 | -0.592813 | -2.517497 |
| N | -0.898118 | 0.592813 | -2.517497 |
| C | 0.000000 | 0.000000 | -1.679728 |
| C | 0.566918 | -0.374422 | -3.846662 |
| C | -0.566918 | 0.374422 | -3.846662 |
| C | -2.059124 | 1.365223 | -2.042449 |

| | | | |
|---|---|---|---|
| C | -3.385277 | 0.728788 | -2.490061 |
| C | -4.582450 | 1.530102 | -1.952088 |
| C | -4.502113 | 3.009125 | -2.360078 |
| C | -3.168310 | 3.635856 | -1.925201 |
| C | -1.967177 | 2.840954 | -2.463512 |
| C | 2.059124 | -1.365223 | -2.042449 |
| C | 1.967177 | -2.840954 | -2.463512 |
| C | 3.168310 | -3.635856 | -1.925201 |
| C | 4.502113 | -3.009125 | -2.360078 |
| C | 4.582450 | -1.530102 | -1.952088 |
| C | 3.385277 | -0.728788 | -2.490061 |
| H | 1.149812 | -0.759574 | -4.668474 |
| H | -1.149812 | 0.759574 | -4.668474 |
| H | -1.994266 | 1.308150 | -0.950005 |
| H | -3.425855 | -0.310648 | -2.143220 |
| H | -3.428030 | 0.703258 | -3.588904 |
| H | -4.601031 | 1.455278 | -0.855508 |
| H | -5.517221 | 1.082753 | -2.311247 |
| H | -5.340998 | 3.566927 | -1.926028 |
| H | -4.603344 | 3.091133 | -3.452743 |
| H | -3.118676 | 3.661066 | -0.827308 |
| H | -3.104417 | 4.676850 | -2.264572 |
| H | -1.946421 | 2.908863 | -3.561200 |
| H | -1.024722 | 3.265719 | -2.097835 |
| H | 1.994266 | -1.308150 | -0.950005 |
| H | 1.946421 | -2.908863 | -3.561200 |
| H | 1.024722 | -3.265719 | -2.097835 |
| H | 3.104417 | -4.676850 | -2.264572 |
| H | 3.118676 | -3.661066 | -0.827308 |
| H | 4.603344 | -3.091133 | -3.452743 |
| H | 5.340998 | -3.566927 | -1.926028 |
| H | 5.517221 | -1.082753 | -2.311247 |
| H | 4.601031 | -1.455278 | -0.855508 |
| H | 3.425855 | 0.310648 | -2.143220 |
| H | 3.428030 | -0.703258 | -3.588904 |
| B | 0.000000 | 0.000000 | 2.290582 |
| O | 0.999288 | -0.550300 | 3.097502 |
| C | 0.553094 | -0.557997 | 4.477104 |
| C | -0.553094 | 0.557997 | 4.477104 |
| O | -0.999288 | 0.550300 | 3.097502 |
| C | 1.757227 | -0.287079 | 5.380410 |
| H | 2.483862 | -1.100152 | 5.275920 |
| H | 1.458808 | -0.234081 | 6.434837 |
| H | 2.259085 | 0.645766 | 5.112818 |
| C | 0.000000 | -1.964461 | 4.759227 |
| H | 0.780237 | -2.701052 | 4.540884 |
| H | -0.858784 | -2.184446 | 4.117470 |
| H | -0.304464 | -2.084821 | 5.805544 |
| C | 0.000000 | 1.964461 | 4.759227 |
| H | 0.858784 | 2.184446 | 4.117470 |
| H | 0.304464 | 2.084821 | 5.805544 |
| H | -0.780237 | 2.701052 | 4.540884 |
| C | -1.757227 | 0.287079 | 5.380410 |
| H | -2.259085 | -0.645766 | 5.112818 |
| H | -2.483862 | 1.100152 | 5.275920 |
| H | -1.458808 | 0.234081 | 6.434837 |

5-TS

B3LYP SCF energy: -1613.82312180 a.u.
B3LYP enthalpy: -1613.093934 a.u.
B3LYP free energy: -1613.198988 a.u.
M06 SCF energy in solution: -1613.23866121 a.u.
M06 enthalpy in solution: -1612.509473 a.u.
M06 free energy in solution: -1612.614527 a.u.
Three lowest frequencies (cm-1): -232.4176 12.1367 19.0193
Imaginary frequency: -232.4176 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.034582 | 0.092255 | -0.805464 |
| N | -1.001385 | -2.436483 | 0.280815 |
| N | 1.079400 | -2.142534 | 0.786820 |
| C | 0.036576 | -1.559904 | 0.126695 |
| C | -0.605614 | -3.546932 | 1.013559 |
| C | 0.698332 | -3.356629 | 1.339172 |
| C | 2.427503 | -1.551578 | 0.883930 |
| C | 3.499116 | -2.502984 | 0.326510 |
| C | 4.894223 | -1.862106 | 0.414004 |
| C | 5.224684 | -1.422717 | 1.848777 |
| C | 4.144635 | -0.481457 | 2.403524 |
| C | 2.747465 | -1.118457 | 2.324500 |
| C | -2.333352 | -2.227670 | -0.308015 |
| C | -2.534384 | -3.088972 | -1.567205 |
| C | -3.908976 | -2.819124 | -2.200262 |
| C | -5.047424 | -3.020965 | -1.188565 |
| C | -4.828716 | -2.173596 | 0.074932 |
| C | -3.458537 | -2.456254 | 0.713790 |
| H | -1.270569 | -4.364665 | 1.240779 |
| H | 1.373394 | -3.974575 | 1.909311 |
| H | 2.391801 | -0.661628 | 0.247417 |
| H | 3.254219 | -2.757918 | -0.711473 |
| H | 3.494113 | -3.441777 | 0.900291 |
| H | 4.932044 | -0.990384 | -0.252189 |
| H | 5.645976 | -2.573135 | 0.048870 |
| H | 6.203530 | -0.928186 | 1.873858 |
| H | 5.303726 | -2.310018 | 2.495765 |
| H | 4.145855 | 0.450996 | 1.823226 |
| H | 4.367407 | -0.210630 | 3.443203 |
| H | 2.704528 | -1.996394 | 2.986765 |
| H | 1.980267 | -0.416017 | 2.671840 |
| H | -2.344371 | -1.170517 | -0.595713 |
| H | -2.454605 | -4.151557 | -1.293689 |
| H | -1.729752 | -2.880304 | -2.282194 |
| H | -4.050076 | -3.470924 | -3.070999 |
| H | -3.934812 | -1.785883 | -2.575125 |
| H | -5.100372 | -4.083615 | -0.908056 |
| H | -6.011529 | -2.771057 | -1.648410 |
| H | -5.623703 | -2.364067 | 0.806364 |
| H | -4.888479 | -1.107558 | -0.186052 |
| H | -3.297121 | -1.813971 | 1.588074 |
| H | -3.436837 | -3.496133 | 1.070443 |
| B | -1.202287 | 1.650434 | -0.217333 |

| | | | |
|---|---|---|---|
| O | -2.571778 | 1.693632 | -0.445364 |
| C | -3.140277 | 2.735734 | 0.401183 |
| C | -2.063924 | 2.856436 | 1.545390 |
| O | -0.847737 | 2.445570 | 0.865402 |
| C | -4.529031 | 2.288965 | 0.854706 |
| H | -5.188613 | 2.199451 | -0.015079 |
| H | -4.973190 | 3.020834 | 1.539820 |
| H | -4.497831 | 1.318869 | 1.356657 |
| C | -3.251565 | 3.998686 | -0.463888 |
| H | -3.863200 | 3.774712 | -1.343845 |
| H | -2.268072 | 4.330317 | -0.811514 |
| H | -3.721795 | 4.824539 | 0.080936 |
| C | -2.290360 | 1.869709 | 2.700146 |
| H | -2.430483 | 0.850609 | 2.326318 |
| H | -3.159926 | 2.144409 | 3.307526 |
| H | -1.405973 | 1.871798 | 3.345165 |
| C | -1.854815 | 4.266452 | 2.096984 |
| H | -1.552701 | 4.965451 | 1.313637 |
| H | -1.064637 | 4.249516 | 2.854820 |
| H | -2.769283 | 4.644018 | 2.570007 |
| C | -0.091114 | 1.825157 | -1.816287 |
| C | 1.092987 | 1.070465 | -2.297841 |
| H | 0.126559 | 2.838077 | -1.461525 |
| H | 0.996760 | 0.598268 | -3.271986 |
| C | 2.442014 | 1.407999 | -1.879883 |
| C | 3.565608 | 0.917346 | -2.596612 |
| C | 2.724001 | 2.231147 | -0.756404 |
| C | 4.867947 | 1.229192 | -2.224804 |
| H | 3.391999 | 0.288304 | -3.468106 |
| C | 4.034507 | 2.540623 | -0.390203 |
| H | 1.905355 | 2.636838 | -0.166673 |
| C | 5.122863 | 2.046240 | -1.113907 |
| H | 5.697125 | 0.840260 | -2.813032 |
| H | 4.204141 | 3.185708 | 0.470166 |
| H | 6.141234 | 2.296858 | -0.829897 |
| H | -0.909780 | 1.834187 | -2.537900 |

6

B3LYP SCF energy: -1613.87835095 a.u.
B3LYP enthalpy: -1613.147018 a.u.
B3LYP free energy: -1613.254971 a.u.
M06 SCF energy in solution: -1613.28810462 a.u.
M06 enthalpy in solution: -1612.556772 a.u.
M06 free energy in solution: -1612.664725 a.u.
Three lowest frequencies (cm-1): 9.5551 11.8869 25.9096

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.463800 | -0.156203 | -0.174606 |
| N | -2.478326 | 1.968338 | 0.108027 |
| N | -0.509916 | 2.843366 | 0.043651 |
| C | -1.157763 | 1.644263 | -0.005553 |
| C | -2.647854 | 3.338608 | 0.226516 |
| C | -1.407723 | 3.891555 | 0.185211 |
| C | 0.952522 | 2.987577 | -0.046916 |

| | | | |
|---|---|---|---|
| C | 1.535505 | 3.612339 | 1.232096 |
| C | 3.064088 | 3.742842 | 1.133200 |
| C | 3.484987 | 4.526605 | -0.119319 |
| C | 2.893468 | 3.902472 | -1.392435 |
| C | 1.364040 | 3.775167 | -1.302397 |
| C | -3.570544 | 0.974952 | 0.104598 |
| C | -4.318723 | 0.954054 | 1.447439 |
| C | -5.428086 | -0.111490 | 1.433040 |
| C | -6.392053 | 0.094752 | 0.254518 |
| C | -5.635582 | 0.128054 | -1.082252 |
| C | -4.528832 | 1.195975 | -1.077063 |
| H | -3.616360 | 3.802126 | 0.328184 |
| H | -1.100228 | 4.923680 | 0.243443 |
| H | 1.323328 | 1.960722 | -0.139910 |
| H | 1.251756 | 3.001888 | 2.097763 |
| H | 1.095968 | 4.608743 | 1.385429 |
| H | 3.511132 | 2.738719 | 1.101711 |
| H | 3.452060 | 4.226580 | 2.037777 |
| H | 4.578868 | 4.567220 | -0.190479 |
| H | 3.138123 | 5.566888 | -0.029880 |
| H | 3.329100 | 2.904527 | -1.545955 |
| H | 3.163011 | 4.497997 | -2.273074 |
| H | 0.916415 | 4.779104 | -1.267568 |
| H | 0.962463 | 3.276521 | -2.192517 |
| H | -3.069070 | 0.010964 | -0.029769 |
| H | -4.761678 | 1.943375 | 1.636447 |
| H | -3.605916 | 0.760570 | 2.258068 |
| H | -5.973730 | -0.085569 | 2.384383 |
| H | -4.969551 | -1.106779 | 1.356810 |
| H | -6.938270 | 1.040821 | 0.389294 |
| H | -7.144926 | -0.702789 | 0.240759 |
| H | -6.328007 | 0.320723 | -1.911063 |
| H | -5.182587 | -0.855362 | -1.267044 |
| H | -3.962139 | 1.172083 | -2.015768 |
| H | -4.984028 | 2.194706 | -1.000615 |
| B | 2.488018 | -2.173420 | 0.396484 |
| O | 3.517487 | -2.412590 | 1.287626 |
| C | 4.716484 | -1.776368 | 0.780671 |
| C | 4.392228 | -1.628662 | -0.756628 |
| O | 2.942873 | -1.576365 | -0.762428 |
| C | 5.916263 | -2.663718 | 1.113256 |
| H | 6.031434 | -2.730858 | 2.200114 |
| H | 6.842110 | -2.246844 | 0.699483 |
| H | 5.786696 | -3.677342 | 0.727274 |
| C | 4.845316 | -0.429537 | 1.507827 |
| H | 4.863857 | -0.609817 | 2.587310 |
| H | 3.989437 | 0.218206 | 1.290414 |
| H | 5.763643 | 0.099405 | 1.229882 |
| C | 4.792390 | -2.859664 | -1.583171 |
| H | 4.418053 | -3.781552 | -1.127059 |
| H | 4.350111 | -2.774552 | -2.580729 |
| C | 4.929447 | -0.361355 | -1.421040 |
| H | 4.546569 | 0.540942 | -0.937602 |
| H | 4.618819 | -0.338598 | -2.470835 |
| H | 6.025066 | -0.335139 | -1.390961 |
| C | -0.037061 | -2.068031 | -0.331685 |
| C | 1.003222 | -2.592565 | 0.678503 |

| | | | |
|---|---|---|---|
| H | 5.879303 | -2.941747 | -1.692222 |
| C | -1.380110 | -2.719646 | -0.265678 |
| C | -3.988934 | -3.883537 | -0.185971 |
| C | -1.934236 | -3.226526 | 0.931552 |
| C | -2.184566 | -2.837223 | -1.425145 |
| C | -3.456797 | -3.402930 | -1.389025 |
| C | -3.210914 | -3.791090 | 0.970763 |
| H | -1.350744 | -3.178557 | 1.847026 |
| H | -1.785490 | -2.476403 | -2.372248 |
| H | -4.032745 | -3.485459 | -2.309104 |
| H | -3.595106 | -4.174348 | 1.914417 |
| H | -4.977303 | -4.334850 | -0.156884 |
| H | 0.358058 | -2.190712 | -1.349364 |
| H | 0.999018 | -3.702336 | 0.710362 |
| H | 0.767299 | -2.301436 | 1.712654 |

7-TS

B3LYP SCF energy: -1613.80323721 a.u.
B3LYP enthalpy: -1613.074632 a.u.
B3LYP free energy: -1613.180822 a.u.
M06 SCF energy in solution: -1613.21943376 a.u.
M06 enthalpy in solution: -1612.490829 a.u.
M06 free energy in solution: -1612.597019 a.u.
Three lowest frequencies (cm-1): -289.7014 13.2413 13.9113
Imaginary frequency: -289.7014 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.219301 | -0.116615 | -1.191108 |
| N | -2.712560 | -1.132913 | -0.063879 |
| N | -1.063032 | -2.452421 | 0.393817 |
| C | -1.365470 | -1.281787 | -0.244384 |
| C | -3.236307 | -2.193285 | 0.665503 |
| C | -2.202877 | -3.026000 | 0.945335 |
| C | 0.282335 | -3.044230 | 0.402478 |
| C | 0.367157 | -4.255278 | -0.542566 |
| C | 1.787394 | -4.843010 | -0.556616 |
| C | 2.267922 | -5.195668 | 0.859661 |
| C | 2.168891 | -3.984858 | 1.800343 |
| C | 0.746191 | -3.401278 | 1.823943 |
| C | -3.464820 | 0.032909 | -0.551962 |
| C | -4.726642 | -0.378955 | -1.327212 |
| C | -5.470916 | 0.862105 | -1.848577 |
| C | -5.808144 | 1.838035 | -0.711006 |
| C | -4.548317 | 2.238070 | 0.071525 |
| C | -3.788080 | 1.008057 | 0.592585 |
| H | -4.281057 | -2.266166 | 0.921991 |
| H | -2.184931 | -3.960993 | 1.482170 |
| H | 0.934171 | -2.251892 | 0.018226 |
| H | 0.061535 | -3.949476 | -1.549926 |
| H | -0.345953 | -5.023091 | -0.207981 |
| H | 2.475469 | -4.109738 | -1.001859 |
| H | 1.816033 | -5.728272 | -1.203577 |
| H | 3.299830 | -5.566785 | 0.828541 |
| H | 1.651883 | -6.015867 | 1.257857 |

| | | | |
|---|---|---|---|
| H | 2.871415 | -3.206923 | 1.469084 |
| H | 2.469887 | -4.264095 | 2.817548 |
| H | 0.061497 | -4.142142 | 2.262006 |
| H | 0.702124 | -2.507765 | 2.457391 |
| H | -2.778758 | 0.527329 | -1.250001 |
| H | -5.399208 | -0.947910 | -0.668784 |
| H | -4.448622 | -1.043029 | -2.154241 |
| H | -6.383574 | 0.551649 | -2.371848 |
| H | -4.842691 | 1.372746 | -2.592602 |
| H | -6.526089 | 1.361980 | -0.026318 |
| H | -6.304506 | 2.729844 | -1.113481 |
| H | -4.809895 | 2.894396 | 0.910630 |
| H | -3.882104 | 2.819192 | -0.582137 |
| H | -2.853211 | 1.312369 | 1.075249 |
| H | -4.397383 | 0.488046 | 1.347061 |
| B | 0.610367 | 1.278734 | 0.123792 |
| O | -0.168571 | 2.346156 | 0.562946 |
| C | 0.462386 | 2.916226 | 1.745069 |
| C | 1.341888 | 1.717002 | 2.265465 |
| O | 1.591768 | 0.963797 | 1.048088 |
| C | -0.632028 | 3.386269 | 2.702784 |
| H | -1.207809 | 4.191556 | 2.234511 |
| H | -0.199239 | 3.777107 | 3.631455 |
| H | -1.324376 | 2.579724 | 2.955891 |
| C | 1.291437 | 4.118869 | 1.272431 |
| H | 0.633259 | 4.815412 | 0.742604 |
| H | 2.082956 | 3.809158 | 0.583765 |
| H | 1.750303 | 4.651898 | 2.112633 |
| C | 0.590780 | 0.782508 | 3.226155 |
| H | -0.369662 | 0.469979 | 2.805188 |
| H | 0.411878 | 1.254219 | 4.198920 |
| H | 1.196700 | -0.114928 | 3.388983 |
| C | 2.688851 | 2.112489 | 2.870867 |
| H | 3.313311 | 2.641299 | 2.147808 |
| H | 3.228708 | 1.212315 | 3.182904 |
| H | 2.552741 | 2.748767 | 3.753851 |
| C | 1.071812 | 1.357502 | -1.841698 |
| C | 0.452547 | 0.525313 | -2.935369 |
| H | -0.250478 | 1.062842 | -3.571310 |
| H | 0.706197 | 2.386510 | -1.845070 |
| C | 2.571834 | 1.315716 | -1.750273 |
| C | 3.308925 | 2.509523 | -1.785014 |
| C | 3.283407 | 0.106627 | -1.682055 |
| C | 4.705276 | 2.499856 | -1.751026 |
| H | 2.779737 | 3.457602 | -1.855630 |
| C | 4.676363 | 0.093380 | -1.648294 |
| H | 2.735283 | -0.832044 | -1.656373 |
| C | 5.397216 | 1.290617 | -1.680158 |
| H | 5.250574 | 3.440165 | -1.785253 |
| H | 5.203659 | -0.856369 | -1.595047 |
| H | 6.483679 | 1.278784 | -1.653013 |
| H | 1.154107 | -0.081877 | -3.504091 |

8
B3LYP SCF energy: -1613.87302708 a.u.

B3LYP enthalpy: -1613.141439 a.u.
B3LYP free energy: -1613.250401 a.u.
M06 SCF energy in solution: -1613.28044171 a.u.
M06 enthalpy in solution: -1612.548854 a.u.
M06 free energy in solution: -1612.657816 a.u.
Three lowest frequencies (cm-1): 10.5239 11.9350 21.2754

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.641882 | -0.596047 | -0.725100 |
| N | -2.466009 | 1.735468 | -0.471200 |
| N | -3.535694 | -0.103825 | -0.136396 |
| C | -2.291108 | 0.383820 | -0.409557 |
| C | -3.790429 | 2.080636 | -0.247746 |
| C | -4.464952 | 0.920934 | -0.033494 |
| C | -3.827980 | -1.537464 | 0.031383 |
| C | -4.829999 | -2.040057 | -1.021135 |
| C | -5.089591 | -3.546077 | -0.849943 |
| C | -5.555080 | -3.881505 | 0.575259 |
| C | -4.559661 | -3.362520 | 1.624220 |
| C | -4.298634 | -1.856119 | 1.460116 |
| C | -1.374403 | 2.680885 | -0.769121 |
| C | -1.530558 | 3.299992 | -2.168243 |
| C | -0.358568 | 4.247041 | -2.476969 |
| C | -0.199231 | 5.323577 | -1.392830 |
| C | -0.062832 | 4.694636 | 0.002492 |
| C | -1.242812 | 3.759679 | 0.316533 |
| H | -4.140194 | 3.100768 | -0.255998 |
| H | -5.507540 | 0.747692 | 0.181732 |
| H | -2.865027 | -2.031928 | -0.138545 |
| H | -4.443854 | -1.823928 | -2.024433 |
| H | -5.778428 | -1.492850 | -0.916760 |
| H | -4.164474 | -4.097664 | -1.070469 |
| H | -5.832800 | -3.878208 | -1.584816 |
| H | -5.688619 | -4.964734 | 0.684297 |
| H | -6.540359 | -3.424918 | 0.752612 |
| H | -3.608731 | -3.905266 | 1.524002 |
| H | -4.928615 | -3.565116 | 2.636978 |
| H | -5.223135 | -1.300154 | 1.674688 |
| H | -3.544277 | -1.512120 | 2.177827 |
| H | -0.468146 | 2.065710 | -0.756324 |
| H | -2.477929 | 3.857162 | -2.217633 |
| H | -1.589156 | 2.499274 | -2.915089 |
| H | -0.507442 | 4.710664 | -3.459726 |
| H | 0.568147 | 3.659916 | -2.544752 |
| H | -1.076400 | 5.987862 | -1.407612 |
| H | 0.672757 | 5.952291 | -1.610957 |
| H | 0.003914 | 5.475759 | 0.769847 |
| H | 0.870949 | 4.117492 | 0.055222 |
| H | -1.108102 | 3.281299 | 1.293590 |
| H | -2.169435 | 4.349935 | 0.370286 |
| B | 2.429096 | -0.202717 | 0.477210 |
| O | 2.165720 | 1.103013 | 0.860147 |
| C | 2.534869 | 1.241980 | 2.258183 |
| C | 2.487775 | -0.249265 | 2.770292 |
| O | 2.753319 | -0.996317 | 1.558082 |
| C | 1.548230 | 2.190698 | 2.937735 |

| | | | |
|---|---|---|---|
| H | 1.633434 | 3.189421 | 2.496139 |
| H | 1.763390 | 2.277391 | 4.009366 |
| H | 0.516172 | 1.852010 | 2.817469 |
| C | 3.945756 | 1.847971 | 2.283386 |
| H | 3.934295 | 2.797974 | 1.739292 |
| H | 4.667893 | 1.188059 | 1.792765 |
| H | 4.288118 | 2.040164 | 3.306104 |
| C | 1.098813 | -0.680834 | 3.264181 |
| H | 0.327439 | -0.449289 | 2.522460 |
| H | 0.835495 | -0.198470 | 4.212100 |
| H | 1.100981 | -1.764686 | 3.417379 |
| C | 3.548257 | -0.614953 | 3.808789 |
| H | 4.559174 | -0.451109 | 3.428688 |
| H | 3.455077 | -1.674594 | 4.068504 |
| H | 3.418459 | -0.028639 | 4.726233 |
| C | 2.327034 | -0.720156 | -1.004516 |
| C | 0.997193 | -1.546188 | -1.129177 |
| H | 0.929754 | -1.920090 | -2.164739 |
| H | 2.236204 | 0.167304 | -1.645878 |
| C | 3.553211 | -1.489940 | -1.478444 |
| C | 4.244944 | -1.090893 | -2.632308 |
| C | 4.015285 | -2.634579 | -0.805165 |
| C | 5.350613 | -1.802961 | -3.103546 |
| H | 3.906433 | -0.207878 | -3.171738 |
| C | 5.119450 | -3.348121 | -1.270492 |
| H | 3.505433 | -2.958216 | 0.097125 |
| C | 5.794169 | -2.937792 | -2.423775 |
| H | 5.863972 | -1.469669 | -4.002932 |
| H | 5.457359 | -4.228909 | -0.728578 |
| H | 6.654003 | -3.495834 | -2.786323 |
| H | 1.083925 | -2.444536 | -0.498862 |

9-TS-BINAP

B3LYP SCF energy: -3485.50674038 a.u.
B3LYP enthalpy: -3484.489323 a.u.
B3LYP free energy: -3484.648841 a.u.
M06 SCF energy in solution: -3484.38377080 a.u.
M06 enthalpy in solution: -3483.366353 a.u.
M06 free energy in solution: -3483.525871 a.u.
Three lowest frequencies (cm-1): -217.8368 13.7452 15.2890
Imaginary frequency: -217.8368 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 3.916525 | -1.981691 | 2.592746 |
| C | 3.563897 | -2.048773 | 1.206539 |
| C | 2.701816 | -1.042601 | 0.633535 |
| C | 2.215815 | -0.014539 | 1.442420 |
| C | 2.431807 | -1.136358 | -0.843278 |
| C | 3.530759 | -0.819603 | -1.726426 |
| C | 3.396962 | -1.021490 | -3.137678 |
| C | 2.172223 | -1.524382 | -3.638746 |
| C | 1.126519 | -1.790562 | -2.795297 |
| C | 1.228372 | -1.606232 | -1.382436 |
| P | 1.118713 | 1.328615 | 0.747228 |

| | | | |
|---|---|---|---|
| P | -0.417176 | -1.684304 | -0.511273 |
| H | 2.062715 | -1.684725 | -4.708446 |
| H | 0.195843 | -2.150234 | -3.216658 |
| C | -1.321988 | -3.022061 | -1.438797 |
| C | -1.028163 | -4.382269 | -1.242106 |
| C | -2.314763 | -2.672650 | -2.366383 |
| C | -1.706405 | -5.367378 | -1.958471 |
| H | -0.275944 | -4.682147 | -0.520977 |
| C | -2.990227 | -3.664555 | -3.085488 |
| H | -2.559505 | -1.629898 | -2.537244 |
| C | -2.690555 | -5.011182 | -2.884207 |
| H | -1.465478 | -6.414210 | -1.792018 |
| H | -3.753627 | -3.374137 | -3.802480 |
| H | -3.219012 | -5.780094 | -3.441914 |
| C | -0.288634 | -2.451950 | 1.160734 |
| C | -1.272306 | -2.069586 | 2.089656 |
| C | 0.639799 | -3.438516 | 1.523995 |
| C | -1.316589 | -2.660278 | 3.354839 |
| H | -2.025116 | -1.336637 | 1.810776 |
| C | 0.598354 | -4.018843 | 2.792660 |
| H | 1.406592 | -3.750647 | 0.824102 |
| C | -0.379038 | -3.630797 | 3.711326 |
| H | -2.086966 | -2.359998 | 4.060650 |
| H | 1.334400 | -4.771750 | 3.061048 |
| H | -0.410481 | -4.085151 | 4.698183 |
| C | 0.661945 | 2.275760 | 2.269086 |
| C | 1.172533 | 3.544209 | 2.575189 |
| C | -0.280551 | 1.698989 | 3.139643 |
| C | 0.757122 | 4.216381 | 3.727839 |
| H | 1.882578 | 4.019515 | 1.908082 |
| C | -0.689630 | 2.369112 | 4.292247 |
| H | -0.689130 | 0.715146 | 2.922603 |
| C | -0.172554 | 3.632982 | 4.588932 |
| H | 1.161221 | 5.201083 | 3.947614 |
| H | -1.416492 | 1.906287 | 4.954406 |
| H | -0.495602 | 4.159019 | 5.483191 |
| C | 2.313516 | 2.385991 | -0.167860 |
| C | 1.967069 | 2.832929 | -1.450629 |
| C | 3.564722 | 2.735318 | 0.371045 |
| C | 2.854270 | 3.634196 | -2.174293 |
| H | 1.013904 | 2.553201 | -1.888183 |
| C | 4.442955 | 3.538444 | -0.354215 |
| H | 3.854012 | 2.375762 | 1.355003 |
| C | 4.086845 | 3.990138 | -1.628778 |
| H | 2.573888 | 3.977234 | -3.165946 |
| H | 5.406413 | 3.806978 | 0.071479 |
| H | 4.774251 | 4.613549 | -2.194739 |
| C | 2.583360 | 0.028766 | 2.818666 |
| C | 3.407624 | -0.916498 | 3.374149 |
| H | 3.679018 | -0.854735 | 4.425437 |
| H | 2.210979 | 0.830772 | 3.443335 |
| C | 4.075700 | -3.142516 | 0.447978 |
| H | 3.820498 | -3.224286 | -0.601843 |
| C | 4.759262 | -2.977206 | 3.157142 |
| H | 5.016429 | -2.901462 | 4.211048 |
| C | 5.236399 | -4.016143 | 2.392490 |
| H | 5.879442 | -4.773098 | 2.833108 |

| | | | |
|---|---|---|---|
| C | 4.884240 | -4.097684 | 1.024020 |
| H | 5.258124 | -4.920162 | 0.420279 |
| C | 4.482894 | -0.719945 | -4.001944 |
| H | 4.355938 | -0.884942 | -5.069191 |
| C | 4.768345 | -0.297925 | -1.250596 |
| H | 4.893410 | -0.112893 | -0.190807 |
| C | 5.802287 | -0.007669 | -2.113092 |
| H | 6.731140 | 0.396877 | -1.720233 |
| C | 5.665687 | -0.225099 | -3.504029 |
| H | 6.490274 | 0.005178 | -4.173148 |
| Cu | -0.810979 | 0.698997 | -0.484347 |
| C | -2.395954 | 2.342887 | -0.793084 |
| H | -3.185543 | 2.427287 | -1.539740 |
| C | -1.649823 | 3.644108 | -0.819030 |
| C | -0.382393 | 6.183292 | -0.958188 |
| C | -1.333821 | 4.244897 | -2.057174 |
| C | -1.315416 | 4.362435 | 0.343279 |
| C | -0.690943 | 5.610784 | 0.274850 |
| C | -0.712317 | 5.488766 | -2.126407 |
| H | -1.580592 | 3.721226 | -2.975830 |
| H | -1.562470 | 3.953278 | 1.316819 |
| H | -0.456551 | 6.139215 | 1.196156 |
| H | -0.492206 | 5.923657 | -3.098907 |
| H | 0.097255 | 7.157313 | -1.011430 |
| C | -3.113431 | 1.988704 | 0.535681 |
| H | -3.648305 | 2.894409 | 0.874080 |
| H | -2.409026 | 1.749435 | 1.342300 |
| B | -4.205983 | 0.860480 | 0.423617 |
| O | -5.477422 | 1.097090 | -0.034912 |
| C | -6.172217 | -0.176482 | -0.128235 |
| C | -5.340404 | -1.086717 | 0.860640 |
| O | -4.034282 | -0.437857 | 0.859083 |
| C | -5.167849 | -2.538166 | 0.418999 |
| H | -4.676302 | -2.609716 | -0.552875 |
| H | -6.139073 | -3.043529 | 0.360916 |
| H | -4.551584 | -3.075389 | 1.147867 |
| C | -5.845710 | -1.034649 | 2.309904 |
| H | -5.957044 | -0.002296 | 2.656829 |
| H | -5.118323 | -1.533635 | 2.958836 |
| H | -6.808753 | -1.543923 | 2.421687 |
| C | -7.631488 | 0.044008 | 0.271077 |
| H | -8.106355 | 0.718932 | -0.448129 |
| H | -7.720342 | 0.494101 | 1.262717 |
| H | -8.185735 | -0.901905 | 0.264067 |
| C | -6.089708 | -0.622677 | -1.593801 |
| H | -6.614433 | -1.570735 | -1.755800 |
| H | -5.052235 | -0.720338 | -1.921743 |
| H | -6.561071 | 0.141724 | -2.219899 |
| C | -1.882855 | 0.975518 | -2.377191 |
| O | -0.802239 | 1.250725 | -2.885677 |
| O | -2.917699 | 0.387024 | -2.628052 |

9-TS-Me-BPE

B3LYP SCF energy: -2339.94547384 a.u.

B3LYP enthalpy: -2339.169966 a.u.

B3LYP free energy: -2339.288057 a.u.
M06 SCF energy in solution: -2339.38991476 a.u.
M06 enthalpy in solution: -2338.614407 a.u.
M06 free energy in solution: -2338.732498 a.u.
Three lowest frequencies (cm-1): -221.6452 14.9707 28.0834
Imaginary frequency: -221.6452 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 0.201290 | 2.270182 | -0.144303 |
| C | 1.306490 | 2.737922 | 1.313600 |
| C | 2.127010 | 3.948214 | 0.823359 |
| C | 2.470615 | 3.700532 | -0.651087 |
| C | 1.170444 | 3.320374 | -1.390574 |
| H | 3.025681 | 4.086240 | 1.438731 |
| H | 1.530803 | 4.867967 | 0.919877 |
| H | 2.938651 | 4.575499 | -1.119575 |
| H | 3.187002 | 2.872422 | -0.726410 |
| P | -2.735278 | 0.776195 | 0.459233 |
| C | -4.001823 | 0.606757 | -0.931440 |
| C | -5.373313 | 0.560098 | -0.229213 |
| C | -5.193370 | -0.235572 | 1.070905 |
| C | -3.990334 | 0.371169 | 1.822565 |
| H | -6.131406 | 0.113062 | -0.884681 |
| H | -5.711328 | 1.581255 | 0.001668 |
| H | -6.092648 | -0.210731 | 1.699520 |
| H | -4.989012 | -1.288523 | 0.835682 |
| H | 1.982222 | 1.877462 | 1.402636 |
| H | 0.574676 | 4.235836 | -1.518020 |
| Cu | -0.627969 | 0.073818 | -0.251185 |
| C | -2.500761 | 2.611466 | 0.797190 |
| H | -3.445008 | 3.151601 | 0.651930 |
| H | -2.275741 | 2.663336 | 1.870114 |
| C | -1.371760 | 3.286969 | -0.000086 |
| H | -3.791927 | -0.391125 | -1.337316 |
| H | -4.302161 | 1.348666 | 2.218120 |
| H | -1.158676 | 4.281323 | 0.412848 |
| H | -1.693892 | 3.442159 | -1.037301 |
| C | 1.389556 | 2.675477 | -2.762093 |
| H | 1.940073 | 1.734839 | -2.677184 |
| H | 1.954221 | 3.358164 | -3.410436 |
| H | 0.440321 | 2.447846 | -3.258446 |
| C | 0.607154 | 2.947815 | 2.659227 |
| H | 0.065335 | 2.051307 | 2.981815 |
| H | -0.101696 | 3.784144 | 2.626725 |
| H | 1.346687 | 3.179189 | 3.436015 |
| C | -3.883392 | 1.619655 | -2.072441 |
| H | -4.033141 | 2.648857 | -1.723639 |
| H | -4.647406 | 1.418914 | -2.833799 |
| H | -2.906095 | 1.551500 | -2.561967 |
| C | -3.462738 | -0.476235 | 2.982294 |
| H | -4.252868 | -0.631765 | 3.728220 |
| H | -2.621751 | 0.011003 | 3.490259 |
| H | -3.126127 | -1.455929 | 2.633576 |
| C | 0.069378 | -2.038845 | -0.434889 |
| H | 0.605817 | -2.622573 | -1.186795 |
| C | -1.278782 | -2.689124 | -0.290113 |

| | | | |
|---|---|---|---|
| C | -3.779711 | -4.029260 | -0.114966 |
| C | -2.067574 | -2.930653 | -1.437588 |
| C | -1.780509 | -3.149551 | 0.942519 |
| C | -3.008897 | -3.811622 | 1.027883 |
| C | -3.295426 | -3.583378 | -1.349968 |
| H | -1.704151 | -2.590445 | -2.402082 |
| H | -1.194879 | -3.007616 | 1.845734 |
| H | -3.355714 | -4.171083 | 1.994544 |
| H | -3.872932 | -3.758052 | -2.255179 |
| H | -4.729716 | -4.553298 | -0.049679 |
| C | 0.971566 | -1.987631 | 0.818250 |
| H | 0.989262 | -2.993875 | 1.273274 |
| H | 0.560506 | -1.322350 | 1.592888 |
| B | 2.486542 | -1.624671 | 0.557972 |
| O | 3.395212 | -2.562763 | 0.133695 |
| C | 4.679977 | -1.912659 | -0.046200 |
| C | 4.523069 | -0.602508 | 0.830505 |
| O | 3.080624 | -0.424282 | 0.893215 |
| C | 5.146046 | 0.652295 | 0.220702 |
| H | 4.719677 | 0.871720 | -0.760502 |
| H | 6.230853 | 0.537596 | 0.112514 |
| H | 4.964545 | 1.511741 | 0.875766 |
| C | 4.999482 | -0.770288 | 2.280857 |
| H | 4.550379 | -1.652446 | 2.747969 |
| H | 4.694068 | 0.108115 | 2.859073 |
| H | 6.089151 | -0.860909 | 2.344481 |
| C | 5.770418 | -2.875041 | 0.428351 |
| H | 5.774386 | -3.762821 | -0.212138 |
| H | 5.604703 | -3.204771 | 1.456784 |
| H | 6.760638 | -2.408624 | 0.365330 |
| C | 4.842625 | -1.640490 | -1.547877 |
| H | 5.813772 | -1.184299 | -1.770925 |
| H | 4.042424 | -1.000842 | -1.925254 |
| H | 4.784161 | -2.594371 | -2.082116 |
| C | 0.482011 | -0.675288 | -1.966449 |
| O | -0.502969 | -0.427489 | -2.657832 |
| O | 1.696103 | -0.603209 | -2.003008 |

9-TS-PCy3

B3LYP SCF energy: -2154.04655304 a.u.
B3LYP enthalpy: -2153.184109 a.u.
B3LYP free energy: -2153.306619 a.u.
M06 SCF energy in solution: -2153.41495929 a.u.
M06 enthalpy in solution: -2152.552515 a.u.
M06 free energy in solution: -2152.675025 a.u.
Three lowest frequencies (cm-1): -186.4247 7.8294 13.5762
Imaginary frequency: -186.4247 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.371007 | 0.749461 | 0.339495 |
| B | 3.757436 | 0.790186 | -0.330468 |
| O | 4.405251 | -0.054435 | -1.200218 |
| C | 5.517923 | -0.659019 | -0.484834 |
| C | 5.750072 | 0.354647 | 0.709158 |

| | | | |
|---|---|---|---|
| O | 4.458560 | 1.004427 | 0.832375 |
| C | 6.691907 | -0.797355 | -1.455110 |
| H | 6.419157 | -1.486560 | -2.261115 |
| H | 7.574425 | -1.203876 | -0.947280 |
| H | 6.960883 | 0.159593 | -1.908885 |
| C | 5.048570 | -2.048210 | -0.029332 |
| H | 4.752738 | -2.624021 | -0.912968 |
| H | 4.180361 | -1.975468 | 0.630156 |
| H | 5.847488 | -2.595798 | 0.483057 |
| C | 6.765105 | 1.461294 | 0.387270 |
| H | 6.528497 | 1.955286 | -0.560565 |
| H | 6.726402 | 2.216610 | 1.178638 |
| C | 6.091056 | -0.292579 | 2.051355 |
| H | 5.304907 | -0.978417 | 2.373960 |
| H | 6.194698 | 0.484614 | 2.815885 |
| H | 7.038631 | -0.841238 | 1.995065 |
| C | 1.520539 | 1.807306 | 0.514088 |
| C | 2.436368 | 1.573083 | -0.685743 |
| H | 7.788035 | 1.073335 | 0.330929 |
| C | 0.408223 | 2.800355 | 0.371501 |
| C | -1.713729 | 4.687108 | 0.166946 |
| C | -0.068239 | 3.248387 | -0.888581 |
| C | -0.233855 | 3.326864 | 1.526831 |
| C | -1.271041 | 4.248774 | 1.421474 |
| C | -1.105568 | 4.179919 | -0.982155 |
| H | 0.413176 | 2.892565 | -1.794469 |
| H | 0.111818 | 3.003262 | 2.504967 |
| H | -1.728435 | 4.641986 | 2.326152 |
| H | -1.427514 | 4.520245 | -1.963728 |
| H | -2.513345 | 5.418597 | 0.090438 |
| H | 2.090914 | 2.048019 | 1.411363 |
| H | 2.747144 | 2.549679 | -1.100856 |
| H | 1.922185 | 1.055178 | -1.505407 |
| P | -1.948693 | -0.716204 | -0.200312 |
| C | 1.302049 | -0.035699 | 1.521197 |
| O | 2.000185 | -0.853961 | 0.949579 |
| O | 0.702968 | 0.138866 | 2.574853 |
| C | -3.406313 | -0.057276 | -1.192526 |
| C | -5.286487 | 1.675434 | -1.256485 |
| C | -4.172061 | 0.964579 | -3.405412 |
| C | -4.851240 | 2.119011 | -2.658477 |
| C | -2.986789 | 0.386971 | -2.611367 |
| C | -4.106412 | 1.103942 | -0.451193 |
| H | -6.073604 | 0.911542 | -1.344384 |
| H | -4.908009 | 0.167484 | -3.588553 |
| H | -4.147130 | 2.959157 | -2.569978 |
| H | -2.198247 | 1.149131 | -2.530966 |
| H | -3.376652 | 1.904019 | -0.262935 |
| H | -4.118319 | -0.889254 | -1.293896 |
| H | -5.728133 | 2.516111 | -0.706852 |
| H | -3.821491 | 1.296504 | -4.390883 |
| H | -5.712983 | 2.487602 | -3.228928 |
| H | -2.560869 | -0.455370 | -3.166867 |
| H | -4.465825 | 0.771323 | 0.527864 |
| C | -2.661013 | -1.534560 | 1.338988 |
| C | -3.220256 | -1.330053 | 3.804677 |
| C | -4.371402 | -3.091308 | 2.390805 |

| | | | |
|---|---|---|---|
| C | -4.507540 | -2.139134 | 3.587860 |
| C | -3.958255 | -2.338475 | 1.113062 |
| C | -2.799012 | -0.566331 | 2.536786 |
| H | -2.406871 | -2.009226 | 4.098230 |
| H | -3.614962 | -3.856682 | 2.618206 |
| H | -5.344943 | -1.448520 | 3.406576 |
| H | -4.770024 | -1.655640 | 0.827266 |
| H | -3.546181 | 0.208221 | 2.320500 |
| H | -1.869218 | -2.241776 | 1.618172 |
| H | -3.347766 | -0.622252 | 4.633174 |
| H | -5.313902 | -3.625904 | 2.215848 |
| H | -4.760197 | -2.704628 | 4.493630 |
| H | -3.839036 | -3.048549 | 0.284295 |
| H | -1.845101 | -0.057976 | 2.711548 |
| C | -1.249185 | -2.119371 | -1.265357 |
| C | 0.451475 | -2.683399 | -3.086332 |
| C | -0.178447 | -4.429319 | -1.373038 |
| C | 0.934593 | -3.900012 | -2.286435 |
| C | -0.744259 | -3.332427 | -0.452004 |
| C | -0.096510 | -1.589732 | -2.154649 |
| H | -0.333792 | -2.994376 | -3.792261 |
| H | -0.994039 | -4.836233 | -1.989980 |
| H | 1.798352 | -3.606558 | -1.673594 |
| H | 0.040741 | -3.000449 | 0.241547 |
| H | 0.712658 | -1.239678 | -1.500667 |
| H | -2.070593 | -2.459684 | -1.914456 |
| H | 1.270807 | -2.271333 | -3.688164 |
| H | 0.191979 | -5.259841 | -0.758868 |
| H | 1.279082 | -4.692507 | -2.962898 |
| H | -1.551113 | -3.762821 | 0.150838 |
| H | -0.421683 | -0.727330 | -2.746759 |

9-TS-PEt3

B3LYP SCF energy: -1685.91197795 a.u.
B3LYP enthalpy: -1685.344211 a.u.
B3LYP free energy: -1685.446503 a.u.
M06 SCF energy in solution: -1685.50365061 a.u.
M06 enthalpy in solution: -1684.935884 a.u.
M06 free energy in solution: -1685.038176 a.u.
Three lowest frequencies (cm-1): -192.2673 15.4186 19.6038
Imaginary frequency: -192.2673 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -1.389238 | 0.058031 | 0.215812 |
| B | 2.647602 | 0.498606 | -0.580089 |
| O | 3.318307 | -0.427507 | -1.341517 |
| C | 4.535292 | -0.789372 | -0.633121 |
| C | 4.737168 | 0.434573 | 0.353808 |
| O | 3.397530 | 0.982224 | 0.465142 |
| C | 5.647815 | -0.978615 | -1.665247 |
| H | 5.391368 | -1.812991 | -2.326357 |
| H | 6.600879 | -1.214792 | -1.177625 |
| H | 5.784209 | -0.089000 | -2.284711 |
| C | 4.255661 | -2.118213 | 0.082756 |

| | | | |
|---|---|---|---|
| H | 3.972824 | -2.866147 | -0.665672 |
| H | 3.428176 | -2.021719 | 0.789356 |
| H | 5.142717 | -2.483524 | 0.612082 |
| C | 5.616748 | 1.553129 | -0.223994 |
| H | 5.275451 | 1.854464 | -1.219608 |
| H | 5.552136 | 2.427301 | 0.431767 |
| C | 5.219821 | 0.061630 | 1.755512 |
| H | 4.521877 | -0.618233 | 2.248610 |
| H | 5.299042 | 0.966130 | 2.367866 |
| H | 6.208515 | -0.410945 | 1.719594 |
| C | 0.329306 | 1.371093 | 0.227550 |
| C | 1.239463 | 1.093883 | -0.968477 |
| H | 6.667673 | 1.251666 | -0.293224 |
| C | -0.895557 | 2.208614 | 0.010879 |
| C | -3.224449 | 3.806682 | -0.328593 |
| C | -1.433313 | 2.470276 | -1.275260 |
| C | -1.581741 | 2.767892 | 1.123766 |
| C | -2.721032 | 3.548679 | 0.952415 |
| C | -2.573640 | 3.261440 | -1.436441 |
| H | -0.924749 | 2.081325 | -2.152246 |
| H | -1.193241 | 2.579646 | 2.120658 |
| H | -3.213014 | 3.972258 | 1.824621 |
| H | -2.944671 | 3.461938 | -2.438884 |
| H | -4.105538 | 4.428961 | -0.458317 |
| H | 0.893430 | 1.793602 | 1.060137 |
| H | 1.438758 | 2.045030 | -1.496054 |
| H | 0.764385 | 0.439601 | -1.710972 |
| P | -2.831293 | -1.563712 | -0.211235 |
| C | 0.342374 | -0.297627 | 1.510785 |
| O | 1.202991 | -1.054786 | 1.110065 |
| O | -0.358826 | -0.072142 | 2.492270 |
| C | -4.199169 | -1.185223 | -1.412352 |
| C | -5.062341 | 0.022028 | -1.020275 |
| H | -4.458599 | 0.930674 | -0.925815 |
| H | -5.581729 | -0.140151 | -0.069587 |
| C | -3.731857 | -2.193732 | 1.288465 |
| C | -2.044291 | -3.088679 | -0.927285 |
| C | -1.213293 | -2.826261 | -2.190583 |
| H | -0.388947 | -2.135899 | -1.983152 |
| H | -1.818321 | -2.404916 | -3.001317 |
| H | -5.826595 | 0.202970 | -1.784464 |
| H | -0.778600 | -3.762553 | -2.557220 |
| H | -4.421936 | -2.986443 | 0.967829 |
| H | -4.346169 | -1.362096 | 1.653227 |
| H | -2.835915 | -3.824709 | -1.123375 |
| H | -1.399730 | -3.505225 | -0.145320 |
| H | -4.816686 | -2.086895 | -1.523007 |
| H | -3.724114 | -1.001137 | -2.383194 |
| C | -2.807568 | -2.688017 | 2.411918 |
| H | -2.092648 | -1.915888 | 2.712894 |
| H | -2.239919 | -3.574221 | 2.108295 |
| H | -3.403442 | -2.965693 | 3.288563 |

9-TS-PPh2Me
B3LYP SCF energy: -1951.43476641 a.u.

B3LYP enthalpy: -1950.844452 a.u.
B3LYP free energy: -1950.952888 a.u.
M06 SCF energy in solution: -1950.89415954 a.u.
M06 enthalpy in solution: -1950.303845 a.u.
M06 free energy in solution: -1950.412281 a.u.
Three lowest frequencies (cm-1): -174.3550 13.1086 16.5856
Imaginary frequency: -174.3550 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.806534 | 0.945118 | 0.403324 |
| B | 3.085312 | 0.380887 | -0.607372 |
| O | 3.482975 | -0.910399 | -0.871087 |
| C | 4.710351 | -1.163631 | -0.130504 |
| C | 5.230564 | 0.300114 | 0.193851 |
| O | 4.030067 | 1.105495 | 0.075428 |
| C | 5.637353 | -1.995015 | -1.018915 |
| H | 5.174051 | -2.966581 | -1.220783 |
| H | 6.597659 | -2.176707 | -0.522406 |
| H | 5.828108 | -1.508271 | -1.978283 |
| C | 4.322902 | -1.971031 | 1.115924 |
| H | 3.843467 | -2.903145 | 0.797218 |
| H | 3.611923 | -1.423377 | 1.738011 |
| H | 5.203229 | -2.230295 | 1.714283 |
| C | 6.223072 | 0.846987 | -0.842557 |
| H | 5.831243 | 0.750660 | -1.860188 |
| H | 6.387253 | 1.911293 | -0.646328 |
| C | 5.792171 | 0.487750 | 1.603705 |
| H | 5.046248 | 0.246202 | 2.363786 |
| H | 6.088082 | 1.532988 | 1.741684 |
| H | 6.677168 | -0.139162 | 1.763664 |
| C | 1.016824 | 1.917044 | -0.188928 |
| C | 1.765499 | 1.028678 | -1.181947 |
| H | 7.189925 | 0.334464 | -0.792345 |
| C | -0.147223 | 2.718223 | -0.674340 |
| C | -2.402037 | 4.242741 | -1.510930 |
| C | -0.834081 | 2.427320 | -1.883897 |
| C | -0.651633 | 3.794898 | 0.109667 |
| C | -1.752450 | 4.536289 | -0.304110 |
| C | -1.936712 | 3.185758 | -2.292007 |
| H | -0.464289 | 1.635211 | -2.528018 |
| H | -0.154032 | 4.031831 | 1.045690 |
| H | -2.102521 | 5.359567 | 0.313709 |
| H | -2.420382 | 2.951593 | -3.237532 |
| H | -3.253400 | 4.834748 | -1.834971 |
| H | 1.696509 | 2.561902 | 0.367712 |
| H | 2.072196 | 1.641961 | -2.049999 |
| H | 1.127959 | 0.236327 | -1.593831 |
| P | -2.040865 | -0.849056 | 0.782673 |
| C | -1.435120 | -2.236542 | -0.266392 |
| C | -0.373036 | -4.278070 | -1.867900 |
| C | -2.288262 | -3.123846 | -0.937018 |
| C | -0.042744 | -2.377933 | -0.406833 |
| C | 0.482023 | -3.395154 | -1.203645 |
| C | -1.755739 | -4.141353 | -1.732388 |
| H | -3.365260 | -3.019736 | -0.848564 |
| H | 0.635671 | -1.695920 | 0.099570 |

| | | | |
|---|---|---|---|
| H | 1.559630 | -3.474927 | -1.313754 |
| H | -2.425046 | -4.823072 | -2.250590 |
| H | 0.036283 | -5.065693 | -2.494982 |
| C | -3.853883 | -0.740315 | 0.527110 |
| C | -6.614052 | -0.492632 | 0.074982 |
| C | -4.351616 | 0.274015 | -0.306534 |
| C | -4.758328 | -1.626455 | 1.135404 |
| C | -6.129784 | -1.501675 | 0.910704 |
| C | -5.723619 | 0.393506 | -0.533613 |
| H | -3.664034 | 0.976248 | -0.771596 |
| H | -4.398537 | -2.417172 | 1.787109 |
| H | -6.819249 | -2.191185 | 1.390170 |
| H | -6.095397 | 1.184576 | -1.178808 |
| H | -7.682608 | -0.395058 | -0.096319 |
| C | 0.942954 | 0.951281 | 1.737308 |
| O | 1.639276 | -0.045957 | 1.667906 |
| O | 0.409775 | 1.699839 | 2.539030 |
| C | -1.813214 | -1.462973 | 2.511914 |
| H | -0.737712 | -1.542137 | 2.694312 |
| H | -2.277487 | -2.440678 | 2.670478 |
| H | -2.228547 | -0.733194 | 3.213416 |

9-TS-PPh3

B3LYP SCF energy: -2143.16442483 a.u.
B3LYP enthalpy: -2142.517457 a.u.
B3LYP free energy: -2142.633919 a.u.
M06 SCF energy in solution: -2142.52482432 a.u.
M06 enthalpy in solution: -2141.877856 a.u.
M06 free energy in solution: -2141.994318 a.u.
Three lowest frequencies (cm-1): -186.2027 12.0962 16.4964
Imaginary frequency: -186.2027 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.493440 | -1.009243 | -0.543397 |
| B | 3.379699 | -0.610416 | 0.481508 |
| O | 3.651595 | 0.552649 | 1.167651 |
| C | 4.837753 | 1.157136 | 0.579299 |
| C | 5.495026 | -0.057083 | -0.204844 |
| O | 4.384530 | -0.973456 | -0.380015 |
| C | 5.690095 | 1.727245 | 1.714861 |
| H | 5.136267 | 2.525022 | 2.221300 |
| H | 6.621191 | 2.158197 | 1.328963 |
| H | 5.940237 | 0.967618 | 2.459366 |
| C | 4.357773 | 2.295797 | -0.331007 |
| H | 3.789223 | 3.012078 | 0.272239 |
| H | 3.699584 | 1.925129 | -1.119180 |
| H | 5.201053 | 2.828779 | -0.784010 |
| C | 6.555821 | -0.813778 | 0.607542 |
| H | 6.169945 | -1.109170 | 1.588397 |
| H | 6.830421 | -1.725362 | 0.067325 |
| C | 6.047381 | 0.290448 | -1.587770 |
| H | 5.268862 | 0.699711 | -2.234802 |
| H | 6.437768 | -0.616446 | -2.061461 |
| H | 6.866768 | 1.015395 | -1.516809 |

| | | | |
|---|---|---|---|
| C | 1.375602 | -2.055299 | -0.404100 |
| C | 2.149805 | -1.544902 | 0.811208 |
| H | 7.461029 | -0.214929 | 0.755520 |
| C | 0.288279 | -3.062806 | -0.183367 |
| C | -1.788976 | -4.975513 | 0.162380 |
| C | -0.261399 | -3.336573 | 1.095584 |
| C | -0.254891 | -3.777861 | -1.286214 |
| C | -1.272291 | -4.711123 | -1.111762 |
| C | -1.276484 | -4.283058 | 1.259916 |
| H | 0.143977 | -2.833028 | 1.967698 |
| H | 0.143168 | -3.583058 | -2.277886 |
| H | -1.657878 | -5.246433 | -1.975893 |
| H | -1.655708 | -4.487220 | 2.258703 |
| H | -2.573707 | -5.715115 | 0.294800 |
| H | 2.050844 | -2.426071 | -1.176473 |
| H | 2.563815 | -2.412790 | 1.357665 |
| H | 1.496567 | -1.030941 | 1.527127 |
| P | -1.932320 | 0.589873 | -0.016285 |
| C | -1.298047 | 1.462185 | 1.476145 |
| C | -0.189761 | 2.735327 | 3.714065 |
| C | -2.123910 | 1.891389 | 2.524869 |
| C | 0.089822 | 1.674117 | 1.558466 |
| C | 0.638440 | 2.306373 | 2.673538 |
| C | -1.568511 | 2.528673 | 3.637437 |
| H | -3.195525 | 1.720909 | 2.481128 |
| H | 0.748605 | 1.342079 | 0.760017 |
| H | 1.715165 | 2.437535 | 2.726618 |
| H | -2.215479 | 2.856447 | 4.446884 |
| H | 0.238722 | 3.221530 | 4.586490 |
| C | -3.645357 | 0.059709 | 0.399747 |
| C | -6.210191 | -0.840036 | 1.099572 |
| C | -3.820143 | -1.200216 | 0.996154 |
| C | -4.771615 | 0.857571 | 0.146018 |
| C | -6.046470 | 0.407648 | 0.495008 |
| C | -5.095062 | -1.642911 | 1.348919 |
| H | -2.960646 | -1.841370 | 1.174432 |
| H | -4.656939 | 1.824495 | -0.333586 |
| H | -6.911492 | 1.032491 | 0.289676 |
| H | -5.216586 | -2.620285 | 1.807645 |
| H | -7.203854 | -1.189232 | 1.367011 |
| C | -2.107264 | 1.893952 | -1.298525 |
| C | -2.396061 | 3.823313 | -3.310364 |
| C | -2.432086 | 3.219790 | -0.967968 |
| C | -1.908700 | 1.547951 | -2.644402 |
| C | -2.056841 | 2.511213 | -3.643947 |
| C | -2.579314 | 4.177687 | -1.971353 |
| H | -2.555978 | 3.506483 | 0.072494 |
| H | -1.605397 | 0.539647 | -2.910894 |
| H | -1.891605 | 2.235479 | -4.681574 |
| H | -2.828648 | 5.201682 | -1.706461 |
| H | -2.504354 | 4.572499 | -4.090057 |
| C | 1.172851 | -0.508542 | -1.854563 |
| O | 1.918235 | 0.387960 | -1.514570 |
| O | 0.537516 | -0.922988 | -2.816871 |

9-TS-Xanphos

B3LYP SCF energy: -3370.20030333 a.u.
B3LYP enthalpy: -3369.210651 a.u.
B3LYP free energy: -3369.366570 a.u.
M06 SCF energy in solution: -3369.16005640 a.u.
M06 enthalpy in solution: -3368.170404 a.u.
M06 free energy in solution: -3368.326323 a.u.
Three lowest frequencies (cm-1): -145.3439 10.3226 15.7008
Imaginary frequency: -145.3439 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -1.314735 | 1.973380 | 0.404556 |
| P | -0.362088 | -2.049542 | 0.486165 |
| O | -2.611466 | -0.489034 | -0.717582 |
| C | -3.127264 | 1.664633 | 0.140006 |
| C | -4.111554 | 2.596643 | 0.506239 |
| H | -3.812968 | 3.531471 | 0.970479 |
| C | -5.461918 | 2.331858 | 0.295436 |
| H | -6.210584 | 3.060821 | 0.592006 |
| C | -5.858273 | 1.132718 | -0.303395 |
| H | -6.914468 | 0.952471 | -0.473110 |
| C | -4.916498 | 0.174227 | -0.683651 |
| C | -3.567381 | 0.459055 | -0.422771 |
| C | -2.972148 | -1.808856 | -0.572211 |
| C | -1.997994 | -2.695627 | -0.089942 |
| C | -2.354647 | -4.051093 | 0.009712 |
| H | -1.621496 | -4.770478 | 0.360466 |
| C | -3.638311 | -4.478196 | -0.320264 |
| H | -3.900341 | -5.528496 | -0.230558 |
| C | -4.595073 | -3.557064 | -0.754096 |
| H | -5.594119 | -3.907854 | -0.990418 |
| C | -4.278784 | -2.204036 | -0.896319 |
| C | -5.239467 | -1.131035 | -1.423826 |
| C | -6.711219 | -1.542028 | -1.250511 |
| H | -6.926844 | -2.458298 | -1.808393 |
| H | -7.376937 | -0.771761 | -1.651381 |
| H | -6.967810 | -1.708607 | -0.198735 |
| C | -4.956123 | -0.918773 | -2.939653 |
| H | -3.916060 | -0.628533 | -3.116691 |
| H | -5.605566 | -0.131046 | -3.338839 |
| H | -5.152077 | -1.844665 | -3.492993 |
| C | -1.301550 | 2.520839 | 2.171250 |
| C | -1.398893 | 3.863668 | 2.564987 |
| H | -1.447878 | 4.648494 | 1.817197 |
| C | -1.413790 | 4.203217 | 3.919313 |
| H | -1.483759 | 5.248409 | 4.209577 |
| C | -1.335204 | 3.208522 | 4.895425 |
| H | -1.343020 | 3.476254 | 5.948779 |
| C | -1.236437 | 1.869724 | 4.511995 |
| H | -1.161806 | 1.086047 | 5.260770 |
| C | -1.214754 | 1.529334 | 3.159531 |
| H | -1.119389 | 0.486512 | 2.874068 |
| C | -1.019140 | 3.542224 | -0.530338 |
| C | -1.937094 | 4.080113 | -1.444356 |
| H | -2.898549 | 3.603273 | -1.599081 |
| C | -1.622936 | 5.230867 | -2.172564 |

| | | | |
|---|---|---|---|
| H | -2.346911 | 5.633028 | -2.876747 |
| C | -0.390459 | 5.860028 | -1.997242 |
| H | -0.147972 | 6.755492 | -2.563440 |
| C | 0.533576 | 5.325452 | -1.095427 |
| H | 1.502058 | 5.799697 | -0.960325 |
| C | 0.229908 | 4.172034 | -0.371757 |
| H | 0.970124 | 3.738302 | 0.292730 |
| C | -0.467235 | -2.233186 | 2.333335 |
| C | 0.574124 | -1.689309 | 3.109822 |
| H | 1.403523 | -1.177266 | 2.629924 |
| C | 0.544445 | -1.790072 | 4.502395 |
| H | 1.362173 | -1.371019 | 5.082702 |
| C | -0.529946 | -2.408698 | 5.144579 |
| H | -0.553057 | -2.480824 | 6.228858 |
| C | -1.578672 | -2.927020 | 4.383662 |
| H | -2.425773 | -3.401747 | 4.872128 |
| C | -1.547938 | -2.843475 | 2.990010 |
| H | -2.374599 | -3.252792 | 2.420915 |
| C | 0.796110 | -3.401320 | -0.035941 |
| C | 0.606957 | -4.066239 | -1.260212 |
| H | -0.265388 | -3.849342 | -1.868608 |
| C | 1.527449 | -5.015781 | -1.705655 |
| H | 1.359213 | -5.521666 | -2.652849 |
| C | 2.657056 | -5.312293 | -0.941324 |
| H | 3.375920 | -6.048922 | -1.289494 |
| C | 2.858890 | -4.650522 | 0.270341 |
| H | 3.738758 | -4.865265 | 0.870380 |
| C | 1.939340 | -3.701746 | 0.719896 |
| H | 2.124154 | -3.191952 | 1.657762 |
| Cu | 0.157124 | 0.167501 | -0.183096 |
| C | 2.015181 | 0.538116 | -1.473776 |
| H | 2.357018 | 1.571427 | -1.522207 |
| C | 0.877750 | 0.359291 | -2.430313 |
| C | -1.194623 | 0.070124 | -4.366910 |
| C | 0.183839 | 1.479248 | -2.954727 |
| C | 0.502081 | -0.911028 | -2.936638 |
| C | -0.514448 | -1.049234 | -3.882302 |
| C | -0.831886 | 1.336990 | -3.895885 |
| H | 0.477742 | 2.472608 | -2.630635 |
| H | 1.044177 | -1.790361 | -2.607403 |
| H | -0.762499 | -2.040171 | -4.257347 |
| H | -1.328800 | 2.225041 | -4.279138 |
| H | -1.973687 | -0.038119 | -5.117163 |
| C | 3.159907 | -0.464743 | -1.658568 |
| H | 3.316891 | -0.643697 | -2.738292 |
| H | 2.906019 | -1.443851 | -1.236004 |
| B | 4.540736 | -0.036052 | -1.041571 |
| O | 4.912770 | 1.271224 | -0.824190 |
| C | 6.160616 | 1.261174 | -0.080459 |
| C | 6.740711 | -0.166974 | -0.425554 |
| O | 5.542883 | -0.928146 | -0.729054 |
| C | 7.476610 | -0.860806 | 0.720539 |
| H | 6.828419 | -0.992654 | 1.589691 |
| H | 8.359670 | -0.286582 | 1.025092 |
| H | 7.812430 | -1.851312 | 0.395317 |
| C | 7.607801 | -0.185400 | -1.693063 |
| H | 7.096735 | 0.301027 | -2.530063 |

| | | | |
|---|---|---|---|
| H | 7.800521 | -1.225537 | -1.975013 |
| H | 8.570415 | 0.313528 | -1.536194 |
| C | 7.011627 | 2.440431 | -0.551219 |
| H | 6.505980 | 3.378063 | -0.298208 |
| H | 7.166853 | 2.423427 | -1.632729 |
| H | 7.990439 | 2.439753 | -0.056976 |
| C | 5.795008 | 1.433125 | 1.400676 |
| H | 6.687792 | 1.495429 | 2.033175 |
| H | 5.162911 | 0.612034 | 1.749985 |
| H | 5.221429 | 2.357946 | 1.515558 |
| C | 2.185681 | 0.746959 | 0.697888 |
| O | 2.012894 | 1.909222 | 1.012138 |
| O | 2.693542 | -0.278132 | 1.130094 |

9-TS

B3LYP SCF energy: -1802.43607837 a.u.
B3LYP enthalpy: -1801.689230 a.u.
B3LYP free energy: -1801.803967 a.u.
M06 SCF energy in solution: -1801.83389836 a.u.
M06 enthalpy in solution: -1801.087050 a.u.
M06 free energy in solution: -1801.201787 a.u.
Three lowest frequencies (cm-1): -196.0012 4.0577 15.4850
Imaginary frequency: -196.0012 cm-1

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.825438 | -0.310898 | 0.232662 |
| N | 3.106172 | 1.560661 | -0.105300 |
| N | 1.197571 | 2.568239 | -0.154837 |
| C | 1.764913 | 1.336872 | -0.029511 |
| C | 3.371004 | 2.911074 | -0.271371 |
| C | 2.168492 | 3.543947 | -0.305657 |
| C | -0.259851 | 2.809904 | -0.129800 |
| C | -0.774389 | 3.307768 | -1.489658 |
| C | -2.303297 | 3.472825 | -1.450757 |
| C | -2.738012 | 4.400079 | -0.304164 |
| C | -2.186214 | 3.921589 | 1.048443 |
| C | -0.657624 | 3.758458 | 1.011284 |
| C | 4.123312 | 0.501570 | 0.023143 |
| C | 5.061477 | 0.462292 | -1.193866 |
| C | 6.085238 | -0.675781 | -1.048982 |
| C | 6.873659 | -0.566474 | 0.265585 |
| C | 5.930566 | -0.505615 | 1.477220 |
| C | 4.906909 | 0.632935 | 1.340261 |
| H | 4.371756 | 3.305117 | -0.348979 |
| H | 1.930768 | 4.589263 | -0.422711 |
| H | -0.704698 | 1.832913 | 0.078234 |
| H | -0.482155 | 2.599245 | -2.274577 |
| H | -0.302164 | 4.271427 | -1.733118 |
| H | -2.765369 | 2.484290 | -1.323696 |
| H | -2.654947 | 3.864723 | -2.413259 |
| H | -3.832885 | 4.459604 | -0.263499 |
| H | -2.377068 | 5.420462 | -0.504479 |
| H | -2.634185 | 2.953858 | 1.308254 |
| H | -2.462219 | 4.624197 | 1.844305 |

| | | | |
|---|---|---|---|
| H | -0.183270 | 4.740512 | 0.864881 |
| H | -0.290465 | 3.357116 | 1.963097 |
| H | 3.550249 | -0.431133 | 0.050368 |
| H | 5.592575 | 1.421232 | -1.282396 |
| H | 4.469835 | 0.336513 | -2.108496 |
| H | 6.767779 | -0.668098 | -1.907589 |
| H | 5.552399 | -1.636255 | -1.076649 |
| H | 7.496416 | 0.340428 | 0.242866 |
| H | 7.561881 | -1.415019 | 0.363964 |
| H | 6.502563 | -0.377303 | 2.404015 |
| H | 5.393398 | -1.460143 | 1.569194 |
| H | 4.205039 | 0.628119 | 2.182514 |
| H | 5.428414 | 1.601165 | 1.359806 |
| B | -3.009871 | -1.291815 | -0.562091 |
| O | -3.820292 | -0.288813 | -1.045943 |
| C | -5.083443 | -0.348923 | -0.325696 |
| C | -5.086435 | -1.827948 | 0.243003 |
| O | -3.677221 | -2.167320 | 0.262202 |
| C | -6.207554 | -0.032278 | -1.313282 |
| H | -6.090623 | 0.992375 | -1.681731 |
| H | -7.188363 | -0.106652 | -0.829174 |
| H | -6.193376 | -0.702065 | -2.176476 |
| C | -5.032928 | 0.725186 | 0.769288 |
| H | -4.885755 | 1.702674 | 0.297438 |
| H | -4.199599 | 0.551727 | 1.453956 |
| H | -5.968321 | 0.761427 | 1.338829 |
| C | -5.766461 | -2.842970 | -0.687711 |
| H | -5.370270 | -2.777127 | -1.706108 |
| H | -5.567074 | -3.852742 | -0.314953 |
| C | -5.633736 | -1.975313 | 1.662958 |
| H | -5.069787 | -1.366491 | 2.372737 |
| H | -5.552855 | -3.021244 | 1.977054 |
| H | -6.690709 | -1.687779 | 1.711778 |
| C | -0.572891 | -1.937783 | 0.070101 |
| C | -1.539144 | -1.571221 | -1.060909 |
| H | -6.851555 | -2.697963 | -0.726950 |
| C | 0.762889 | -2.524351 | -0.289528 |
| C | 3.284132 | -3.685300 | -0.899350 |
| C | 1.297459 | -2.481045 | -1.599956 |
| C | 1.544548 | -3.162654 | 0.709393 |
| C | 2.778948 | -3.728788 | 0.407070 |
| C | 2.536070 | -3.056214 | -1.895851 |
| H | 0.719329 | -2.021118 | -2.395612 |
| H | 1.159075 | -3.199177 | 1.724019 |
| H | 3.345669 | -4.223742 | 1.192249 |
| H | 2.907761 | -3.024064 | -2.917415 |
| H | 4.237727 | -4.149462 | -1.136599 |
| H | -1.056245 | -2.617409 | 0.774023 |
| H | -1.606465 | -2.422092 | -1.763051 |
| H | -1.182130 | -0.721593 | -1.657387 |
| C | -0.814011 | -0.645393 | 1.640322 |
| O | -1.816927 | 0.017852 | 1.412188 |
| O | -0.066356 | -0.934917 | 2.564478 |

CO2

B3LYP SCF energy: -188.57757052 a.u.
B3LYP enthalpy: -188.562367 a.u.
B3LYP free energy: -188.586668 a.u.
M06 SCF energy in solution: -188.55995572 a.u.
M06 enthalpy in solution: -188.544752 a.u.
M06 free energy in solution: -188.569053 a.u.
Three lowest frequencies (cm-1): 646.8590 646.8590 1370.4469

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.000000 | 0.000000 | 0.000000 |
| O | 0.000000 | 0.000000 | 1.169583 |
| O | 0.000000 | 0.000000 | -1.169583 |

ICyCu-OtBu
B3LYP SCF energy: -1126.03309410 a.u.
B3LYP enthalpy: -1125.505116 a.u.
B3LYP free energy: -1125.591827 a.u.
M06 SCF energy in solution: -1125.64508025 a.u.
M06 enthalpy in solution: -1125.117102 a.u.
M06 free energy in solution: -1125.203813 a.u.
Three lowest frequencies (cm-1): 2.2170 17.1671 23.3272

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.000063 | 1.062691 | 0.313676 |
| N | 1.078704 | -1.625690 | -0.123089 |
| N | -1.078575 | -1.625747 | -0.123106 |
| C | 0.000039 | -0.799497 | 0.008775 |
| C | 0.679265 | -2.937127 | -0.328808 |
| C | -0.679062 | -2.937165 | -0.328814 |
| C | -2.475830 | -1.168335 | -0.025854 |
| C | -3.165741 | -1.731423 | 1.227870 |
| C | -4.608118 | -1.210413 | 1.335869 |
| C | -5.415775 | -1.512948 | 0.064385 |
| C | -4.712851 | -0.963801 | -1.186740 |
| C | -3.271158 | -1.486732 | -1.302364 |
| C | 2.475931 | -1.168203 | -0.025821 |
| C | 3.165901 | -1.731349 | 1.227844 |
| C | 4.608240 | -1.210245 | 1.335868 |
| C | 5.415900 | -1.512612 | 0.064343 |
| C | 4.712917 | -0.963409 | -1.186725 |
| C | 3.271260 | -1.486437 | -1.302372 |
| H | 1.377974 | -3.748182 | -0.459055 |
| H | -1.377728 | -3.748249 | -0.459113 |
| H | -2.398783 | -0.080254 | 0.076978 |
| H | -2.586029 | -1.455401 | 2.116726 |
| H | -3.175190 | -2.830198 | 1.177769 |
| H | -4.585864 | -0.124311 | 1.504294 |
| H | -5.094758 | -1.651699 | 2.214017 |
| H | -6.424344 | -1.089892 | 0.147144 |
| H | -5.539734 | -2.601574 | -0.037073 |
| H | -4.694149 | 0.134403 | -1.141570 |
| H | -5.274483 | -1.229007 | -2.090610 |
| H | -3.291905 | -2.574544 | -1.463348 |

| | | | |
|---|---|---|---|
| H | -2.765588 | -1.044246 | -2.169014 |
| H | 2.398822 | -0.080135 | 0.077103 |
| H | 3.175431 | -2.830120 | 1.177651 |
| H | 2.586179 | -1.455447 | 2.116732 |
| H | 5.094926 | -1.651576 | 2.213967 |
| H | 4.585913 | -0.124161 | 1.504387 |
| H | 5.539937 | -2.601220 | -0.037208 |
| H | 6.424440 | -1.089488 | 0.147125 |
| H | 5.274555 | -1.228496 | -2.090626 |
| H | 4.694133 | 0.134789 | -1.141461 |
| H | 2.765643 | -1.043910 | -2.168974 |
| H | 3.292079 | -2.574234 | -1.463449 |
| C | 0.001310 | 5.180658 | 0.861838 |
| C | -0.000216 | 3.950020 | -0.069685 |
| H | -0.883589 | 5.158286 | 1.507877 |
| H | 0.887819 | 5.157784 | 1.505651 |
| H | 0.000873 | 6.124932 | 0.301797 |
| C | 1.259030 | 3.985061 | -0.963378 |
| C | -1.261515 | 3.985937 | -0.960440 |
| H | 1.264092 | 3.119394 | -1.638658 |
| H | 1.312463 | 4.896721 | -1.574130 |
| H | 2.158014 | 3.933911 | -0.337995 |
| H | -1.315714 | 4.897624 | -1.571083 |
| H | -1.268741 | 3.120263 | -1.635692 |
| H | -2.159085 | 3.935429 | -0.332980 |
| O | 0.000313 | 2.811618 | 0.746852 |

ICyCuH

B3LYP SCF energy: -893.52360736 a.u.
B3LYP enthalpy: -893.122270 a.u.
B3LYP free energy: -893.189148 a.u.
M06 SCF energy in solution: -893.22836436 a.u.
M06 enthalpy in solution: -892.827027 a.u.
M06 free energy in solution: -892.893905 a.u.
Three lowest frequencies (cm-1): 13.3524 36.9675 44.9804

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.000033 | 2.168365 | -0.000209 |
| N | 1.076710 | -0.617944 | -0.000129 |
| N | -1.076695 | -0.617945 | -0.000132 |
| C | 0.000008 | 0.219941 | -0.000147 |
| C | 0.679122 | -1.946772 | -0.000082 |
| C | -0.679104 | -1.946772 | -0.000104 |
| C | -2.473867 | -0.149974 | -0.000066 |
| C | -3.216476 | -0.590398 | 1.272230 |
| C | -4.663252 | -0.069038 | 1.268151 |
| C | -5.416297 | -0.500054 | 0.000277 |
| C | -4.663509 | -0.069372 | -1.267864 |
| C | -3.216729 | -0.590729 | -1.272095 |
| C | 2.473880 | -0.149968 | -0.000065 |
| C | 3.216493 | -0.590388 | 1.272230 |
| C | 4.663267 | -0.069021 | 1.268149 |
| C | 5.416313 | -0.500034 | 0.000274 |
| C | 4.663521 | -0.069357 | -1.267866 |

| | | | |
|---|---|---|---|
| C | 3.216744 | -0.590719 | -1.272095 |
| H | 1.377721 | -2.768534 | -0.000057 |
| H | -1.377701 | -2.768536 | -0.000098 |
| H | -2.395454 | 0.942976 | -0.000212 |
| H | -2.675136 | -0.228019 | 2.154197 |
| H | -3.225556 | -1.688761 | 1.329189 |
| H | -4.649962 | 1.028568 | 1.328171 |
| H | -5.185506 | -0.424005 | 2.164808 |
| H | -6.428698 | -0.077962 | 0.000323 |
| H | -5.533062 | -1.594203 | 0.000433 |
| H | -4.650240 | 1.028218 | -1.328186 |
| H | -5.185937 | -0.424585 | -2.164323 |
| H | -3.225831 | -1.689106 | -1.328765 |
| H | -2.675570 | -0.228583 | -2.154267 |
| H | 2.395462 | 0.942982 | -0.000211 |
| H | 3.225579 | -1.688751 | 1.329188 |
| H | 2.675153 | -0.228013 | 2.154198 |
| H | 5.185524 | -0.423985 | 2.164806 |
| H | 4.649972 | 1.028585 | 1.328168 |
| H | 5.533083 | -1.594182 | 0.000431 |
| H | 6.428712 | -0.077938 | 0.000320 |
| H | 5.185950 | -0.424568 | -2.164325 |
| H | 4.650247 | 1.028233 | -1.328188 |
| H | 2.675582 | -0.228576 | -2.154267 |
| H | 3.225850 | -1.689097 | -1.328764 |
| H | -0.000030 | 3.692401 | -0.000256 |

NaOtBu

B3LYP SCF energy: -395.37573272 a.u.
B3LYP enthalpy: -395.241987 a.u.
B3LYP free energy: -395.284398 a.u.
M06 SCF energy in solution: -395.29194665 a.u.
M06 enthalpy in solution: -395.158201 a.u.
M06 free energy in solution: -395.200612 a.u.
Three lowest frequencies (cm-1): 40.9258 46.7484 229.7604

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.144402 | 1.053818 | -1.005463 |
| C | 0.619125 | -0.000255 | -0.000219 |
| H | 0.775114 | 0.819732 | -2.011798 |
| H | 0.765841 | 2.046220 | -0.730064 |
| H | 2.241493 | 1.101190 | -1.042791 |
| C | 1.144741 | 0.347195 | 1.414242 |
| C | 1.152884 | -1.395548 | -0.407325 |
| H | 0.773869 | -0.390506 | 2.136898 |
| H | 2.241888 | 0.364696 | 1.471504 |
| H | 0.768586 | 1.332819 | 1.716079 |
| H | 2.250319 | -1.447434 | -0.420432 |
| H | 0.780394 | -2.151960 | 0.294836 |
| H | 0.783536 | -1.654120 | -1.407676 |
| O | -0.759478 | -0.005430 | -0.001656 |
| Na | -2.697466 | -0.000769 | -0.000065 |