**Supporting Information**

For

# Mechanism of the Reduction of the Native Intermediate in the Multicopper Oxidases: Insights into Rapid Intramolecular Electron Transfer in Turnover

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**Table S1** – Fit parameters used in modeling the 614 nm band with 50 electron equivalents (1.25 mM) $H_2Q$. Graphical representations are featured in Figure 4. Rate constants in units of $s^{-1}$.

| Fit | A | B | C | D |
|---|---|---|---|---|
| $k^{red}_1$ | 0.207 | 0.207 | 0.207 | 0.207 |
| $k^{IET}_1$ | 700 | 700 | 700 | 700 |
| $k^{red}_2$ | 0.207 | 0.400 | 0.207 | 0.400 |
| $k^{IET}_{+2}$ | *fast* | *fast* | 1000 | 1000 |
| $k^{IET}_{-2}$ | 0 | 0 | 1000 | 1000 |
| $k^{red}_3$ | 0.207 | 0.400 | 0.207 | 0.400 |
| $k^{IET}_3$ | *fast* | *fast* | *fast* | *fast* |
| $k^{red}_4$ | 0.207 | 0.400 | 0.207 | 0.400 |

**Table S2**– Fit parameters used in the global fit of the 614 nm band. Rate constants in units of $s^{-1}$.

| $[H_2Q]$ mM | 0.125 | 0.250 | 0.500 | 1.250 |
|---|---|---|---|---|
| $k^{red}_1$ | 0.0268 | 0.0475 | 0.0879 | 0.207 |
| $k^{IET}_1$ | 700 | 700 | 700 | 700 |
| $k^{red}_{2,3,4}$ | 0.0536 | 0.0800 | 0.160 | 0.400 |
| $k^{IET}_2$ | 1000 | 1000 | 1000 | 1000 |
| $k^{IET}_{-2}$ | 1000 | 1000 | 1000 | 1000 |
| $k^{IET}_3$ | 500 | 500 | 500 | 500 |

| $[H_2Q]$ mM | 42.8 | 85.5 | 145 |
|---|---|---|---|
| $k^{ox}{}_1$ * | 52.0 | 56.0 | 65.0 |
| $k^{red}{}_1$ | 6.86 | 13.1 | 22.5 |
| $k^{IET}{}_1$ | 700 | 700 | 700 |
| $k^{red}{}_{2,3,4}$ | 13.7 | 30.0 | 50.0 |
| $k^{IET}{}_2$ | 1000 | 1000 | 1000 |
| $k^{IET}{}_{-2}$ | 1000 | 1000 | 1000 |
| $k^{IET}{}_3$ | 500 | 500 | 500 |

*- Average of the NI formation rates gives a second order rate of $1.2 \times 10^6$ $M^{-1}s^{-1}$.

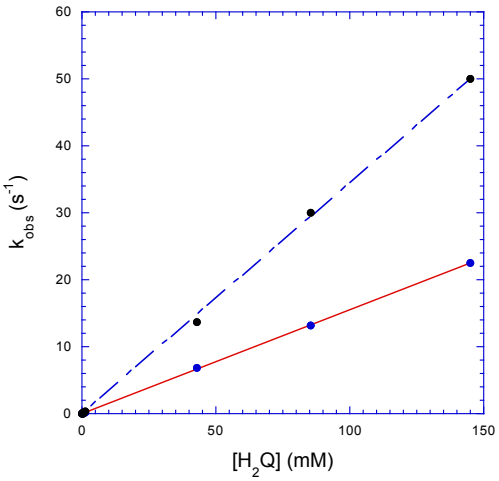


**Figure S1** – Plot of rate constants $k^{red}{}_1$ (blue dots) and $k^{red}{}_{2,3,4}$ (black dots) from 614 nm fits affording second order T1 rates of 154.7 $M^{-1}s^{-1}$ and 346.0 $M^{-1}s^{-1}$, respectively.

*EPR*

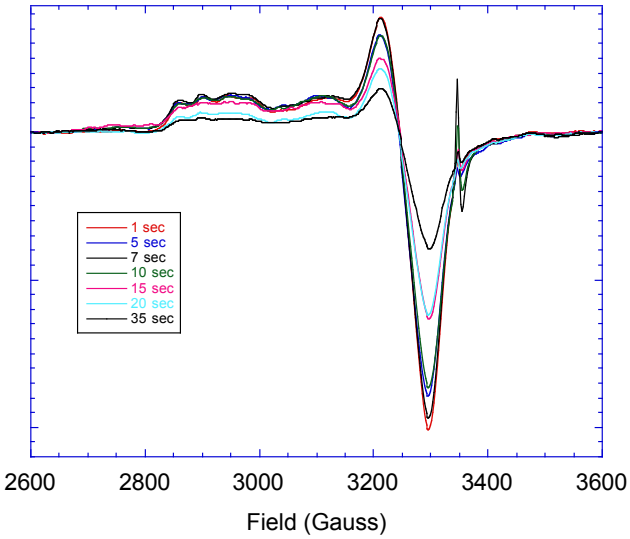


**Figure S2** – 77 K X-Band EPR spectra of the reduction of NI. Quench time given in figure legend. Radical attributed to $H_2Q$.

The overall integrated signal intensity of these spectra are scaled to the integrated intensity of NI at the same conditions. The quench times for the FQ-EPR time points were scaled slower by four since the $H_2Q$ concentration is four times higher in the FQ-EPR reaction as it is in SF experiment and the rates of T1 reduction vary linearly with $[H_2Q]$. To estimate the relative contribution of the T1 and the 1-hole intermediate in the FQ-EPR spectra, the obtained Red NI spectra (Figure S2) were subtracted from an experimental T1 spectrum composed of 50/50 combination the 77 K X-band spectra of NI and met T2D, which best matches the $A_{//}$ hyperfine of the T1 signal in the intermediate. Since the exact spectrum of the 1-hole form is somewhat underdetermined, an average percentage of the T1 and 1-hole species was obtained by obtaining of the subtractions from matching the intensities of the top (~3200 G) and bottom (~3300 G) of the $g_{\perp}$ region of the intermediate to obtain an integrated ratio of the T1 and intermediate.

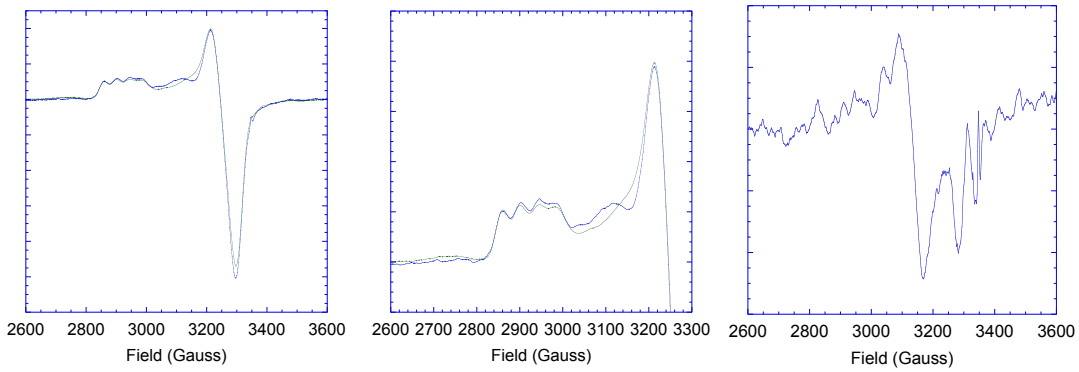


**Figure S3** – Example of FQ-EPR subtracted spectra (left) T1 (black) and 1sec Red NI (blue) FQ-EPR X-band spectra (middle), same as (left) but expanded to low field, (right) residual spectrum from the subtraction featuring intensity at g ≈ 2.14 (derivative) and g ≈ 2.05.

**Table S3** – Percent compositions of Red NI X-band EPR signal.

| FQ Time (sec) | Percent T1 | Percent 1-hole |
|---|---|---|
| 1 | 86.7% | 6.4% |
| 5 | 72.5% | 15.7% |
| 7 | 81.9% | 9.2% |
| 10 | 70.2% | 18.2% |
| 15 | 58.9% | 15.9% |
| 20 | 54.9% | 9.3% |
| 35 | 39.4% | 14.5% |

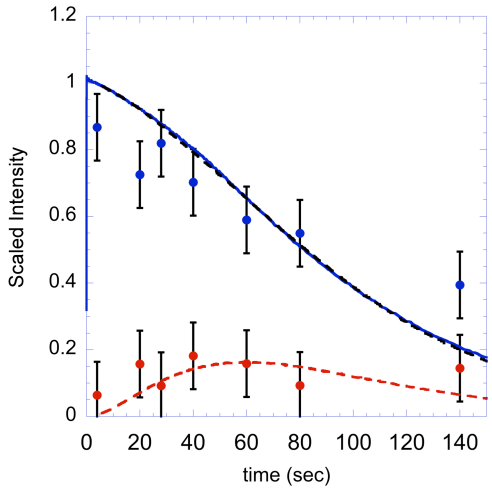


**Figure S4** – Correlation of spin-integrated speciation of T1 (blue dots) and 1-electron hole intermediate (red dots) with the SF absorption spectra. Correlation of the kinetics of the ±10% error bars on spin integrated points. Quench times of FQ-EPR points are scaled slower by 4× due to the higher $H_2Q$ concentration in the FQ-EPR compared to the SF conditions. Note the correlation of the T1 signal from EPR correlated with the 614 nm absorption. We attempt to estimate the time dependence of the 1-hole intermediate overtime, which is difficult due to its low concentration and large errors.

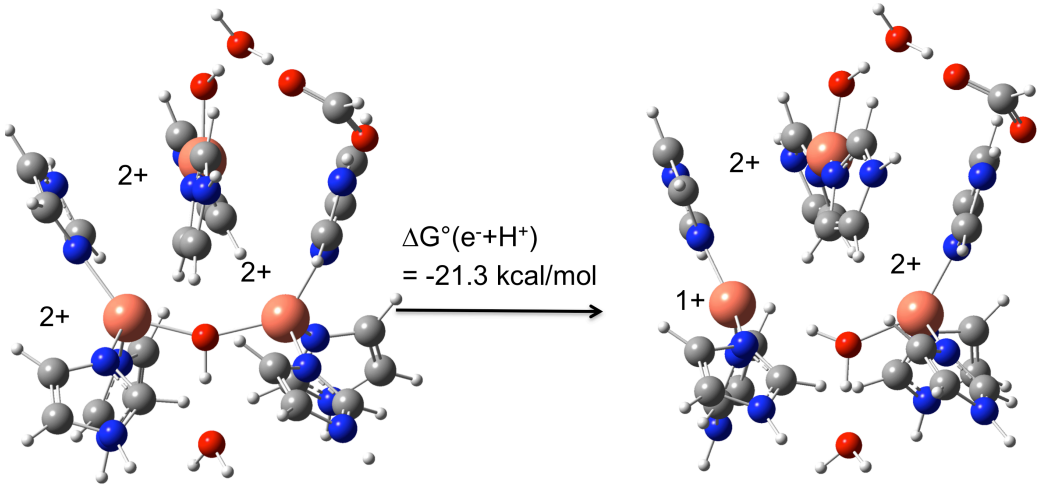


**Figure S5**– Optimized structures of EPT for Resting. Colors: Cu – orange, O – red, N – blue, C – gray, and H – white.

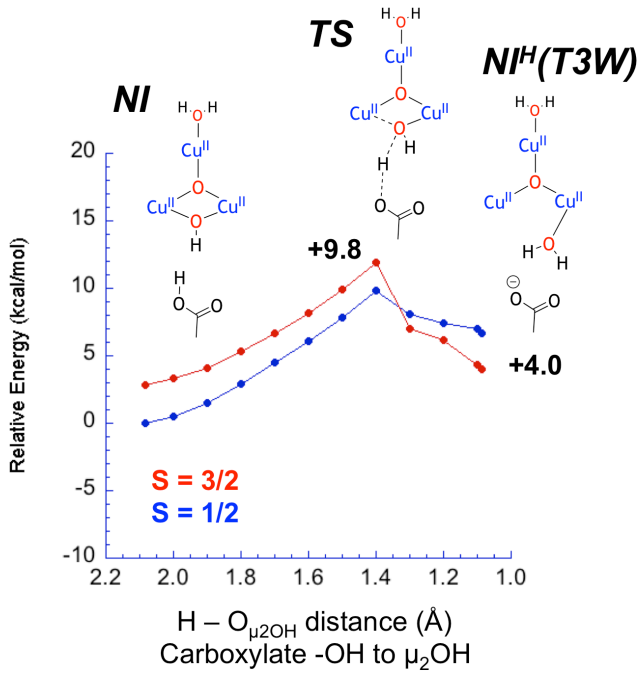


**Figure S6**– Potential energy surfaces of proton transfer from a carboxylate to the $\mu_2$-OH of NI (left) and from the T3b-$OH_2$ to the $\mu_3$-oxo of NI. Energies in blue and red correspond to S = 1/2 and 3/2 spin states, respectively.

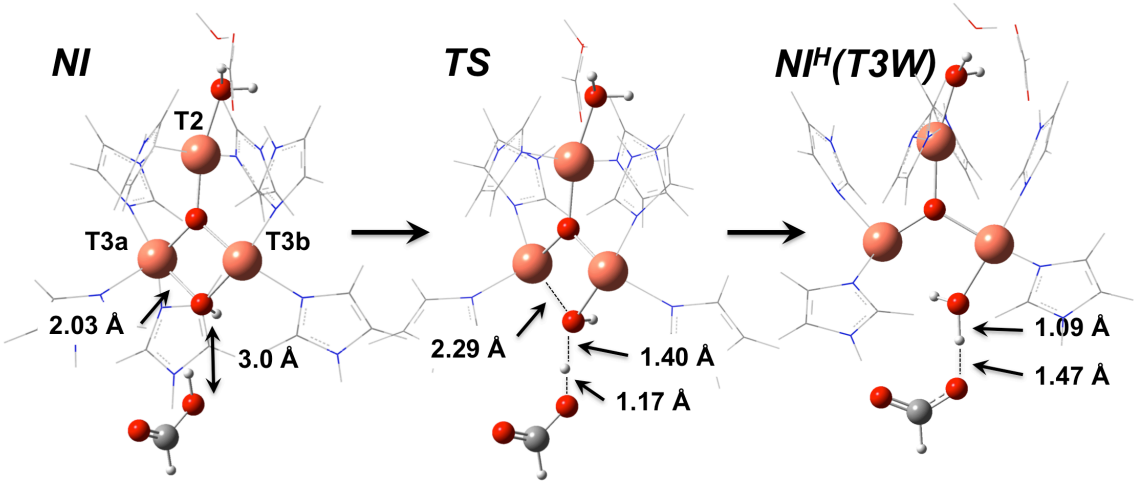


**Figure S7** – Optimized structures along the Proton Transfer coordinate from the carboxylate donor to the $\mu_2$-OH of NI. These structures are correlated to the energy surfaces in Figure S5. Some histidines omitted for clarity. Colors: Cu – orange, O – red, N – blue, C – gray, and H – white.

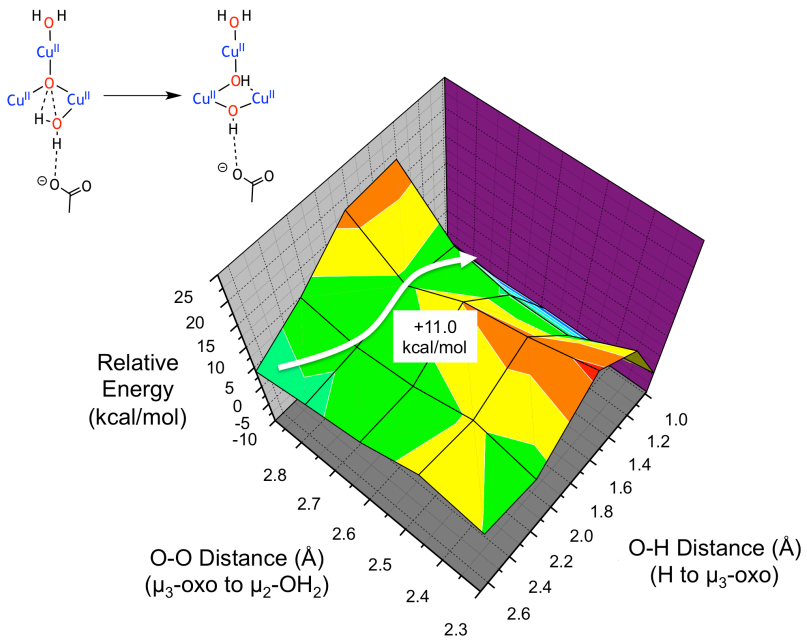


**Figure S8**– 2D potential energy surface for Proton Transfer from the $\mu_2$-$OH_2$ donor to the $\mu_3$-oxo of NI as a function of the donor-acceptor O-O distance and H-$O_{oxo}$ distance. The reaction starts at +4.0 kcal/mol proceeding through a TS at +11.0 kcal/mol and forms product with an energy of -7.7 kcal/mol. Structures along this path are presented in Figure S9.

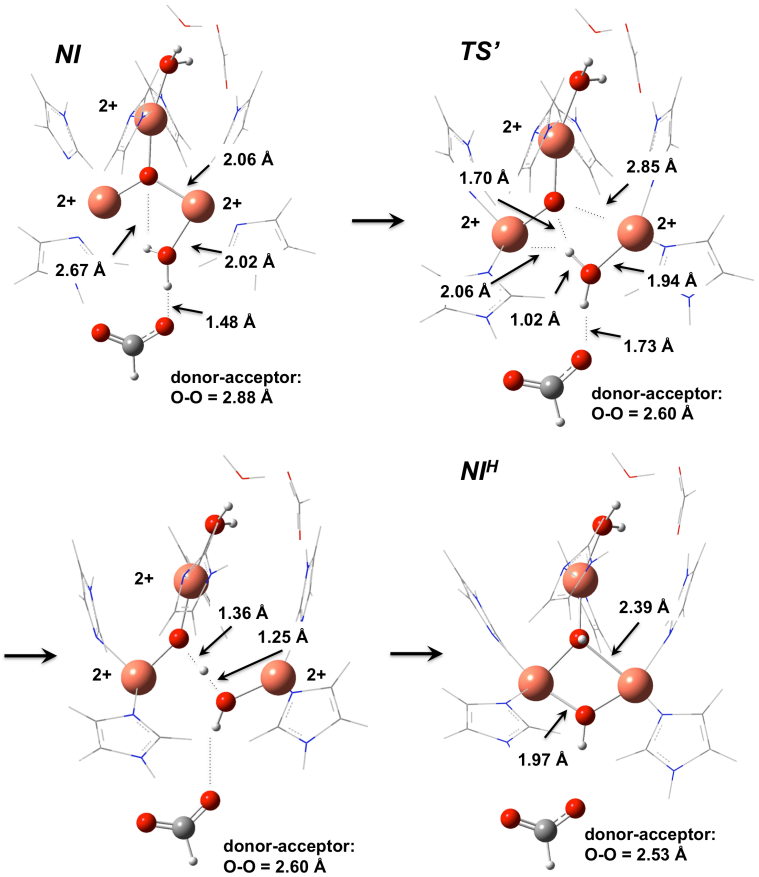


**Figure S9** – Optimized structures from the 2D proton transfer coordinate from the T3b-$OH_2$ to the $\mu_3$-oxo of NI. Colors: Cu – orange, O – red, N – blue, C – gray, and H – white.

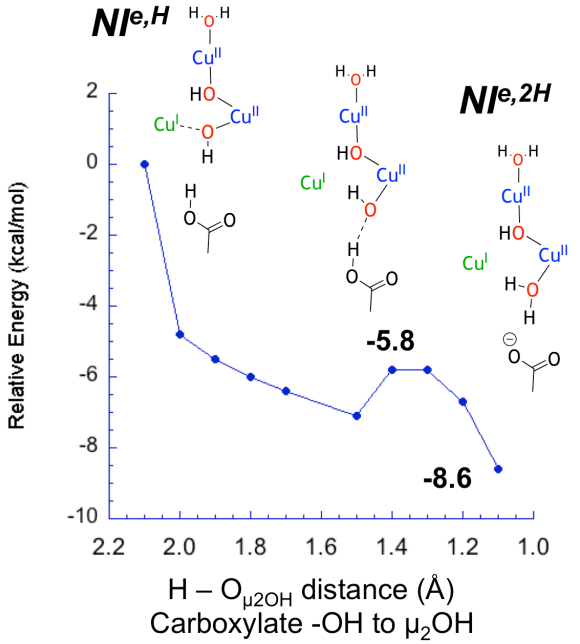


**Figure S10** – Potential energy surface of proton transfer from a carboxylate to the $\mu_2$-OH of **NI**$^{e,H}$. The energy is of the S = 0 state. Structures in Figure S11.

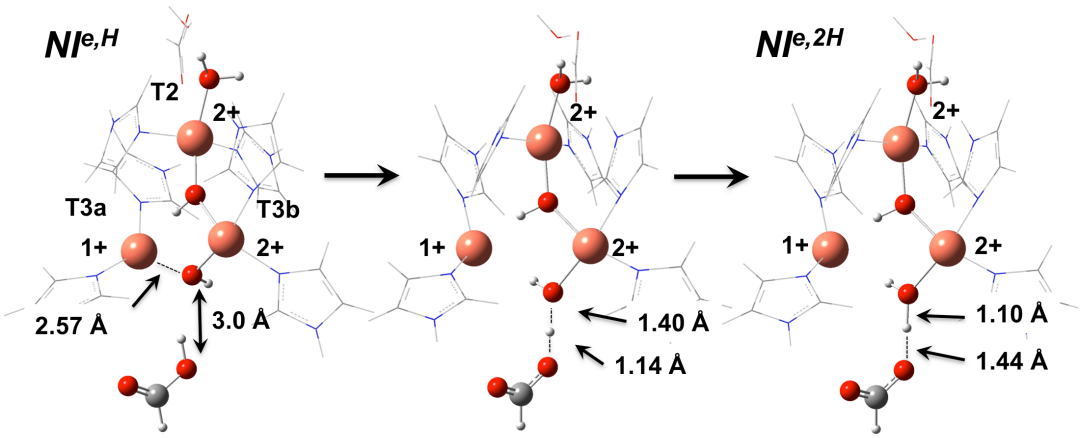


**Figure S11** – Optimized structures along the proton transfer coordinate from the carboxylate to the $\mu_2$-OH$_2$ of **NI**$^{e,H}$. Colors: Cu – orange, O – red, N – blue, C – gray, and H – white.

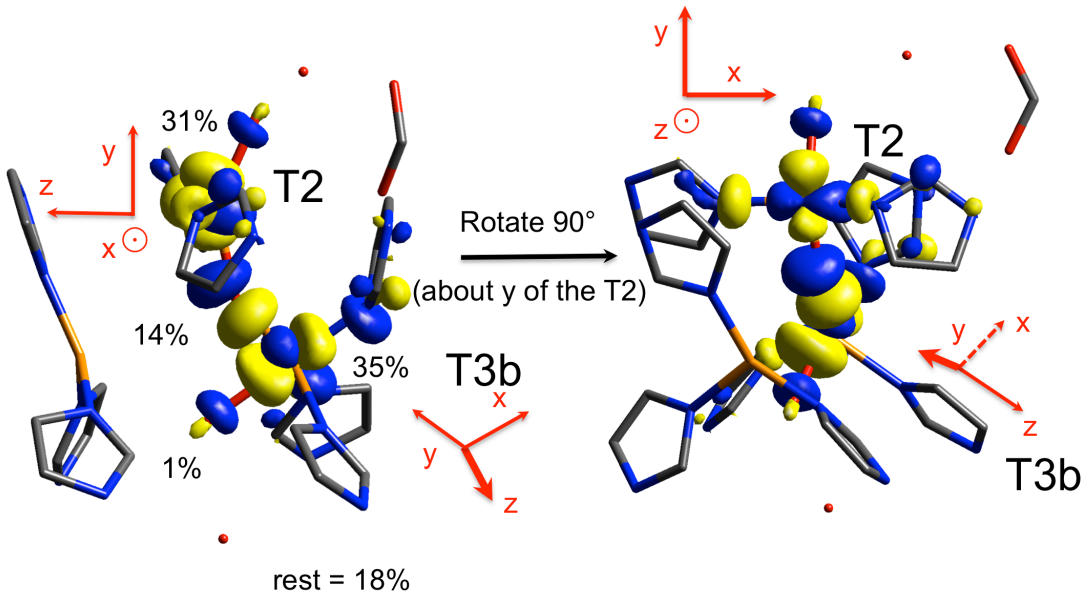


**Figure S12** – β-LUMO of **$NI^{2e,2H}$(MV)** (isodensity value = 0.035). The approximate g-tensor directions are given with axis in red where bold arrow indicates when the axis is directed out of the plane or dashed when directed into the plane.

Complete Gaussian 09 Citation:

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

XYZ Coordinates:

NI

| | | | |
|---|---|---|---|
| Cu | -1.54858 | 0.81540 | 0.94698 |
| Cu | -0.36923 | -1.24178 | -0.86063 |
| Cu | 1.68810 | 1.45040 | -0.14380 |
| O | 0.11047 | 0.44514 | 0.05440 |
| O | -1.86815 | -0.96218 | 0.26929 |
| C | 2.27840 | -0.81589 | 3.03405 |
| N | 3.58984 | -0.66252 | 2.60366 |
| C | 1.55654 | 0.15992 | 2.41738 |
| C | 3.62719 | 0.37194 | 1.72921 |
| N | 2.39786 | 0.88620 | 1.58874 |
| H | 0.50227 | 0.35190 | 2.46241 |
| H | 4.51199 | 0.71871 | 1.20966 |
| C | -0.39963 | 3.85865 | 2.07483 |
| N | -1.07502 | 2.95769 | 1.24570 |
| C | -0.35027 | 5.09571 | 1.50381 |
| C | -1.42524 | 3.67568 | 0.17899 |
| N | -1.00412 | 4.96446 | 0.30108 |
| H | 0.07128 | 6.02264 | 1.85481 |
| H | -1.94356 | 3.31131 | -0.68876 |
| C | -2.80569 | -0.66502 | 5.05260 |
| N | -2.62961 | -1.78228 | 4.24171 |
| C | -2.48183 | 0.41653 | 4.26535 |
| C | -2.21478 | -1.34414 | 3.01723 |
| N | -2.11556 | -0.01576 | 2.99641 |
| H | -2.48724 | 1.46349 | 4.52746 |
| H | -2.00059 | -1.97630 | 2.17338 |
| C | -0.01315 | -4.66358 | 1.79725 |
| N | -0.36931 | -5.49600 | 0.74439 |
| C | 0.06294 | -3.40035 | 1.27583 |
| C | -0.49141 | -4.69826 | -0.37222 |
| N | -0.23917 | -3.42818 | -0.07475 |
| H | 0.31215 | -2.47877 | 1.77547 |
| H | -0.75270 | -5.07650 | -1.35038 |
| C | -0.71672 | 2.68334 | -3.17720 |
| N | -0.01739 | 3.86481 | -2.99245 |
| C | -0.12982 | 1.75874 | -2.37233 |
| C | 0.97018 | 3.62411 | -2.08329 |
| N | 0.90728 | 2.35555 | -1.68771 |
| H | -0.39557 | 0.73407 | -2.21706 |
| H | 1.67958 | 4.36019 | -1.73348 |
| C | 3.43331 | -0.69887 | -2.43423 |
| N | 3.64927 | -1.42072 | -1.27807 |
| C | 2.07363 | -0.70443 | -2.64692 |
| C | 2.44424 | -1.83293 | -0.81627 |

| | | | |
|---|---|---|---|
| N | 1.46366 | -1.41085 | -1.61925 |
| H | 1.50395 | -0.25653 | -3.44507 |
| H | 2.31292 | -2.40176 | 0.09009 |
| C | -2.18461 | -2.58109 | -4.68019 |
| N | -3.25483 | -2.21965 | -3.86998 |
| C | -1.06183 | -2.28364 | -3.93581 |
| C | -2.76882 | -1.73606 | -2.69527 |
| N | -1.43833 | -1.75584 | -2.70098 |
| H | -0.02301 | -2.41791 | -4.19436 |
| H | -3.40758 | -1.48857 | -1.86286 |
| C | -5.16690 | 1.30728 | -1.27280 |
| N | -5.77561 | 0.83707 | -0.11729 |
| C | -3.86317 | 1.55395 | -0.94458 |
| C | -4.81350 | 0.84165 | 0.87326 |
| N | -3.64715 | 1.26304 | 0.39289 |
| H | -3.07037 | 1.89295 | -1.59116 |
| H | -4.99800 | 0.53820 | 1.89403 |
| C | 6.66174 | -1.54033 | 0.63861 |
| O | 5.44058 | -1.89599 | 0.52738 |
| O | 7.20233 | -0.45288 | 0.22605 |
| O | 3.45265 | 2.25081 | -0.73155 |
| O | 5.72007 | 1.53611 | -0.03692 |
| H | 3.42829 | 2.28429 | -1.71030 |
| H | 6.17605 | 2.23588 | 0.50501 |
| H | 6.33881 | 0.64136 | -0.04184 |
| H | 4.41688 | 1.91127 | -0.47558 |
| H | -2.79636 | -1.25378 | 0.10145 |
| H | 7.31697 | -2.25454 | 1.15783 |
| H | 1.96074 | -1.63897 | 3.62329 |
| H | 0.02493 | 3.70461 | 3.03368 |
| H | -3.13187 | -0.75930 | 6.07314 |
| H | 0.14897 | -5.00584 | 2.79485 |
| H | -1.56761 | 2.58056 | -3.79957 |
| H | 4.26072 | -0.24591 | -2.93820 |
| H | -2.35722 | -3.01659 | -5.65986 |
| H | -5.69825 | 1.46090 | -2.18610 |
| H | -2.78359 | -2.77218 | 4.52441 |
| H | -0.48972 | -6.53469 | 0.81540 |
| H | -4.25235 | -2.28959 | -4.10935 |
| H | 4.55591 | -1.54134 | -0.73551 |
| H | -6.78160 | 0.53353 | -0.07810 |
| H | -1.12997 | 5.74009 | -0.34218 |
| H | -0.21050 | 4.73793 | -3.50160 |
| H | 4.37626 | -1.29063 | 2.83880 |
| O | -4.29942 | -1.98971 | -0.11899 |
| H | -5.16568 | -1.58608 | 0.17371 |

| | | | |
|---|---|---|---|
| H | -4.27934 | -2.94141 | 0.19891 |

NIe

| | | | |
|---|---|---|---|
| Cu | -1.74631 | 1.00903 | 1.18332 |
| Cu | -0.29745 | -1.21609 | -0.82242 |
| Cu | 1.38450 | 1.51911 | -0.11393 |
| O | -0.13765 | 0.40056 | 0.19733 |
| O | -1.83719 | -1.92659 | 0.04789 |
| C | 2.36337 | -0.53932 | 3.01941 |
| N | 3.65934 | -0.30643 | 2.57448 |
| C | 1.55473 | 0.36352 | 2.40817 |
| C | 3.59411 | 0.73443 | 1.69684 |
| N | 2.32551 | 1.14455 | 1.56829 |
| H | 0.48198 | 0.44712 | 2.41668 |
| H | 4.43293 | 1.14185 | 1.16376 |
| C | -0.67372 | 3.96367 | 1.81844 |
| N | -1.57929 | 3.09127 | 1.23053 |
| C | -0.52575 | 5.10011 | 1.08027 |
| C | -1.99786 | 3.72035 | 0.13585 |
| N | -1.37723 | 4.92982 | 0.01214 |
| H | 0.07517 | 5.98135 | 1.22902 |
| H | -2.72295 | 3.34818 | -0.56702 |
| C | -2.74040 | -0.63311 | 4.96878 |
| N | -2.47574 | -1.77033 | 4.21037 |
| C | -2.49000 | 0.43454 | 4.14309 |
| C | -2.07496 | -1.34965 | 2.96422 |
| N | -2.07770 | -0.01858 | 2.89616 |
| H | -2.57608 | 1.48839 | 4.35906 |
| H | -1.82622 | -1.97966 | 2.11930 |
| C | 0.48292 | -4.61555 | 1.92400 |
| N | 0.22093 | -5.54370 | 0.92447 |
| C | 0.65998 | -3.41995 | 1.27523 |
| C | 0.25822 | -4.87521 | -0.27498 |
| N | 0.51655 | -3.59022 | -0.09209 |
| H | 0.84028 | -2.44567 | 1.70248 |
| H | 0.09098 | -5.35803 | -1.22753 |
| C | -0.89753 | 2.46332 | -3.31094 |
| N | -0.25583 | 3.68547 | -3.20923 |
| C | -0.41115 | 1.68421 | -2.31211 |
| C | 0.60994 | 3.60673 | -2.15409 |
| N | 0.51569 | 2.40501 | -1.59564 |
| H | -0.65778 | 0.67700 | -2.04860 |
| H | 1.26012 | 4.40423 | -1.82780 |
| C | 3.54818 | -0.51039 | -2.39833 |
| N | 3.77205 | -1.08296 | -1.15792 |
| C | 2.18395 | -0.51184 | -2.58827 |

| | | | |
|---|---|---|---|
| C | 2.56540 | -1.40916 | -0.63976 |
| N | 1.57878 | -1.07532 | -1.47560 |
| H | 1.60577 | -0.15269 | -3.42517 |
| H | 2.44171 | -1.87775 | 0.31961 |
| C | -1.88729 | -2.98167 | -4.65843 |
| N | -2.98574 | -2.62977 | -3.87781 |
| C | -0.79021 | -2.53800 | -3.94969 |
| C | -2.52906 | -2.00929 | -2.75218 |
| N | -1.20031 | -1.93508 | -2.76361 |
| H | 0.25539 | -2.61844 | -4.20396 |
| H | -3.15845 | -1.66467 | -1.94695 |
| C | -5.14667 | 0.83132 | -1.47371 |
| N | -5.75344 | 0.40388 | -0.29829 |
| C | -3.84631 | 1.11337 | -1.14243 |
| C | -4.79651 | 0.44012 | 0.68673 |
| N | -3.63341 | 0.87573 | 0.21078 |
| H | -3.05398 | 1.46464 | -1.78113 |
| H | -4.97950 | 0.14184 | 1.70424 |
| C | 6.71897 | -1.18066 | 0.69749 |
| O | 6.00754 | -1.87444 | -0.10005 |
| O | 6.62510 | 0.07184 | 0.96301 |
| O | 3.13573 | 2.41971 | -0.86237 |
| O | 5.54503 | 1.98211 | -0.30249 |
| H | 3.07298 | 2.32895 | -1.83442 |
| H | 5.91555 | 2.77038 | 0.23991 |
| H | 5.98543 | 1.11138 | 0.10022 |
| H | 4.12106 | 2.18051 | -0.63017 |
| H | -1.75171 | -2.87352 | -0.19098 |
| H | 7.50999 | -1.73375 | 1.23533 |
| H | 2.09852 | -1.35055 | 3.62646 |
| H | -0.18385 | 3.81180 | 2.73777 |
| H | -3.06750 | -0.68739 | 5.98942 |
| H | 0.52486 | -4.87096 | 2.96662 |
| H | -1.62445 | 2.22271 | -4.03657 |
| H | 4.37049 | -0.15517 | -2.98438 |
| H | -2.01810 | -3.50561 | -5.60015 |
| H | -5.68798 | 0.91443 | -2.39491 |
| H | -2.56874 | -2.75137 | 4.55320 |
| H | 0.01114 | -6.54213 | 1.06745 |
| H | -3.97403 | -2.82678 | -4.10430 |
| H | 4.72750 | -1.30948 | -0.71176 |
| H | -6.72945 | 0.02916 | -0.24808 |
| H | -1.43611 | 5.58322 | -0.75042 |
| H | -0.41792 | 4.47933 | -3.84505 |
| H | 4.49360 | -0.88240 | 2.84164 |
| O | -4.36924 | -2.29367 | 0.75693 |

| | | | |
|---|---|---|---|
| H | -4.22513 | -2.57657 | 1.70588 |
| H | -3.43682 | -2.02377 | 0.43654 |

NIH (T3W)

| | | | |
|---|---|---|---|
| Cu | -1.65695 | 0.92428 | 1.13173 |
| Cu | -0.33597 | -1.26733 | -0.88652 |
| Cu | 1.53878 | 1.46442 | -0.13673 |
| O | -0.14894 | 0.39875 | 0.16336 |
| O | -2.01448 | -1.79719 | 0.17129 |
| C | 2.37506 | -0.62591 | 3.05113 |
| N | 3.66695 | -0.47251 | 2.57874 |
| C | 1.60426 | 0.29081 | 2.41783 |
| C | 3.64878 | 0.51911 | 1.65271 |
| N | 2.39550 | 0.98867 | 1.52657 |
| H | 0.54637 | 0.44900 | 2.49747 |
| H | 4.50847 | 0.86711 | 1.09004 |
| C | -0.40006 | 4.01494 | 1.89068 |
| N | -1.29064 | 3.15681 | 1.25373 |
| C | -0.23852 | 5.16761 | 1.18190 |
| C | -1.67574 | 3.81304 | 0.15990 |
| N | -1.05487 | 5.02116 | 0.08448 |
| H | 0.34676 | 6.05090 | 1.37630 |
| H | -2.38125 | 3.46645 | -0.57606 |
| C | -2.74083 | -0.42732 | 5.04380 |
| N | -2.53415 | -1.58720 | 4.30160 |
| C | -2.49083 | 0.61116 | 4.17135 |
| C | -2.17089 | -1.23554 | 3.04429 |
| N | -2.13527 | 0.09462 | 2.92244 |
| H | -2.53450 | 1.67454 | 4.35151 |
| H | -1.94961 | -1.93026 | 2.25734 |
| C | 0.19507 | -4.55897 | 1.98754 |
| N | -0.13734 | -5.44792 | 0.97627 |
| C | 0.33548 | -3.33699 | 1.38923 |
| C | -0.17791 | -4.73600 | -0.19612 |
| N | 0.09638 | -3.45046 | 0.02595 |
| H | 0.59456 | -2.39284 | 1.84041 |
| H | -0.40139 | -5.17727 | -1.15777 |
| C | -0.76128 | 2.57726 | -3.25181 |
| N | -0.06338 | 3.76163 | -3.12776 |
| C | -0.27369 | 1.72955 | -2.31550 |
| C | 0.83496 | 3.60313 | -2.11245 |
| N | 0.70605 | 2.37785 | -1.60343 |
| H | -0.55545 | 0.71644 | -2.12078 |
| H | 1.53126 | 4.35702 | -1.77486 |
| C | 3.49477 | -0.67414 | -2.40718 |
| N | 3.71208 | -1.31591 | -1.20727 |

| | | | |
|---|---|---|---|
| C | 2.13193 | -0.62648 | -2.59210 |
| C | 2.50935 | -1.63869 | -0.68497 |
| N | 1.52312 | -1.23055 | -1.49771 |
| H | 1.56090 | -0.21223 | -3.40802 |
| H | 2.38408 | -2.15218 | 0.25324 |
| C | -2.07722 | -2.79625 | -4.57367 |
| N | -3.15159 | -2.37585 | -3.79881 |
| C | -0.95558 | -2.43373 | -3.85637 |
| C | -2.67423 | -1.78743 | -2.67748 |
| N | -1.34068 | -1.80830 | -2.66839 |
| H | 0.08476 | -2.58087 | -4.10257 |
| H | -3.32367 | -1.43470 | -1.89965 |
| C | -5.08118 | 1.12465 | -1.35651 |
| N | -5.68476 | 0.69031 | -0.17866 |
| C | -3.75684 | 1.30383 | -1.05622 |
| C | -4.71505 | 0.64815 | 0.79491 |
| N | -3.53459 | 1.00166 | 0.28580 |
| H | -2.95780 | 1.62603 | -1.70332 |
| H | -4.89645 | 0.36047 | 1.82079 |
| C | 6.73510 | -1.44379 | 0.63681 |
| O | 5.58168 | -1.95003 | 0.42220 |
| O | 7.16439 | -0.29607 | 0.26085 |
| O | 3.27592 | 2.19688 | -0.84843 |
| O | 5.59962 | 1.56693 | -0.27339 |
| H | 3.20954 | 2.21725 | -1.82594 |
| H | 6.06460 | 2.35394 | 0.12432 |
| H | 6.25240 | 0.69737 | -0.16208 |
| H | 4.26291 | 1.86823 | -0.63784 |
| H | -3.02479 | -1.77656 | 0.03022 |
| H | 7.42784 | -2.07329 | 1.22042 |
| H | 2.07003 | -1.41166 | 3.67058 |
| H | 0.05965 | 3.87040 | 2.82864 |
| H | -3.02755 | -0.48329 | 6.09103 |
| H | 0.30177 | -4.83859 | 3.01199 |
| H | -1.53501 | 2.39443 | -3.93691 |
| H | 4.33320 | -0.30733 | -2.95784 |
| H | -2.25280 | -3.29648 | -5.52104 |
| H | -5.64541 | 1.29849 | -2.25733 |
| H | -2.65579 | -2.56348 | 4.64035 |
| H | -0.32009 | -6.47085 | 1.11132 |
| H | -4.15322 | -2.52116 | -4.00077 |
| H | 4.65219 | -1.49150 | -0.69665 |
| H | -6.71073 | 0.46014 | -0.10353 |
| H | -1.13162 | 5.72357 | -0.63826 |
| H | -0.20661 | 4.58174 | -3.74823 |
| H | 4.47843 | -1.06898 | 2.86198 |

| | | | |
|---|---|---|---|
| O | -4.48745 | -2.14999 | -0.13783 |
| H | -5.28951 | -1.57573 | -0.28982 |
| H | -4.76416 | -3.11375 | -0.16920 |
| H | -1.80715 | -2.75442 | 0.23513 |

NIH

| | | | |
|---|---|---|---|
| Cu | -1.64197 | 0.92727 | 0.91706 |
| Cu | -0.42089 | -1.56368 | -0.91669 |
| Cu | 1.77578 | 1.60715 | -0.14369 |
| O | 0.23720 | 0.48852 | 0.20264 |
| O | -1.81577 | -0.85044 | 0.14583 |
| C | 2.36041 | -0.61100 | 3.07886 |
| N | 3.64759 | -0.53198 | 2.57007 |
| C | 1.67892 | 0.44713 | 2.54574 |
| C | 3.70733 | 0.51297 | 1.71095 |
| N | 2.51365 | 1.12279 | 1.64987 |
| H | 0.67039 | 0.76913 | 2.74998 |
| H | 4.58193 | 0.80165 | 1.13448 |
| C | -0.32471 | 3.94794 | 1.81024 |
| N | -1.13409 | 3.04918 | 1.09430 |
| C | -0.21946 | 5.12931 | 1.13752 |
| C | -1.51089 | 3.72579 | 0.00509 |
| N | -0.97128 | 4.97253 | -0.00218 |
| H | 0.29446 | 6.04167 | 1.39173 |
| H | -2.15033 | 3.36491 | -0.77985 |
| C | -2.70805 | -0.33811 | 5.09677 |
| N | -2.56968 | -1.50751 | 4.35481 |
| C | -2.39722 | 0.68275 | 4.22369 |
| C | -2.19524 | -1.16584 | 3.09032 |
| N | -2.07727 | 0.15657 | 2.97361 |
| H | -2.38290 | 1.74585 | 4.40961 |
| H | -2.03200 | -1.87363 | 2.29569 |
| C | -0.01235 | -4.55539 | 2.05421 |
| N | -0.40499 | -5.43324 | 1.05478 |
| C | 0.06641 | -3.31815 | 1.48003 |
| C | -0.55269 | -4.69106 | -0.09379 |
| N | -0.27797 | -3.40580 | 0.14342 |
| H | 0.33938 | -2.38565 | 1.94516 |
| H | -0.84492 | -5.10647 | -1.04812 |
| C | -0.79206 | 2.49648 | -3.26843 |
| N | -0.06411 | 3.67685 | -3.20674 |
| C | -0.23650 | 1.66709 | -2.33328 |
| C | 0.89757 | 3.53602 | -2.25435 |
| N | 0.80780 | 2.32590 | -1.70296 |
| H | -0.51555 | 0.66248 | -2.08316 |
| H | 1.61570 | 4.29950 | -1.98881 |

| | | | |
|---|---|---|---|
| C | 3.37723 | -0.89977 | -2.47875 |
| N | 3.61525 | -1.55625 | -1.28646 |
| C | 2.01215 | -0.93387 | -2.66918 |
| C | 2.42914 | -1.96742 | -0.78373 |
| N | 1.42836 | -1.60367 | -1.59746 |
| H | 1.42085 | -0.53662 | -3.47904 |
| H | 2.32970 | -2.52221 | 0.13659 |
| C | -2.29790 | -2.83383 | -4.51309 |
| N | -3.34294 | -2.39853 | -3.70738 |
| C | -1.15118 | -2.49013 | -3.83442 |
| C | -2.82570 | -1.82232 | -2.59513 |
| N | -1.49371 | -1.85783 | -2.64021 |
| H | -0.12174 | -2.65505 | -4.11215 |
| H | -3.42274 | -1.49069 | -1.76439 |
| C | -5.16304 | 1.24991 | -1.28784 |
| N | -5.74589 | 0.85314 | -0.09060 |
| C | -3.84502 | 1.47986 | -1.01965 |
| C | -4.75964 | 0.88673 | 0.87041 |
| N | -3.59931 | 1.25393 | 0.32619 |
| H | -3.06627 | 1.76499 | -1.70708 |
| H | -4.91407 | 0.63927 | 1.91092 |
| C | 6.63899 | -1.58293 | 0.60562 |
| O | 5.40670 | -1.91873 | 0.57683 |
| O | 7.16198 | -0.52142 | 0.10346 |
| O | 3.47128 | 2.23621 | -0.88101 |
| O | 5.69421 | 1.44969 | -0.20848 |
| H | 3.41021 | 2.25303 | -1.86016 |
| H | 6.22209 | 2.19699 | 0.18667 |
| H | 6.31499 | 0.52638 | -0.19076 |
| H | 4.45444 | 1.85252 | -0.63657 |
| H | -2.70992 | -1.28223 | 0.20655 |
| H | 7.32375 | -2.27620 | 1.12112 |
| H | 2.02481 | -1.45068 | 3.64814 |
| H | 0.13147 | 3.86827 | 2.76995 |
| H | -3.00824 | -0.36565 | 6.13838 |
| H | 0.16288 | -4.84133 | 3.06324 |
| H | -1.60969 | 2.34688 | -3.94916 |
| H | 4.20599 | -0.48725 | -3.02991 |
| H | -2.49308 | -3.34421 | -5.44700 |
| H | -5.71808 | 1.37458 | -2.18983 |
| H | -2.71156 | -2.47318 | 4.70946 |
| H | -0.53092 | -6.48096 | 1.19410 |
| H | -4.34912 | -2.50241 | -3.90739 |
| H | 4.53245 | -1.64918 | -0.75823 |
| H | -6.76801 | 0.59009 | -0.00821 |
| H | -1.07067 | 5.70659 | -0.70118 |

| | | | |
|---|---|---|---|
| H | -0.22522 | 4.50291 | -3.81048 |
| H | 4.42749 | -1.17847 | 2.79689 |
| H | 0.55060 | -0.13683 | 0.88658 |
| O | -4.16243 | -2.01532 | 0.21114 |
| H | -5.05048 | -1.56582 | 0.11313 |
| H | -4.31718 | -2.92802 | 0.59767 |

NIe,H

| | | | |
|---|---|---|---|
| Cu | -1.98234 | 1.11297 | 1.14783 |
| Cu | -0.26399 | -1.49549 | -0.86902 |
| Cu | 1.95387 | 1.44130 | -0.33441 |
| O | 0.58770 | 0.17461 | -0.21848 |
| O | -1.70201 | -0.69798 | 0.12069 |
| C | 2.14225 | -0.54609 | 3.14248 |
| N | 3.48194 | -0.38755 | 2.79667 |
| C | 1.46392 | 0.38001 | 2.39570 |
| C | 3.57957 | 0.58592 | 1.86357 |
| N | 2.36600 | 1.07351 | 1.58779 |
| H | 0.40483 | 0.57000 | 2.34654 |
| H | 4.49846 | 0.90880 | 1.39017 |
| C | -0.57992 | 3.99279 | 1.77782 |
| N | -1.13039 | 2.99353 | 0.96438 |
| C | -0.56691 | 5.19509 | 1.13557 |
| C | -1.42906 | 3.62432 | -0.17466 |
| N | -1.10939 | 4.94640 | -0.10316 |
| H | -0.23097 | 6.16726 | 1.45484 |
| H | -1.83172 | 3.17138 | -1.06066 |
| C | -3.03508 | -0.35931 | 4.98906 |
| N | -2.80495 | -1.52150 | 4.26224 |
| C | -2.73776 | 0.67989 | 4.14276 |
| C | -2.38094 | -1.14671 | 3.01508 |
| N | -2.33096 | 0.18035 | 2.91309 |
| H | -2.78363 | 1.74079 | 4.33422 |
| H | -2.12616 | -1.82706 | 2.22179 |
| C | -0.05623 | -4.51899 | 2.14739 |
| N | -0.36029 | -5.43202 | 1.14659 |
| C | -0.01633 | -3.29060 | 1.54671 |
| C | -0.49249 | -4.71786 | -0.02151 |
| N | -0.29252 | -3.42183 | 0.19813 |
| H | 0.19845 | -2.32931 | 1.98258 |
| H | -0.71947 | -5.16695 | -0.97804 |
| C | -0.64809 | 2.40780 | -3.40008 |
| N | 0.02579 | 3.61731 | -3.29561 |
| C | -0.01279 | 1.55206 | -2.54757 |
| C | 1.03561 | 3.46306 | -2.39407 |
| N | 1.02646 | 2.21962 | -1.91858 |

| | | | |
|---|---|---|---|
| H | -0.24560 | 0.53042 | -2.32588 |
| H | 1.72402 | 4.24436 | -2.10458 |
| C | 3.52410 | -0.89954 | -2.28580 |
| N | 3.71724 | -1.54423 | -1.07518 |
| C | 2.20646 | -1.10620 | -2.62471 |
| C | 2.53673 | -2.11030 | -0.71939 |
| N | 1.59395 | -1.86053 | -1.63263 |
| H | 1.66471 | -0.76380 | -3.49246 |
| H | 2.38581 | -2.64949 | 0.20300 |
| C | -2.00399 | -2.99142 | -4.53684 |
| N | -3.10457 | -2.59460 | -3.78736 |
| C | -0.90881 | -2.66225 | -3.77213 |
| C | -2.66088 | -2.05658 | -2.61903 |
| N | -1.33129 | -2.07719 | -2.58274 |
| H | 0.13775 | -2.81250 | -3.98483 |
| H | -3.31433 | -1.76872 | -1.80965 |
| C | -5.19870 | 1.17584 | -1.52252 |
| N | -5.85459 | 0.77040 | -0.36903 |
| C | -3.95255 | 1.57333 | -1.12274 |
| C | -4.98756 | 0.96008 | 0.68300 |
| N | -3.82369 | 1.43163 | 0.25068 |
| H | -3.14002 | 1.91058 | -1.74307 |
| H | -5.23438 | 0.74389 | 1.71288 |
| C | 6.65226 | -1.31751 | 1.00969 |
| O | 5.42003 | -1.62726 | 0.89130 |
| O | 7.24528 | -0.27759 | 0.54466 |
| O | 3.63601 | 2.31429 | -0.82913 |
| O | 5.78585 | 1.68782 | 0.15841 |
| H | 3.70884 | 2.33998 | -1.80654 |
| H | 6.20823 | 2.42849 | 0.67103 |
| H | 6.41985 | 0.79256 | 0.21234 |
| H | 4.59226 | 2.01497 | -0.44487 |
| H | -2.56613 | -1.16640 | 0.09861 |
| H | 7.27387 | -2.01736 | 1.58684 |
| H | 1.82026 | -1.33258 | 3.80858 |
| H | -0.18665 | 3.91312 | 2.75836 |
| H | -3.37400 | -0.38024 | 6.00461 |
| H | 0.10002 | -4.78709 | 3.16669 |
| H | -1.50587 | 2.26102 | -4.02567 |
| H | 4.33572 | -0.37582 | -2.75199 |
| H | -2.12720 | -3.47196 | -5.49522 |
| H | -5.67280 | 1.17829 | -2.48168 |
| H | -2.93322 | -2.49326 | 4.62177 |
| H | -0.43775 | -6.46909 | 1.28386 |
| H | -4.09088 | -2.67225 | -4.07096 |
| H | 4.57233 | -1.50059 | -0.45071 |

| | | | |
|---|---|---|---|
| H | -6.81663 | 0.38548 | -0.35084 |
| H | -1.25215 | 5.67276 | -0.79713 |
| H | -0.19914 | 4.46157 | -3.83945 |
| H | 4.25649 | -0.99332 | 3.08674 |
| O | -4.09848 | -1.99409 | 0.03999 |
| H | -4.95546 | -1.48700 | 0.12283 |
| H | -4.20289 | -2.85386 | 0.54573 |
| H | -0.18632 | 0.58562 | 0.21925 |

NI2e,H

| | | | |
|---|---|---|---|
| Cu | 1.97341 | -1.19599 | 1.03928 |
| Cu | 0.15565 | 1.56535 | -0.88866 |
| Cu | -1.80180 | -1.62306 | -0.28118 |
| O | -0.85759 | 0.16782 | -0.09587 |
| O | 1.64073 | 0.54843 | -0.06764 |
| C | -2.19973 | 0.18961 | 3.21121 |
| N | -3.52079 | 0.07478 | 2.78868 |
| C | -1.50455 | -0.75141 | 2.49244 |
| C | -3.57527 | -0.88875 | 1.82082 |
| N | -2.35870 | -1.40390 | 1.60366 |
| H | -0.44777 | -0.96868 | 2.50814 |
| H | -4.46708 | -1.16140 | 1.27092 |
| C | 0.65943 | -4.13704 | 1.42190 |
| N | 1.33247 | -3.10665 | 0.76460 |
| C | 0.60733 | -5.26351 | 0.65624 |
| C | 1.68011 | -3.63613 | -0.40656 |
| N | 1.26491 | -4.92733 | -0.50434 |
| H | 0.17495 | -6.23210 | 0.84050 |
| H | 2.18945 | -3.13644 | -1.20600 |
| C | 2.99130 | -0.00148 | 4.99301 |
| N | 2.75542 | 1.21714 | 4.36714 |
| C | 2.72662 | -0.96460 | 4.04906 |
| C | 2.36010 | 0.94688 | 3.08048 |
| N | 2.33284 | -0.36604 | 2.85878 |
| H | 2.78414 | -2.03782 | 4.14457 |
| H | 2.11022 | 1.69775 | 2.35136 |
| C | -0.02192 | 4.33036 | 2.51114 |
| N | 0.27785 | 5.34176 | 1.60598 |
| C | 0.01046 | 3.16110 | 1.79446 |
| C | 0.47994 | 4.74341 | 0.38495 |
| N | 0.33121 | 3.42788 | 0.47463 |
| H | -0.20239 | 2.15516 | 2.11995 |
| H | 0.71457 | 5.29098 | -0.51707 |
| C | 0.81653 | -2.13050 | -3.47973 |
| N | 0.12899 | -3.34074 | -3.54040 |

| | | | |
|---|---|---|---|
| C | 0.30729 | -1.47536 | -2.38243 |
| C | -0.76791 | -3.36267 | -2.50194 |
| N | -0.67812 | -2.25197 | -1.77763 |
| H | 0.59286 | -0.52883 | -1.96035 |
| H | -1.44243 | -4.18244 | -2.30613 |
| C | -3.58073 | 1.13864 | -2.28923 |
| N | -3.78275 | 1.65852 | -1.01999 |
| C | -2.30388 | 1.48452 | -2.65379 |
| C | -2.63001 | 2.28086 | -0.65777 |
| N | -1.70729 | 2.19655 | -1.62153 |
| H | -1.77048 | 1.25265 | -3.56307 |
| H | -2.47693 | 2.73048 | 0.31022 |
| C | 1.96598 | 3.44315 | -4.26481 |
| N | 3.06458 | 2.98103 | -3.55110 |
| C | 0.86734 | 3.04312 | -3.54368 |
| C | 2.61079 | 2.32607 | -2.44477 |
| N | 1.28101 | 2.34541 | -2.41678 |
| H | -0.17804 | 3.21000 | -3.74696 |
| H | 3.25717 | 1.92548 | -1.68006 |
| C | 5.21705 | -0.91724 | -1.60141 |
| N | 5.86732 | -0.62205 | -0.41516 |
| C | 3.96459 | -1.33574 | -1.24391 |
| C | 4.99383 | -0.88536 | 0.60903 |
| N | 3.83110 | -1.31592 | 0.13523 |
| H | 3.14926 | -1.59952 | -1.89434 |
| H | 5.23941 | -0.76229 | 1.65443 |
| C | -6.71919 | 1.10126 | 1.04428 |
| O | -5.48352 | 1.41157 | 0.95963 |
| O | -7.32366 | 0.11152 | 0.50126 |
| O | -3.60456 | -2.20585 | -1.29390 |
| O | -5.79398 | -1.79801 | -0.11558 |
| H | -3.61507 | -1.79730 | -2.18121 |
| H | -6.16040 | -2.59115 | 0.36620 |
| H | -6.43464 | -0.96343 | 0.05099 |
| H | -4.51758 | -2.00905 | -0.87133 |
| H | 2.45413 | 1.07765 | 0.05790 |
| H | -7.33413 | 1.76413 | 1.67374 |
| H | -1.88347 | 0.98393 | 3.87055 |
| H | 0.22510 | -4.11418 | 2.38281 |
| H | 3.31316 | -0.06539 | 6.01626 |
| H | -0.22227 | 4.51092 | 3.54600 |
| H | 1.55721 | -1.85311 | -4.22049 |
| H | -4.33938 | 0.55950 | -2.76815 |
| H | 2.08375 | 3.99631 | -5.17966 |
| H | 5.69387 | -0.83646 | -2.55506 |
| H | 2.84301 | 2.15225 | 4.81948 |

| | | | |
|---|---|---|---|
| H | 0.29719 | 6.36004 | 1.82138 |
| H | 4.05237 | 3.10987 | -3.81490 |
| H | -4.61099 | 1.47552 | -0.37959 |
| H | 6.80941 | -0.21284 | -0.35426 |
| H | 1.34479 | -5.53758 | -1.30383 |
| H | 0.28932 | -4.08396 | -4.23733 |
| H | -4.30851 | 0.66636 | 3.10262 |
| H | -0.13387 | -0.21352 | 0.43841 |
| O | 3.86316 | 2.19687 | 0.31230 |
| H | 4.34079 | 1.86558 | 1.12855 |
| H | 3.34068 | 3.00697 | 0.59316 |

NIe,2H

| | | | |
|---|---|---|---|
| Cu | 1.97341 | -1.19599 | 1.03928 |
| Cu | 0.15565 | 1.56535 | -0.88866 |
| Cu | -1.80180 | -1.62306 | -0.28118 |
| O | -0.85759 | 0.16782 | -0.09587 |
| O | 1.64073 | 0.54843 | -0.06764 |
| C | -2.19973 | 0.18961 | 3.21121 |
| N | -3.52079 | 0.07478 | 2.78868 |
| C | -1.50455 | -0.75141 | 2.49244 |
| C | -3.57527 | -0.88875 | 1.82082 |
| N | -2.35870 | -1.40390 | 1.60366 |
| H | -0.44777 | -0.96868 | 2.50814 |
| H | -4.46708 | -1.16140 | 1.27092 |
| C | 0.65943 | -4.13704 | 1.42190 |
| N | 1.33247 | -3.10665 | 0.76460 |
| C | 0.60733 | -5.26351 | 0.65624 |
| C | 1.68011 | -3.63613 | -0.40656 |
| N | 1.26491 | -4.92733 | -0.50434 |
| H | 0.17495 | -6.23210 | 0.84050 |
| H | 2.18945 | -3.13644 | -1.20600 |
| C | 2.99130 | -0.00148 | 4.99301 |
| N | 2.75542 | 1.21714 | 4.36714 |
| C | 2.72662 | -0.96460 | 4.04906 |
| C | 2.36010 | 0.94688 | 3.08048 |
| N | 2.33284 | -0.36604 | 2.85878 |
| H | 2.78414 | -2.03782 | 4.14457 |
| H | 2.11022 | 1.69775 | 2.35136 |
| C | -0.02192 | 4.33036 | 2.51114 |
| N | 0.27785 | 5.34176 | 1.60598 |
| C | 0.01046 | 3.16110 | 1.79446 |
| C | 0.47994 | 4.74341 | 0.38495 |
| N | 0.33121 | 3.42788 | 0.47463 |
| H | -0.20239 | 2.15516 | 2.11995 |
| H | 0.71457 | 5.29098 | -0.51707 |

| | | | |
|---|---|---|---|
| C | 0.81653 | -2.13050 | -3.47973 |
| N | 0.12899 | -3.34074 | -3.54040 |
| C | 0.30729 | -1.47536 | -2.38243 |
| C | -0.76791 | -3.36267 | -2.50194 |
| N | -0.67812 | -2.25197 | -1.77763 |
| H | 0.59286 | -0.52883 | -1.96035 |
| H | -1.44243 | -4.18244 | -2.30613 |
| C | -3.58073 | 1.13864 | -2.28923 |
| N | -3.78275 | 1.65852 | -1.01999 |
| C | -2.30388 | 1.48452 | -2.65379 |
| C | -2.63001 | 2.28086 | -0.65777 |
| N | -1.70729 | 2.19655 | -1.62153 |
| H | -1.77048 | 1.25265 | -3.56307 |
| H | -2.47693 | 2.73048 | 0.31022 |
| C | 1.96598 | 3.44315 | -4.26481 |
| N | 3.06458 | 2.98103 | -3.55110 |
| C | 0.86734 | 3.04312 | -3.54368 |
| C | 2.61079 | 2.32607 | -2.44477 |
| N | 1.28101 | 2.34541 | -2.41678 |
| H | -0.17804 | 3.21000 | -3.74696 |
| H | 3.25717 | 1.92548 | -1.68006 |
| C | 5.21705 | -0.91724 | -1.60141 |
| N | 5.86732 | -0.62205 | -0.41516 |
| C | 3.96459 | -1.33574 | -1.24391 |
| C | 4.99383 | -0.88536 | 0.60903 |
| N | 3.83110 | -1.31592 | 0.13523 |
| H | 3.14926 | -1.59952 | -1.89434 |
| H | 5.23941 | -0.76229 | 1.65443 |
| C | -6.71919 | 1.10126 | 1.04428 |
| O | -5.48352 | 1.41157 | 0.95963 |
| O | -7.32366 | 0.11152 | 0.50126 |
| O | -3.60456 | -2.20585 | -1.29390 |
| O | -5.79398 | -1.79801 | -0.11558 |
| H | -3.61507 | -1.79730 | -2.18121 |
| H | -6.16040 | -2.59115 | 0.36620 |
| H | -6.43464 | -0.96343 | 0.05099 |
| H | -4.51758 | -2.00905 | -0.87133 |
| H | 2.45413 | 1.07765 | 0.05790 |
| H | -7.33413 | 1.76413 | 1.67374 |
| H | -1.88347 | 0.98393 | 3.87055 |
| H | 0.22510 | -4.11418 | 2.38281 |
| H | 3.31316 | -0.06539 | 6.01626 |
| H | -0.22227 | 4.51092 | 3.54600 |
| H | 1.55721 | -1.85311 | -4.22049 |
| H | -4.33938 | 0.55950 | -2.76815 |
| H | 2.08375 | 3.99631 | -5.17966 |

| | | | |
|---|---|---|---|
| H | 5.69387 | -0.83646 | -2.55506 |
| H | 2.84301 | 2.15225 | 4.81948 |
| H | 0.29719 | 6.36004 | 1.82138 |
| H | 4.05237 | 3.10987 | -3.81490 |
| H | -4.61099 | 1.47552 | -0.37959 |
| H | 6.80941 | -0.21284 | -0.35426 |
| H | 1.34479 | -5.53758 | -1.30383 |
| H | 0.28932 | -4.08396 | -4.23733 |
| H | -4.30851 | 0.66636 | 3.10262 |
| H | -0.13387 | -0.21352 | 0.43841 |
| O | 3.86316 | 2.19687 | 0.31230 |
| H | 4.34079 | 1.86558 | 1.12855 |
| H | 3.34068 | 3.00697 | 0.59316 |

NI2e,2H (MV)

| | | | |
|---|---|---|---|
| Cu | -2.29349 | 1.54947 | 1.24890 |
| Cu | -0.01248 | -1.75677 | -0.90629 |
| Cu | 1.69553 | 1.54559 | -0.35845 |
| O | 0.55412 | -0.04138 | -0.14597 |
| O | -1.92484 | -1.32347 | 0.09018 |
| C | 2.13688 | 0.01451 | 3.22906 |
| N | 3.45954 | 0.15893 | 2.82964 |
| C | 1.41749 | 0.88541 | 2.45497 |
| C | 3.49909 | 1.06624 | 1.81593 |
| N | 2.26605 | 1.51745 | 1.55205 |
| H | 0.35791 | 1.08826 | 2.46891 |
| H | 4.38991 | 1.34779 | 1.26595 |
| C | -0.83665 | 4.26759 | 1.27607 |
| N | -1.71342 | 3.32783 | 0.74859 |
| C | -0.64321 | 5.29167 | 0.40184 |
| C | -2.05995 | 3.80050 | -0.44899 |
| N | -1.42634 | 4.97297 | -0.68347 |
| H | -0.04464 | 6.18451 | 0.46507 |
| H | -2.74341 | 3.34194 | -1.14140 |
| C | -3.06263 | 0.10823 | 4.90255 |
| N | -2.76667 | -1.11179 | 4.31504 |
| C | -2.76730 | 1.06508 | 3.97178 |
| C | -2.31096 | -0.86364 | 3.05345 |
| N | -2.29951 | 0.45048 | 2.81315 |
| H | -2.84096 | 2.13792 | 4.06080 |
| H | -2.02103 | -1.62720 | 2.35796 |
| C | 0.17206 | -4.19909 | 2.58690 |
| N | -0.07185 | -5.24278 | 1.70248 |
| C | 0.22783 | -3.06399 | 1.82021 |
| C | -0.14472 | -4.70038 | 0.44212 |
| N | 0.01909 | -3.38605 | 0.49277 |

| | | | |
|---|---|---|---|
| H | 0.42518 | -2.04860 | 2.12314 |
| H | -0.30419 | -5.28299 | -0.45466 |
| C | -0.78291 | 2.08136 | -3.59659 |
| N | -0.13595 | 3.31009 | -3.64827 |
| C | -0.29902 | 1.44293 | -2.48754 |
| C | 0.72155 | 3.36756 | -2.58119 |
| N | 0.63444 | 2.25289 | -1.86153 |
| H | -0.52604 | 0.46720 | -2.09584 |
| H | 1.37369 | 4.20177 | -2.36904 |
| C | 3.70490 | -1.01930 | -2.19659 |
| N | 3.89683 | -1.50338 | -0.91519 |
| C | 2.46530 | -1.45076 | -2.59589 |
| C | 2.77988 | -2.20124 | -0.57987 |
| N | 1.88496 | -2.18474 | -1.57265 |
| H | 1.95399 | -1.27839 | -3.53065 |
| H | 2.63717 | -2.67007 | 0.38097 |
| C | -1.72409 | -3.53547 | -4.27250 |
| N | -2.84917 | -3.05926 | -3.61729 |
| C | -0.64931 | -3.06929 | -3.56293 |
| C | -2.42822 | -2.32322 | -2.55070 |
| N | -1.10026 | -2.31773 | -2.49103 |
| H | 0.40269 | -3.22952 | -3.73593 |
| H | -3.08142 | -1.81708 | -1.86217 |
| C | -5.13070 | 0.69836 | -1.79897 |
| N | -5.80023 | 0.39087 | -0.62330 |
| C | -3.86216 | 1.06074 | -1.41640 |
| C | -4.94195 | 0.58225 | 0.41755 |
| N | -3.75540 | 0.99404 | -0.03051 |
| H | -3.02350 | 1.34124 | -2.03132 |
| H | -5.19928 | 0.40916 | 1.45340 |
| C | 6.71885 | -0.81354 | 1.21769 |
| O | 5.49314 | -1.16785 | 1.15198 |
| O | 7.28000 | 0.16903 | 0.61422 |
| O | 3.44369 | 2.20710 | -1.22776 |
| O | 5.65496 | 1.93570 | -0.10982 |
| H | 3.48150 | 1.92365 | -2.16265 |
| H | 6.01378 | 2.78916 | 0.25426 |
| H | 6.35313 | 1.13955 | 0.10122 |
| H | 4.38733 | 2.05394 | -0.82092 |
| H | -2.52353 | -2.06533 | 0.41513 |
| H | 7.36172 | -1.41867 | 1.87752 |
| H | 1.83255 | -0.75340 | 3.91039 |
| H | -0.39262 | 4.23364 | 2.22935 |
| H | -3.44952 | 0.18718 | 5.89152 |
| H | 0.29090 | -4.33875 | 3.63996 |
| H | -1.47729 | 1.75639 | -4.34180 |

| | | | |
|---|---|---|---|
| H | 4.45047 | -0.42832 | -2.67183 |
| H | -1.79624 | -4.13035 | -5.15324 |
| H | -5.62336 | 0.65365 | -2.75646 |
| H | -2.87895 | -2.04561 | 4.76864 |
| H | -0.12467 | -6.24876 | 1.95393 |
| H | -3.82720 | -3.27062 | -3.86476 |
| H | 4.68634 | -1.27064 | -0.25273 |
| H | -6.77754 | 0.05377 | -0.56888 |
| H | -1.45733 | 5.52226 | -1.52296 |
| H | -0.27940 | 4.02522 | -4.38697 |
| H | 4.26620 | -0.37959 | 3.19695 |
| O | -3.31462 | -3.30045 | 0.97030 |
| H | -3.95628 | -3.73388 | 0.33067 |
| H | -2.66932 | -4.01429 | 1.25093 |
| H | 0.00756 | 0.07566 | 0.65597 |
| H | -2.33811 | -0.46535 | 0.30075 |

NI2e,2H (L)

| | | | |
|---|---|---|---|
| Cu | 2.00403 | -1.26687 | 1.06130 |
| Cu | 0.18734 | 1.77889 | -0.88286 |
| Cu | -1.84766 | -1.82580 | -0.31208 |
| O | -0.90100 | 0.20495 | -0.06585 |
| O | 1.49301 | 0.57330 | -0.06482 |
| C | -2.18795 | 0.13301 | 3.18219 |
| N | -3.50929 | 0.02752 | 2.76112 |
| C | -1.49907 | -0.81371 | 2.45887 |
| C | -3.57890 | -0.93154 | 1.79046 |
| N | -2.36440 | -1.45460 | 1.56138 |
| H | -0.44919 | -1.06435 | 2.49683 |
| H | -4.47936 | -1.20082 | 1.24399 |
| C | 0.63452 | -4.17876 | 1.31575 |
| N | 1.39376 | -3.17137 | 0.71893 |
| C | 0.53654 | -5.26717 | 0.50196 |
| C | 1.75617 | -3.67953 | -0.45932 |
| N | 1.25478 | -4.93159 | -0.62214 |
| H | 0.04394 | -6.21541 | 0.63574 |
| H | 2.34968 | -3.18971 | -1.20772 |
| C | 2.96047 | -0.15707 | 5.00553 |
| N | 2.76484 | 1.08120 | 4.40549 |
| C | 2.65864 | -1.08783 | 4.04037 |
| C | 2.36852 | 0.86215 | 3.11479 |
| N | 2.28997 | -0.44400 | 2.86221 |
| H | 2.67861 | -2.16445 | 4.10985 |
| H | 2.21233 | 1.64545 | 2.39445 |
| C | 0.00276 | 4.26567 | 2.60390 |
| N | 0.29770 | 5.28952 | 1.71456 |

| | | | |
|---|---|---|---|
| C | -0.01367 | 3.11078 | 1.86904 |
| C | 0.44302 | 4.71819 | 0.47505 |
| N | 0.26389 | 3.40214 | 0.54549 |
| H | -0.21037 | 2.10451 | 2.20190 |
| H | 0.66110 | 5.27695 | -0.42443 |
| C | 0.83386 | -2.05906 | -3.52952 |
| N | 0.15028 | -3.26932 | -3.61177 |
| C | 0.32080 | -1.43024 | -2.41478 |
| C | -0.73959 | -3.32445 | -2.57248 |
| N | -0.65655 | -2.22955 | -1.81747 |
| H | 0.61827 | -0.48863 | -1.98796 |
| H | -1.40764 | -4.15489 | -2.39761 |
| C | -3.52635 | 1.21577 | -2.28631 |
| N | -3.74685 | 1.73746 | -1.02267 |
| C | -2.24552 | 1.56917 | -2.63697 |
| C | -2.61724 | 2.39583 | -0.65541 |
| N | -1.67485 | 2.30144 | -1.60488 |
| H | -1.69905 | 1.33882 | -3.53877 |
| H | -2.49858 | 2.89838 | 0.29361 |
| C | 2.05001 | 3.50621 | -4.19389 |
| N | 3.13366 | 3.01957 | -3.47606 |
| C | 0.93439 | 3.09742 | -3.51277 |
| C | 2.65828 | 2.33982 | -2.39716 |
| N | 1.32663 | 2.36895 | -2.39987 |
| H | -0.10459 | 3.27838 | -3.73618 |
| H | 3.27451 | 1.93105 | -1.61208 |
| C | 5.21839 | -0.87177 | -1.60928 |
| N | 5.86436 | -0.61687 | -0.41132 |
| C | 3.93404 | -1.20775 | -1.27304 |
| C | 4.96587 | -0.83154 | 0.60053 |
| N | 3.78555 | -1.18573 | 0.10382 |
| H | 3.11149 | -1.43248 | -1.93002 |
| H | 5.20301 | -0.73421 | 1.65085 |
| C | -6.67215 | 1.14131 | 1.02991 |
| O | -5.42767 | 1.43908 | 0.96963 |
| O | -7.26959 | 0.17050 | 0.44751 |
| O | -3.62809 | -2.21968 | -1.32819 |
| O | -5.75635 | -1.75909 | -0.09082 |
| H | -3.64616 | -1.85035 | -2.23335 |
| H | -6.21168 | -2.56771 | 0.26849 |
| H | -6.40034 | -0.90870 | 0.02898 |
| H | -4.54131 | -2.01092 | -0.89715 |
| H | 2.30413 | 1.07607 | 0.17684 |
| H | -7.30102 | 1.78888 | 1.66787 |
| H | -1.87048 | 0.90309 | 3.87450 |
| H | 0.19684 | -4.17862 | 2.27680 |

| | | | |
|---|---|---|---|
| H | 3.30370 | -0.24801 | 6.02226 |
| H | -0.17340 | 4.42031 | 3.64305 |
| H | 1.58755 | -1.77419 | -4.26346 |
| H | -4.29338 | 0.66099 | -2.78545 |
| H | 2.17610 | 4.09096 | -5.07994 |
| H | 5.72453 | -0.83816 | -2.55219 |
| H | 2.86173 | 2.00200 | 4.87624 |
| H | 0.37357 | 6.30478 | 1.96585 |
| H | 4.12839 | 3.15296 | -3.72625 |
| H | -4.56937 | 1.52241 | -0.37720 |
| H | 6.83378 | -0.27809 | -0.33121 |
| H | 1.32319 | -5.52479 | -1.43671 |
| H | 0.29821 | -3.99144 | -4.34028 |
| H | -4.29416 | 0.62771 | 3.08626 |
| H | -0.05291 | -0.12228 | 0.34581 |
| O | 3.63548 | 2.10071 | 0.46625 |
| H | 4.51362 | 1.78565 | 0.83004 |
| H | 3.55858 | 3.08212 | 0.65881 |
| H | -1.45716 | 0.50509 | 0.68285 |

NI2e,3H

| | | | |
|---|---|---|---|
| Cu | 2.16102 | -1.80167 | 1.35203 |
| Cu | 0.37405 | 1.99759 | -0.76634 |
| Cu | -2.00762 | -1.79367 | -0.40557 |
| O | 0.21822 | 0.11250 | 0.11423 |
| O | 2.19112 | 1.92362 | 0.19160 |
| C | -2.20282 | 0.20064 | 3.13658 |
| N | -3.52607 | 0.17176 | 2.71025 |
| C | -1.52670 | -0.64688 | 2.29871 |
| C | -3.61463 | -0.64295 | 1.62719 |
| N | -2.40488 | -1.14791 | 1.33663 |
| H | -0.48518 | -0.92088 | 2.31026 |
| H | -4.52637 | -0.86863 | 1.07921 |
| C | 0.42988 | -4.34065 | 1.29616 |
| N | 1.43491 | -3.50629 | 0.81923 |
| C | 0.14500 | -5.31560 | 0.39141 |
| C | 1.75742 | -3.99067 | -0.38229 |
| N | 0.99425 | -5.07041 | -0.66248 |
| H | -0.55207 | -6.13636 | 0.41863 |
| H | 2.52330 | -3.60974 | -1.03719 |
| C | 2.91529 | -0.41755 | 5.01601 |
| N | 2.75585 | 0.82524 | 4.42203 |
| C | 2.57192 | -1.34458 | 4.07320 |
| C | 2.33568 | 0.61968 | 3.13784 |
| N | 2.21075 | -0.68964 | 2.90026 |
| H | 2.54554 | -2.41983 | 4.16210 |

| | | | |
|---|---|---|---|
| H | 2.13419 | 1.40501 | 2.42598 |
| C | 0.04216 | 4.18554 | 2.66250 |
| N | 0.36629 | 5.21640 | 1.79216 |
| C | -0.17636 | 3.08675 | 1.88100 |
| C | 0.32481 | 4.72504 | 0.52260 |
| N | 0.00216 | 3.43637 | 0.55398 |
| H | -0.45183 | 2.08533 | 2.16782 |
| H | 0.51245 | 5.31190 | -0.36542 |
| C | 0.63127 | -2.09670 | -3.58146 |
| N | -0.08076 | -3.28677 | -3.64167 |
| C | 0.11313 | -1.41233 | -2.51259 |
| C | -0.99173 | -3.28963 | -2.62596 |
| N | -0.89246 | -2.16615 | -1.91094 |
| H | 0.38441 | -0.43762 | -2.15506 |
| H | -1.69253 | -4.09165 | -2.44279 |
| C | -3.48672 | 1.17964 | -2.18320 |
| N | -3.67342 | 1.67419 | -0.90728 |
| C | -2.13755 | 1.28803 | -2.44806 |
| C | -2.47658 | 2.06858 | -0.42952 |
| N | -1.51327 | 1.85237 | -1.33794 |
| H | -1.58368 | 1.00819 | -3.33006 |
| H | -2.34041 | 2.49027 | 0.55185 |
| C | 2.10394 | 3.34861 | -4.18384 |
| N | 3.17348 | 2.74945 | -3.53220 |
| C | 0.97575 | 2.89157 | -3.55518 |
| C | 2.67716 | 1.93791 | -2.56804 |
| N | 1.34630 | 2.01865 | -2.53846 |
| H | -0.05918 | 3.12437 | -3.75400 |
| H | 3.29989 | 1.32617 | -1.93953 |
| C | 5.07786 | -1.09017 | -1.64067 |
| N | 5.73495 | -0.83601 | -0.44741 |
| C | 3.76456 | -1.30661 | -1.29834 |
| C | 4.82601 | -0.91102 | 0.56473 |
| N | 3.61576 | -1.20322 | 0.08221 |
| H | 2.92800 | -1.53223 | -1.94013 |
| H | 5.07144 | -0.76314 | 1.60762 |
| C | -6.66614 | 1.43859 | 1.04170 |
| O | -5.43063 | 1.76776 | 0.96549 |
| O | -7.26997 | 0.51489 | 0.39366 |
| O | -3.80721 | -2.25385 | -1.32596 |
| O | -5.85828 | -1.46555 | -0.15565 |
| H | -3.82363 | -2.06763 | -2.28609 |
| H | -6.33647 | -2.20904 | 0.30338 |
| H | -6.45439 | -0.57208 | -0.05934 |
| H | -4.69930 | -1.90602 | -0.92746 |
| H | 2.78801 | 2.72994 | -0.02362 |

| | | | |
|---|---|---|---|
| H | -7.26919 | 2.01495 | 1.75957 |
| H | -1.86906 | 0.86301 | 3.91820 |
| H | -0.03493 | -4.28122 | 2.23840 |
| H | 3.26100 | -0.54125 | 6.01606 |
| H | -0.02105 | 4.30581 | 3.72206 |
| H | 1.41973 | -1.85060 | -4.27791 |
| H | -4.34113 | 0.81791 | -2.72856 |
| H | 2.25816 | 3.99340 | -5.01999 |
| H | 5.60283 | -1.11723 | -2.58162 |
| H | 2.91441 | 1.74197 | 4.90322 |
| H | 0.59620 | 6.18836 | 2.06713 |
| H | 4.17622 | 2.95430 | -3.69122 |
| H | -4.56406 | 1.65706 | -0.30695 |
| H | 6.75072 | -0.63979 | -0.36088 |
| H | 1.00912 | -5.62478 | -1.49984 |
| H | 0.03422 | -4.00823 | -4.37571 |
| H | -4.30720 | 0.70459 | 3.14222 |
| H | -0.55219 | -0.50218 | -0.03973 |
| H | 2.71461 | 1.09903 | 0.08139 |
| O | 3.52256 | 3.98069 | -0.37645 |
| H | 3.44612 | 4.39596 | -1.27833 |
| H | 3.61917 | 4.70772 | 0.29977 |
| H | 0.86918 | -0.38837 | 0.65644 |

NI3e,2H

| | | | |
|---|---|---|---|
| Cu | 1.73702 | -1.28688 | 1.08634 |
| Cu | 0.26600 | 1.65500 | -1.14318 |
| Cu | -2.10150 | -1.61852 | -0.01994 |
| O | 0.54516 | 0.04315 | 0.05819 |
| O | 4.12057 | 2.27547 | -0.10072 |
| C | -1.99971 | 0.92483 | 3.10510 |
| N | -3.36425 | 0.85138 | 2.84748 |
| C | -1.40761 | -0.01381 | 2.30528 |
| C | -3.56377 | -0.10507 | 1.90019 |
| N | -2.39103 | -0.64931 | 1.55283 |
| H | -0.36468 | -0.24119 | 2.15812 |
| H | -4.52465 | -0.38933 | 1.48317 |
| C | 0.24826 | -4.00758 | 1.93519 |
| N | 1.08482 | -3.21527 | 1.15427 |
| C | -0.05480 | -5.17886 | 1.30600 |
| C | 1.28546 | -3.92850 | 0.04715 |
| N | 0.61361 | -5.11481 | 0.10601 |
| H | -0.65648 | -6.01893 | 1.60911 |
| H | 1.88905 | -3.63438 | -0.79339 |
| C | 3.24301 | 0.31867 | 4.68295 |

| | | | |
|---|---|---|---|
| N | 3.11279 | 1.45384 | 3.88492 |
| C | 2.75362 | -0.72383 | 3.93815 |
| C | 2.53980 | 1.05188 | 2.69985 |
| N | 2.30994 | -0.25716 | 2.70448 |
| H | 2.67979 | -1.76686 | 4.20330 |
| H | 2.34748 | 1.72877 | 1.88365 |
| C | 0.47576 | 4.55905 | 1.79734 |
| N | 0.80709 | 5.38932 | 0.73396 |
| C | 0.35926 | 3.29877 | 1.27461 |
| C | 0.88987 | 4.59040 | -0.38680 |
| N | 0.63137 | 3.31941 | -0.08441 |
| H | 0.09972 | 2.37794 | 1.76686 |
| H | 1.14338 | 4.95972 | -1.36974 |
| C | 0.14388 | -2.71378 | -3.24449 |
| N | -0.64311 | -3.84637 | -3.05492 |
| C | -0.22753 | -1.82774 | -2.26647 |
| C | -1.45796 | -3.61257 | -1.98333 |
| N | -1.21871 | -2.40209 | -1.47966 |
| H | 0.15730 | -0.84527 | -2.03987 |
| H | -2.18706 | -4.31506 | -1.60806 |
| C | -3.73789 | 1.01913 | -2.14933 |
| N | -3.80215 | 1.75299 | -0.98158 |
| C | -2.41428 | 1.02314 | -2.53377 |
| C | -2.54271 | 2.17649 | -0.69844 |
| N | -1.67473 | 1.75142 | -1.61452 |
| H | -1.94680 | 0.55674 | -3.38678 |
| H | -2.29277 | 2.75705 | 0.17622 |
| C | 1.77589 | 2.47837 | -4.91191 |
| N | 2.88270 | 1.98878 | -4.23556 |
| C | 0.71208 | 2.25772 | -4.06982 |
| C | 2.46823 | 1.49959 | -3.03032 |
| N | 1.15685 | 1.65639 | -2.89503 |
| H | -0.33006 | 2.49607 | -4.21217 |
| H | 3.13776 | 1.08199 | -2.29459 |
| C | 4.77623 | -1.63300 | -1.87844 |
| N | 5.54309 | -1.22251 | -0.79974 |
| C | 3.48477 | -1.68557 | -1.41369 |
| C | 4.70111 | -1.04536 | 0.27191 |
| N | 3.44415 | -1.32592 | -0.07300 |
| H | 2.58672 | -1.93386 | -1.95427 |
| H | 5.02921 | -0.62322 | 1.20749 |
| C | -6.59677 | 1.93327 | 1.26791 |
| O | -5.35810 | 2.14012 | 1.05802 |
| O | -7.31721 | 0.95869 | 0.85491 |
| O | -4.07885 | -2.19487 | -0.77154 |
| O | -6.01558 | -1.15838 | 0.48618 |

| | | | |
|---|---|---|---|
| H | -4.07076 | -1.89935 | -1.70324 |
| H | -6.43076 | -1.77717 | 1.16200 |
| H | -6.56819 | -0.24442 | 0.50282 |
| H | -4.89214 | -1.74648 | -0.33786 |
| H | 4.63524 | 1.90317 | 0.66123 |
| H | -7.10060 | 2.70106 | 1.86574 |
| H | -1.58285 | 1.65764 | 3.76497 |
| H | -0.10734 | -3.79563 | 2.90660 |
| H | 3.65283 | 0.36929 | 5.67192 |
| H | 0.37542 | 4.90472 | 2.80316 |
| H | 0.86777 | -2.64184 | -4.03658 |
| H | -4.62505 | 0.56927 | -2.54722 |
| H | 1.86924 | 2.92386 | -5.88972 |
| H | 5.20942 | -1.85077 | -2.83579 |
| H | 3.29778 | 2.43378 | 4.19455 |
| H | 0.92081 | 6.42791 | 0.79141 |
| H | 3.85263 | 2.03260 | -4.54940 |
| H | -4.60362 | 1.83697 | -0.30844 |
| H | 6.56344 | -1.04710 | -0.83637 |
| H | 0.55208 | -5.83553 | -0.59706 |
| H | -0.60523 | -4.70368 | -3.63218 |
| H | -4.08378 | 1.49723 | 3.22531 |
| H | -0.31762 | -0.40919 | -0.00893 |
| H | 3.28247 | 1.77393 | -0.12131 |
| O | 5.57853 | 1.30101 | 1.95302 |
| H | 6.49600 | 1.70967 | 1.97420 |
| H | 5.13230 | 1.51593 | 2.82560 |

NI3e,3H (FR)

| | | | |
|---|---|---|---|
| Cu | 2.15531 | 1.67087 | -1.30187 |
| Cu | 0.08391 | -1.93322 | 1.15020 |
| Cu | -2.16065 | 1.65571 | 0.17322 |
| O | 1.61669 | -0.90434 | 0.11376 |
| O | 4.00033 | -2.21904 | 0.15055 |
| C | -2.07086 | -0.67378 | -3.13443 |
| N | -3.43490 | -0.55878 | -2.89021 |
| C | -1.45770 | 0.19482 | -2.26519 |
| C | -3.61123 | 0.35048 | -1.89156 |
| N | -2.42582 | 0.82523 | -1.48877 |
| H | -0.40860 | 0.41043 | -2.13900 |
| H | -4.56712 | 0.65008 | -1.47552 |
| C | 0.38702 | 4.15470 | -1.65289 |
| N | 1.37925 | 3.41408 | -1.02987 |
| C | 0.00659 | 5.20504 | -0.87703 |
| C | 1.60729 | 4.02832 | 0.13040 |
| N | 0.79340 | 5.10184 | 0.24732 |

| | | | |
|---|---|---|---|
| H | -0.72097 | 5.98433 | -1.02821 |
| H | 2.33469 | 3.74306 | 0.87048 |
| C | 3.19647 | -0.15485 | -4.67545 |
| N | 2.98695 | -1.32586 | -3.95834 |
| C | 2.77085 | 0.87215 | -3.88739 |
| C | 2.43231 | -0.96611 | -2.75500 |
| N | 2.29750 | 0.35950 | -2.68572 |
| H | 2.75431 | 1.92816 | -4.10855 |
| H | 2.15153 | -1.65677 | -1.98179 |
| C | 0.23632 | -4.48238 | -2.09462 |
| N | 0.49933 | -5.41333 | -1.10098 |
| C | 0.13013 | -3.27585 | -1.45078 |
| C | 0.54195 | -4.74883 | 0.09530 |
| N | 0.32575 | -3.45121 | -0.08690 |
| H | -0.09620 | -2.30644 | -1.85987 |
| H | 0.72012 | -5.23187 | 1.04541 |
| C | 0.18788 | 2.43331 | 3.42798 |
| N | -0.54941 | 3.60641 | 3.31636 |
| C | -0.19501 | 1.64620 | 2.36812 |
| C | -1.35373 | 3.49110 | 2.21595 |
| N | -1.15597 | 2.31622 | 1.61692 |
| H | 0.12816 | 0.64889 | 2.10967 |
| H | -2.05272 | 4.24887 | 1.89407 |
| C | -3.83982 | -0.97595 | 2.02957 |
| N | -3.91916 | -1.62343 | 0.81694 |
| C | -2.50276 | -0.92925 | 2.35283 |
| C | -2.66076 | -1.93881 | 0.43116 |
| N | -1.77460 | -1.53307 | 1.33829 |
| H | -2.01815 | -0.50920 | 3.21947 |
| H | -2.42857 | -2.43384 | -0.49776 |
| C | 1.57690 | -2.90558 | 4.77824 |
| N | 2.70102 | -2.41551 | 4.13477 |
| C | 0.51371 | -2.54221 | 3.99336 |
| C | 2.29749 | -1.78256 | 2.99928 |
| N | 0.97665 | -1.85392 | 2.88193 |
| H | -0.53834 | -2.73068 | 4.14035 |
| H | 2.97207 | -1.32412 | 2.29621 |
| C | 4.77172 | 1.34379 | 2.01519 |
| N | 5.53165 | 0.95320 | 0.92440 |
| C | 3.51942 | 1.60143 | 1.51698 |
| C | 4.73924 | 0.97789 | -0.18206 |
| N | 3.51046 | 1.37508 | 0.14359 |
| H | 2.62757 | 1.89499 | 2.04514 |
| H | 5.05978 | 0.60038 | -1.14025 |
| C | -6.71057 | -1.63276 | -1.41170 |
| O | -5.48203 | -1.92239 | -1.22138 |

| | | | |
|---|---|---|---|
| O | -7.37092 | -0.64104 | -0.94076 |
| O | -4.04889 | 2.32183 | 0.83513 |
| O | -6.01615 | 1.40574 | -0.43293 |
| H | -4.15712 | 2.17498 | 1.79616 |
| H | -6.41303 | 2.08104 | -1.04752 |
| H | -6.59047 | 0.50137 | -0.51809 |
| H | -4.89108 | 1.93207 | 0.38953 |
| H | 4.56790 | -1.97072 | -0.64052 |
| H | -7.25334 | -2.32325 | -2.06851 |
| H | -1.68593 | -1.36143 | -3.86316 |
| H | -0.00659 | 3.95331 | -2.60432 |
| H | 3.60897 | -0.14405 | -5.64899 |
| H | 0.13839 | -4.74384 | -3.13174 |
| H | 0.87378 | 2.26199 | 4.24071 |
| H | -4.72837 | -0.61552 | 2.49830 |
| H | 1.64587 | -3.45826 | 5.68846 |
| H | 5.18997 | 1.39080 | 3.00411 |
| H | 3.16391 | -2.29479 | -4.32728 |
| H | 0.60995 | -6.42904 | -1.23371 |
| H | 3.67178 | -2.55052 | 4.42502 |
| H | -4.74016 | -1.71713 | 0.17334 |
| H | 6.52601 | 0.68186 | 0.95734 |
| H | 0.70638 | 5.70651 | 1.04116 |
| H | -0.51539 | 4.40375 | 3.98097 |
| H | -4.18260 | -1.14301 | -3.32407 |
| H | 1.79549 | 0.01288 | -0.17230 |
| H | 3.78408 | -3.16904 | 0.05612 |
| O | 5.47004 | -1.42338 | -1.86545 |
| H | 6.43846 | -1.69377 | -1.87032 |
| H | 5.11294 | -1.57801 | -2.78837 |
| H | 2.50935 | -1.34775 | 0.14545 |

NI3e,3H (innerwater)

| | | | |
|---|---|---|---|
| Cu | 2.91908 | -1.43411 | 1.12023 |
| Cu | -0.86106 | 2.43365 | -0.82702 |
| Cu | -1.37912 | -2.01418 | -0.53253 |
| O | -1.10854 | 0.28847 | -0.29946 |
| O | 1.41790 | 0.77673 | -0.05373 |
| C | -1.85903 | -0.71662 | 3.23251 |
| N | -3.14794 | -1.11556 | 2.90364 |
| C | -1.04182 | -1.25517 | 2.26743 |
| C | -3.08349 | -1.86134 | 1.76032 |
| N | -1.81452 | -1.96031 | 1.34077 |
| H | 0.03110 | -1.19427 | 2.17709 |
| H | -3.93867 | -2.27774 | 1.23687 |
| C | 1.79036 | -4.22703 | 0.77776 |

| | | | |
|---|---|---|---|
| N | 2.64180 | -3.19367 | 0.42493 |
| C | 1.62906 | -5.09651 | -0.25479 |
| C | 3.00634 | -3.44337 | -0.83319 |
| N | 2.40796 | -4.57653 | -1.26353 |
| H | 1.04910 | -5.99845 | -0.35168 |
| H | 3.68249 | -2.85414 | -1.42931 |
| C | 3.37068 | -0.11623 | 4.81338 |
| N | 2.86830 | 1.08996 | 4.35893 |
| C | 3.25443 | -1.00912 | 3.79267 |
| C | 2.47586 | 0.90032 | 3.05862 |
| N | 2.69459 | -0.37004 | 2.69385 |
| H | 3.51259 | -2.05677 | 3.78327 |
| H | 2.13591 | 1.70244 | 2.42350 |
| C | -0.76460 | 3.75690 | 3.12308 |
| N | -0.78314 | 4.93118 | 2.38710 |
| C | -0.71002 | 2.74679 | 2.19266 |
| C | -0.75040 | 4.61014 | 1.06275 |
| N | -0.69961 | 3.28729 | 0.91370 |
| H | -0.68379 | 1.68179 | 2.35263 |
| H | -0.78072 | 5.33753 | 0.26365 |
| C | 1.04027 | -1.47130 | -3.79902 |
| N | 0.64679 | -2.79125 | -3.98049 |
| C | 0.50341 | -1.07992 | -2.59780 |
| C | -0.11217 | -3.14985 | -2.89597 |
| N | -0.21048 | -2.13596 | -2.03593 |
| H | 0.58106 | -0.12238 | -2.11329 |
| H | -0.56649 | -4.12113 | -2.77098 |
| C | -4.03456 | 0.74228 | -1.96419 |
| N | -4.22156 | 0.99371 | -0.61532 |
| C | -3.17426 | 1.70519 | -2.42664 |
| C | -3.48373 | 2.09581 | -0.31008 |
| N | -2.80674 | 2.54218 | -1.38017 |
| H | -2.78138 | 1.83902 | -3.42298 |
| H | -3.44891 | 2.53598 | 0.67575 |
| C | 0.92998 | 4.29087 | -3.79799 |
| N | 2.13007 | 3.95555 | -3.19658 |
| C | -0.05304 | 3.61571 | -3.14386 |
| C | 1.82578 | 3.07206 | -2.18475 |
| N | 0.50905 | 2.85989 | -2.12861 |
| H | -1.11380 | 3.62369 | -3.33266 |
| H | 2.55579 | 2.63293 | -1.53012 |
| C | 5.19852 | 0.40555 | -1.96755 |
| N | 5.85638 | 0.71219 | -0.78673 |
| C | 4.09456 | -0.31896 | -1.58928 |
| C | 5.15982 | 0.17313 | 0.24890 |
| N | 4.08315 | -0.45998 | -0.20534 |

| | | | |
|---|---|---|---|
| H | 3.30027 | -0.71601 | -2.19931 |
| H | 5.45484 | 0.26209 | 1.28536 |
| C | -6.61274 | -0.60342 | 1.53260 |
| O | -5.46044 | -0.04950 | 1.47791 |
| O | -7.04050 | -1.58502 | 0.82926 |
| O | -3.10856 | -2.71167 | -1.50218 |
| O | -5.17192 | -2.97739 | -0.10555 |
| H | -3.29622 | -2.32543 | -2.38061 |
| H | -5.37185 | -3.91424 | 0.16323 |
| H | -5.98674 | -2.34356 | 0.19344 |
| H | -4.00642 | -2.79843 | -1.00580 |
| H | 1.76887 | 1.64763 | 0.29103 |
| H | -7.31471 | -0.19506 | 2.27979 |
| H | -1.66278 | -0.06537 | 4.06429 |
| H | 1.33512 | -4.32599 | 1.71657 |
| H | 3.79345 | -0.24421 | 5.76948 |
| H | -0.80408 | 3.74875 | 4.20017 |
| H | 1.63324 | -0.93799 | -4.52224 |
| H | -4.50076 | -0.09222 | -2.43419 |
| H | 0.85122 | 4.96067 | -4.60376 |
| H | 5.58734 | 0.71492 | -2.92477 |
| H | 2.77717 | 1.96147 | 4.94895 |
| H | -0.82115 | 5.88690 | 2.75402 |
| H | 3.06428 | 4.34434 | -3.48749 |
| H | -4.76448 | 0.40306 | 0.07641 |
| H | 6.72124 | 1.25592 | -0.71155 |
| H | 2.42738 | -4.94736 | -2.19388 |
| H | 0.86050 | -3.36710 | -4.81694 |
| H | -4.02196 | -0.79446 | 3.37581 |
| H | -0.14548 | 0.32463 | -0.03430 |
| O | 2.35827 | 2.98359 | 0.91837 |
| H | 3.29276 | 3.33110 | 0.80343 |
| H | 1.72142 | 3.75241 | 0.86245 |
| H | -1.62146 | 0.29502 | 0.53227 |
| H | 2.04296 | 0.09707 | 0.26260 |

NI3e,3H (innerwater partial optimization)

| | | | |
|---|---|---|---|
| Cu | 2.69153 | -1.68529 | 0.98936 |
| Cu | -0.80552 | 2.43527 | -0.96833 |
| Cu | -1.73550 | -1.91607 | -0.38571 |
| O | -0.10908 | 0.53454 | -0.04634 |
| O | 3.47142 | 2.55901 | 0.31526 |
| C | -1.85622 | -0.38001 | 3.31772 |
| N | -3.19550 | -0.66396 | 3.08474 |
| C | -1.15575 | -1.04824 | 2.34200 |
| C | -3.27386 | -1.47170 | 1.98523 |

| | | | |
|---|---|---|---|
| N | -2.04853 | -1.71991 | 1.50248 |
| H | -0.08951 | -1.10052 | 2.18889 |
| H | -4.19587 | -1.82691 | 1.53528 |
| C | 1.27731 | -4.36454 | 0.87409 |
| N | 2.20226 | -3.44221 | 0.41471 |
| C | 0.96940 | -5.26661 | -0.09526 |
| C | 2.46333 | -3.79335 | -0.84491 |
| N | 1.73227 | -4.88163 | -1.17434 |
| H | 0.29951 | -6.10944 | -0.10687 |
| H | 3.15605 | -3.30745 | -1.51107 |
| C | 3.49375 | -0.22660 | 4.56830 |
| N | 3.08447 | 0.99840 | 4.07260 |
| C | 3.22905 | -1.15584 | 3.60963 |
| C | 2.59687 | 0.78099 | 2.80942 |
| N | 2.66817 | -0.52248 | 2.50803 |
| H | 3.38285 | -2.22320 | 3.64727 |
| H | 2.29849 | 1.57842 | 2.14794 |
| C | -0.33991 | 3.94857 | 2.88610 |
| N | -0.28881 | 5.07829 | 2.08480 |
| C | -0.44084 | 2.89044 | 2.01481 |
| C | -0.36833 | 4.68618 | 0.78175 |
| N | -0.45583 | 3.35893 | 0.70780 |
| H | -0.50877 | 1.83814 | 2.23514 |
| H | -0.37631 | 5.36976 | -0.05566 |
| C | 0.52154 | -1.79256 | -3.80750 |
| N | -0.00899 | -3.07392 | -3.88930 |
| C | 0.09961 | -1.28632 | -2.60334 |
| C | -0.73172 | -3.29659 | -2.74523 |
| N | -0.67815 | -2.23401 | -1.94189 |
| H | 0.29958 | -0.31724 | -2.18077 |
| H | -1.27003 | -4.20924 | -2.53860 |
| C | -4.19212 | 1.01435 | -1.82682 |
| N | -4.27113 | 1.35412 | -0.48670 |
| C | -3.27192 | 1.86001 | -2.39184 |
| C | -3.41221 | 2.39090 | -0.28787 |
| N | -2.76148 | 2.70978 | -1.41814 |
| H | -2.92936 | 1.90087 | -3.41455 |
| H | -3.27461 | 2.87671 | 0.66705 |
| C | 0.97340 | 3.94342 | -4.13767 |
| N | 2.16955 | 3.52116 | -3.58513 |
| C | -0.02900 | 3.40610 | -3.39164 |
| C | 1.84288 | 2.72742 | -2.50793 |
| N | 0.51765 | 2.65216 | -2.36660 |
| H | -1.09347 | 3.51086 | -3.52147 |
| H | 2.56515 | 2.25220 | -1.87007 |
| C | 4.94676 | -0.24988 | -2.32244 |

| | | | |
|---|---|---|---|
| N | 5.70216 | 0.05083 | -1.19989 |
| C | 3.80260 | -0.83861 | -1.84178 |
| C | 5.02088 | -0.36000 | -0.09747 |
| N | 3.86195 | -0.90458 | -0.45347 |
| H | 2.93769 | -1.18531 | -2.38253 |
| H | 5.38570 | -0.24677 | 0.91409 |
| C | -6.67107 | 0.12137 | 1.88031 |
| O | -5.47578 | 0.55280 | 1.72948 |
| O | -7.23451 | -0.84791 | 1.26044 |
| O | -3.58057 | -2.48608 | -1.21548 |
| O | -5.57096 | -2.46868 | 0.30657 |
| H | -3.78292 | -2.12978 | -2.10325 |
| H | -5.84445 | -3.36516 | 0.64040 |
| H | -6.30041 | -1.74116 | 0.61267 |
| H | -4.45066 | -2.45570 | -0.66585 |
| H | 3.34119 | 3.52539 | 0.37765 |
| H | -7.28303 | 0.63715 | 2.64009 |
| H | -1.54710 | 0.29113 | 4.09779 |
| H | 0.87269 | -4.36751 | 1.84089 |
| H | 3.95955 | -0.34589 | 5.50534 |
| H | -0.31423 | 4.00126 | 3.96235 |
| H | 1.11843 | -1.36055 | -4.59247 |
| H | -4.76520 | 0.20740 | -2.22059 |
| H | 0.91126 | 4.57432 | -4.97565 |
| H | 5.30476 | -0.03216 | -3.31621 |
| H | 3.11484 | 1.90452 | 4.61473 |
| H | -0.21108 | 6.05100 | 2.39669 |
| H | 3.11769 | 3.79806 | -3.94964 |
| H | -4.82580 | 0.85844 | 0.26747 |
| H | 6.61884 | 0.50793 | -1.20474 |
| H | 1.65870 | -5.30109 | -2.08104 |
| H | 0.09619 | -3.71167 | -4.70116 |
| H | -4.00366 | -0.23204 | 3.58504 |
| H | -0.59845 | -0.32551 | -0.06098 |
| O | 5.46828 | 1.87792 | 1.93330 |
| H | 6.29250 | 2.45223 | 1.96551 |
| H | 5.16446 | 1.75641 | 2.88006 |
| H | 0.83487 | 0.29873 | 0.10413 |
| H | 4.24198 | 2.34694 | 0.91275 |

Proton PES
NI

| | | | |
|---|---|---|---|
| Cu | 1.32805 | 1.03875 | -0.92415 |
| Cu | 0.29449 | -1.01851 | 1.04779 |
| Cu | -2.02171 | 1.25936 | -0.09632 |

| | | | |
|---|---|---|---|
| O | -0.30195 | 0.43804 | -0.13282 |
| O | 2.00382 | -0.51089 | 0.20245 |
| C | -2.12926 | -1.36690 | -3.00506 |
| N | -3.47358 | -1.36136 | -2.65769 |
| C | -1.59262 | -0.23048 | -2.48573 |
| C | -3.71150 | -0.24882 | -1.92186 |
| N | -2.57715 | 0.45453 | -1.79196 |
| H | -0.57410 | 0.10519 | -2.50343 |
| H | -4.66562 | 0.01905 | -1.48420 |
| C | -0.18021 | 3.71324 | -2.41333 |
| N | 0.58854 | 3.02924 | -1.46563 |
| C | -0.46039 | 4.97664 | -1.98469 |
| C | 0.76476 | 3.90549 | -0.47543 |
| N | 0.14472 | 5.08234 | -0.75445 |
| H | -1.00623 | 5.77897 | -2.45210 |
| H | 1.29595 | 3.73193 | 0.44131 |
| C | 3.02350 | -0.70770 | -4.69873 |
| N | 2.94410 | -1.74842 | -3.78021 |
| C | 2.51459 | 0.39469 | -4.04713 |
| C | 2.41832 | -1.25090 | -2.62644 |
| N | 2.13620 | 0.04523 | -2.75408 |
| H | 2.39801 | 1.40187 | -4.41678 |
| H | 2.26753 | -1.83625 | -1.73764 |
| C | 0.58145 | -4.69381 | -1.18826 |
| N | 0.97454 | -5.34079 | -0.02489 |
| C | 0.32186 | -3.39603 | -0.84314 |
| C | 0.94290 | -4.39809 | 0.98111 |
| N | 0.55330 | -3.21464 | 0.50864 |
| H | -0.02068 | -2.58903 | -1.47068 |
| H | 1.19820 | -4.61120 | 2.00930 |
| C | -0.07771 | 3.16459 | 2.91994 |
| N | -0.91938 | 4.20388 | 2.56236 |
| C | -0.43595 | 2.09582 | 2.16199 |
| C | -1.76249 | 3.73637 | 1.59590 |
| N | -1.47187 | 2.46449 | 1.33379 |
| H | -0.01915 | 1.11023 | 2.14211 |
| H | -2.53616 | 4.31931 | 1.11739 |
| C | -3.68342 | -0.83008 | 2.33947 |
| N | -3.71368 | -1.69052 | 1.26076 |
| C | -2.35040 | -0.60724 | 2.61396 |
| C | -2.43614 | -1.95966 | 0.90134 |
| N | -1.57778 | -1.31400 | 1.69775 |
| H | -1.90256 | -0.00031 | 3.38452 |
| H | -2.16758 | -2.59208 | 0.06983 |
| C | 1.94782 | -1.68037 | 5.12390 |
| N | 3.02682 | -1.29514 | 4.34046 |

| | | | |
|---|---|---|---|
| C | 0.86278 | -1.64552 | 4.26942 |
| C | 2.58827 | -1.06710 | 3.07810 |
| N | 1.27472 | -1.25415 | 2.99558 |
| H | -0.16983 | -1.88172 | 4.47395 |
| H | 3.27111 | -0.83540 | 2.27664 |
| C | 4.62706 | 2.26951 | 1.46918 |
| N | 5.38167 | 1.78270 | 0.41497 |
| C | 3.33409 | 2.31003 | 1.02424 |
| C | 4.52211 | 1.55139 | -0.63072 |
| N | 3.27340 | 1.86740 | -0.29080 |
| H | 2.45705 | 2.61633 | 1.57041 |
| H | 4.82896 | 1.15748 | -1.58864 |
| C | -6.53480 | -2.46926 | -0.77125 |
| O | -5.29835 | -2.65756 | -0.51586 |
| O | -7.23094 | -1.41870 | -0.53355 |
| O | -3.90580 | 1.82062 | 0.36062 |
| O | -6.02573 | 0.75809 | -0.35011 |
| H | -3.93635 | 1.96375 | 1.32877 |
| H | -6.54114 | 1.35662 | -0.95653 |
| H | -6.52804 | -0.20722 | -0.30636 |
| H | -4.80561 | 1.33070 | 0.10340 |
| H | 2.52602 | -0.00361 | 0.85184 |
| H | -7.04900 | -3.31034 | -1.25989 |
| H | -1.65591 | -2.19862 | -3.45660 |
| H | -0.51181 | 3.39909 | -3.36988 |
| H | 3.43942 | -0.86282 | -5.68345 |
| H | 0.52872 | -5.16511 | -2.14066 |
| H | 0.70158 | 3.24018 | 3.62987 |
| H | -4.60832 | -0.46510 | 2.75269 |
| H | 2.10082 | -1.95904 | 6.16392 |
| H | 5.05477 | 2.55889 | 2.40392 |
| H | 3.25197 | -2.72976 | -3.93724 |
| H | 1.21763 | -6.37064 | 0.03549 |
| H | 3.99044 | -1.13641 | 4.65510 |
| H | -4.55951 | -2.01551 | 0.70066 |
| H | 6.40893 | 1.57941 | 0.48466 |
| H | 0.10014 | 5.92267 | -0.18716 |
| H | -0.90935 | 5.13759 | 3.00598 |
| H | -4.14826 | -2.11841 | -2.86213 |
| O | 5.19128 | -2.71304 | -1.68172 |
| H | 3.85566 | -1.41768 | -0.09843 |
| C | 5.61228 | -2.15830 | -0.67149 |
| O | 4.83450 | -1.44072 | 0.20122 |
| H | 6.67008 | -2.15862 | -0.33782 |

TS

| | | | |
|---|---|---|---|
| Cu | 1.42715 | 1.06292 | -0.96182 |
| Cu | 0.33908 | -1.10424 | 0.99920 |
| Cu | -1.92338 | 1.26504 | -0.08536 |
| O | -0.14464 | 0.43461 | -0.11417 |
| O | 2.29779 | -0.70386 | 0.21407 |
| C | -2.19368 | -1.30307 | -3.00218 |
| N | -3.53258 | -1.27286 | -2.64404 |
| C | -1.61101 | -0.20530 | -2.45893 |
| C | -3.72666 | -0.17355 | -1.87389 |
| N | -2.56565 | 0.48755 | -1.73820 |
| H | -0.58127 | 0.09628 | -2.48105 |
| H | -4.66833 | 0.11432 | -1.42148 |
| C | -0.16584 | 3.75230 | -2.35544 |
| N | 0.63706 | 3.06537 | -1.43734 |
| C | -0.45257 | 5.00478 | -1.89965 |
| C | 0.82673 | 3.92944 | -0.44004 |
| N | 0.18397 | 5.09968 | -0.68480 |
| H | -1.01941 | 5.80718 | -2.34137 |
| H | 1.39367 | 3.75795 | 0.45528 |
| C | 2.95784 | -0.68983 | -4.70392 |
| N | 2.86235 | -1.74561 | -3.80609 |
| C | 2.47445 | 0.40773 | -4.02625 |
| C | 2.36088 | -1.26936 | -2.63952 |
| N | 2.10015 | 0.03366 | -2.73724 |
| H | 2.37356 | 1.42529 | -4.37125 |
| H | 2.22642 | -1.87766 | -1.76475 |
| C | 0.45719 | -4.68508 | -1.24401 |
| N | 0.84597 | -5.34753 | -0.08872 |
| C | 0.21976 | -3.38718 | -0.89162 |
| C | 0.83906 | -4.41243 | 0.92376 |
| N | 0.46410 | -3.21969 | 0.45891 |
| H | -0.11104 | -2.57169 | -1.51393 |
| H | 1.10181 | -4.63280 | 1.94842 |
| C | -0.04504 | 3.13951 | 2.95340 |
| N | -0.87515 | 4.18981 | 2.60714 |
| C | -0.37436 | 2.09062 | 2.16029 |
| C | -1.69005 | 3.74662 | 1.60373 |
| N | -1.38407 | 2.48272 | 1.31502 |
| H | 0.04382 | 1.10515 | 2.12891 |
| H | -2.45339 | 4.33795 | 1.11939 |
| C | -3.72579 | -0.77380 | 2.32696 |
| N | -3.77286 | -1.61557 | 1.23233 |
| C | -2.38301 | -0.55048 | 2.57468 |
| C | -2.50113 | -1.87432 | 0.84153 |
| N | -1.62208 | -1.23868 | 1.62656 |
| H | -1.91916 | 0.04090 | 3.34807 |

| | | | |
|---|---|---|---|
| H | -2.25145 | -2.50122 | -0.00026 |
| C | 1.88160 | -1.78526 | 5.10315 |
| N | 2.97236 | -1.41066 | 4.33409 |
| C | 0.81041 | -1.73481 | 4.23000 |
| C | 2.56570 | -1.17670 | 3.06918 |
| N | 1.25011 | -1.34721 | 2.96203 |
| H | -0.22878 | -1.95682 | 4.41636 |
| H | 3.26993 | -0.96713 | 2.28226 |
| C | 4.62134 | 2.18571 | 1.49547 |
| N | 5.37039 | 1.70715 | 0.43410 |
| C | 3.33165 | 2.24996 | 1.04551 |
| C | 4.52037 | 1.49877 | -0.61816 |
| N | 3.27443 | 1.83109 | -0.28075 |
| H | 2.45543 | 2.56156 | 1.59003 |
| H | 4.82487 | 1.10098 | -1.57517 |
| C | -6.60651 | -2.36837 | -0.77299 |
| O | -5.38804 | -2.62174 | -0.48661 |
| O | -7.25420 | -1.28669 | -0.53975 |
| O | -3.81124 | 1.85056 | 0.39870 |
| O | -5.98433 | 0.84641 | -0.25733 |
| H | -3.82127 | 1.98233 | 1.36904 |
| H | -6.49320 | 1.48120 | -0.83249 |
| H | -6.51072 | -0.10638 | -0.25509 |
| H | -4.72383 | 1.37797 | 0.16388 |
| H | 2.56756 | -0.02157 | 0.85622 |
| H | -7.14771 | -3.17863 | -1.28585 |
| H | -1.74016 | -2.12259 | -3.47449 |
| H | -0.50786 | 3.45474 | -3.31421 |
| H | 3.37315 | -0.83741 | -5.68988 |
| H | 0.39887 | -5.14051 | -2.20130 |
| H | 0.71052 | 3.18276 | 3.68119 |
| H | -4.65809 | -0.42632 | 2.76133 |
| H | 2.03039 | -2.07141 | 6.14347 |
| H | 5.05109 | 2.44952 | 2.44054 |
| H | 3.15821 | -2.72445 | -3.96862 |
| H | 1.07106 | -6.38586 | -0.04241 |
| H | 3.93110 | -1.25846 | 4.64335 |
| H | -4.63597 | -1.94962 | 0.68863 |
| H | 6.38754 | 1.47470 | 0.50655 |
| H | 0.14727 | 5.92541 | -0.09874 |
| H | -0.87098 | 5.11352 | 3.08490 |
| H | -4.23029 | -2.01112 | -2.87575 |
| O | 5.04079 | -2.67203 | -1.68028 |
| H | 3.58473 | -1.23516 | 0.06741 |
| C | 5.47033 | -2.15230 | -0.64095 |
| O | 4.72025 | -1.43739 | 0.23269 |

| | | | |
|---|---|---|---|
| H | 6.58883 | -2.25560 | -0.36633 |

$NI^{H}$(T3W)

| | | | |
|---|---|---|---|
| Cu | 1.39806 | 1.14229 | -1.10019 |
| Cu | 0.29262 | -1.28627 | 0.97907 |
| Cu | -1.83127 | 1.31428 | 0.00216 |
| O | -0.02034 | 0.43288 | -0.11417 |
| O | 2.23867 | -1.31894 | 0.22433 |
| C | -2.23834 | -1.03076 | -3.07490 |
| N | -3.57073 | -0.98817 | -2.70567 |
| C | -1.61325 | -0.00485 | -2.45080 |
| C | -3.72201 | 0.05013 | -1.84393 |
| N | -2.53623 | 0.65615 | -1.66551 |
| H | -0.57299 | 0.25524 | -2.46480 |
| H | -4.64973 | 0.33353 | -1.35930 |
| C | -0.05905 | 3.97335 | -2.10162 |
| N | 0.88443 | 3.27839 | -1.35446 |
| C | -0.40225 | 5.14183 | -1.49124 |
| C | 1.12092 | 4.04876 | -0.29292 |
| N | 0.35438 | 5.17165 | -0.34226 |
| H | -1.07569 | 5.93059 | -1.78207 |
| H | 1.81649 | 3.83822 | 0.50064 |
| C | 2.93737 | -0.40287 | -4.74127 |
| N | 2.79456 | -1.52023 | -3.92177 |
| C | 2.50234 | 0.66470 | -3.98995 |
| C | 2.31162 | -1.11215 | -2.72403 |
| N | 2.10666 | 0.21017 | -2.73007 |
| H | 2.44611 | 1.70820 | -4.25915 |
| H | 2.14778 | -1.75781 | -1.87938 |
| C | 0.28939 | -4.59561 | -1.57764 |
| N | 0.65285 | -5.35541 | -0.47485 |
| C | 0.02704 | -3.33777 | -1.11459 |
| C | 0.60344 | -4.52172 | 0.61880 |
| N | 0.22514 | -3.29708 | 0.25409 |
| H | -0.28719 | -2.46920 | -1.66957 |
| H | 0.84462 | -4.83204 | 1.62556 |
| C | 0.06676 | 2.94124 | 3.13985 |
| N | -0.74834 | 4.02644 | 2.88138 |
| C | -0.22894 | 1.98677 | 2.22557 |
| C | -1.52851 | 3.69847 | 1.80831 |
| N | -1.21100 | 2.47107 | 1.39602 |
| H | 0.18288 | 1.00300 | 2.11485 |
| H | -2.27801 | 4.33872 | 1.36704 |
| C | -3.75075 | -0.83080 | 2.26929 |
| N | -3.82255 | -1.58484 | 1.11417 |
| C | -2.40185 | -0.65236 | 2.52278 |

| | | | |
|---|---|---|---|
| C | -2.56275 | -1.84435 | 0.69526 |
| N | -1.66508 | -1.28880 | 1.52009 |
| H | -1.91639 | -0.13233 | 3.33377 |
| H | -2.33441 | -2.42415 | -0.18474 |
| C | 1.82089 | -2.16247 | 4.97382 |
| N | 2.90403 | -1.69431 | 4.24220 |
| C | 0.73341 | -1.99862 | 4.14140 |
| C | 2.46769 | -1.28415 | 3.03045 |
| N | 1.15061 | -1.45059 | 2.92801 |
| H | -0.30257 | -2.23958 | 4.32247 |
| H | 3.13039 | -0.94097 | 2.25661 |
| C | 4.63367 | 1.88721 | 1.66756 |
| N | 5.36778 | 1.42190 | 0.58326 |
| C | 3.32625 | 1.89916 | 1.25841 |
| C | 4.49946 | 1.16702 | -0.44023 |
| N | 3.24464 | 1.44626 | -0.05960 |
| H | 2.44962 | 2.18053 | 1.81727 |
| H | 4.78939 | 0.65529 | -1.34755 |
| C | -6.66609 | -2.14827 | -0.91874 |
| O | -5.47336 | -2.49126 | -0.61687 |
| O | -7.25659 | -1.04664 | -0.63203 |
| O | -3.69503 | 1.87982 | 0.57981 |
| O | -5.90618 | 0.98659 | -0.10946 |
| H | -3.68631 | 1.95917 | 1.55595 |
| H | -6.40392 | 1.70254 | -0.59253 |
| H | -6.46963 | 0.05796 | -0.21364 |
| H | -4.62245 | 1.44042 | 0.33288 |
| H | 2.50657 | -0.38753 | 0.11054 |
| H | -7.23729 | -2.89079 | -1.49892 |
| H | -1.80603 | -1.81201 | -3.61658 |
| H | -0.43427 | 3.70591 | -3.04952 |
| H | 3.33674 | -0.49544 | -5.74347 |
| H | 0.25738 | -4.96784 | -2.57365 |
| H | 0.78031 | 2.88986 | 3.90409 |
| H | -4.67750 | -0.50659 | 2.73381 |
| H | 1.96923 | -2.56243 | 5.97018 |
| H | 5.10047 | 2.14168 | 2.60275 |
| H | 3.07554 | -2.49774 | -4.16484 |
| H | 0.89907 | -6.38505 | -0.51371 |
| H | 3.88914 | -1.68904 | 4.52962 |
| H | -4.69450 | -1.87365 | 0.55485 |
| H | 6.41113 | 1.27875 | 0.59927 |
| H | 0.28423 | 5.91616 | 0.33729 |
| H | -0.75259 | 4.89808 | 3.45498 |
| H | -4.29228 | -1.68276 | -3.00542 |
| O | 5.23559 | -1.33455 | -1.75560 |

| | | | |
|---|---|---|---|
| H | 3.20239 | -1.81998 | 0.21880 |
| C | 5.46018 | -1.98982 | -0.69708 |
| O | 4.60916 | -2.25732 | 0.25659 |
| H | 6.51829 | -2.38113 | -0.54587 |

TS’

| | | | |
|---|---|---|---|
| Cu | 1.65691 | 1.33887 | -1.01920 |
| Cu | 0.04480 | -1.87268 | 1.12038 |
| Cu | -1.60862 | 1.52977 | -0.00775 |
| O | 0.11704 | 0.61137 | -0.26829 |
| O | 1.71651 | -1.39021 | 0.17404 |
| C | -2.28381 | -0.50877 | -3.23852 |
| N | -3.61013 | -0.41502 | -2.85232 |
| C | -1.58935 | 0.42460 | -2.54699 |
| C | -3.68349 | 0.56056 | -1.90552 |
| N | -2.45876 | 1.07580 | -1.69604 |
| H | -0.53253 | 0.61287 | -2.53840 |
| H | -4.58319 | 0.85119 | -1.37543 |
| C | 0.28726 | 4.19592 | -1.68400 |
| N | 1.28651 | 3.44643 | -1.08117 |
| C | -0.05255 | 5.26678 | -0.91411 |
| C | 1.56467 | 4.08160 | 0.05489 |
| N | 0.76891 | 5.17432 | 0.18626 |
| H | -0.76176 | 6.06341 | -1.06448 |
| H | 2.30714 | 3.79277 | 0.77969 |
| C | 2.99544 | -0.13812 | -4.71990 |
| N | 2.75604 | -1.31567 | -4.02090 |
| C | 2.67237 | 0.88211 | -3.86109 |
| C | 2.32211 | -0.98603 | -2.77799 |
| N | 2.24542 | 0.34222 | -2.65088 |
| H | 2.71889 | 1.94821 | -4.02242 |
| H | 2.08376 | -1.70368 | -2.01268 |
| C | -0.08771 | -4.43852 | -2.06331 |
| N | 0.17160 | -5.35288 | -1.05372 |
| C | -0.30684 | -3.23806 | -1.45263 |
| C | 0.10060 | -4.68947 | 0.13505 |
| N | -0.18922 | -3.40786 | -0.08668 |
| H | -0.52796 | -2.27791 | -1.88955 |
| H | 0.26424 | -5.14631 | 1.10110 |
| C | 0.25014 | 2.57919 | 3.39495 |
| N | -0.48786 | 3.74245 | 3.26430 |
| C | -0.03236 | 1.80531 | 2.31487 |
| C | -1.20890 | 3.63940 | 2.10820 |
| N | -0.92898 | 2.47855 | 1.51843 |
| H | 0.33783 | 0.83276 | 2.05057 |
| H | -1.89447 | 4.38665 | 1.73738 |

| | | | |
|---|---|---|---|
| C | -3.89019 | -0.86690 | 2.16131 |
| N | -3.99462 | -1.47448 | 0.92565 |
| C | -2.55848 | -0.94428 | 2.51780 |
| C | -2.77112 | -1.90575 | 0.55988 |
| N | -1.86383 | -1.59561 | 1.49898 |
| H | -2.05705 | -0.58563 | 3.40307 |
| H | -2.57373 | -2.42540 | -0.36295 |
| C | 1.53296 | -2.78776 | 4.77291 |
| N | 2.64872 | -2.32421 | 4.09213 |
| C | 0.45242 | -2.40857 | 4.02118 |
| C | 2.23950 | -1.69777 | 2.96619 |
| N | 0.90583 | -1.73376 | 2.89169 |
| H | -0.59781 | -2.58282 | 4.19634 |
| H | 2.91394 | -1.29731 | 2.22636 |
| C | 4.71751 | 1.37131 | 1.89763 |
| N | 5.43536 | 0.94191 | 0.79057 |
| C | 3.44677 | 1.61197 | 1.44236 |
| C | 4.59739 | 0.91327 | -0.28610 |
| N | 3.38191 | 1.32846 | 0.07727 |
| H | 2.58664 | 1.95040 | 1.99449 |
| H | 4.87025 | 0.44185 | -1.22420 |
| C | -6.80642 | -1.55121 | -1.21852 |
| O | -5.65286 | -2.02884 | -0.94508 |
| O | -7.29717 | -0.43942 | -0.81105 |
| O | -3.45482 | 2.00184 | 0.75539 |
| O | -5.76260 | 1.36393 | 0.03288 |
| H | -3.40830 | 1.94823 | 1.73131 |
| H | -6.21058 | 2.19098 | -0.29839 |
| H | -6.39951 | 0.52423 | -0.22272 |
| H | -4.40634 | 1.65838 | 0.48765 |
| H | 1.41625 | -0.46351 | -0.05213 |
| H | -7.43347 | -2.17033 | -1.88515 |
| H | -1.89693 | -1.28890 | -3.81284 |
| H | -0.12680 | 4.01456 | -2.63370 |
| H | 3.37004 | -0.14866 | -5.72705 |
| H | -0.09619 | -4.68741 | -3.09694 |
| H | 0.88910 | 2.36408 | 4.20287 |
| H | -4.78431 | -0.45873 | 2.60983 |
| H | 1.62616 | -3.35383 | 5.67638 |
| H | 5.16531 | 1.43176 | 2.87551 |
| H | 2.92925 | -2.28338 | -4.37863 |
| H | 0.39770 | -6.36310 | -1.19644 |
| H | 3.63355 | -2.48014 | 4.36066 |
| H | -4.86178 | -1.57794 | 0.29502 |
| H | 6.44600 | 0.69175 | 0.80461 |
| H | 0.68992 | 5.78581 | 0.98123 |

| | | | |
|---|---|---|---|
| H | -0.48013 | 4.52040 | 3.95803 |
| H | -4.37782 | -1.03621 | -3.21870 |
| O | 5.40118 | -1.39631 | -1.89309 |
| H | 2.70810 | -1.60972 | 0.06323 |
| C | 5.35536 | -2.17090 | -0.88597 |
| O | 4.38383 | -2.28553 | -0.03001 |
| H | 6.30060 | -2.82084 | -0.73061 |

$NI^{H}$

| | | | |
|---|---|---|---|
| Cu | 1.52945 | 0.95672 | -0.81868 |
| Cu | 0.33596 | -1.41256 | 1.13079 |
| Cu | -2.04714 | 1.45386 | -0.07380 |
| O | -0.37599 | 0.43544 | -0.21192 |
| O | 1.82232 | -0.75592 | 0.10970 |
| C | -2.24104 | -1.03052 | -3.12474 |
| N | -3.56373 | -1.03253 | -2.70747 |
| C | -1.69008 | 0.11693 | -2.63083 |
| C | -3.77006 | 0.05766 | -1.93144 |
| N | -2.63761 | 0.77332 | -1.84273 |
| H | -0.69503 | 0.50441 | -2.78210 |
| H | -4.70246 | 0.30464 | -1.43338 |
| C | -0.07397 | 3.86330 | -2.11263 |
| N | 0.77784 | 3.12025 | -1.27969 |
| C | -0.35151 | 5.07659 | -1.55497 |
| C | 1.01112 | 3.92108 | -0.23904 |
| N | 0.33914 | 5.09976 | -0.36628 |
| H | -0.94066 | 5.90266 | -1.91745 |
| H | 1.63935 | 3.69781 | 0.60371 |
| C | 2.90624 | -0.46766 | -4.79489 |
| N | 2.80674 | -1.57750 | -3.96285 |
| C | 2.43338 | 0.58728 | -4.04443 |
| C | 2.31888 | -1.17121 | -2.76468 |
| N | 2.06416 | 0.13637 | -2.77816 |
| H | 2.34314 | 1.62616 | -4.32177 |
| H | 2.18969 | -1.81944 | -1.91572 |
| C | 0.36100 | -4.62967 | -1.55567 |
| N | 0.74104 | -5.37543 | -0.45015 |
| C | 0.12609 | -3.36044 | -1.11258 |
| C | 0.72894 | -4.52545 | 0.62884 |
| N | 0.35945 | -3.30084 | 0.24849 |
| H | -0.18279 | -2.50072 | -1.68366 |
| H | 0.99002 | -4.81942 | 1.63560 |
| C | 0.10410 | 2.91729 | 3.11108 |
| N | -0.70994 | 4.01343 | 2.86741 |
| C | -0.28051 | 1.95190 | 2.22595 |
| C | -1.55757 | 3.68941 | 1.85092 |

| | | | |
|---|---|---|---|
| N | -1.30666 | 2.44526 | 1.44073 |
| H | 0.10770 | 0.95818 | 2.10887 |
| H | -2.30994 | 4.34851 | 1.44158 |
| C | -3.67519 | -0.91093 | 2.33932 |
| N | -3.75918 | -1.70238 | 1.20750 |
| C | -2.32875 | -0.80308 | 2.62805 |
| C | -2.50304 | -2.05405 | 0.84259 |
| N | -1.60162 | -1.51869 | 1.67784 |
| H | -1.83978 | -0.27680 | 3.43287 |
| H | -2.28244 | -2.68399 | -0.00549 |
| C | 1.95644 | -2.11054 | 4.96572 |
| N | 3.02213 | -1.65202 | 4.20163 |
| C | 0.84452 | -1.93102 | 4.17504 |
| C | 2.55510 | -1.22645 | 3.00367 |
| N | 1.23115 | -1.37628 | 2.95647 |
| H | -0.18702 | -2.16526 | 4.38682 |
| H | 3.18769 | -0.87970 | 2.19995 |
| C | 4.72072 | 1.94394 | 1.57176 |
| N | 5.42834 | 1.46143 | 0.48409 |
| C | 3.41377 | 1.99829 | 1.19049 |
| C | 4.53515 | 1.21810 | -0.52487 |
| N | 3.30554 | 1.55551 | -0.12167 |
| H | 2.55712 | 2.29107 | 1.77427 |
| H | 4.80712 | 0.65121 | -1.41190 |
| C | -6.62285 | -2.16789 | -0.87382 |
| O | -5.36938 | -2.36743 | -0.72736 |
| O | -7.28633 | -1.13366 | -0.49864 |
| O | -3.85389 | 1.95961 | 0.52054 |
| O | -5.97868 | 0.96337 | -0.22129 |
| H | -3.84846 | 2.02977 | 1.49874 |
| H | -6.51173 | 1.63669 | -0.72690 |
| H | -6.53348 | 0.00645 | -0.21847 |
| H | -4.78102 | 1.48753 | 0.24890 |
| H | 2.74343 | -1.12719 | 0.09319 |
| H | -7.18699 | -2.96650 | -1.38695 |
| H | -1.79016 | -1.87928 | -3.58675 |
| H | -0.44005 | 3.65064 | -3.08864 |
| H | 3.31690 | -0.55588 | -5.79399 |
| H | 0.30349 | -5.01469 | -2.54264 |
| H | 0.87126 | 2.90496 | 3.85531 |
| H | -4.58371 | -0.53024 | 2.78926 |
| H | 2.11637 | -2.52198 | 5.95542 |
| H | 5.17767 | 2.16716 | 2.50333 |
| H | 3.08717 | -2.54516 | -4.19405 |
| H | 0.98010 | -6.40949 | -0.47862 |
| H | 4.01193 | -1.65189 | 4.48116 |

| | | | |
|---|---|---|---|
| H | -4.62254 | -1.91717 | 0.62317 |
| H | 6.46607 | 1.29242 | 0.49046 |
| H | 0.31172 | 5.89578 | 0.26795 |
| H | -0.67805 | 4.90107 | 3.40841 |
| H | -4.26871 | -1.75720 | -2.94369 |
| O | 5.58142 | -1.12276 | -1.89353 |
| H | -0.60760 | -0.26493 | -0.85369 |
| C | 5.60855 | -1.78883 | -0.80576 |
| O | 4.68840 | -1.85453 | 0.09674 |
| H | 6.57753 | -2.37726 | -0.62269 |

$NI^{e,H}$

| | | | |
|---|---|---|---|
| Cu | 1.79264 | 1.50761 | -1.26867 |
| Cu | 0.21976 | -1.34412 | 1.09585 |
| Cu | -2.24115 | 1.26161 | 0.12800 |
| O | -0.69424 | 0.18443 | 0.17232 |
| O | 1.76878 | -0.58487 | 0.22169 |
| C | -2.04320 | -0.98281 | -3.14737 |
| N | -3.40681 | -0.97430 | -2.87068 |
| C | -1.52458 | 0.08445 | -2.46917 |
| C | -3.67333 | 0.05504 | -2.03622 |
| N | -2.54442 | 0.71927 | -1.76209 |
| H | -0.50165 | 0.41635 | -2.40277 |
| H | -4.64790 | 0.29359 | -1.62854 |
| C | 0.00247 | 3.97882 | -2.03491 |
| N | 0.70109 | 3.16106 | -1.14319 |
| C | -0.25241 | 5.19712 | -1.48200 |
| C | 0.85419 | 3.90989 | -0.04902 |
| N | 0.29405 | 5.13439 | -0.22195 |
| H | -0.74789 | 6.06854 | -1.87551 |
| H | 1.33122 | 3.61361 | 0.86554 |
| C | 3.16492 | -0.29445 | -4.71308 |
| N | 3.02922 | -1.40974 | -3.90008 |
| C | 2.69533 | 0.76853 | -3.98748 |
| C | 2.50101 | -0.99008 | -2.71176 |
| N | 2.28005 | 0.32513 | -2.73688 |
| H | 2.62483 | 1.80577 | -4.27599 |
| H | 2.31114 | -1.63084 | -1.87110 |
| C | 0.53390 | -4.55796 | -1.66803 |
| N | 0.88036 | -5.33758 | -0.57378 |
| C | 0.28119 | -3.30477 | -1.18419 |
| C | 0.82829 | -4.52307 | 0.53238 |
| N | 0.46954 | -3.28988 | 0.18534 |
| H | -0.02799 | -2.42273 | -1.72022 |
| H | 1.04727 | -4.85620 | 1.53688 |
| C | -0.04574 | 2.82793 | 3.24446 |

| | | | |
|---|---|---|---|
| N | -0.85772 | 3.92590 | 2.99500 |
| C | -0.48764 | 1.83465 | 2.42121 |
| C | -1.75886 | 3.57004 | 2.03525 |
| N | -1.54546 | 2.30809 | 1.66542 |
| H | -0.11789 | 0.83581 | 2.30799 |
| H | -2.51830 | 4.22493 | 1.63223 |
| C | -3.72065 | -1.06092 | 2.21750 |
| N | -3.75424 | -1.82663 | 1.06462 |
| C | -2.40984 | -1.05410 | 2.63760 |
| C | -2.49162 | -2.25618 | 0.81982 |
| N | -1.64658 | -1.80283 | 1.75067 |
| H | -1.97196 | -0.57120 | 3.49720 |
| H | -2.21657 | -2.85165 | -0.03681 |
| C | 1.85983 | -2.24679 | 4.95342 |
| N | 2.94838 | -1.77316 | 4.23625 |
| C | 0.78360 | -2.11893 | 4.10718 |
| C | 2.52159 | -1.39122 | 3.00667 |
| N | 1.20890 | -1.58013 | 2.89935 |
| H | -0.24874 | -2.38263 | 4.27388 |
| H | 3.19094 | -1.05072 | 2.23410 |
| C | 4.70519 | 2.00104 | 1.76238 |
| N | 5.48269 | 1.60419 | 0.68826 |
| C | 3.43342 | 2.13452 | 1.26930 |
| C | 4.66965 | 1.51283 | -0.40586 |
| N | 3.41956 | 1.83456 | -0.08743 |
| H | 2.54245 | 2.41204 | 1.80739 |
| H | 5.00694 | 1.20893 | -1.38627 |
| C | -6.55169 | -2.15182 | -1.18646 |
| O | -5.30233 | -2.29921 | -0.97246 |
| O | -7.28785 | -1.15623 | -0.84526 |
| O | -4.04990 | 1.92485 | 0.48754 |
| O | -6.07334 | 0.98237 | -0.52149 |
| H | -4.17179 | 2.01554 | 1.45605 |
| H | -6.54666 | 1.63631 | -1.10346 |
| H | -6.60341 | 0.01818 | -0.54572 |
| H | -4.94888 | 1.48646 | 0.09374 |
| H | 2.22426 | -0.00194 | 0.85491 |
| H | -7.04659 | -2.96701 | -1.73627 |
| H | -1.58388 | -1.77585 | -3.70767 |
| H | -0.30628 | 3.75082 | -3.01822 |
| H | 3.58715 | -0.35093 | -5.69101 |
| H | 0.50054 | -4.91908 | -2.66843 |
| H | 0.75783 | 2.83587 | 3.94759 |
| H | -4.62119 | -0.61778 | 2.59401 |
| H | 1.97792 | -2.63280 | 5.95164 |
| H | 5.11773 | 2.17106 | 2.73628 |

| | | | |
|---|---|---|---|
| H | 3.31866 | -2.38316 | -4.15233 |
| H | 1.11477 | -6.36119 | -0.61743 |
| H | 3.91771 | -1.70817 | 4.57099 |
| H | -4.56747 | -1.94822 | 0.39314 |
| H | 6.48689 | 1.36048 | 0.75009 |
| H | 0.30072 | 5.91401 | 0.42016 |
| H | -0.79334 | 4.82936 | 3.49566 |
| H | -4.08531 | -1.69223 | -3.15314 |
| O | 4.92182 | -2.67983 | -1.77833 |
| H | 3.63565 | -1.50924 | -0.04341 |
| C | 5.36955 | -2.19511 | -0.74312 |
| O | 4.62338 | -1.56962 | 0.21589 |
| H | 6.43468 | -2.19110 | -0.45182 |
| H | 0.04983 | 0.57615 | -0.32570 |

$NI^{2e,H}$

| | | | |
|---|---|---|---|
| Cu | 1.94785 | 1.68490 | -1.33644 |
| Cu | 0.21257 | -1.52050 | 1.04384 |
| Cu | -2.06891 | 1.30236 | 0.15759 |
| O | -0.47677 | 0.18587 | 0.14170 |
| O | 2.03658 | -1.18225 | 0.17531 |
| C | -2.12472 | -0.75856 | -3.18946 |
| N | -3.47279 | -0.75095 | -2.85412 |
| C | -1.55379 | 0.27139 | -2.50262 |
| C | -3.67980 | 0.23933 | -1.95645 |
| N | -2.52426 | 0.87520 | -1.70924 |
| H | -0.52838 | 0.60372 | -2.50778 |
| H | -4.63129 | 0.47486 | -1.49431 |
| C | 0.08088 | 4.12325 | -1.83792 |
| N | 1.02997 | 3.39496 | -1.12795 |
| C | -0.29540 | 5.23208 | -1.14397 |
| C | 1.23111 | 4.08243 | -0.00290 |
| N | 0.44328 | 5.18326 | 0.01558 |
| H | -0.98232 | 6.02681 | -1.38152 |
| H | 1.92793 | 3.83145 | 0.77765 |
| C | 3.04805 | -0.13741 | -4.73299 |
| N | 2.89491 | -1.28691 | -3.97604 |
| C | 2.57333 | 0.89171 | -3.96748 |
| C | 2.36900 | -0.93060 | -2.77479 |
| N | 2.14639 | 0.38831 | -2.73850 |
| H | 2.50226 | 1.93985 | -4.21427 |
| H | 2.21262 | -1.61253 | -1.96035 |
| C | 0.32650 | -4.48744 | -1.86164 |
| N | 0.65468 | -5.32836 | -0.80967 |
| C | 0.05790 | -3.26877 | -1.31018 |
| C | 0.57884 | -4.59072 | 0.34224 |

| | | | |
|---|---|---|---|
| N | 0.21763 | -3.34262 | 0.06039 |
| H | -0.23523 | -2.35420 | -1.79854 |
| H | 0.78753 | -4.98117 | 1.32811 |
| C | 0.02793 | 2.70205 | 3.37015 |
| N | -0.76849 | 3.81812 | 3.17445 |
| C | -0.35412 | 1.77970 | 2.44774 |
| C | -1.61608 | 3.54108 | 2.14073 |
| N | -1.37184 | 2.31212 | 1.68166 |
| H | 0.02900 | 0.79272 | 2.28093 |
| H | -2.36171 | 4.22104 | 1.75454 |
| C | -3.77348 | -1.03218 | 2.18786 |
| N | -3.83379 | -1.74316 | 1.00236 |
| C | -2.44732 | -1.03112 | 2.56785 |
| C | -2.57952 | -2.15247 | 0.69726 |
| N | -1.70840 | -1.73619 | 1.62356 |
| H | -1.98484 | -0.59084 | 3.43738 |
| H | -2.33434 | -2.71753 | -0.18762 |
| C | 1.76545 | -2.49775 | 4.86625 |
| N | 2.86098 | -2.00026 | 4.17650 |
| C | 0.68882 | -2.28467 | 4.03978 |
| C | 2.44362 | -1.52034 | 2.98138 |
| N | 1.12494 | -1.67535 | 2.86816 |
| H | -0.34868 | -2.53522 | 4.19507 |
| H | 3.11604 | -1.14097 | 2.23071 |
| C | 4.69064 | 1.75100 | 1.87372 |
| N | 5.45355 | 1.36439 | 0.78302 |
| C | 3.40407 | 1.84379 | 1.40934 |
| C | 4.62646 | 1.22436 | -0.28696 |
| N | 3.37346 | 1.52799 | 0.05410 |
| H | 2.50765 | 2.09465 | 1.95241 |
| H | 4.95042 | 0.89903 | -1.26524 |
| C | -6.63669 | -1.94026 | -1.22682 |
| O | -5.39208 | -2.15227 | -1.03485 |
| O | -7.32290 | -0.93728 | -0.81072 |
| O | -3.88236 | 1.92211 | 0.62559 |
| O | -5.99681 | 1.10315 | -0.31583 |
| H | -3.95595 | 1.97682 | 1.60146 |
| H | -6.45838 | 1.82378 | -0.82515 |
| H | -6.57409 | 0.16862 | -0.41459 |
| H | -4.81166 | 1.52394 | 0.26402 |
| H | 2.15217 | -0.23795 | -0.05475 |
| H | -7.17283 | -2.69584 | -1.82383 |
| H | -1.68864 | -1.54361 | -3.75851 |
| H | -0.27358 | 3.90999 | -2.80644 |
| H | 3.50980 | -0.15023 | -5.69249 |
| H | 0.32107 | -4.78367 | -2.88243 |

| | | | |
|---|---|---|---|
| H | 0.78958 | 2.63088 | 4.10205 |
| H | -4.67686 | -0.62045 | 2.60513 |
| H | 1.88106 | -2.95716 | 5.83235 |
| H | 5.12792 | 1.91989 | 2.84092 |
| H | 3.19590 | -2.24787 | -4.25331 |
| H | 0.90610 | -6.33862 | -0.90673 |
| H | 3.83865 | -2.01401 | 4.48991 |
| H | -4.66280 | -1.84281 | 0.34175 |
| H | 6.47077 | 1.17364 | 0.81194 |
| H | 0.39718 | 5.88769 | 0.73073 |
| H | -0.71359 | 4.68126 | 3.75432 |
| H | -4.18555 | -1.42610 | -3.18978 |
| O | 4.78008 | -2.48970 | -1.90321 |
| H | 3.06806 | -1.56536 | 0.17611 |
| C | 5.20450 | -2.21557 | -0.75501 |
| O | 4.48306 | -1.80916 | 0.26980 |
| H | 6.32712 | -2.31252 | -0.56124 |
| H | 0.09928 | 0.41850 | -0.61606 |