Supporting Information

"Spectroscopic Definition of the Cu_Z^o Intermediate in Turnover of Nitrous Oxide Reductase and Molecular Insight into the Catalytic Mechanism"

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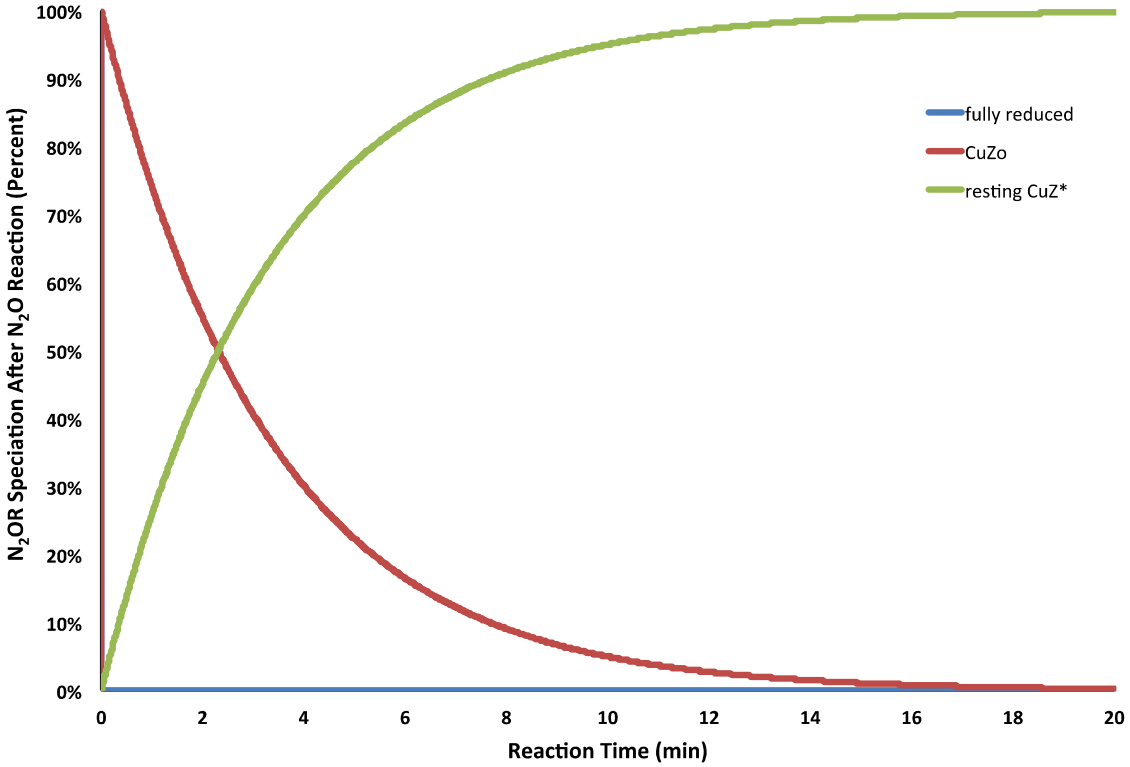


Figure S1: Calculated time dependence of the decay of the Cu_Z^o intermediate formed upon N_2O reduction by fully reduced Cu_Z* ($k_{formation}$ of 200 s^{-1} and k_{decay} of 0.005 s^{-1}).[1,2] Note that fully reduced N_2OR is consumed in the first 50 μs, yielding 99.97% Cu_Z^o with a t_{max} of 52.2 μs.

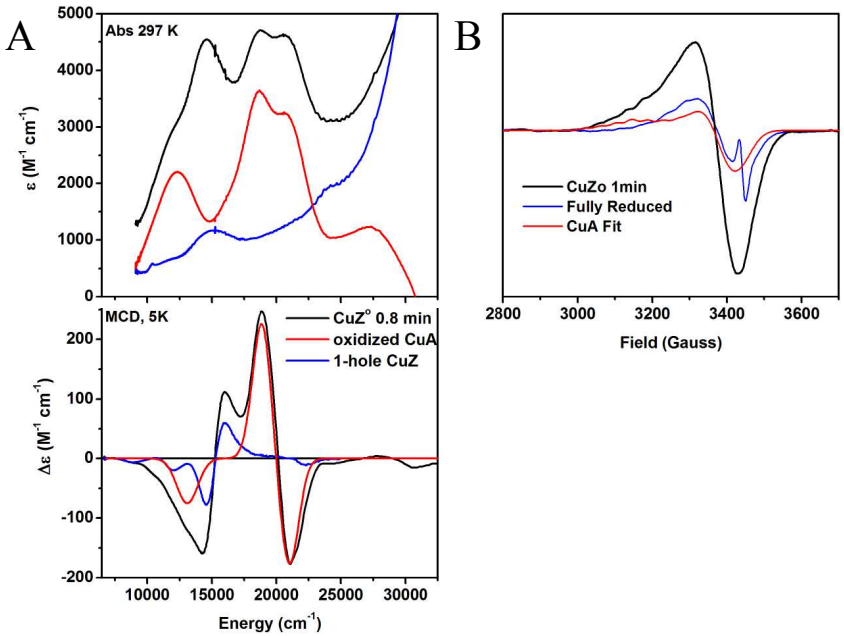


Figure S2: Spectra of the reaction of fully reduced N_2OR with N_2O (black), containing contributions from Cu_Z^o, Cu_A, and 1-hole Cu_Z. Additional spectra in red and blue show the separately determined spectral contributions of oxidized Cu_A (red) and 1-hole Cu_Z (blue), which are subtracted as described in the text to obtain the clean EPR, absorption, and MCD spectra of Cu_Z^o reported in Figures 2 and 3. A) Absorption spectra at 297 K and MCD spectra at 5 K and 7 T, after 50 s of reaction. B) EPR spectra at 77 K after 60 s of reaction.

1-hole Cu_Z^o				**1-hole Cu_Z***		
Energy (cm^{-1})	*C_0/D_0*	*Assignment*	*Band #*	*Energy (cm^{-1})*	*C_0/D_0*	*Assignment*
			1	8,015	-0.016	d-d (z^2)
			2	10,000	---	IT
11,100	0.764	d-d	**3**	11,140	-0.218	d-d (xz)
			4	12,900	-0.194	d-d (yz)
14,200	0.092	S $p_{y'}$	**5**	14,300	-0.327	S $p_{y'}$
15,600	0.123	S $p_{x'}$	**6**	15,675	0.196	S $p_{x'}$
16,800	0.188	S $p_{z'}$	**7**	16,520	0.091	S $p_{z'}$
			8	17,980	0.170	d-d (xy)
24,300	---	His π_1	**9**	19,775	-0.029	His π_1
31,000	---	His π_1	**10**	20,985	-0.045	His π_1
			11	22,270	0.193	His π_1
			12	24,030	-0.047	His π_1
			13	28,055	-0.002	His π_2

Table S1: Band energies, C/D ratios, and assignments from simultaneous fitting of the absorption and MCD spectra of Cu_Z^o and Cu_Z* (band numbers, energies, and assignments for Cu_Z* reproduced from Ref. [3]).

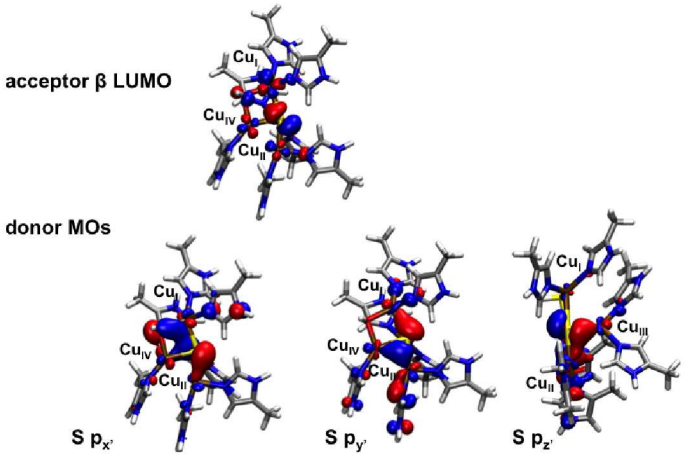


Figure S3: Molecular orbital contours of the acceptor β LUMO and donor μ_4S^{2-} 3p orbitals involved in S to Cu CT transitions for resting 1-hole Cu_Z*, based on a computational model with a hydroxide bridged edge (B3LYP, tzvp on Cu_4SON_7, sv on remainder, PCM=4.0).

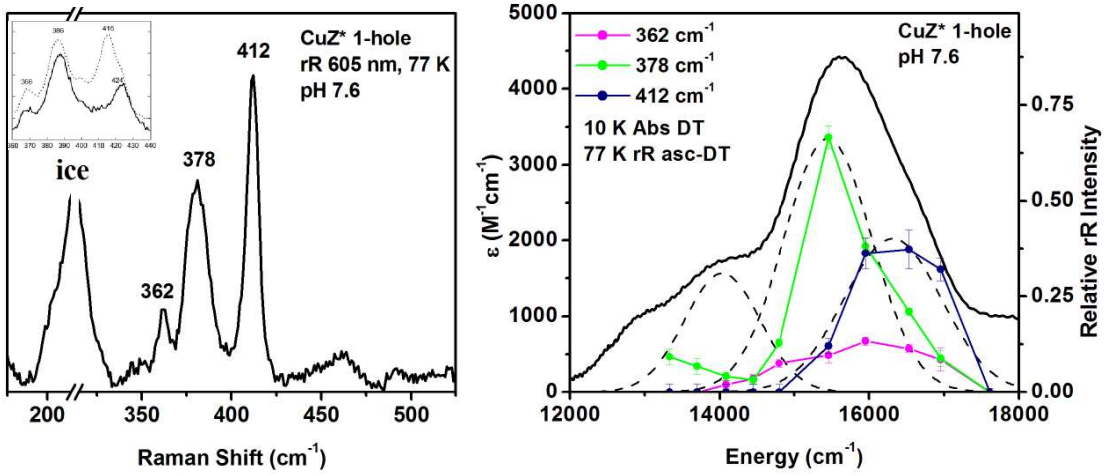


Figure S4: Resonance Raman spectrum of resting Cu_Z* at 77 K and 605 nm excitation; excitation profile of resting Cu_Z*. Inset: H_2O^{16}/H_2O^{18} dependence at pH 10.5 reproduced from Reference [3]; no O^{16}/O^{18} is observed at pH 7.6.

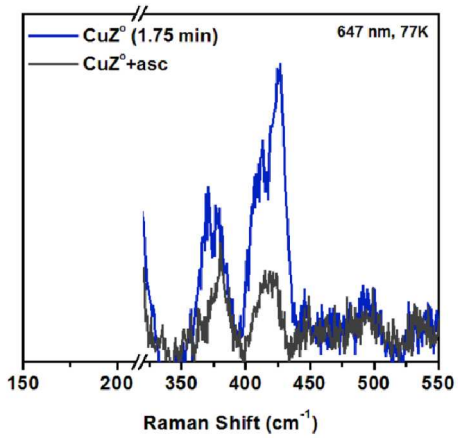
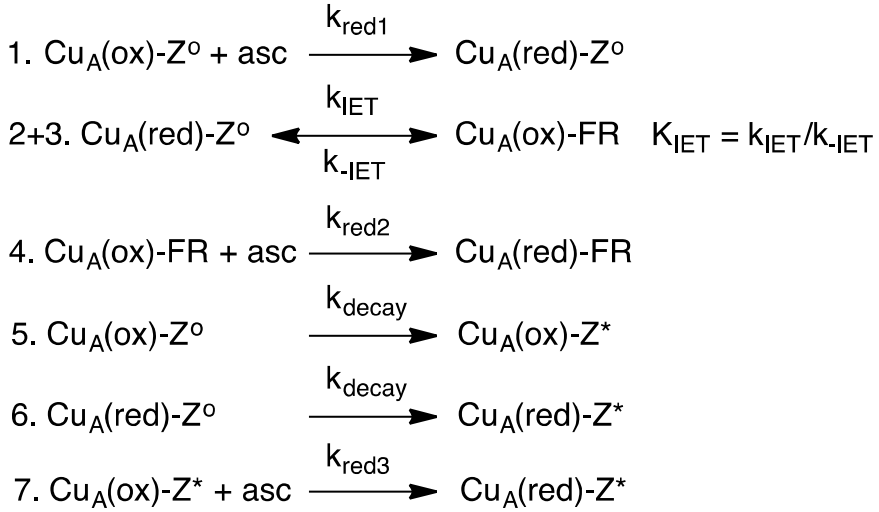


Figure S5: Resonance Raman spectra before (blue) and after (grey) sodium ascorbate addition to a sample of Cu_Z^o (77 K, 647 nm excitation energy).

*S1. Supplementary Discussion of Kinetic Modeling and Fitting of Ascorbate Reduction of Cu_Z^o and Cu_Z**

S1.1 Kinetic Modeling of the Sodium Ascorbate Reduction of Cu_Z^o

Two possible routes for reduction of Cu_Z^o are considered: (1) reduction via intramolecular electron transfer (IET) from Cu_A (which is reduced by sodium ascorbate in a bimolecular step), or (2) direct bimolecular reduction of Cu_Z^o by sodium ascorbate, independent of the concomitant reduction of Cu_A. Kinetic models have been developed for both these possible pathways. The IET model is shown in Scheme 1.

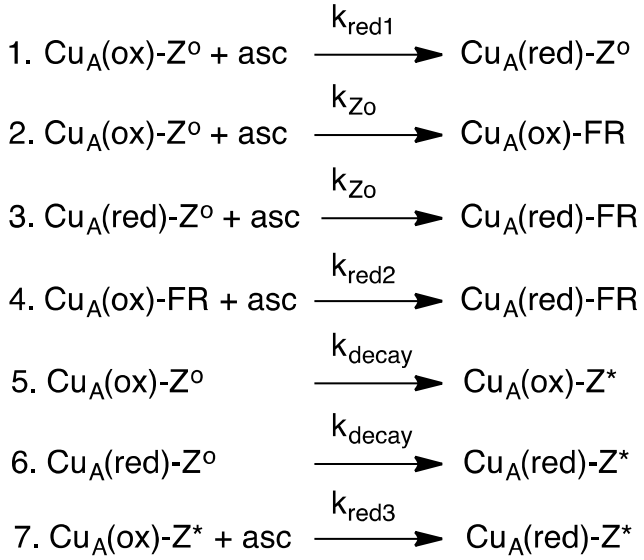


Scheme S1: Kinetic model for reduction of 1-hole Cu_Z^o via IET from Cu_A.

The IET model has 7 steps: 1) bimolecular reduction of Cu_A by sodium ascorbate in the presence of Cu_Z^o, 2) IET from Cu_A to Cu_Z^o, 3) IET from Cu_Z^o to Cu_A (since electron transfer between two copper sites has been shown to be potentially reversible in other enzymes with multiple copper sites),[4] 4) bimolecular reduction of Cu_A by sodium ascorbate in the presence of the fully reduced Cu_4S cluster, 5) decay of Cu_Z^o to Cu_Z* in the presence of oxidized Cu_A (which has been experimentally shown to occur in the

absence of a reductant, vide infra), 6) decay of Cu_Z^o to Cu_Z* in the presence of reduced Cu_A (assumed to be the same as in 5, since the Cu_Z^o decay to Cu_Z* is likely unaffected by the difference in Cu_A redox state), and 7) bimolecular reduction of Cu_A by sodium ascorbate in the presence of Cu_Z*.

The direct reduction model for Cu_Z^o reduction by sodium ascorbate is presented in Scheme S2.



Scheme S2: Kinetic model for reduction of 1-hole Cu_Z^o directly by sodium ascorbate.

The direct reduction model also contains 7 steps: 1) bimolecular reduction of Cu_A by sodium ascorbate in the presence of Cu_Z^o, 2) bimolecular reduction of Cu_Z^o by sodium ascorbate in the presence of oxidized Cu_A, 3) bimolecular reduction of Cu_Z^o by sodium ascorbate in the presence of reduced Cu_A, 4) bimolecular reduction of Cu_A by sodium ascorbate in the presence of the fully reduced Cu_4S cluster, 5) decay of Cu_Z^o to Cu_Z* in the presence of oxidized Cu_A, 6) decay of Cu_Z^o to Cu_Z* in the presence of reduced Cu_A, and 7) bimolecular reduction of Cu_A by sodium ascorbate in the presence of Cu_Z*. Note that both models include five identical steps, (1), (4), (5), (6), and (7), which involve the bimolecular reduction of Cu_A or the decay of Cu_Z^o to Cu_Z*. The difference in the two is the nature of steps (2) and (3), which involve the reduction of Cu_Z^o.

To determine whether one of these kinetic models provides a better fit for the reduction of Cu_Z^o by sodium ascorbate (data in Figure 5A and 5B), two initial simplifying assumptions were made. First, we assumed that the rate of the bimolecular reduction of Cu_A by sodium ascorbate is independent of the state of the Cu_4S site. This assumption is reasonable, since the two sites are separated by ~10 Å with a large solvent-filled cavity between them. This allows the rate constant for steps (1), (4), and (7) in both models to be determined experimentally, by measuring the bimolecular rate of Cu_A reduction in the presence of Cu_Z*. This experiment has been performed and the data is reported in Figures 5C and 5D, with details of the kinetic fit below. From this experiment, the bimolecular rate of Cu_A reduction in the presence of Cu_Z* is 1.4 M^{-1} s^{-1} (R^2 = 0.9516 for Cu_A reduction). The second simplifying assumption is that the rate of decay of Cu_Z^o to Cu_Z* is independent of the redox state of Cu_A (which is also reasonable, due to the separation between the two sites, vide supra). This allows the rate constant for steps (5) and (6) in

both models to be determined by measuring the rate of decay of Cu_Z^o in the presence of oxidized Cu_A (in situ formation of Cu_Z^o without addition of sodium ascorbate, Figure S6).

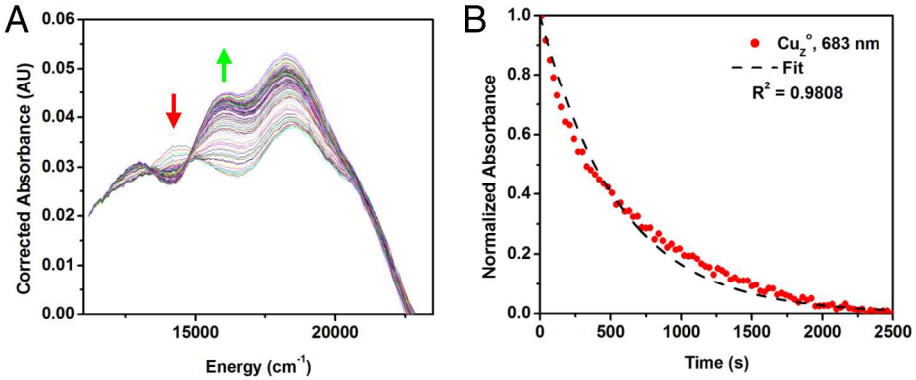


Figure S6: A) Decay of Cu_Z^o (red arrow) to Cu_Z* (green arrow). [N_2OR] = 30 μM (60% Cu_4S, 40% Cu_4S_2), [N_2O] = 30.5 μM. B) Normalized time dependence at 683 nm showing decay of Cu_Z^o, with single exponential fit (black line, R^2 = 0.9808).

The decay of Cu_Z^o to Cu_Z* can be observed at 683 nm and fit with a single exponential decay function, yielding a k_{decay} value of 1.8×10^{-3} s^{-1} (Figure S6B, black line, R^2 = 0.9808).

Using the experimentally determined values of $k_{red1} = k_{red2} = k_{red3}$ =1.4 M^{-1} s^{-1} and k_{decay} = 1.8×10^{-3} s^{-1}, the IET kinetic model (Scheme S1) was used to fit the time dependence of Cu_Z^o and Cu_A reduction by sodium ascorbate by optimizing the rates of intramolecular electron transfer (k_{IET} and k_{-IET}). The best fit is obtained with k_{IET} = 0.1 s^{-1} and k_{-IET} = 0.06 s^{-1} (R^2 = 0.9829, Figure S7A). This provides a good fit for the reduction

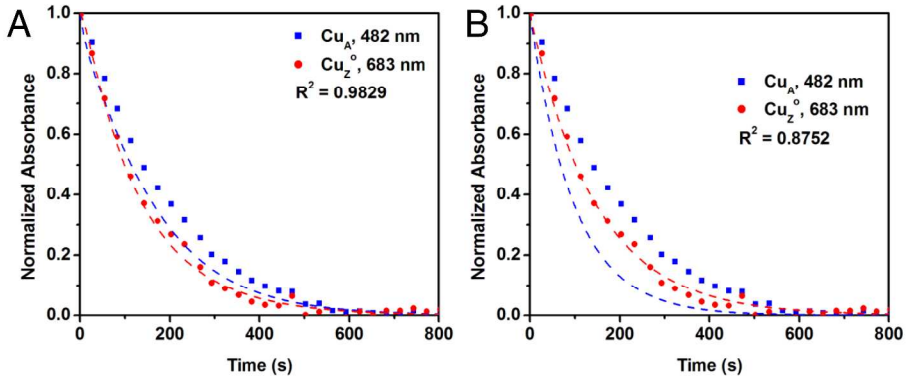


Figure S7: A) Fit of the reduction of Cu_Z^o and Cu_A by sodium ascorbate with the IET kinetic model, using experimentally determined values for $k_{red1} = k_{red2} = k_{red3}$ = 1.4 M^{-1} s^{-1} and $k_{decay} = k_{decay}$ = 1.8×10^{-3} s^{-1}. The fit was obtained using the chemical kinetics program Tenua with k_{IET} = 0.1 s^{-1} and K_{IET} = 3.3 (R^2 = 0.9829). B) Fit of the reduction of Cu_Z^o and Cu_A by sodium ascorbate with the direct reduction kinetic model, using experimentally determined values for $k_{red1} = k_{red2} = k_{red3}$ = 1.4 M^{-1} s^{-1} and $k_{decay} = k_{decay}$ = 1.8×10^{-3} s^{-1}. The fit was obtained using the chemical kinetics program Tenua with k_{Zo} = 0.69 M^{-1} s^{-1} (R^2 = 0.8752). For both, [N_2OR] = 20 μM, [asc] = 7.285 mM.

of Cu_Z^o (red line in Figure S7A) but predicts a slightly faster reduction of Cu_A (blue line in Figure S7A) than is observed experimentally. The same approach was also used to fit the data using the direct reduction model (Scheme S2), optimizing the bimolecular rate of Cu_Z^o reduction by sodium ascorbate (k_{Zo}). The best fit is obtained with a k_{Zo} of 0.69 M^{-1} s^{-1} (R^2 = 0.8752, Figure S7B). This yields a significantly worse fit for the experimental time dependence of Cu_A (blue line in Figure S7B) compared to the IET model, since the reduction of Cu_A is predicted to proceed much more quickly than experimentally observed (indeed, faster than the reduction of Cu_Z^o, red line in Figure S7B).

It is possible to improve the fits obtained with both kinetic models by allowing the rate of bimolecular reduction of Cu_A in the presence of Cu_Z^o (k_{red1}) to vary somewhat from the rate obtained experimentally in the presence of Cu_Z*, and then reoptimizing the rates of Cu_Z^o reduction (k_{IET} and k_{-IET} for the IET model, k_{Zo} for the direct reduction model). This leads to much better fits for the experimental data using both the IET model and the direct reduction model (Figure S8A and S8B, respectively).

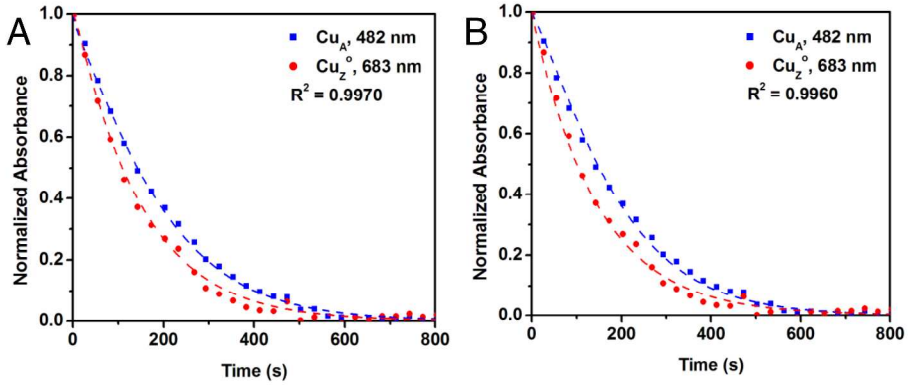


Figure S8: A) Fit of the reduction of Cu_Z^o and Cu_A by sodium ascorbate with Scheme 1, the reduction of Cu_Z^o via IET from Cu_A (R^2 = 0.9970). The fit was obtained using the chemical kinetics program Tenua with k_{red1} = 0.9 M^{-1} s^{-1}, k_{IET} > 0.1 s^{-1}, K_{IET} = 2.5, k_{decay} = 1.8×10^{-3} s^{-1}, k_{red2} = k_{red3} = 1.4 M^{-1} s^{-1}. B) Fit of the reduction of Cu_Z^o and Cu_A by sodium ascorbate with Scheme 2, the direct reduction of Cu_Z^o by sodium ascorbate (R^2 = 0.9960). The fit was obtained using the chemical kinetics program Tenua with k_{red1} = 0.17 M^{-1} s^{-1}, k_{Zo} = 0.69 M^{-1} s^{-1}, k_{red2} = k_{red3} = 1.4 M^{-1} s^{-1}, k_{decay} = 1.8×10^{-3} s^{-1}. For both, [N_2OR] = 20 μM, [asc] = 7.285 mM.

Note that the fit does not change as k_{IET} increases above 0.1 s^{-1}, as long as the same equilibrium constant for the IET is maintained (K_{IET} of 2.5). Thus, the k_{IET} value of 0.1 s^{-1} provided by this model represents a lower limit on the rate of IET from Cu_A to Cu_Z^o. In the case of the IET model, to obtain a good fit it is necessary to decrease k_{red1} from 1.4 M^{-1} s^{-1} to 0.9 M^{-1} s^{-1}, a decrease of ~35% (R^2 = 0.9970), within the range of reasonable variation in kinetic parameters. In contrast, for the direct reduction model, it is necessary to decrease k_{red1} from 1.4 M^{-1} s^{-1} to 0.17 M^{-1} s^{-1} to obtain a good fit for the data, with no change to the value of k_{Zo} (R^2 = 0.9960). An order of magnitude perturbation in the rate of reduction of Cu_A in the presence of Cu_Z^o versus resting 1-hole Cu_Z* is not chemically reasonable, since the two sites differ only in the position of the edge hydroxide ligand (vida infra), which is ~7 Å away from Cu_A. Thus, on the basis of these fits we strongly prefer the IET model as the best kinetic model for the reduction of Cu_Z^o.

*S1.2 Kinetic model for fitting the reduction of Cu_A in the presence of Cu_Z**

$$Cu_A(ox)\text{-}Z^* + asc \xrightarrow{k_1} Cu_A(red)\text{-}Z^*$$

$$Cu_A(red)\text{-}Z^* \xrightarrow{k_{IET}} Cu_A(ox)\text{-}FR$$

$$Cu_A(ox)\text{-}FR + asc \xrightarrow{k_2 = k_1} Cu_A(red)\text{-}FR$$

Scheme S3: Kinetic model for the reduction of Cu_A in the presence of Cu_Z*. To obtain an upper limit for rate of the unobserved reduction of Cu_Z* by intramolecular electron transfer from Cu_A, the possibility of IET was included in Step 2. The fit shown in Figure 5D was obtained from this model using the chemical kinetics program Tenua with $k_1 = k_2 = 1.4\ M^{-1}\ s^{-1}$, $k_{IET} < 1\times10^{-5}\ s^{-1}$.

S1.3 Details of Data Normalization For Kinetics Fitting:

Normalized time dependence for the reduction of Cu_A, Cu_Z^o, and Cu_Z* were generated as follows. For Cu_A, absorption data at 482 nm, in a band of Cu_A that has no overlap with other components of the spectra, were normalized. For Cu_Z^o, data were used from 683 nm, and for Cu_Z*, 653 nm, near the absorption maxima of the two species. At these wavelengths, some overlap with the bands of Cu_A contributes to the change with time. To correct for the contribution of Cu_A to the change with time at 683 nm and 653 nm, the absorption spectrum of Cu_A (Figure S2A, red) was used to estimate the amount of Cu_A present at each wavelength with respect to the intensity of Cu_A at 482 nm (0.5 and 0.35 at 683 nm and 653 nm, respectively). This Cu_A contribution was subtracted from the time dependent data at 683 nm and 653 nm and the data normalized to generate time dependence for the reduction of Cu_Z^o and Cu_Z*.

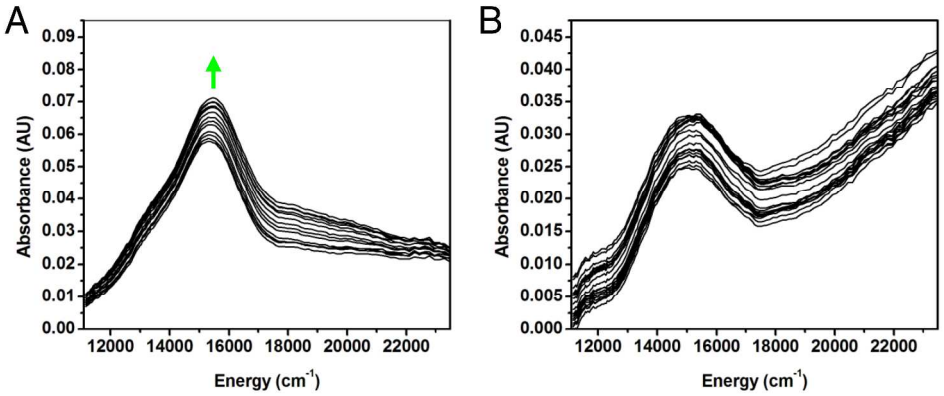


Figure S9: A) Second phase of reactivity observed after reduction of Cu_Z^o and Cu_A by sodium ascorbate (20 μM N_2OR, 7.3 mM ascorbate), from 800-1500 s, spectra shown every 5 minutes. B) Reaction of 20 μM fully reduced N_2OR with 200 μM N_2O (in the presence of excess sodium ascorbate (10 mM). Spectra shown every 5 minutes for 300 min. Note that the only change observed is spectral noise.

Linear Regression Statistics	**Arrhenius Plot** (1/T vs lnk, Figure 6A)	**Eyring Plot** (1/T vs ln(k/T), Figure 6B)
R^2	0.8298	0.8119
Uncertainty of Regression ($s_{y/x}$)	0.526	0.347
Slope ($b \pm s_b$)	$(-5.1 \pm 0.8) \times 10^3$	$(-4.8 \pm 0.5) \times 10^3$
Intercept ($a \pm s_a$)	24±3	18±2
Degrees of Freedom (n-2)	21	21

Table S2: Details of linear regression analyses for Arrhenius and Eyring plots in Figures 6A and 6B (respectively).

S2. Error Propagation for Thermodynamic Values Derived from Linear Regression Analysis.

Arrhenius Plot (Figure 6A)

$\Delta E_A = -Rb$ $\qquad$ $s_{Ea} = -Rs_b$

R is the ideal gas constant (1.9872 kcal K^{-1} mol^{-1})

Eyring Plot (Figure 6B)

$\Delta H^{\ddagger} = -Rb$ $\qquad$ $s_H = -Rs_b$

$\Delta S^{\ddagger} = R\left[a - \ln\frac{\kappa_B}{h}\right]$ $\qquad$ $s_S = Rs_a$

$\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$ $\qquad$ $s_G = \sqrt{(s_H)^2 + (Ts_S)^2}$

κ_B is Boltzmann's Constant (1.3807×10^{-34} J K^{-1})

h is Planck's Constant (6.626×10^{-34} J s)

R is the ideal gas constant (1.9872 kcal K^{-1} mol^{-1})

T is the temperature in Kelvin. The reported value of $\Delta G^{\ddagger}$ is calculated with T = 293 K

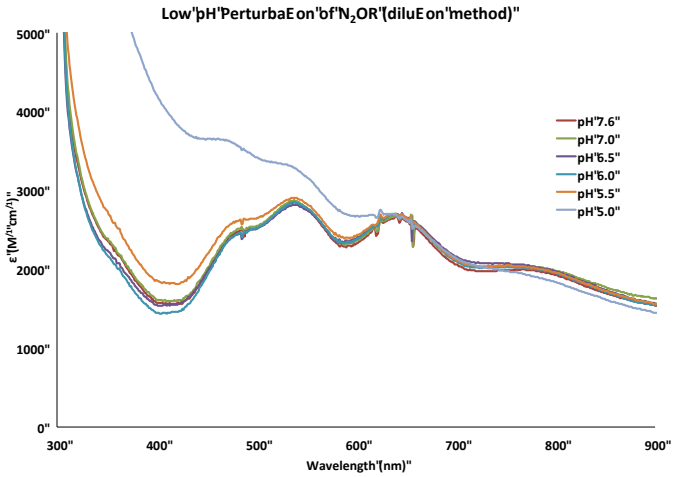


Figure S10: Absorption spectra of resting oxidized N_2OR, containing 1-hole Cu_Z* and oxidized Cu_A, obtained by diluting concentrated aliquots of N_2OR in buffer with different pH values. Indicates no pH dependence of the spectral features of Cu_A up to pH 5.5 and denaturation of the protein at pH 5.0.

S3. Computational modeling of resting Cu_Z*

The spectral features of resting 1-hole Cu_Z* have been previously described and correlated to a computational model in Ref. [3]. A simple computational model with a hydroxide bridged Cu_I-Cu_{IV} edge and 7 ligating His residues was found to reproduce the spin distribution and absorption spectrum of Cu_Z*, which are close to identical at low and high pH (pH 6 and 10.5). However, a pH effect on the vibrations of resting Cu_Z* is observed with a pKa of 9.2. A Cu-S vibration observed at 415 cm^{-1} in low pH Cu_Z* shifts up in energy to 424 cm^{-1} and shows O^{18} isotope sensitivity (-9 cm^{-1}), while there is no O^{18} isotope sensitivity in low pH Cu_Z*. This indicates that at high pH there is coupling between one of the Cu-S stretches and a vibration of the edge hydroxide, which does not occur at low pH. This pH effect was attributed to the deprotonation of Lys397 near the Cu_I-Cu_{IV} edge. When a protonated Lys397 was added to model low pH Cu_Z*, this residue moves from its crystallographic position to directly hydrogen bond to the edge hydroxide ligand, which then coordinates terminally to Cu_I. Upon deprotonation of Lys397, this residue remains in its crystallographic position and the hydroxide ligand bridges the Cu_I-Cu_{IV} edge. This structural change does not significantly perturb the calculated spin distribution, but is predicted to affect the kinematic coupling between the Cu-OH and Cu-S vibrations. While this previously proposed model reproduces the spectral features of low and high pH Cu_Z*, the significant movement of Lys397 is not consistent with the structural characterization by X-ray crystallography.

In this study, we extend the active site model in Ref. [3] to include Glu435, which is the hydrogen-bonding partner of Lys397 in all published crystal structures of N_2OR. When Glu435 is included, after optimization the protonated form of Lys397 remains hydrogen-bonded to Glu435 and does not interact with the edge hydroxide. This refined model reproduces well the spin distribution (Table S3), vibrations (Figure S11A) and absorption spectrum (Figure S12) of low pH Cu_Z*. In addition, when the protonated Lys is required to interact with the hydroxide, as in the previous computational model, a

significant perturbation of the spin distribution in the cluster is observed, inconsistent with the lack of change in the EPR between low and high pH Cu_Z*. Thus, we modeled the low pH Cu_Z* site with a hydroxide ligand bridging the Cu_I-Cu_{IV} edge and the protonated Lys397 4.02 Å away from and not interacting with the hydroxide. In this model, deprotonation of Lys397 leads to a change in the position of the edge hydroxide ligand due to a through-space charge effect (the presence or absence of a +1 charge near the edge ligand). Both the Cu_I-OH and Cu_{IV}-OH bonds become shorter by 0.02 Å, leading to a 10 cm^{-1} increase in energy of the Cu_I-OH vibration (Figure S11). The Cu-S vibrations are only slightly perturbed in energy and do not show new O^{18} sensitivity, indicating that the Cu-OH and Cu-S vibrations are insufficiently coupled in this model. The spin distribution and TD DFT predicted absorption spectrum (Table S3, Figure S12) remain close to identical to the low pH model with the protonated Lys397. Thus, the hydroxide bridged model with a protonated Lys397 hydrogen-bonded to Glu435 produces a small pH effect between low and high pH that involves perturbation only of the vibrations, where one vibration shifts up in energy. Since this model also reproduces the crystallographic position of Lys397, it is used as the model for resting 1-hole Cu_Z*.

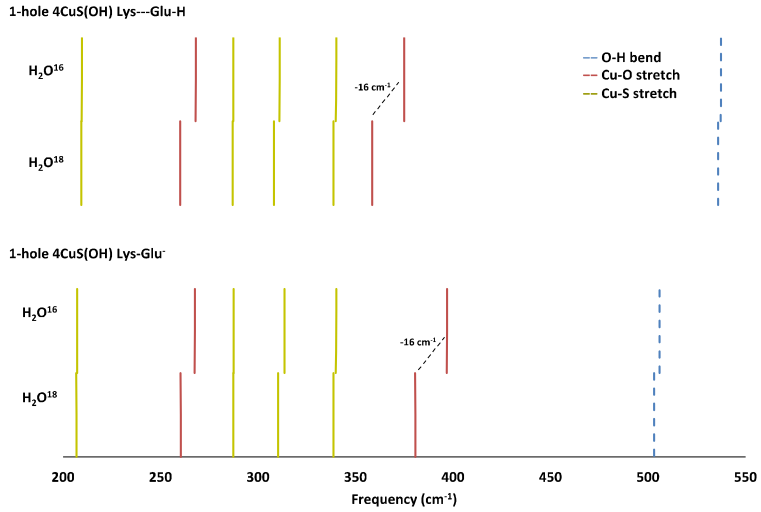


Figure S11: Energies of important vibrations of OH bridged models and their O^{16}/O^{18} sensitivies with protonated (top) and deprotonated (bottom) Lys397 in its crystallographic position and hydrogen bonded to Glu435. Vibrations are described as Cu-S stretches (yellow), Cu-OH stretches (red) or OH bending (blue dashes). (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

Edge Ligand	Mulliken Atomic Spin Density					
	Cu_I	Cu_{II}	Cu_{III}	Cu_{IV}	S^{2-}	OH
OH^-	**0.30**	0.09	0.04	**0.10**	0.30	0.09
OH^- $LysH^+$	**0.26**	**0.12**	0.07	**0.12**	0.26	0.08
OH^- Lys	**0.24**	**0.10**	0.05	**0.14**	0.31	0.09
OH^----$LysH^+$	**0.16**	**0.16**	0.07	**0.14**	0.31	0.06

Table S3: Mulliken atomic spin density distributions for Cu_Z* models with a hydroxide bridged edge and A) no Lys397 or Glu435, B) Lys397 protonated and not interacting with the hydroxide, C) Lys397 deprotonated and not interacting with the hydroxide, and D) Lys397 protonated and directly hydrogen bonding with the hydroxide. (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

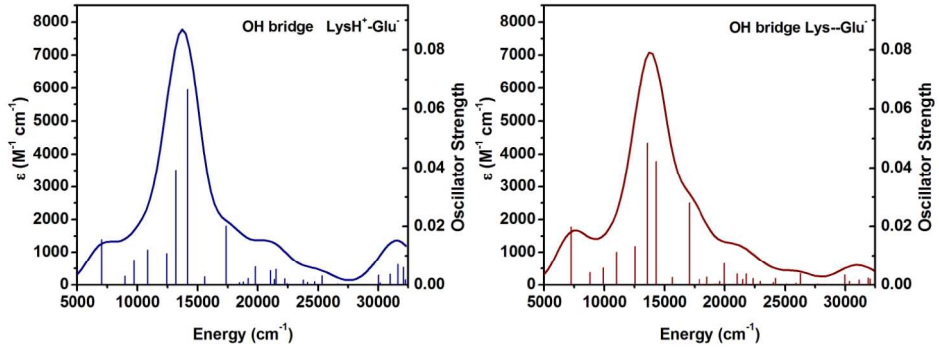


Figure S12: TD DFT predicted absorption spectra of OH bridged models with protonated (blue) and deprotonated (red) Lys397 at its crystallographic position and hydrogen-bonded to Glu435. (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

Bond Lengths (Å)	**OH bridge $LysH^+$-Glu**	**OH bridge Lys-Glu**	**OH_2 near Cu_{IV} $LysH^+$-Glu^-**	**Cu_{IV}-OH $LysH^+$-Glu^-**
Cu_I-S_1	2.440	2.456	2.362	2.331
Cu_{II}-S_1	2.258	2.259	2.275	2.265
Cu_{III}-S_1	2.237	2.236	2.229	2.267
Cu_{IV}-S_1	2.250	2.256	2.183	2.191
Cu_I-O	2.002	1.978	3.386	3.503
Cu_{IV}-O	2.093	2.077	2.264	1.931
OH---Lys	4.022	4.501	3.334	2.640

Table S4: Important bond lengths for computational models with different Cu_I-Cu_{IV} edge ligands. (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

Cu_Z* (OH bridge)		**OH_2**		**Cu_{IV}-OH**	
Energy (cm^{-1}) (O^{18} shift)	*Vibration*	*Energy (cm^{-1}) (O^{18} shift)*	*Vibration*	*Energy (cm^{-1}) (O^{18} shift)*	*Vibration*
375 (-16)	Cu_I-OH			467 (-16)	Cu_{IV}-OH
340 (-1)	Cu_{IV}-S-Cu_{II}	392 (0)	Cu_{IV}-S	386 (-2)	Cu_{IV}-S
311 (-2)	Cu_{III}-S-Cu_{IV} sym	338 (0)	Cu_{III}-S	333 (0)	Cu_I-S-Cu_{IV}
287 (0)	Cu_{III}-S-Cu_{IV} antisym	296 (0)	Cu_{II}-S	281 (0)	Cu_{III}-S
268 (-8)	Cu_{IV}-OH				
210 (0)	Cu_I-S	210 (0)	Cu_I-S	234 (0)	Cu_I-S
		202 (-16)	Cu_{IV}-OH_2		
		121 (-2)	Cu_I-OH_2		

Table S5: Energies of vibrational frequencies computationally predicted for the Cu_Z* model and the Cu_Z^o models, with their predicted H_2O^{16}/H_2O^{18} isotope shifts and the nature of the vibration. (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

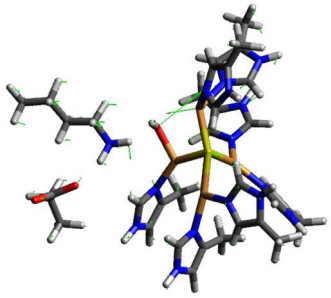


Figure S13: Transition state obtained for decay of Cu_Z^o to Cu_Z*, $\Delta G^{\ddagger}$ = 6 kcal/mol. (B3LYP, tzvp on Cu_4SON_7, NH_3^+ and CO_2^-, sv on remainder, PCM=10)

S4. Estimates of λ_{total}, H_{DA}, and $\Delta\Delta G^o$ values for reduction of Cu_Z^o and Cu_Z* by Cu_A

In order to determine the total reorganization energy (λ_{total}) for PCET from Cu_A to Cu_Z^o or Cu_Z*, estimates of $\lambda_{total} = \lambda_i + \lambda_o$ for Cu_A, Cu_Z^o, and Cu_Z* are required. The total reorganization energy of Cu_A has been experimentally determined to be 0.3-0.4 eV[5] and values for Cu_Z^o and Cu_Z* can be estimated from the computational models in Figure 8. The reduction of Cu_Z^o and resting Cu_Z* to fully reduced Cu_Z* is a proton-coupled electron transfer (PCET) process. The inner sphere reorganization energy for a PCET process is given by ½[E_{ox}(red geom) - E_{ox}(ox geom) + E_{red}(ox geom) - E_{red}(red geom)]. For a concerted PCET process, following Refs [6] and [7], E_{ox}(red geom) is obtained by calculating the oxidized energy at a reduced geometry without the additional proton, and E_{red}(ox geom) is obtained by calculating the reduced energy at an oxidized geometry with the addition of the proton., These calculations yield λ_i values of 0.32 eV for Cu_Z^o and 0.42 eV for Cu_Z*. These values seem low relative to the inner sphere reorganization energies observed for other multinuclear copper sites (e.g. λ_i = 1.1 eV for the one electron reduction of the $3Cu^{II}$ NI intermediate in the multicopper oxidases).[4] However, in Cu_Z^o and Cu_Z* the nuclear reorganization is distributed over four coppers, with spin dominantly on two, which may contribute to the lower calculated inner sphere reorganization energy.[8] λ_o for Cu_Z^o is dependent on charge delocalization[8] and is estimated to be midway between that of the blue copper center (localized, λ_o of 0.32 eV)[5] and Cu_A (delocalized, λ_o of 0.15 eV)[5] leading to a λ_o contribution of 0.24 eV for Cu_Z^o and Cu_Z*. This produces calculated $\lambda_{total} = \lambda_i + \lambda_o$ values of 0.56 eV for Cu_Z^o and 0.61 eV for Cu_Z*. The difference between these values is small, justifying treating λ_{total} for these as equal. The total reorganization energy for PCET from Cu_A to Cu_Z^o or Cu_Z* is the average of the reorganization energies of Cu_A (0.3-0.4 eV) and Cu_Z^o (0.56-1.24 eV). This leads to a $\lambda_{A->Z}$ range of 0.5 to 0.75 eV, and the following analysis considers the wider range of 0.5-1 eV.

We assume that the H_{DA} values for ET from Cu_A to both Cu_Z^o and Cu_Z* are similar as there are only small structural changes that would not change the electron transfer pathway. A range of H_{DA} values of 0.001-0.5 cm^{-1} was evaluated based on experimental and calculated values for the superexchange pathway in the multicopper oxidases.[9]

For all pairs of H_{DA} and λ values in these ranges, a ΔG^o range for Cu_Z^o relative to Cu_A between -4.6 kcal/mol (for the limit where λ=1 eV and H_{DA}=0.001 cm^{-1}) and +11.1 kcal/mol (for the limit where λ=0.5 eV and H_{DA}=0.5 cm^{-1}) is obtained that will produce a k_{ET} greater than 0.1 s^{-1}. Then sets of ΔG^o, λ, and H_{DA} values were used to determine the range of $\Delta\Delta G^o$ values between Cu_Z^o and resting Cu_Z* that reproduce the observed ratio of ET rate differences of at least 4 orders of magnitude (Figure S14). This approach gives a range of $\Delta\Delta G^o$ of +5-10 kcal/mol. This is comparable to the calculated $\Delta\Delta G^o$ of 6.4 kcal/mol between the computational models of Cu_Z^o and resting Cu_Z*.

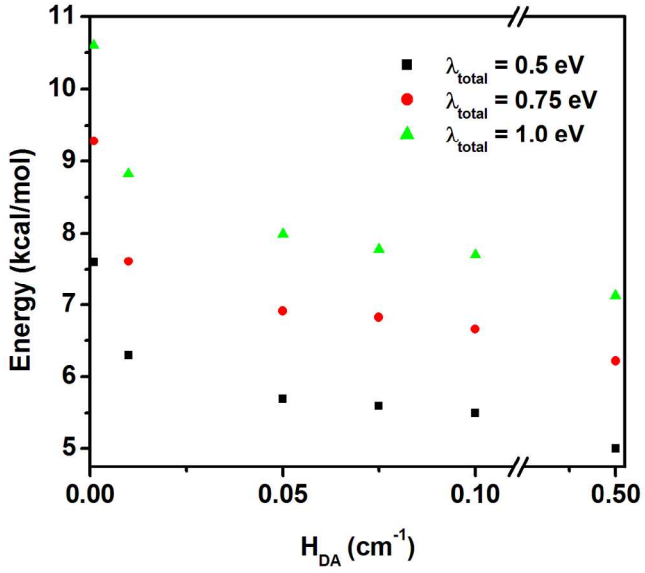


Figure S14: Dependence of calculated $\Delta\Delta G^{o}$ (Cu_Z^{o}-Cu_Z*) on H_{DA} for different values of λ_{total}**.** Black: λ=0.5 eV (the calculated value from DFT models), Red: λ=0.75 eV, Blue: λ=1 eV.

S5. Supporting Discussion of the Computational Reaction Coordinate for N-O Bond Cleavage.

S5.1 Isomers of N_2O bound to the fully reduced Cu_4S cluster. The lowest energy isomer formed from N_2O coordination to the fully reduced Cu_4S cluster has a linear N_2O molecule terminally N-coordinated to Cu_I. However, upon N-O bond elongation by 0.1-0.2 Å to start the N-O bond cleavage reaction, the structure rearranges to form a μ-1,3 coordination geometry, with the O of N_2O coordinating to Cu_{IV} and hydrogen-bonded to Lys397. This suggests that the N-O bond cleavage reaction proceeds via the μ-1,3 isomer, consistent with the formation of a terminal Cu_{IV}-OH intermediate as the product. The μ-1,3 isomer is not stable with the functional B3LYP, but is stable with the functional BP86 with 10% Hartree-Fock exchange (hereafter called B10HFP86). The lower amount of Hartree-Fock (10% relative to 20% in B3LYP) increases the covalency of the metal-ligand bonds, resulting in a cluster with somewhat stronger backbonding to N_2O from Cu_I and Cu_{IV}, enhancing the stability of the bent μ-1,3 isomer and producing stable reactant structures for both the terminal Cu_I-N and μ-1,3 N_2O isomers (Figure S15). The terminal Cu_I-N isomer is lower in electronic energy by 1.7 kcal/mol and lower in free energy by 6.8 kcal/mol, but rearranges to the μ-1,3 during N-O bond elongation with both B3LYP and BP8610HF.

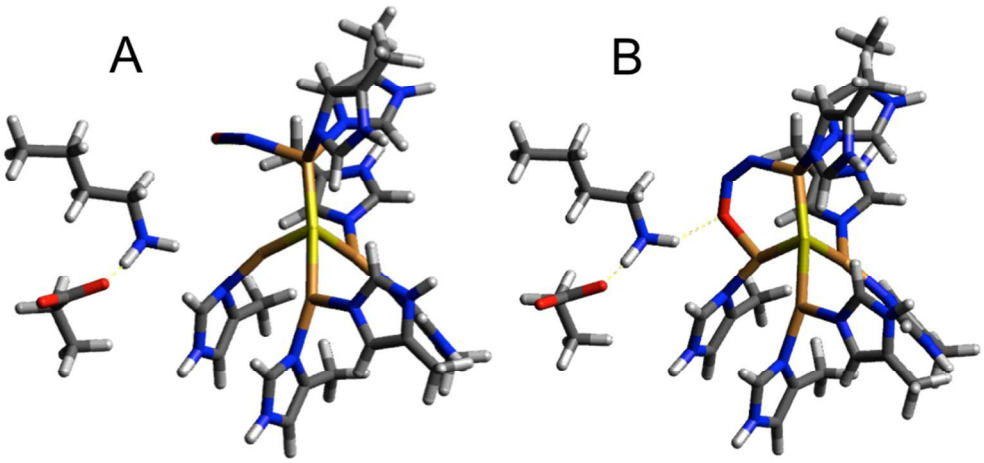


Figure S15: Structures of two isomers for N_2O coordination to fully reduced Cu_4S, (A) the lowest energy isomer, terminal Cu_I-N, and (B) μ-1,3. BP86 and 10% HF, PCM = 10.

S5.2 Comparison of μ-1,3 and terminal Cu_I-O transition states. After N-O bond elongation from the μ-1,3 isomer, a transition state (TS) for N-O bond cleavage is obtained at an N-O bond length of 1.81 Å (Figure 9C, 1.68 Å for B3LYP), as discussed in the main text. This TS occurs at a $\Delta G^{\ddagger}$ of 17.7 kcal/mol and a $\Delta E^{\ddagger}$ of 6.1 kcal/mol (relative to fully reduced and free N_2O; 17.3 kcal/mol and 10.3 kcal/mol, respectively, for B3LYP). An alternative possibility to μ-1,3 binding and cleavage of N-O, proposed previously in two studies, is the coordination and cleavage of N_2O via a μ-1,1-O or terminal Cu_I-O isomer.[10,11] While our computational model does not yield a stable point for end-on N_2O coordination via O to the fully reduced cluster in either a terminal or μ-1,1 mode, N_2O can be positioned near the Cu_I-Cu_{IV} edge with O oriented towards Cu_I and upon N-O elongation a TS is found for terminal N-O bond cleavage which has an N-O bond length of 1.34 Å, a Cu_I-O bond length of 2.07 and a Cu_{IV}-O distance of 2.42 Å (Figure S16). The terminal TS is ~9 kcal/mol higher in energy compared to the μ-1,3 TS described in the main text, with a $\Delta G^{\ddagger}$ of 26.4 kcal/mol and a $\Delta E^{\ddagger}$ of 19.7 kcal/mol using

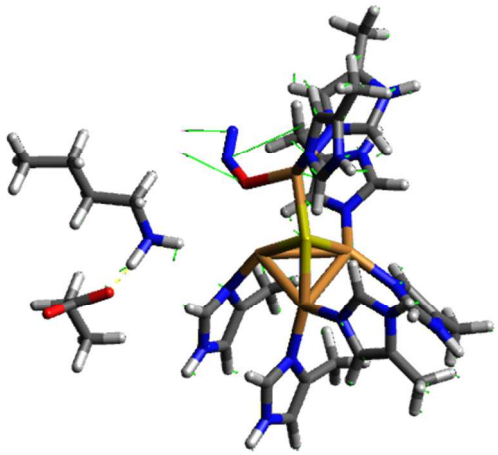


Figure S16: Transition state for N-O bond cleavage in a terminal Cu_I-O geometry. B3LYP, PCM = 10.

the B3LYP functional. The higher energy of the terminal TS arises from the absence of a hydrogen bond to the O of N_2O, as Lys397 is 4.25 Å away. A prior computational study found the μ-1,3 and terminal TS to be at similar energies, utilizing H_2O to hydrogen bond to the O in both transition states.[11] However, Lys397 is constrained by the protein and is only available as a hydrogen bond donor to N_2O in the μ-1,3 binding mode (to the O coordinated to Cu_{IV}). Additionally, a terminal Cu_I-O or μ-1,1-O-bridged structure would give a bridging oxo or hydroxo product after N-O cleavage, which would result in resting 1-hole Cu_Z* rather than 1-hole Cu_Z^o, where only the latter is capable of turnover. Thus, our model and the experimental identification of the Cu_Z^o intermediate as a terminal Cu_{IV}-OH hydrogen bonded to Lys397 indicate that N-O bond cleavage in nitrous oxide reductase proceeds via the μ-1,3 TS.

		Mulliken Atomic Spin Density						
		Cu_I	Cu_{II}	Cu_{III}	Cu_{IV}	S^{2-}	N_2	O
μ-1,3 N_2O	α,β LUMO	*0.14*	0.05	0.02	0.09	0.12	**0.43**	**0.09**
μ-1,3 TS	α LUMO	0.09	**0.14**	0.05	**0.20**	**0.18**	0.05	0.16
	β LUMO	*0.11*	0.05	0.03	*0.15*	0.11	**0.16**	**0.28**
Before H^+ transfer N-O 2.1 Å	α LUMO	0.09	**0.19**	0.08	**0.20**	**0.20**	0.01	0.11
	β LUMO	0.05	0.02	0.01	*0.16*	0.05	**0.12**	**0.48**
After H^+ transfer N-O 2.1 Å	α LUMO	**0.11**	**0.16**	**0.14**	**0.12**	**0.20**	0.01	0.09
	β LUMO	0.08	0.08	0.02	**0.27**	0.14	0.03	**0.24**
2-hole Cu_{IV}-OH after protonation	α LUMO	**0.29**	0.08	**0.17**	0.07	0.15	0.00	0.04
	β LUMO	0.06	**0.18**	0.03	**0.28**	0.17	0.00	0.13

Table S6: Mulliken distribution of α and β LUMOs of key structures along the N-O bond cleavage, O-H bond formation, and N_2 loss 3D potential energy surface, and for the 2-hole Cu_{IV}-OH intermediate after Lys397 protonation. BP86 with 10% HF, PCM of 10.

	Total Mulliken Atomic Spin Density						
	Cu_I	Cu_{II}	Cu_{III}	Cu_{IV}	S^{2-}	N_2	O
μ-1,3 TS N-O 1.81 Å, O-H 1.6 Å, Cu-N 2.0 Å	0.02	-0.08	-0.02	-0.04	-0.08	0.06	0.18
N-O 2.1 Å, O-H 1.6 Å, Cu-N 2.0 Å	-0.04	-0.16	-0.06	-0.04	-0.18	0.03	0.50
N-O 2.1 Å, O-H 1.02 Å, Cu-N 2.0 Å	-0.05	-0.14	-0.12	0.13	-0.13	0.01	0.32
2-hole Cu_{IV}-OH $LysH^+$	-0.24	0.10	-0.14	0.21	0.02	0.00	0.10

Table S7: Total Mulliken spin distribution for key structures along the N-O bond cleavage, O-H bond formation, and N_2 loss 3D potential energy surface, and for the 2-hole Cu_{IV}-OH intermediate after Lys397 protonation. BP86 with 10% HF, PCM of 10.

	Mulliken Charge						
	Cu_I	Cu_{II}	Cu_{III}	Cu_{IV}	S^{2-}	N_2	O
μ-1,3 N_2O	-0.17	0.04	0.04	0.08	-0.15	0.06	-0.34
μ-1,3 TS N-O 1.81 Å, O-H 1.6 Å, Cu-N 2.0 Å	-0.14	0.05	0.04	0.10	-0.13	0.09	-0.59
N-O 2.1 Å, O-H 1.6 Å, Cu-N 2.0 Å	-0.05	0.07	0.04	0.10	-0.17	0.09	-0.61
N-O 2.1 Å, O-H 1.02 Å, Cu-N 2.0 Å	-0.06	0.07	0.06	0.13	-0.13	0.10	-0.54
2-hole Cu_{IV}-OH $LysH^+$	0.15	0.13	0.07	0.10	-0.04	0.00	-0.61

Table S8: Atomic charges for key structures along the N-O bond cleavage, O-H bond formation, and N_2 loss 3D potential energy surface, and for the 2-hole Cu_{IV}-OH intermediate after Lys397 protonation. BP86 with 10% HF, PCM of 10.

S5.3 Stabilization of a Cu_{IV}-OH intermediate via rapid protonation or reduction. After proton transfer occurs at an N-O distance of 2.1 Å to form a hydroxide at Cu_{IV}, cleavage of the Cu_I-N bond is still required. A wider 2D potential energy scan of the N-O and Cu_I-N bond lengths shows that after the proton transfer from Lys397, further N-O elongation to 2.6 Å before loss of N_2 becomes energetically feasible (costing <2

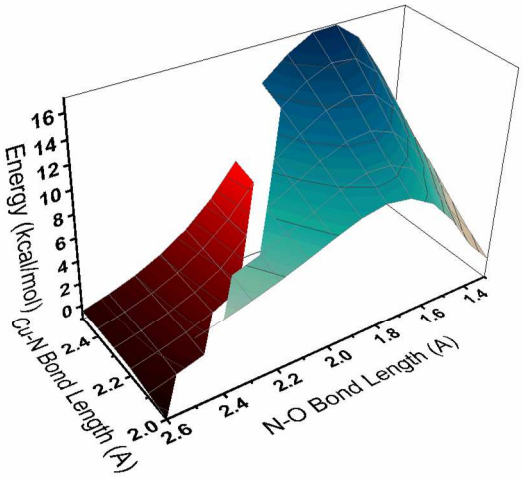


Figure S17: 2D potential energy surfaces for N-O bond cleavage and N_2 loss (Cu_I-N elongation) before (blue) and after (green) proton transfer from Lys397 to Cu_{IV}-OH. Red arrows track the lowest energy path from reactants to products. BP86 with 10% Hartree-Fock, PCM = 10.

kcal/mol, Figure S17). Further, the surfaces show that N_2 loss from Cu_I is coupled to movement of the hydroxide ligand from terminal coordination at Cu_{IV} to bridging Cu_{IV} and Cu_I, generating the undesired 2-hole μOH precursor to resting 1-hole Cu_Z*. However, these calculations neglect the possibility of a rapid proton uptake from solvent and electron transfer from Cu_A, both of which should take place after the proton transfer from Lys397 to form the Cu_{IV}-OH product. When an extra proton or electron is added to the model after proton transfer from Lys397, intermediates are formed with a hydroxide ligand terminally coordinated to Cu_{IV} and hydrogen bonded to Lys397 in either the 2-hole or 1-hole redox state (respectively, Figure S18). Further reduction or protonation, v respectively, yields the 1-hole Cu_{IV}-OH structure identified above as Cu_Z^o from

spectroscopy, with loss of N_2. The total proton and electron transfer process to form the 1-hole Cu_{IV}-OH with a protonated Lys is highly favorable, with $\Delta G = -51$ kcal/mol and $\Delta E = -50$ kcal/mol (Figure S18).Thus, a terminally coordinated hydroxide is obtained as the product of μ-1,3 N-O bond cleavage, as long as proton uptake from solvent is facile. This emphasizes the importance of the hydrogen bond from Lys397 to the Cu_{IV}-OH and the Lys397-Glu435 salt bridge, which anchors the position of Lys397. The hydrogen bond stabilizes the higher energy Cu_{IV}-OH product of N-O cleavage, which is required for rapid reduction of the catalytic site in turnover.

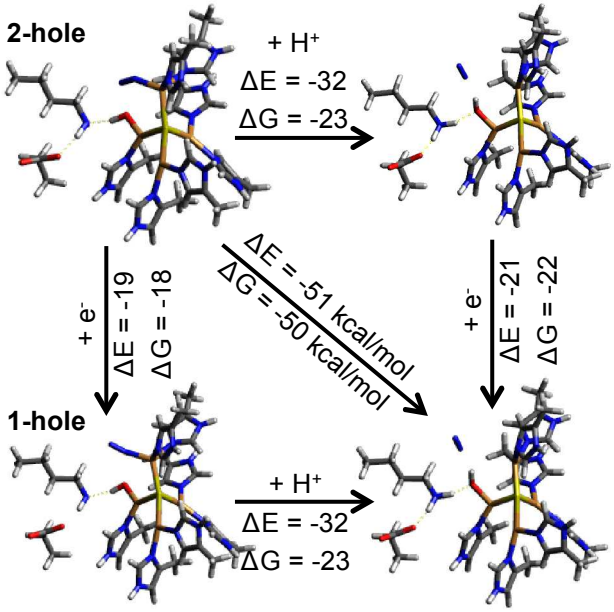


Figure S18: Scheme and energies for sequential protonation and reduction of the transient species with N-O 2.1 Å, O-H 1.02 Å, and Cu_I-N 2.0 Å formed after proton transfer from Lys397.

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X,Y,Z Coordinates for DFT Optimized Structures

Structures for Modeling of Cu_Z^o (Section 3.3.1)

1-hole μOH (resting Cu_Z* model, Figure 8A)

C 21.7600010000 43.4680050000 13.8479930000
C 22.4558030000 42.8488360000 15.0339310000
N 22.2113020000 41.5359110000 15.4628730000
C 23.3900370000 43.4111490000 15.8898950000
C 22.9694080000 41.3240390000 16.5404370000
N 23.7059930000 42.4349990000 16.8339960000
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H 20.7459450000 43.8166890000 14.1129460000
H 23.8447260000 44.3974740000 15.8999130000
H 23.0143350000 40.4056250000 17.1180540000
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C 26.3109760000 33.5561760000 10.6733760000
C 26.4405640000 35.0881410000 10.7661850000
C 25.1257750000 35.7975280000 11.1094070000
N 25.3724850000 37.2590480000 11.3849390000
H 27.5874530000 31.7799550000 10.4636470000
H 28.3222420000 33.0993550000 11.4207910000
H 25.7990660000 33.1764780000 11.5804540000
H 25.6675520000 33.2826060000 9.8132480000
H 27.1813960000 35.3283120000 11.5507030000
H 26.8425450000 35.4832660000 9.8116740000
H 24.3816970000 35.7087010000 10.2993380000
H 24.6873210000 35.3781540000 12.0304510000
H 25.7139260000 37.7359660000 10.5525880000
H 26.1270630000 37.3533340000 12.2044490000
H 24.5188520000 37.7399240000 11.6757860000
C 29.1669970000 39.2720060000 12.4009950000
C 29.0154040000 37.7536750000 12.1757540000
C 28.2650660000 37.0888630000 13.3425270000
O 26.9880670000 37.2504160000 13.3766800000
O 28.9169880000 36.4759890000 14.1999930000
H 28.1799220000 39.7657170000 12.4813370000
H 29.7298910000 39.4808120000 13.3302030000
H 28.4706530000 37.5724930000 11.2292400000
H 30.0105280000 37.2860680000 12.0826760000
C 23.2859940000 41.3879980000 11.0910050000
C 23.9386020000 40.8155630000 12.3282840000
N 23.5723070000 39.5785480000 12.8944380000
C 24.9382110000 41.3623870000 13.1152740000
C 24.3319840000 39.4051590000 13.9819850000
N 25.1660320000 40.4670240000 14.1610390000
H 23.6823880000 42.3966560000 10.8859070000
H 22.1914710000 41.4668120000 11.2144990000
H 25.4842740000 42.2963050000 13.0220680000
H 24.3036900000 38.5484870000 14.6487370000
H 25.8649390000 40.5607320000 14.8919850000
Cu 19.4269520000 36.8300150000 12.0251680000
Cu 20.8408900000 40.1837380000 14.8200160000
Cu 19.3413470000 40.4802630000 12.4452760000
Cu 21.7633410000 38.6505700000 12.7674420000
S 19.6944480000 38.6290700000 13.6510570000
O 21.3619250000 37.0024330000 11.5412770000
H 13.8799290000 34.4762830000 13.7295330000
H 18.2150450000 43.4462860000 18.7205060000
H 29.7149980000 39.7450310000 11.5641330000
H 28.2230190000 33.2330130000 9.6402860000
H 15.4279730000 35.4599150000 7.2361400000
H 20.1074390000 37.8802690000 6.8027230000
H 19.2079990000 46.6137020000 11.9841920000
H 22.3302560000 44.3374130000 13.4782430000
H 23.4805890000 40.7601930000 10.2013400000
H 21.8174810000 36.2553780000 11.9463480000

1-hole Cu_{IV}-OH_2 (Figure 8B)

C 21.7599990000 43.4680090000 13.8480060000
C 22.4459820000 42.8403980000 15.0355390000
N 22.1964310000 41.5290740000 15.4780600000
C 23.3872530000 43.4026060000 15.8830460000
C 22.9635360000 41.3241920000 16.5554410000
N 23.7060010000 42.4350060000 16.8339910000
H 21.6530710000 42.7463610000 13.0242090000
H 20.7497590000 43.8294190000 14.1093680000
H 23.8453260000 44.3873090000 15.8801520000
H 23.0069370000 40.4114740000 17.1422170000
H 24.3626240000 42.5393100000 17.6024830000
C 18.5339900000 45.9070000000 11.4619970000
C 18.5120850000 44.5774640000 12.1244580000
N 18.0960000000 44.3620030000 13.4380070000
C 18.8771480000 43.3327800000 11.6542680000
C 18.2205360000 43.0268340000 13.7181420000
N 18.6954010000 42.3816670000 12.6540780000
H 17.5290390000 46.3705560000 11.4295660000
H 18.8914720000 45.8067090000 10.4240430000
H 19.2605510000 43.0703000000 10.6733780000
H 17.9725700000 42.5871290000 14.6794280000
H 17.7517680000 45.0723300000 14.0783810000
C 17.4769980000 42.6500010000 18.5279980000
C 18.0603400000 41.6230030000 17.6330730000
N 17.3850150000 40.4789900000 17.2109920000
C 19.2959630000 41.5601010000 17.0225030000
C 18.2081010000 39.7781800000 16.3741300000
N 19.3704220000 40.4130850000 16.2405960000
H 16.5697060000 43.1115370000 18.0917540000
H 17.1874140000 42.2289820000 19.5103950000
H 20.1170040000 42.2659880000 17.0945500000
H 17.9243050000 38.8517370000 15.8869800000
H 16.4458610000 40.2050250000 17.4874070000
C 14.7849920000 33.8559930000 13.5820040000
C 16.0874110000 34.5921570000 13.6212840000
N 16.4240110000 35.4899720000 14.6370120000
C 17.1906730000 34.5881880000 12.7859030000
C 17.6810370000 35.9593790000 14.4140340000
N 18.1723750000 35.4486360000 13.2859380000
H 14.6646060000 33.1919130000 14.4595010000
H 14.7307300000 33.2301600000 12.6758280000
H 17.3332040000 34.0336850000 11.8619380000
H 18.1911050000 36.6525190000 15.0767620000
H 15.8458640000 35.7056620000 15.4453450000
C 16.3109890000 36.1229920000 7.1490050000
C 16.7885730000 36.5794000000 8.4923160000
N 16.0009960000 37.3420050000 9.3539940000
C 17.9823510000 36.4035470000 9.1751820000
C 16.7093710000 37.5992650000 10.4905030000
N 17.9180430000 37.0461630000 10.4108930000
H 16.0518530000 36.9771990000 6.4948470000
H 17.0964020000 35.5363120000 6.6445480000
H 18.8656930000 35.8576650000 8.8557970000
H 16.3144500000 38.1687520000 11.3268280000
H 15.0485150000 37.6463040000 9.1697000000
C 20.5880090000 38.8280660000 7.1139890000
C 19.9521760000 39.4021670000 8.3369930000
N 18.6039750000 39.7309910000 8.4179790000
C 20.4655980000 39.7552970000 9.5712210000
C 18.3497130000 40.2753500000 9.6420130000
N 19.4599220000 40.2980430000 10.3682920000

H 20.5347940000 39.5285580000 6.2585100000
H 21.6520500000 38.6091840000 7.3040150000
H 21.4944850000 39.6897810000 9.9054650000
H 17.3710860000 40.6328550000 9.9479840000
H 17.9250350000 39.6210030000 7.6696080000
C 27.6859860000 32.8789820000 10.5420250000
C 26.3467050000 33.6312350000 10.5290640000
C 26.5538900000 35.1520740000 10.6498650000
C 25.2505090000 35.9223880000 10.8797840000
N 25.5288890000 37.3620830000 11.2235650000
H 27.5369290000 31.7872500000 10.4436680000
H 28.2343680000 33.0608840000 11.4863400000
H 25.7196530000 33.2794650000 11.3731700000
H 25.7851860000 33.3963090000 9.6026280000
H 27.2290930000 35.3442360000 11.5032410000
H 27.0642930000 35.5319290000 9.7425160000
H 24.5888790000 35.8899330000 9.9978470000
H 24.7023900000 35.5004650000 11.7384800000
H 25.9511690000 37.8512600000 10.4367480000
H 26.2278820000 37.4009740000 12.1073280000
H 24.6643310000 37.8530680000 11.4568640000
C 29.1670110000 39.2719820000 12.4010040000
C 29.0711350000 37.7500140000 12.1806060000
C 28.2887650000 37.0781420000 13.3194040000
O 27.0074560000 37.2261940000 13.3084980000
O 28.9169400000 36.4760800000 14.1999790000
H 28.1639920000 39.7381810000 12.4351600000
H 29.6816620000 39.5028280000 13.3526530000
H 28.5786990000 37.5436460000 11.2113140000
H 30.0820640000 37.3105000000 12.1389880000
C 23.2860320000 41.3879620000 11.0909510000
C 23.9586650000 40.8286480000 12.3229000000
N 23.6301540000 39.5719820000 12.8604660000
C 24.9337740000 41.3821850000 13.1326650000
C 24.3744500000 39.3882650000 13.9556320000
N 25.1660540000 40.4669650000 14.1610660000
H 23.6901540000 42.3878340000 10.8602000000
H 22.1964350000 41.4905820000 11.2335010000
H 25.4617680000 42.3287140000 13.0693910000
H 24.3645110000 38.5139550000 14.5996400000
H 25.8610620000 40.5632460000 14.8965390000
Cu 18.9626520000 36.9103590000 12.1079000000
Cu 20.8248920000 40.1499670000 14.8427770000
Cu 19.3468520000 40.5185510000 12.4066230000
Cu 21.8653680000 38.7491510000 12.7827000000
S 19.8052290000 38.6279380000 13.4936820000
O 22.1994290000 37.2079190000 11.1580620000
H 13.9222630000 34.5495650000 13.5690710000
H 18.2089110000 43.4534070000 18.7120900000
H 29.7379220000 39.7569770000 11.5866420000
H 28.3373830000 33.2044130000 9.7074570000
H 15.4114900000 35.4833770000 7.2319720000
H 20.0960390000 37.8868460000 6.8027410000
H 19.2052960000 46.6169070000 11.9830480000
H 22.3429850000 44.3308800000 13.4842230000
H 23.4603560000 40.7450670000 10.2086690000
H 22.0413290000 36.2987380000 11.4463150000
H 21.6318700000 37.3342950000 10.3850560000

1-hole Cu_{IV}-OH---Lys397-Glu (Cu_Z^0 model, Figure 8C)

C 21.7599990000 43.4680020000 13.8479980000
C 22.4523200000 42.8441320000 15.0334940000
N 22.1964360000 41.5356720000 15.4744090000
C 23.3947850000 43.4042640000 15.8817350000
C 22.9575020000 41.3278560000 16.5528830000
N 23.7060000000 42.4350030000 16.8340020000
H 21.6478480000 42.7425980000 13.0278930000
H 20.7498030000 43.8267150000 14.1144150000
H 23.8581720000 44.3865290000 15.8797200000
H 22.9963880000 40.4142420000 17.1385950000
H 24.3635130000 42.5348330000 17.6018780000
C 18.5339990000 45.9070010000 11.4619990000
C 18.5106670000 44.5709980000 12.1224510000
N 18.0959970000 44.3620020000 13.4380000000
C 18.8680060000 43.3188980000 11.6598590000
C 18.2147350000 43.0263220000 13.7233700000
N 18.6837800000 42.3708620000 12.6645750000
H 17.5290140000 46.3707510000 11.4318160000
H 18.8912250000 45.8095940000 10.4234990000
H 19.2487300000 43.0462780000 10.6803470000
H 17.9679460000 42.5942730000 14.6885420000
H 17.7579980000 45.0767570000 14.0764360000
C 17.4769990000 42.6500010000 18.5280040000
C 18.0550520000 41.6260490000 17.6320580000
N 17.3850000000 40.4790030000 17.2109940000
C 19.2879720000 41.5728400000 17.0175480000
C 18.2132130000 39.7877290000 16.3694200000
N 19.3681610000 40.4312250000 16.2341710000
H 16.5671080000 43.1136750000 18.0985370000
H 17.1918840000 42.2313390000 19.5131000000
H 20.1047020000 42.2843270000 17.0880550000
H 17.9372470000 38.8615830000 15.8771320000
H 16.4485970000 40.1987630000 17.4892070000
C 14.7849990000 33.8559990000 13.5820000000
C 16.0767950000 34.6106410000 13.6086000000
N 16.4240050000 35.4900020000 14.6369970000
C 17.1597560000 34.6431790000 12.7471760000
C 17.6691410000 35.9840440000 14.3911150000
N 18.1392200000 35.5072640000 13.2415160000
H 14.6880670000 33.1794510000 14.4530990000
H 14.7249080000 33.2400550000 12.6692700000
H 17.2881540000 34.1129070000 11.8069850000
H 18.1837380000 36.6773720000 15.0496900000
H 15.8622190000 35.6820290000 15.4621910000
C 16.3109970000 36.1229970000 7.1490030000
C 16.7874810000 36.5796060000 8.4906830000
N 16.0010030000 37.3420050000 9.3539980000
C 17.9823240000 36.4024680000 9.1703040000
C 16.7138240000 37.5955620000 10.4893150000
N 17.9199780000 37.0418130000 10.4053280000
H 16.0561960000 36.9760260000 6.4909420000
H 17.0957900000 35.5328450000 6.6472990000
H 18.8692800000 35.8647640000 8.8470020000
H 16.3232430000 38.1664060000 11.3265040000
H 15.0490280000 37.6476630000 9.1715140000
C 20.5880010000 38.8279970000 7.1139970000
C 19.9472490000 39.3756760000 8.3460420000
N 18.6040010000 39.7310030000 8.4180000000
C 20.4539470000 39.6844510000 9.5939220000
C 18.3524820000 40.2589580000 9.6514840000
N 19.4550190000 40.2382800000 10.3897290000

H 20.5555470000 39.5528480000 6.2772400000
H 21.6462510000 38.5889290000 7.3117750000
H 21.4593130000 39.5129530000 9.9618000000
H 17.3798720000 40.6353570000 9.9544090000
H 17.9305720000 39.6493650000 7.6618760000
C 27.6860020000 32.8789990000 10.5420080000
C 26.2773210000 33.4563070000 10.6811080000
C 26.3223000000 34.9857810000 10.8080850000
C 24.9565680000 35.5808510000 11.1250000000
N 25.0273810000 37.0530550000 11.3984880000
H 27.6694870000 31.7770460000 10.4410590000
H 28.3051700000 33.1251350000 11.4262890000
H 25.7847390000 33.0271850000 11.5768400000
H 25.6539560000 33.1656170000 9.8114530000
H 27.0262870000 35.2614560000 11.6149750000
H 26.7187110000 35.4259580000 9.8705780000
H 24.2411750000 35.4296130000 10.2985090000
H 24.5268150000 35.1189400000 12.0302320000
H 25.3824120000 37.5507620000 10.5842000000
H 25.6920220000 37.2393370000 12.1932480000
H 24.0158060000 37.3588000000 11.5527160000
C 29.1670050000 39.2719840000 12.4010110000
C 28.9458580000 37.7601960000 12.1718720000
C 28.2192440000 37.0834040000 13.3575720000
O 26.9499870000 37.2161630000 13.4019360000
O 28.9169650000 36.4760630000 14.1999830000
H 28.2039150000 39.8010240000 12.5354840000
H 29.7841020000 39.4513660000 13.3020100000
H 28.3483950000 37.6134510000 11.2517200000
H 29.9209020000 37.2629690000 12.0227700000
C 23.2859700000 41.3880150000 11.0909900000
C 23.9365500000 40.8553400000 12.3448640000
N 23.5147940000 39.6704790000 12.9554540000
C 24.9839590000 41.3554690000 13.0996240000
C 24.2737370000 39.4576290000 14.0261850000
N 25.1660560000 40.4669240000 14.1610160000
H 23.6815180000 42.3886500000 10.8480140000
H 22.1917140000 41.4702720000 11.2110660000
H 25.5939970000 42.2452700000 12.9774340000
H 24.2016720000 38.6179760000 14.7098730000
H 25.8898430000 40.5316960000 14.8708350000
Cu 19.0066650000 36.9774010000 12.0819750000
Cu 20.8223540000 40.1739600000 14.8116030000
Cu 19.3372210000 40.4785300000 12.4515630000
Cu 21.8064780000 38.7079860000 12.7703620000
S 19.7811080000 38.5718980000 13.5949750000
O 22.4174880000 37.4517010000 11.4373620000
H 13.9112140000 34.5359900000 13.5910280000
H 18.2098910000 43.4537190000 18.7082540000
H 29.6887550000 39.7326930000 11.5403300000
H 28.2008410000 33.2870790000 9.6499790000
H 15.4091100000 35.4859750000 7.2295520000
H 20.0905700000 37.9008700000 6.7689260000
H 19.2068160000 46.6134530000 11.9858030000
H 22.3382540000 44.3314780000 13.4773640000
H 23.4813630000 40.7275370000 10.2260720000
H 21.8744140000 36.6633010000 11.3442120000

Transition state for 1-hole Cu_{IV}-OH decay to 1-hole μOH

C 21.7600010000 43.4680030000 13.8480010000
C 22.4524990000 42.8479970000 15.0352370000
N 22.1965180000 41.5402690000 15.4755920000
C 23.3957660000 43.4064530000 15.8834810000
C 22.9576830000 41.3289800000 16.5524210000
N 23.7059820000 42.4349840000 16.8339830000
H 21.6471670000 42.7383470000 13.0316910000
H 20.7500420000 43.8284720000 14.1131870000
H 23.8605200000 44.3880680000 15.8831650000
H 22.9960670000 40.4144260000 17.1365510000
H 24.3643770000 42.5337250000 17.6012710000
C 18.5340090000 45.9070120000 11.4620020000
C 18.5064880000 44.5736140000 12.1219230000
N 18.0959800000 44.3619940000 13.4379910000
C 18.8588410000 43.3236140000 11.6529730000
C 18.2124270000 43.0251170000 13.7181540000
N 18.6756480000 42.3740660000 12.6544180000
H 17.5314420000 46.3762800000 11.4337860000
H 18.8878780000 45.8074260000 10.4225810000
H 19.2358240000 43.0544620000 10.6710930000
H 17.9676750000 42.5890840000 14.6822080000
H 17.7619830000 45.0755980000 14.0798070000
C 17.4770120000 42.6499860000 18.5280060000
C 18.0584090000 41.6190650000 17.6459070000
N 17.3849780000 40.4790230000 17.2109900000
C 19.3059250000 41.5492890000 17.0652190000
C 18.2279060000 39.7733170000 16.3987790000
N 19.3937470000 40.4029120000 16.2913910000
H 16.5767990000 43.1201870000 18.0852620000
H 17.1746170000 42.2384500000 19.5111420000
H 20.1286340000 42.2520010000 17.1545870000
H 17.9533010000 38.8479890000 15.9054940000
H 16.4387250000 40.2109850000 17.4667660000
C 14.7850420000 33.8559990000 13.5819990000
C 16.0502560000 34.6603680000 13.5775140000
N 16.4240130000 35.4900800000 14.6369440000
C 17.0782050000 34.7927420000 12.6568670000
C 17.6312780000 36.0575080000 14.3418190000
N 18.0511560000 35.6689940000 13.1431810000
H 14.7597320000 33.1394840000 14.4257570000
H 14.6995860000 33.2784380000 12.6464550000
H 17.1706470000 34.3218330000 11.6818310000
H 18.1543500000 36.7374920000 15.0062720000
H 15.9038980000 35.6167210000 15.5007100000
C 16.3110220000 36.1230040000 7.1490170000
C 16.7906430000 36.5980840000 8.4770200000
N 16.0010200000 37.3419840000 9.3540700000
C 18.0026450000 36.4429140000 9.1292280000
C 16.7436740000 37.5953900000 10.4820900000
N 17.9607120000 37.0693380000 10.3707260000
H 16.0148450000 36.9627900000 6.4905440000
H 17.1077470000 35.5588500000 6.6361510000
H 18.8906520000 35.9237690000 8.7785190000
H 16.3613740000 38.1476820000 11.3353890000
H 15.0381280000 37.6260650000 9.1979840000
C 20.5879950000 38.8279900000 7.1140010000
C 19.9489790000 39.3818470000 8.3443080000
N 18.6039940000 39.7310060000 8.4179540000
C 20.4575380000 39.7031160000 9.5886750000
C 18.3530980000 40.2650780000 9.6484080000
N 19.4583270000 40.2576380000 10.3829140000

H 20.5400170000 39.5432780000 6.2699640000
H 21.6506110000 38.6038460000 7.3055100000
H 21.4718600000 39.5682060000 9.9471180000
H 17.3787600000 40.6349610000 9.9533390000
H 17.9279280000 39.6362020000 7.6657510000
C 27.6859910000 32.8790260000 10.5419990000
C 26.2528560000 33.2712860000 10.9175390000
C 26.0942880000 34.7985130000 10.9906240000
C 24.7118400000 35.2236550000 11.4786620000
N 24.6329110000 36.7135480000 11.6824640000
H 27.8042820000 31.7805540000 10.4819810000
H 28.4100380000 33.2544460000 11.2908360000
H 25.9896320000 32.8273110000 11.8986080000
H 25.5370610000 32.8521000000 10.1818140000
H 26.8543750000 35.2127960000 11.6787790000
H 26.2897850000 35.2377250000 9.9915450000
H 23.9153460000 34.9468810000 10.7679910000
H 24.4760170000 34.7637110000 12.4531980000
H 24.8492820000 37.2042100000 10.8152270000
H 25.3492190000 37.0111460000 12.3822970000
H 23.6376070000 36.9531740000 11.9286320000
C 29.1669760000 39.2718980000 12.4010470000
C 28.9116240000 37.7625500000 12.1679230000
C 28.1989000000 37.0623340000 13.3540200000
O 26.9253630000 37.1450610000 13.3842860000
O 28.9169080000 36.4762030000 14.1998820000
H 28.2174800000 39.8185390000 12.5605560000
H 29.8087220000 39.4345940000 13.2879150000
H 28.2919730000 37.6351910000 11.2597470000
H 29.8768840000 37.2541030000 11.9913270000
C 23.2860110000 41.3879000000 11.0910460000
C 23.9269060000 40.8290540000 12.3407800000
N 23.5374240000 39.6143630000 12.9303550000
C 24.9524520000 41.3564170000 13.1073020000
C 24.3070420000 39.4259230000 14.0048380000
N 25.1660650000 40.4669080000 14.1610670000
H 23.6888940000 42.3915300000 10.8743310000
H 22.1905230000 41.4737380000 11.2013700000
H 25.5288250000 42.2695610000 12.9933510000
H 24.2657070000 38.5768630000 14.6805060000
H 25.8832690000 40.5470320000 14.8758070000
Cu 19.2947280000 36.9498740000 11.9775750000
Cu 20.8177820000 40.1947620000 14.8323250000
Cu 19.3313740000 40.4903240000 12.4312170000
Cu 21.7603550000 38.6793460000 12.8954190000
S 19.6830250000 38.6479380000 13.6461010000
O 21.8447480000 36.8965070000 11.9607520000
H 13.8887500000 34.5005660000 13.6661450000
H 18.2139440000 43.4483300000 18.7155330000
H 29.6765480000 39.7251790000 11.5293180000
H 27.9721950000 33.3003490000 9.5583880000
H 15.4329760000 35.4545970000 7.2427820000
H 20.0987470000 37.8914790000 6.7833820000
H 19.2113380000 46.6114230000 11.9829000000
H 22.3383470000 44.3295320000 13.4729000000
H 23.4877100000 40.7460440000 10.2129660000
H 21.6920460000 36.2165700000 12.6289690000

Structures for Computational Reaction Coordinate (Section 3.3.3)

Cu_I-N_2O bound to Fully Reduced Cu_4S, B3LYP

C 21.7600470000 43.4678640000 13.8481050000
C 22.4547060000 42.8507350000 15.0353240000
N 22.2245960000 41.5306190000 15.4477070000
C 23.3789300000 43.4172970000 15.8998800000
C 22.9829620000 41.3170060000 16.5238530000
N 23.7058300000 42.4348890000 16.8338710000
H 21.6751430000 42.7444590000 13.0234440000
H 20.7379980000 43.7975430000 14.1053670000
H 23.8204100000 44.4095200000 15.9220560000
H 23.0380440000 40.3928510000 17.0914500000
H 24.3531790000 42.5355180000 17.6100170000
C 18.5341170000 45.9070850000 11.4620310000
C 18.5160930000 44.5706130000 12.1241480000
N 18.0958640000 44.3619410000 13.4379620000
C 18.8855280000 43.3193090000 11.6674420000
C 18.2249580000 43.0271570000 13.7274540000
N 18.7045130000 42.3719100000 12.6734840000
H 17.5263670000 46.3645210000 11.4263470000
H 18.8969980000 45.8109490000 10.4252770000
H 19.2733090000 43.0463180000 10.6909310000
H 17.9788170000 42.5959660000 14.6935040000
H 17.7498260000 45.0755430000 14.0731950000
C 17.4771320000 42.6498610000 18.5278860000
C 18.0676900000 41.6087920000 17.6562080000
N 17.3847190000 40.4790020000 17.2111980000
C 19.3202830000 41.5183590000 17.0852980000
C 18.2257890000 39.7650690000 16.3985820000
N 19.3999810000 40.3740310000 16.3050420000
H 16.5934460000 43.1305300000 18.0634820000
H 17.1474300000 42.2419090000 19.5037340000
H 20.1538060000 42.2078950000 17.1830230000
H 17.9425520000 38.8482490000 15.8908470000
H 16.4302610000 40.2270380000 17.4519650000
C 14.7852770000 33.8559890000 13.5820830000
C 16.0792090000 34.5960850000 13.6215430000
N 16.4243590000 35.4905730000 14.6363970000
C 17.1624540000 34.6076820000 12.7619120000
C 17.6714760000 35.9837770000 14.3708000000
N 18.1395540000 35.4800260000 13.2343710000
H 14.6583120000 33.1959440000 14.4623650000
H 14.7385860000 33.2231910000 12.6799550000
H 17.2876360000 34.0566840000 11.8333590000
H 18.1862700000 36.7010350000 15.0034200000
H 15.8600480000 35.7059580000 15.4535300000
C 16.3112600000 36.1227520000 7.1492710000
C 16.7685860000 36.5584140000 8.4964660000
N 16.0009640000 37.3423380000 9.3544620000
C 17.9461310000 36.3279640000 9.1840350000
C 16.7209460000 37.5534510000 10.5031290000
N 17.9032520000 36.9536350000 10.4245520000
H 16.1063460000 36.9826650000 6.4823240000
H 17.0851120000 35.5021580000 6.6674710000
H 18.8045950000 35.7488200000 8.8559050000
H 16.3494450000 38.1312570000 11.3441430000
H 15.0628890000 37.6858240000 9.1686920000
C 20.5879570000 38.8279360000 7.1140930000
C 19.9513530000 39.3940350000 8.3384420000
N 18.6039270000 39.7310620000 8.4177350000
C 20.4660710000 39.7360400000 9.5749930000

C 18.3612910000 40.2730010000 9.6509210000
N 19.4708400000 40.2857780000 10.3759290000
H 20.5283080000 39.5280700000 6.2578750000
H 21.6533420000 38.6153930000 7.3025220000
H 21.4852030000 39.6121750000 9.9249160000
H 17.3851580000 40.6334270000 9.9624310000
H 17.9208160000 39.6199330000 7.6741750000
C 27.6859660000 32.8790370000 10.5420260000
C 26.3497530000 33.6396820000 10.5397160000
C 26.5675160000 35.1587080000 10.6638460000
C 25.2740120000 35.9501160000 10.8871840000
N 25.5851190000 37.3885700000 11.2081670000
H 27.5295620000 31.7884550000 10.4419650000
H 28.2411190000 33.0554260000 11.4834880000
H 25.7253650000 33.2890830000 11.3861200000
H 25.7815520000 33.4112160000 9.6158090000
H 27.2421100000 35.3427180000 11.5193790000
H 27.0850990000 35.5341700000 9.7583670000
H 24.6142120000 35.9146620000 10.0037400000
H 24.7186060000 35.5505410000 11.7523210000
H 26.0130950000 37.8568120000 10.4120750000
H 26.2869000000 37.4188030000 12.1003710000
H 24.7457210000 37.9166390000 11.4569220000
C 29.1670100000 39.2719650000 12.4010110000
C 29.0946570000 37.7497910000 12.1832330000
C 28.3015550000 37.0818260000 13.3155670000
O 27.0215290000 37.2419720000 13.3001160000
O 28.9170100000 36.4760310000 14.1999680000
H 28.1579780000 39.7256730000 12.4122420000
H 29.6571910000 39.5113990000 13.3634490000
H 28.6203530000 37.5310700000 11.2074490000
H 30.1101270000 37.3193270000 12.1619030000
C 23.2860400000 41.3878790000 11.0911210000
C 23.9886780000 40.8184350000 12.2998030000
N 23.7390070000 39.5143660000 12.7686230000
C 24.8935630000 41.4070410000 13.1633270000
C 24.4657810000 39.3411130000 13.8820050000
N 25.1655190000 40.4667980000 14.1607770000
H 23.6413630000 42.4130040000 10.8915520000
H 22.1934940000 41.4289250000 11.2447980000
H 25.3429240000 42.3952110000 13.1614740000
H 24.5102110000 38.4382470000 14.4843010000
H 25.8241580000 40.5838420000 14.9256330000
Cu 19.2132960000 36.8045090000 11.9990880000
Cu 20.8295030000 40.1844440000 14.8122030000
Cu 19.3888980000 40.4826720000 12.5076430000
Cu 21.9364550000 38.8303150000 12.8657910000
S 19.8972080000 38.4854530000 13.4766570000
H 13.9165490000 34.5427930000 13.5583260000
H 18.2193970000 43.4393960000 18.7321870000
H 29.7495990000 39.7632400000 11.5985980000
H 28.3336860000 33.2030890000 9.7039740000
H 15.3831470000 35.5209870000 7.2021910000
H 20.1067970000 37.8811870000 6.8008650000
H 19.1999250000 46.6182980000 11.9884840000
H 22.3193640000 44.3494210000 13.4899170000
H 23.4799650000 40.7802700000 10.1879320000
N 21.5106580000 35.9189730000 10.0511880000
N 20.8628610000 35.7448300000 10.9540640000
O 22.1879240000 36.1387180000 9.1029380000

Cu_I-N N_2O bound to Fully Reduced Cu_4S, BP86 10% HF

C 21.7600510000 43.4678330000 13.8480980000
C 22.4558210000 42.8515760000 15.0302910000
N 22.2112990000 41.5327690000 15.4453990000
C 23.3885820000 43.4168510000 15.8946960000
C 22.9707490000 41.3168310000 16.5289520000
N 23.7058220000 42.4348800000 16.8338690000
H 21.6475000000 42.7292640000 13.0320870000
H 20.7415330000 43.8207700000 14.1145000000
H 23.8406930000 44.4099910000 15.9135180000
H 23.0181990000 40.3903660000 17.1030600000
H 24.3577380000 42.5330210000 17.6132030000
C 18.5341200000 45.9070700000 11.4620320000
C 18.5293320000 44.5740440000 12.1267110000
N 18.0958760000 44.3619190000 13.4379620000
C 18.9276340000 43.3242100000 11.6744010000
C 18.2488260000 43.0261630000 13.7344560000
N 18.7532470000 42.3743070000 12.6810210000
H 17.5157570000 46.3509460000 11.4105000000
H 18.9137050000 45.8132100000 10.4260570000
H 19.3307300000 43.0546880000 10.6967770000
H 18.0008600000 42.5892520000 14.7033230000
H 17.7286150000 45.0747420000 14.0703640000
C 17.4771350000 42.6498570000 18.5278870000
C 18.0624600000 41.6190920000 17.6437200000
N 17.3847340000 40.4790130000 17.2111710000
C 19.3065790000 41.5511190000 17.0401650000
C 18.2165580000 39.7804790000 16.3702830000
N 19.3843550000 40.4107020000 16.2510720000
H 16.5784150000 43.1277400000 18.0781880000
H 17.1648800000 42.2348890000 19.5118920000
H 20.1366050000 42.2555410000 17.1222800000
H 17.9343510000 38.8592510000 15.8596520000
H 16.4354870000 40.2108680000 17.4760540000
C 14.7852890000 33.8560100000 13.5820680000
C 16.0482970000 34.6497220000 13.5852450000
N 16.4243590000 35.4905680000 14.6364200000
C 17.0780780000 34.7633640000 12.6600800000
C 17.6361950000 36.0536980000 14.3316300000
N 18.0514840000 35.6417200000 13.1338870000
H 14.7405800000 33.1431550000 14.4347430000
H 14.7094480000 33.2669210000 12.6472500000
H 17.1677660000 34.2757020000 11.6870940000
H 18.1698610000 36.7484070000 14.9821220000
H 15.8999340000 35.6310840000 15.5014800000
C 16.3112550000 36.1227500000 7.1492770000
C 16.7900930000 36.5941750000 8.4790730000
N 16.0010030000 37.3423480000 9.3544630000
C 18.0005120000 36.4313220000 9.1423580000
C 16.7363510000 37.5967950000 10.4889950000
N 17.9529120000 37.0592680000 10.3843860000
H 16.0195320000 36.9671550000 6.4867220000
H 17.1103260000 35.5528280000 6.6362010000
H 18.8921510000 35.9032200000 8.7977650000
H 16.3516510000 38.1570670000 11.3423930000
H 15.0365840000 37.6344520000 9.1888650000
C 20.5879560000 38.8279340000 7.1140910000
C 19.9491780000 39.3741110000 8.3482860000
N 18.6039350000 39.7310620000 8.4177500000
C 20.4560290000 39.6895210000 9.6017670000
C 18.3531450000 40.2618470000 9.6582570000
N 19.4597750000 40.2476400000 10.4001740000

H 20.5489280000 39.5547080000 6.2728650000
H 21.6530270000 38.5934010000 7.3075300000
H 21.4731630000 39.5417660000 9.9671580000
H 17.3756420000 40.6383850000 9.9636690000
H 17.9246080000 39.6375940000 7.6615920000
C 27.6859330000 32.8790790000 10.5420420000
C 26.3671810000 33.6715710000 10.4797030000
C 26.6054570000 35.1898670000 10.5931220000
C 25.3261130000 36.0216630000 10.7774410000
N 25.6597660000 37.4419140000 11.1083250000
H 27.5085500000 31.7859630000 10.4488610000
H 28.2121920000 33.0554780000 11.5058940000
H 25.6996390000 33.3432360000 11.3093160000
H 25.8255910000 33.4399100000 9.5340780000
H 27.2671920000 35.3690560000 11.4683250000
H 27.1619760000 35.5477800000 9.6958590000
H 24.6798920000 35.9540980000 9.8723800000
H 24.7409580000 35.6196190000 11.6318870000
H 26.0823990000 37.9012680000 10.3005790000
H 26.5453070000 37.4097600000 12.4169900000
H 24.8101140000 37.9673400000 11.3277670000
C 29.1670200000 39.2719650000 12.4010040000
C 29.0449980000 37.7501920000 12.1581940000
C 28.3181500000 37.0598730000 13.3089610000
O 26.9903490000 37.1726060000 13.3441790000
O 28.9169880000 36.4760360000 14.1999540000
H 28.1690120000 39.7565730000 12.4617150000
H 29.7126590000 39.4836360000 13.3446870000
H 28.5101210000 37.5632170000 11.2030400000
H 30.0514530000 37.2944580000 12.0766980000
C 23.2860220000 41.3878760000 11.0911250000
C 23.9647540000 40.8316430000 12.3144050000
N 23.6374260000 39.5663800000 12.8345530000
C 24.9312660000 41.3912950000 13.1390090000
C 24.3811180000 39.3770220000 13.9377840000
N 25.1655010000 40.4668010000 14.1607840000
H 23.6513200000 42.4120470000 10.8778060000
H 22.1853770000 41.4363310000 11.2298590000
H 25.4514870000 42.3488180000 13.0898930000
H 24.3678220000 38.4957360000 14.5812180000
H 25.8496350000 40.5668250000 14.9120430000
Cu 19.2554920000 36.8626110000 11.9546510000
Cu 20.7911310000 40.2460100000 14.7813760000
Cu 19.4277410000 40.5052510000 12.4961130000
Cu 21.8426940000 38.9197650000 12.8924510000
S 19.8256450000 38.5205720000 13.4907300000
H 13.8848100000 34.5057740000 13.6467460000
H 18.2189780000 43.4482610000 18.7243870000
H 29.7272940000 39.7514510000 11.5709300000
H 28.3756310000 33.1788770000 9.7219340000
H 15.4264480000 35.4547510000 7.2397230000
H 20.0923280000 37.8940170000 6.7694630000
H 19.1843900000 46.6342960000 11.9961000000
H 22.3322080000 44.3376960000 13.4674740000
H 23.4880840000 40.7622620000 10.1953810000
N 21.3395770000 34.6760020000 11.6359170000
N 20.7524820000 35.6060180000 11.3497760000
O 21.9458400000 33.7075500000 11.9624810000

μ-1,3 N_2O bound to Fully Reduced Cu_4S, BP86 10% HF

C 21.7600380000 43.4678370000 13.8480950000
C 22.4538500000 42.8456450000 15.0288850000
N 22.1915680000 41.5348000000 15.4620270000
C 23.3984190000 43.4077480000 15.8824980000
C 22.9528330000 41.3236930000 16.5468330000
N 23.7058100000 42.4348740000 16.8338600000
H 21.6411550000 42.7341870000 13.0285450000
H 20.7450910000 43.8284520000 14.1180360000
H 23.8642840000 44.3946190000 15.8852220000
H 22.9893690000 40.4047470000 17.1338650000
H 24.3635580000 42.5324570000 17.6085020000
C 18.5341280000 45.9070880000 11.4620340000
C 18.5321300000 44.5732670000 12.1272110000
N 18.0958740000 44.3619130000 13.4379550000
C 18.9311970000 43.3227620000 11.6763810000
C 18.2460710000 43.0260510000 13.7351740000
N 18.7531190000 42.3720520000 12.6833400000
H 17.5138480000 46.3458840000 11.4073840000
H 18.9178240000 45.8148900000 10.4275070000
H 19.3361210000 43.0534330000 10.6995130000
H 17.9938930000 42.5902510000 14.7032290000
H 17.7266180000 45.0747550000 14.0693200000
C 17.4771380000 42.6498720000 18.5278430000
C 18.0515020000 41.6370020000 17.6125810000
N 17.3847330000 40.4790150000 17.2112460000
C 19.2686770000 41.6004950000 16.9524130000
C 18.1920900000 39.7996990000 16.3337410000
N 19.3384920000 40.4598150000 16.1598250000
H 16.5490060000 43.1054360000 18.1170320000
H 17.2171200000 42.2200440000 19.5202330000
H 20.0847180000 42.3233670000 16.9982540000
H 17.9087010000 38.8674690000 15.8460080000
H 16.4562100000 40.1856910000 17.5199170000
C 14.7852420000 33.8559770000 13.5820870000
C 16.0272590000 34.6820190000 13.5681780000
N 16.4243410000 35.4905410000 14.6364190000
C 17.0177610000 34.8583190000 12.6128520000
C 17.6064790000 36.0941450000 14.3219200000
N 17.9837960000 35.7395020000 13.0954410000
H 14.7990900000 33.1010780000 14.3986660000
H 14.6807700000 33.3124140000 12.6229960000
H 17.0896150000 34.4124510000 11.6192890000
H 18.1493120000 36.7662480000 14.9871000000
H 15.9266710000 35.5804590000 15.5240350000
C 16.3112430000 36.1226860000 7.1493010000
C 16.7874820000 36.5900350000 8.4804100000
N 16.0010950000 37.3424290000 9.3544690000
C 17.9904710000 36.4128680000 9.1518380000
C 16.7215800000 37.5841720000 10.4947700000
N 17.9299290000 37.0348100000 10.3922880000
H 16.0212430000 36.9684040000 6.4878360000
H 17.1111970000 35.5534420000 6.6370490000
H 18.8828740000 35.8771920000 8.8221730000
H 16.3334600000 38.1404980000 11.3491060000
H 15.0413170000 37.6449660000 9.1789430000
C 20.5879600000 38.8279450000 7.1140840000
C 19.9515910000 39.3856930000 8.3436890000
N 18.6039290000 39.7310430000 8.4177340000
C 20.4611310000 39.7083190000 9.5932510000
C 18.3492640000 40.2597700000 9.6560600000
N 19.4598610000 40.2549270000 10.3941420000

H 20.5314960000 39.5386480000 6.2603760000
H 21.6574960000 38.6117550000 7.3032120000
H 21.4802550000 39.5687050000 9.9543160000
H 17.3695140000 40.6283900000 9.9635240000
H 17.9242260000 39.6336090000 7.6622550000
C 27.6859180000 32.8791300000 10.5420030000
C 26.3430890000 33.6200190000 10.5406500000
C 26.5460630000 35.1374940000 10.6943730000
C 25.2353810000 35.8888220000 10.9298350000
N 25.4816930000 37.3283950000 11.2823190000
H 27.5490800000 31.7833030000 10.4170770000
H 28.2317040000 33.0440530000 11.4967840000
H 25.7104700000 33.2465070000 11.3781650000
H 25.7814900000 33.4031980000 9.6034710000
H 27.2196980000 35.3173040000 11.5601350000
H 27.0628370000 35.5385050000 9.7926870000
H 24.5699120000 35.8466170000 10.0441110000
H 24.6852180000 35.4499890000 11.7858350000
H 25.8937540000 37.8323460000 10.4940290000
H 26.1817450000 37.3854650000 12.1756440000
H 24.5718500000 37.7676730000 11.4906620000
C 29.1669840000 39.2719460000 12.4010490000
C 29.0192800000 37.7542870000 12.1688310000
C 28.2642560000 37.0828810000 13.3320890000
O 26.9793070000 37.2352770000 13.3594140000
O 28.9169780000 36.4760580000 14.1999510000
H 28.1743920000 39.7672650000 12.4715230000
H 29.7202530000 39.4791460000 13.3423350000
H 28.4799040000 37.5750480000 11.2126490000
H 30.0198060000 37.2839240000 12.0798630000
C 23.2860900000 41.3878950000 11.0911360000
C 23.9487330000 40.8694140000 12.3389270000
N 23.5325720000 39.6753690000 12.9334420000
C 24.9904550000 41.3698160000 13.1086710000
C 24.2817910000 39.4509320000 14.0160440000
N 25.1654990000 40.4667550000 14.1607330000
H 23.6650890000 42.3981610000 10.8386160000
H 22.1859090000 41.4560960000 11.2197060000
H 25.6029510000 42.2661550000 13.0034040000
H 24.2051760000 38.6016700000 14.6951840000
H 25.8857980000 40.5322600000 14.8816190000
Cu 19.2324700000 36.8493340000 11.9597220000
Cu 20.7792520000 40.2163150000 14.7566610000
Cu 19.4104930000 40.4926280000 12.4545970000
Cu 21.7977200000 38.9052940000 12.8447240000
S 19.8016650000 38.5109370000 13.4775310000
H 13.8738460000 34.4777670000 13.7208760000
H 18.2059620000 43.4658560000 18.6982490000
H 29.7275420000 39.7513780000 11.5695000000
H 28.3420060000 33.2308970000 9.7150700000
H 15.4260820000 35.4547530000 7.2366040000
H 20.1028270000 37.8808730000 6.7914440000
H 19.1794510000 46.6363550000 11.9990380000
H 22.3382730000 44.3339720000 13.4689980000
H 23.4870300000 40.7253010000 10.2225050000
N 21.9004620000 36.6463940000 10.9283870000
N 20.7793020000 36.2963270000 11.0000610000
O 22.5811960000 37.6261450000 11.4225910000

μ-1,3 TS for N-O cleavage, BP86 10% HF

C 21.7600370000 43.4678600000 13.8481050000
C 22.4502630000 42.8415530000 15.0288970000
N 22.1622280000 41.5437370000 15.4882020000
C 23.4134930000 43.3958670000 15.8663570000
C 22.9262220000 41.3359860000 16.5738870000
N 23.7058070000 42.4348740000 16.8338580000
H 21.6237680000 42.7341120000 13.0311780000
H 20.7534270000 43.8481970000 14.1225100000
H 23.9005210000 44.3721900000 15.8473160000
H 22.9450080000 40.4284010000 17.1792070000
H 24.3713550000 42.5312390000 17.6021800000
C 18.5341380000 45.9071020000 11.4620360000
C 18.5308390000 44.5728560000 12.1265240000
N 18.0958720000 44.3618880000 13.4379420000
C 18.9240480000 43.3212580000 11.6734290000
C 18.2387520000 43.0254010000 13.7334510000
N 18.7416040000 42.3701350000 12.6797470000
H 17.5141300000 46.3464710000 11.4085910000
H 18.9170800000 45.8150990000 10.4273000000
H 19.3269390000 43.0517060000 10.6957480000
H 17.9831160000 42.5896830000 14.7004760000
H 17.7300720000 45.0756310000 14.0704410000
C 17.4771280000 42.6498780000 18.5278510000
C 18.0493460000 41.6400900000 17.6079490000
N 17.3847230000 40.4790140000 17.2112600000
C 19.2637600000 41.6081440000 16.9430320000
C 18.1886550000 39.7995960000 16.3333780000
N 19.3328960000 40.4647450000 16.1532390000
H 16.5431230000 43.0994680000 18.1242850000
H 17.2280690000 42.2175940000 19.5218140000
H 20.0769890000 42.3337660000 16.9842000000
H 17.9050320000 38.8649710000 15.8517610000
H 16.4591610000 40.1820440000 17.5257400000
C 14.7852310000 33.8559700000 13.5820970000
C 16.0026130000 34.7228310000 13.5486900000
N 16.4243570000 35.4905700000 14.6364090000
C 16.9488440000 34.9730170000 12.5642560000
C 17.5760120000 36.1415630000 14.3101010000
N 17.9114060000 35.8559090000 13.0549950000
H 14.8709530000 33.0551730000 14.3487190000
H 14.6404070000 33.3674370000 12.5990460000
H 16.9957160000 34.5750180000 11.5493360000
H 18.1305000000 36.7879770000 14.9899640000
H 15.9619320000 35.5214730000 15.5468250000
C 16.3112290000 36.1226950000 7.1492640000
C 16.7970840000 36.6142820000 8.4685350000
N 16.0010860000 37.3424150000 9.3544660000
C 18.0205830000 36.4924290000 9.1144680000
C 16.7365570000 37.6265620000 10.4742890000
N 17.9646790000 37.1262580000 10.3507350000
H 15.9882660000 36.9553900000 6.4864050000
H 17.1172500000 35.5703570000 6.6281810000
H 18.9244720000 35.9890100000 8.7653610000
H 16.3447200000 38.1747530000 11.3321240000
H 15.0268260000 37.6063380000 9.1973430000
C 20.5879380000 38.8279610000 7.1141220000
C 19.9431600000 39.3486930000 8.3584160000
N 18.6039300000 39.7310320000 8.4177160000
C 20.4405430000 39.6296420000 9.6236470000
C 18.3432560000 40.2555060000 9.6534890000
N 19.4406580000 40.2037180000 10.4095490000

H 20.5979700000 39.5934150000 6.3071060000
H 21.6372010000 38.5403280000 7.3205940000
H 21.4380730000 39.4217370000 10.0165770000
H 17.3711930000 40.6543100000 9.9470760000
H 17.9376880000 39.6719900000 7.6464350000
C 27.6859590000 32.8790890000 10.5419880000
C 26.3146970000 33.5593980000 10.6155940000
C 26.4464570000 35.0765760000 10.8366800000
C 25.0918190000 35.7414410000 11.0759200000
N 25.2010870000 37.2014840000 11.3963150000
H 27.5924280000 31.7844910000 10.3730010000
H 28.2561990000 33.0268780000 11.4852960000
H 25.7221510000 33.1169280000 11.4490730000
H 25.7365870000 33.3626010000 9.6836190000
H 27.1022530000 35.2600330000 11.7155390000
H 26.9491980000 35.5396540000 9.9564870000
H 24.4266310000 35.6336180000 10.1961410000
H 24.5751500000 35.2721320000 11.9373770000
H 25.5897060000 37.7130890000 10.6010540000
H 25.8675910000 37.3394450000 12.2257260000
H 24.1780600000 37.5634940000 11.5649760000
C 29.1669730000 39.2718930000 12.4010680000
C 28.9229650000 37.7652480000 12.1697830000
C 28.2140250000 37.1060850000 13.3763870000
O 26.9452380000 37.2836750000 13.4671030000
O 28.9170050000 36.4761010000 14.1999340000
H 28.2084620000 39.8143920000 12.5526660000
H 29.8015470000 39.4397830000 13.2982560000
H 28.3020690000 37.6255260000 11.2569750000
H 29.8908290000 37.2489610000 11.9993820000
C 23.2860710000 41.3878740000 11.0911440000
C 23.9209170000 40.8906080000 12.3604200000
N 23.4406810000 39.7662080000 13.0309390000
C 25.0220820000 41.3383860000 13.0790140000
C 24.2069040000 39.5165080000 14.0924160000
N 25.1655150000 40.4667880000 14.1607390000
H 23.6879840000 42.3838700000 10.8190580000
H 22.1853340000 41.4757220000 11.1975100000
H 25.6972250000 42.1789960000 12.9148630000
H 24.0930280000 38.6970130000 14.8007850000
H 25.9169150000 40.5033270000 14.8513760000
Cu 19.2308240000 36.8415200000 11.9364400000
Cu 20.7714060000 40.2033010000 14.7702330000
Cu 19.3674820000 40.4849650000 12.4327360000
Cu 21.8059990000 38.8786660000 12.8346830000
S 19.7821310000 38.5599960000 13.5156090000
H 13.8674620000 34.4401230000 13.8109740000
H 18.2026400000 43.4698230000 18.6923280000
H 29.6848680000 39.7337880000 11.5322530000
H 28.2988010000 33.2950840000 9.7116560000
H 15.4454020000 35.4329590000 7.2570890000
H 20.0613550000 37.9325610000 6.7180270000
H 19.1805260000 46.6350810000 11.9993120000
H 22.3515310000 44.3213310000 13.4616380000
H 23.4875370000 40.6964760000 10.2455910000
N 21.8959950000 36.2904450000 10.8652640000
N 20.7954570000 36.1428410000 11.0919310000
O 22.6387670000 37.7713580000 11.6007570000

μ-1,3 TS for N-O cleavage, B3LYP

C 21.7600480000 43.4678410000 13.8480750000
C 22.4498000000 42.8410030000 15.0335220000
N 22.1846630000 41.5356760000 15.4807240000
C 23.3979450000 43.3999970000 15.8765690000
C 22.9474760000 41.3306680000 16.5593440000
N 23.7058390000 42.4348930000 16.8338800000
H 21.6401590000 42.7423190000 13.0292000000
H 20.7532330000 43.8351040000 14.1157430000
H 23.8666950000 44.3797230000 15.8675200000
H 22.9813920000 40.4203600000 17.1507460000
H 24.3644900000 42.5344770000 17.6008310000
C 18.5341150000 45.9070890000 11.4620300000
C 18.5138310000 44.5711840000 12.1234250000
N 18.0958680000 44.3619420000 13.4379650000
C 18.8754640000 43.3197540000 11.6624330000
C 18.2160880000 43.0266570000 13.7243990000
N 18.6899510000 42.3713750000 12.6673330000
H 17.5272330000 46.3663690000 11.4281400000
H 18.8953100000 45.8104440000 10.4248570000
H 19.2592310000 43.0476290000 10.6841240000
H 17.9666280000 42.5945930000 14.6886940000
H 17.7538820000 45.0760550000 14.0750140000
C 17.4771240000 42.6498760000 18.5278770000
C 18.0538490000 41.6315050000 17.6185060000
N 17.3847410000 40.4789780000 17.2112050000
C 19.2749660000 41.5841780000 16.9781120000
C 18.1970500000 39.7910540000 16.3529960000
N 19.3458600000 40.4401890000 16.1929050000
H 16.5569270000 43.1041060000 18.1109590000
H 17.2107870000 42.2237740000 19.5147670000
H 20.0899130000 42.2987760000 17.0312390000
H 17.9144610000 38.8620410000 15.8703780000
H 16.4552950000 40.1935420000 17.5073930000
C 14.7852370000 33.8559830000 13.5820750000
C 16.0511630000 34.6438040000 13.5921170000
N 16.4243390000 35.4905240000 14.6364860000
C 17.0792130000 34.7492160000 12.6753940000
C 17.6299530000 36.0497240000 14.3413240000
N 18.0451490000 35.6305930000 13.1536700000
H 14.7279550000 33.1565710000 14.4386040000
H 14.7179110000 33.2599540000 12.6568420000
H 17.1756980000 34.2598280000 11.7105920000
H 18.1557160000 36.7399820000 14.9923520000
H 15.8996070000 35.6322020000 15.4953300000
C 16.3112220000 36.1227200000 7.1492540000
C 16.7821090000 36.5849830000 8.4836170000
N 16.0009710000 37.3423860000 9.3543990000
C 17.9760560000 36.3947800000 9.1552490000
C 16.7232740000 37.5701510000 10.4961030000
N 17.9219910000 37.0121970000 10.3982890000
H 16.0360550000 36.9683050000 6.4892240000
H 17.1053580000 35.5476460000 6.6445740000
H 18.8575530000 35.8539250000 8.8215070000
H 16.3404890000 38.1252040000 11.3476740000
H 15.0492160000 37.6533270000 9.1805050000
C 20.5879590000 38.8279350000 7.1140920000
C 19.9503550000 39.3892700000 8.3417040000
N 18.6039230000 39.7310620000 8.4177230000
C 20.4607710000 39.7186580000 9.5825040000
C 18.3521140000 40.2686970000 9.6456540000
N 19.4592260000 40.2697170000 10.3770490000

H 20.5342530000 39.5346290000 6.2630490000
H 21.6522060000 38.6110390000 7.3050630000
H 21.4695600000 39.5620570000 9.9480150000
H 17.3760400000 40.6342680000 9.9505730000
H 17.9266650000 39.6298850000 7.6673980000
C 27.6859730000 32.8790340000 10.5420160000
C 26.3347900000 33.5948610000 10.4883650000
C 26.4956590000 35.1037980000 10.7314170000
C 25.1497670000 35.8024440000 10.8924450000
N 25.2891230000 37.2498420000 11.2663370000
H 27.5813840000 31.7935540000 10.3536370000
H 28.1628520000 33.0029670000 11.5335770000
H 25.6582890000 33.1693090000 11.2569240000
H 25.8444940000 33.4193180000 9.5095630000
H 27.0926900000 35.2576600000 11.6488730000
H 27.0660080000 35.5571500000 9.8959330000
H 24.5470940000 35.7471780000 9.9713260000
H 24.5642480000 35.3333340000 11.7001960000
H 25.7015860000 37.7839110000 10.5040510000
H 25.9254200000 37.3487490000 12.1158740000
H 24.3084580000 37.6096380000 11.4284820000
C 29.1670110000 39.2719760000 12.4010110000
C 28.9808710000 37.7577430000 12.1745420000
C 28.2388510000 37.0909840000 13.3528410000
O 26.9694060000 37.2477300000 13.3922900000
O 28.9170450000 36.4760160000 14.1999940000
H 28.1908850000 39.7839580000 12.5025010000
H 29.7514900000 39.4670940000 13.3202680000
H 28.4092520000 37.5920110000 11.2411610000
H 29.9658420000 37.2732610000 12.0544410000
C 23.2860560000 41.3879380000 11.0911420000
C 23.9397430000 40.8722780000 12.3478780000
N 23.5010970000 39.7074340000 12.9770830000
C 25.0014290000 41.3527260000 13.0940130000
C 24.2561950000 39.4771020000 14.0451490000
N 25.1655300000 40.4668120000 14.1607770000
H 23.6894130000 42.3799020000 10.8263140000
H 22.1939510000 41.4836690000 11.2171030000
H 25.6331740000 42.2258360000 12.9634650000
H 24.1666800000 38.6435450000 14.7335900000
H 25.8955280000 40.5229560000 14.8654220000
Cu 19.2797250000 36.6827440000 11.9554260000
Cu 20.7963570000 40.1513850000 14.7908770000
Cu 19.3286560000 40.4788760000 12.4355840000
Cu 21.8268730000 38.8201840000 12.7980500000
S 19.7945520000 38.5315510000 13.4927310000
H 13.8923780000 34.5093690000 13.6294280000
H 18.2043030000 43.4604730000 18.7000680000
H 29.7077060000 39.7391490000 11.5556050000
H 28.3846980000 33.2830820000 9.7831990000
H 15.4218970000 35.4675800000 7.2301130000
H 20.1029650000 37.8855180000 6.7936390000
H 19.2021530000 46.6165310000 11.9878390000
H 22.3443490000 44.3260290000 13.4747660000
H 23.4694450000 40.7078550000 10.2395270000
N 21.9339830000 36.3805970000 10.7369790000
N 20.8570130000 36.1288290000 10.9847810000
O 22.6248750000 37.7370380000 11.4383790000

Terminal Cu_I-O TS for N-O cleavage, B3LYP

C 21.7600440000 43.4678280000 13.8480900000
C 22.4574120000 42.8522060000 15.0343970000
N 22.2225800000 41.5353040000 15.4531810000
C 23.3848810000 43.4160900000 15.8966330000
C 22.9794110000 41.3202730000 16.5302800000
N 23.7058290000 42.4348780000 16.8338680000
H 21.6656050000 42.7419730000 13.0266220000
H 20.7420730000 43.8063110000 14.1103290000
H 23.8322250000 44.4056520000 15.9155540000
H 23.0302280000 40.3977630000 17.1008150000
H 24.3558390000 42.5349240000 17.6080170000
C 18.5341030000 45.9071180000 11.4620270000
C 18.5164710000 44.5711420000 12.1241810000
N 18.0959070000 44.3618740000 13.4379490000
C 18.8863100000 43.3204680000 11.6662750000
C 18.2251720000 43.0266670000 13.7261940000
N 18.7052640000 42.3721790000 12.6714850000
H 17.5261910000 46.3640890000 11.4263320000
H 18.8970470000 45.8109480000 10.4253510000
H 19.2734510000 43.0491090000 10.6889790000
H 17.9780480000 42.5944100000 14.6914140000
H 17.7492130000 45.0748030000 14.0736630000
C 17.4771530000 42.6498530000 18.5279000000
C 18.0608300000 41.6175990000 17.6446920000
N 17.3847450000 40.4789450000 17.2111480000
C 19.3045210000 41.5465240000 17.0534920000
C 18.2212810000 39.7771170000 16.3857700000
N 19.3859200000 40.4036040000 16.2722660000
H 16.5807420000 43.1233320000 18.0808630000
H 17.1686530000 42.2368710000 19.5084930000
H 20.1294430000 42.2475580000 17.1389100000
H 17.9414920000 38.8564200000 15.8859850000
H 16.4389590000 40.2122700000 17.4698320000
C 14.7852760000 33.8559960000 13.5820590000
C 16.0182590000 34.7030740000 13.5575860000
N 16.4243120000 35.4905440000 14.6365400000
C 16.9854370000 34.9174140000 12.5912260000
C 17.5897790000 36.1164660000 14.3115240000
N 17.9499670000 35.8009660000 13.0742030000
H 14.8371850000 33.0790980000 14.3693430000
H 14.6576950000 33.3449410000 12.6132720000
H 17.0429240000 34.4978290000 11.5910400000
H 18.1300250000 36.7793090000 14.9789830000
H 15.9462330000 35.5545340000 15.5310090000
C 16.3111870000 36.1227310000 7.1492300000
C 16.7819840000 36.5924170000 8.4757970000
N 16.0010390000 37.3423700000 9.3544300000
C 17.9915150000 36.4210600000 9.1224160000
C 16.7447090000 37.5858210000 10.4800320000
N 17.9531160000 37.0443190000 10.3616550000
H 16.0258290000 36.9629600000 6.4862490000
H 17.1085670000 35.5531850000 6.6434700000
H 18.8767870000 35.9001880000 8.7700650000
H 16.3697040000 38.1385410000 11.3359020000
H 15.0422550000 37.6394920000 9.1971520000
C 20.5879350000 38.8279600000 7.1141180000
C 19.9518270000 39.3951800000 8.3396180000
N 18.6039310000 39.7310530000 8.4177350000
C 20.4602270000 39.7230090000 9.5821080000
C 18.3524140000 40.2595600000 9.6524820000
N 19.4593520000 40.2620810000 10.3842280000

H 20.5024510000 39.5160980000 6.2505210000
H 21.6590920000 38.6412610000 7.2940740000
H 21.4759420000 39.5950580000 9.9374990000
H 17.3752830000 40.6186280000 9.9616110000
H 17.9254520000 39.6287380000 7.6687590000
C 27.6855800000 32.8796570000 10.5420510000
C 26.3326900000 33.6086980000 10.5851070000
C 26.5183500000 35.1309360000 10.7213070000
C 25.2120300000 35.8867820000 10.9853190000
N 25.4937190000 37.3345500000 11.2943470000
H 27.5518370000 31.7870530000 10.4314960000
H 28.2613850000 33.0568780000 11.4709070000
H 25.7390330000 33.2337100000 11.4430110000
H 25.7451580000 33.3785290000 9.6738270000
H 27.2110980000 35.3226290000 11.5609060000
H 27.0031870000 35.5268730000 9.8063510000
H 24.5223440000 35.8336280000 10.1262730000
H 24.6924020000 35.4755020000 11.8663140000
H 25.8926650000 37.8093010000 10.4869360000
H 26.2115180000 37.3927180000 12.1616900000
H 24.6444420000 37.8404530000 11.5534460000
C 29.1669720000 39.2719930000 12.4009930000
C 29.0448190000 37.7524510000 12.1783460000
C 28.2794230000 37.0885220000 13.3341790000
O 27.0012070000 37.2554800000 13.3530960000
O 28.9171050000 36.4759970000 14.2000510000
H 28.1712850000 39.7518920000 12.4534320000
H 29.7008790000 39.4929120000 13.3444640000
H 28.5250680000 37.5575670000 11.2207610000
H 30.0476260000 37.2971680000 12.1111310000
C 23.2863980000 41.3873760000 11.0908500000
C 23.9641810000 40.8195700000 12.3147190000
N 23.6535620000 39.5479900000 12.8323630000
C 24.9193210000 41.3865660000 13.1391760000
C 24.3959400000 39.3725590000 13.9332520000
N 25.1654870000 40.4668300000 14.1609610000
H 23.6669300000 42.4012300000 10.8811260000
H 22.1934180000 41.4548300000 11.2317540000
H 25.4218810000 42.3477510000 13.0915540000
H 24.4014160000 38.4906080000 14.5672430000
H 25.8471820000 40.5705100000 14.9071580000
Cu 19.2627910000 36.9766120000 11.9681000000
Cu 20.8400350000 40.1973800000 14.8218140000
Cu 19.3679120000 40.4686570000 12.4712650000
Cu 21.8498640000 38.7795120000 12.8526610000
S 19.7916640000 38.5490320000 13.6074250000
H 13.8759110000 34.4587200000 13.7703630000
H 18.2154830000 43.4457790000 18.7207790000
H 29.7305790000 39.7512490000 11.5780570000
H 28.3032130000 33.2295440000 9.6917320000
H 15.4277060000 35.4598630000 7.2331290000
H 20.1258120000 37.8660140000 6.8219230000
H 19.1996280000 46.6185580000 11.9884480000
H 22.3231150000 44.3436810000 13.4822860000
H 23.4754050000 40.7636410000 10.1974680000
O 21.2730940000 36.8947000000 11.4540200000
N 21.7850060000 36.3631420000 10.3383700000
N 21.4506760000 36.0929060000 9.2709610000

3D PES Before H^+ transfer (N-O 2.1 Å, O-H 1.6 Å, Cu_I-N 2.0 Å) - Figure 11A

C 1.9848920000 4.8856450000 0.3403240000
C 2.6742960000 4.2582450000 1.5212440000
N 2.3847220000 2.9614450000 1.9831820000
C 3.6390040000 4.8123330000 2.3571120000
C 3.1492950000 2.7546570000 3.0688040000
N 3.9306630000 3.8526620000 3.3260760000
H 1.8493900000 4.1524520000 -0.4773150000
H 0.9781180000 5.2657360000 0.6144610000
H 4.1273640000 5.7879400000 2.3360090000
H 3.1670970000 1.8483170000 3.6760190000
H 4.5968240000 3.9494310000 4.0938100000
C -1.2410060000 7.3248850000 -2.0457450000
C -1.2469240000 5.9919360000 -1.3817410000
N -1.6792780000 5.7796770000 -0.0698390000
C -0.8566550000 4.7413620000 -1.8384360000
C -1.5374220000 4.4426750000 0.2230180000
N -1.0381610000 3.7897440000 -0.8336560000
H -2.2594860000 7.7681580000 -2.0970230000
H -0.8609430000 7.2314450000 -3.0814090000
H -0.4561160000 4.4731030000 -2.8174290000
H -1.7910500000 4.0050210000 1.1897430000
H -2.0423420000 6.4930460000 0.5646380000
C -2.2980200000 4.0676630000 5.0200720000
C -1.7222680000 3.0538600000 4.1063900000
N -2.3904260000 1.8968030000 3.7034790000
C -0.5008940000 3.0133900000 3.4543480000
C -1.5805770000 1.2112170000 2.8349670000
N -0.4299210000 1.8685600000 2.6666000000
H -3.2263280000 4.5211160000 4.6077790000
H -2.5578160000 3.6377040000 6.0123230000
H 0.3158470000 3.7345610000 3.5033530000
H -1.8646250000 0.2784670000 2.3494010000
H -3.3210320000 1.6057320000 4.0083880000
C -4.9899090000 -4.7262570000 0.0743190000
C -3.7443810000 -3.9007860000 0.0600250000
N -3.3507800000 -3.0916210000 1.1285940000
C -2.7459430000 -3.7285110000 -0.8893490000
C -2.1640300000 -2.4917890000 0.8220700000
N -1.7787090000 -2.8490130000 -0.4010610000
H -4.9756690000 -5.4800380000 0.8917700000
H -5.0952920000 -5.2703840000 -0.8843060000
H -2.6684880000 -4.1766040000 -1.8816140000
H -1.6236220000 -1.8232840000 1.4926630000
H -3.8519970000 -3.0012890000 2.0141900000
C -3.4639070000 -2.4595110000 -6.3585110000
C -2.9782220000 -1.9721950000 -5.0356480000
N -3.7740420000 -1.2398140000 -4.1532920000
C -1.7590360000 -2.1031880000 -4.3825700000
C -3.0428090000 -0.9632390000 -3.0273620000
N -1.8158780000 -1.4714450000 -3.1429040000
H -3.7825160000 -1.6236070000 -7.0192550000
H -2.6591260000 -3.0136670000 -6.8795540000
H -0.8575720000 -2.6110460000 -4.7312620000
H -3.4363270000 -0.4131140000 -2.1714120000
H -4.7460430000 -0.9699600000 -4.3140180000
C 0.8127920000 0.2457450000 -6.3936550000
C 0.1668610000 0.7615250000 -5.1464050000
N -1.1712180000 1.1488190000 -5.0900690000
C 0.6617170000 1.0378240000 -3.8785560000

C -1.4343550000 1.6740800000 -3.8557690000
N -0.3395920000 1.6171460000 -3.0967730000
H 0.8363130000 1.0199890000 -7.1920160000
H 1.8574610000 -0.0560680000 -6.1840380000
H 1.6515880000 0.8090110000 -3.4738860000
H -2.4057740000 2.0770570000 -3.5657290000
H -1.8347610000 1.0945910000 -5.8640700000
C 7.9108140000 -5.7031290000 -2.9657920000
C 6.5498380000 -4.9991470000 -2.9297790000
C 6.7032450000 -3.4859650000 -2.6970760000
C 5.3554450000 -2.7937000000 -2.4991010000
N 5.4901830000 -1.3377680000 -2.1681410000
H 7.8033730000 -6.7950920000 -3.1432510000
H 8.4551190000 -5.5697810000 -2.0051760000
H 5.9246890000 -5.4347710000 -2.1167680000
H 5.9968420000 -5.1809210000 -3.8798840000
H 7.3326230000 -3.3189010000 -1.7959620000
H 7.2442770000 -3.0297120000 -3.5576740000
H 4.7173450000 -2.8817270000 -3.4006670000
H 4.8015730000 -3.2538350000 -1.6562330000
H 5.9017060000 -0.8286480000 -2.9536150000
H 6.1433890000 -1.2167010000 -1.3213660000
H 4.4826730000 -0.9586120000 -2.0180710000
C 9.3918210000 0.6896690000 -1.1067130000
C 9.1661010000 -0.8196540000 -1.3376280000
C 8.4463700000 -1.4793430000 -0.1393450000
O 7.1761710000 -1.3049150000 -0.0623340000
O 9.1418370000 -2.1061040000 0.6921380000
H 8.4260460000 1.2223380000 -0.9669820000
H 10.0146480000 0.8658130000 -0.2029880000
H 8.5601300000 -0.9674370000 -2.2588420000
H 10.1410170000 -1.3267980000 -1.4928700000
C 3.5109240000 2.8056530000 -2.4166330000
C 4.1406950000 2.3088540000 -1.1445560000
N 3.6506680000 1.1924230000 -0.4664780000
C 5.2477920000 2.7522590000 -0.4319430000
C 4.4205600000 0.9422560000 0.5920240000
N 5.3903600000 1.8845650000 0.6529510000
H 3.9236420000 3.7951500000 -2.6959620000
H 2.4108730000 2.9040680000 -2.3107180000
H 5.9277750000 3.5877030000 -0.6027420000
H 4.3023710000 0.1270350000 1.3046720000
H 6.1420660000 1.9198830000 1.3431660000
Cu -0.5627080000 -1.7537740000 -1.5627650000
Cu 1.0057160000 1.6073050000 1.2680520000
Cu -0.4176450000 1.9101310000 -1.0789960000
Cu 2.0340710000 0.2542190000 -0.7424750000
S 0.0000000000 0.0000000000 0.0000000000
H -5.8994780000 -4.1020660000 0.2130230000
H -1.5701550000 4.8844000000 5.1900630000
H 9.9144890000 1.1552950000 -1.9705990000
H 8.5552330000 -5.2939390000 -3.7753050000
H -4.3324000000 -3.1461020000 -6.2526770000
H 0.2779740000 -0.6390570000 -6.8023100000
H -0.5909650000 8.0512690000 -1.5106210000
H 2.5770320000 5.7392230000 -0.0448120000
H 3.7018640000 2.1031190000 -3.2551190000
N 2.0753280000 -2.4677850000 -2.8355720000
N 1.0391070000 -2.5674400000 -2.4414840000
O 2.9031330000 -0.7054250000 -2.0489170000

3D PES After H^+ transfer (N-O 2.1 Å, O-H 1.0 Å, Cu_I-N 2.0 Å) - Figure 11B

C 1.9760480000 4.8694100000 0.3417790000
C 2.6628710000 4.2407180000 1.5234300000
N 2.3763230000 2.9429600000 1.9875470000
C 3.6276780000 4.7948940000 2.3585300000
C 3.1435300000 2.7369210000 3.0729910000
N 3.9218140000 3.8364270000 3.3275410000
H 1.8396980000 4.1367770000 -0.4762560000
H 0.9712290000 5.2556120000 0.6144760000
H 4.1153960000 5.7706880000 2.3353790000
H 3.1641400000 1.8303390000 3.6796050000
H 4.5908000000 3.9336770000 4.0930020000
C -1.2498550000 7.3086550000 -2.0442850000
C -1.2567420000 5.9773580000 -1.3805140000
N -1.6881020000 5.7634030000 -0.0683860000
C -0.8695230000 4.7285060000 -1.8427080000
C -1.5505150000 4.4253180000 0.2201400000
N -1.0537250000 3.7747340000 -0.8407880000
H -2.2681010000 7.7522620000 -2.0957630000
H -0.8696360000 7.2147240000 -3.0797120000
H -0.4703210000 4.4640600000 -2.8231240000
H -1.8060940000 3.9845980000 1.1848470000
H -2.0493520000 6.4756370000 0.5686100000
C -2.3068680000 4.0514320000 5.0215300000
C -1.7328710000 3.0411340000 4.1012740000
N -2.3992540000 1.8805560000 3.7049390000
C -0.5162460000 3.0052850000 3.4397160000
C -1.5959790000 1.1956950000 2.8320780000
N -0.4479740000 1.8578560000 2.6531250000
H -3.2414030000 4.4985050000 4.6169440000
H -2.5548490000 3.6175610000 6.0148740000
H 0.2984540000 3.7288770000 3.4821450000
H -1.8825850000 0.2593400000 2.3560630000
H -3.3257620000 1.5853790000 4.0189600000
C -4.9987210000 -4.7424970000 0.0757960000
C -3.7738380000 -3.8819540000 0.0441910000
N -3.3596500000 -3.1078360000 1.1300100000
C -2.8129130000 -3.6443460000 -0.9301250000
C -2.2000160000 -2.4664860000 0.8158090000
N -1.8499790000 -2.7634090000 -0.4321630000
H -4.9204590000 -5.5387390000 0.8477380000
H -5.1412580000 -5.2358350000 -0.9051040000
H -2.7545920000 -4.0508930000 -1.9411760000
H -1.6508670000 -1.8216760000 1.5016800000
H -3.8318740000 -3.0699600000 2.0353020000
C -3.4727470000 -2.4757330000 -6.3570510000
C -2.9821080000 -1.9726300000 -5.0431810000
N -3.7828470000 -1.2560740000 -4.1517890000
C -1.7510060000 -2.0716720000 -4.4080810000
C -3.0449690000 -0.9559080000 -3.0390330000
N -1.8070770000 -1.4350440000 -3.1712220000
H -3.8182590000 -1.6498530000 -7.0168170000
H -2.6624200000 -3.0140490000 -6.8858120000
H -0.8428260000 -2.5601830000 -4.7666040000
H -3.4404960000 -0.4131750000 -2.1794140000
H -4.7631530000 -1.0099910000 -4.3008360000
C 0.8039480000 0.2295170000 -6.3922020000
C 0.1609440000 0.7577560000 -5.1478160000
N -1.1800650000 1.1325720000 -5.0886010000
C 0.6569330000 1.0506460000 -3.8846080000
C -1.4483070000 1.6659730000 -3.8614510000
N -0.3496690000 1.6253560000 -3.1051250000

H 0.8239910000 0.9963930000 -7.1974480000
H 1.8490820000 -0.0702110000 -6.1829810000
H 1.6531590000 0.8440530000 -3.4888010000
H -2.4224630000 2.0632270000 -3.5732560000
H -1.8436410000 1.0698270000 -5.8622280000
C 7.9019120000 -5.7192890000 -2.9643110000
C 6.5477070000 -4.9940680000 -2.9494020000
C 6.6923440000 -3.4772770000 -2.7228750000
C 5.3386310000 -2.7586410000 -2.5915900000
N 5.4070900000 -1.3064850000 -2.2882160000
H 7.7813970000 -6.8121630000 -3.1300650000
H 8.4394230000 -5.5811400000 -2.0002200000
H 5.9055160000 -5.4229620000 -2.1450330000
H 6.0072060000 -5.1795070000 -3.9069940000
H 7.2840960000 -3.2997910000 -1.7969930000
H 7.2740940000 -3.0274380000 -3.5614400000
H 4.7463840000 -2.8927650000 -3.5228300000
H 4.7493400000 -3.2371880000 -1.7788020000
H 5.8649460000 -0.8202090000 -3.0603010000
H 6.0077880000 -1.1629370000 -1.4548910000
H 3.7454150000 -0.8488030000 -2.0855410000
C 9.3829790000 0.6733770000 -1.1052240000
C 9.0904850000 -0.8225400000 -1.3259550000
C 8.4106580000 -1.4431730000 -0.0820740000
O 7.1742180000 -1.1831230000 0.0816360000
O 9.1329000000 -2.1222720000 0.6935220000
H 8.4442960000 1.2369670000 -0.9127040000
H 10.0576480000 0.8249950000 -0.2340730000
H 8.4217660000 -0.9458770000 -2.2059890000
H 10.0346940000 -1.3680520000 -1.5361550000
C 3.5020940000 2.7893450000 -2.4151730000
C 4.1284260000 2.2885110000 -1.1419820000
N 3.6560970000 1.1576750000 -0.4715530000
C 5.2282420000 2.7403790000 -0.4250460000
C 4.4309000000 0.9099910000 0.5853070000
N 5.3815670000 1.8683470000 0.6544670000
H 3.9287790000 3.7726960000 -2.6947270000
H 2.4036440000 2.9069100000 -2.3129490000
H 5.8989560000 3.5838060000 -0.5926870000
H 4.3335060000 0.0814370000 1.2857600000
H 6.1448410000 1.8964980000 1.3323250000
Cu -0.5912150000 -1.7447520000 -1.5848970000
Cu 1.0034430000 1.5949130000 1.2883690000
Cu -0.4432010000 1.8972730000 -1.1091470000
Cu 2.0291790000 0.2453990000 -0.7143150000
S -0.0071210000 0.0239480000 0.0008030000
H -5.9130660000 -4.1503640000 0.2967210000
H -1.5826220000 4.8723050000 5.1860080000
H 9.8758810000 1.1293000000 -1.9924460000
H 8.5596620000 -5.3274860000 -3.7720350000
H -4.3243420000 -3.1808750000 -6.2375840000
H 0.2665150000 -0.6587700000 -6.7888410000
H -0.5997680000 8.0349330000 -1.5092540000
H 2.5726850000 5.7194890000 -0.0436730000
H 3.6899610000 2.0850830000 -3.2531020000
N 2.0094110000 -2.6742770000 -2.7577380000
N 0.9588570000 -2.7139210000 -2.3960530000
O 2.7269460000 -0.8255180000 -2.0669260000

2-hole Cu_{IV}-OH---$LysH^+$

C 21.7600610000 43.4678340000 13.8481000000
C 22.4537680000 42.8490020000 15.0339730000
N 22.2034230000 41.5382640000 15.4684780000
C 23.3919620000 43.4086520000 15.8865930000
C 22.9640920000 41.3268320000 16.5484080000
N 23.7057800000 42.4348630000 16.8338220000
H 21.6761360000 42.7506090000 13.0182700000
H 20.7414490000 43.8049180000 14.1078670000
H 23.8506010000 44.3930820000 15.8918300000
H 23.0039740000 40.4120960000 17.1325080000
H 24.3599730000 42.5358450000 17.6049270000
C 18.5341270000 45.9070910000 11.4620230000
C 18.5157850000 44.5833110000 12.1268380000
N 18.0958620000 44.3618940000 13.4379630000
C 18.9013360000 43.3479510000 11.6535910000
C 18.2406550000 43.0282100000 13.7174350000
N 18.7313540000 42.3929120000 12.6511160000
H 17.5283960000 46.3685260000 11.4257790000
H 18.8941590000 45.8045620000 10.4253310000
H 19.2933800000 43.0971540000 10.6730610000
H 17.9974430000 42.5820550000 14.6772570000
H 17.7381750000 45.0657220000 14.0784120000
C 17.4771480000 42.6498610000 18.5278570000
C 18.0659570000 41.6189670000 17.6323560000
N 17.3847310000 40.4789610000 17.2112030000
C 19.3023030000 41.5386710000 17.0222650000
C 18.2000450000 39.7653350000 16.3793970000
N 19.3681900000 40.3851920000 16.2430900000
H 16.5711050000 43.1089870000 18.0870970000
H 17.1856680000 42.2268330000 19.5086260000
H 20.1316040000 42.2352390000 17.0925380000
H 17.9040550000 38.8366630000 15.9035250000
H 16.4422680000 40.2152930000 17.4869920000
C 14.7852340000 33.8559830000 13.5820560000
C 16.0235510000 34.7039490000 13.5550990000
N 16.4244230000 35.4905960000 14.6364470000
C 17.0079530000 34.9070080000 12.6021280000
C 17.6041440000 36.0958410000 14.3396920000
N 17.9806760000 35.7742640000 13.1050610000
H 14.8514250000 33.0673570000 14.3558890000
H 14.6434600000 33.3617810000 12.6068460000
H 17.0776070000 34.4886660000 11.6021370000
H 18.1477110000 36.7283380000 15.0353040000
H 15.9368380000 35.5509930000 15.5267890000
C 16.3112200000 36.1226720000 7.1492550000
C 16.8022850000 36.6025400000 8.4837710000
N 16.0010430000 37.3424410000 9.3544940000
C 18.0139970000 36.4763580000 9.1504330000
C 16.7161090000 37.6285710000 10.4792090000
N 17.9441250000 37.1239350000 10.3840950000
H 16.0138470000 36.9662390000 6.4975390000
H 17.1038560000 35.5570320000 6.6324000000
H 18.9152880000 35.9677480000 8.8196720000
H 16.3097380000 38.1818270000 11.3202560000
H 15.0343110000 37.6083520000 9.1855930000
C 20.5879520000 38.8279250000 7.1140850000
C 19.9534680000 39.4100440000 8.3288590000
N 18.6039350000 39.7310710000 8.4177360000
C 20.4812040000 39.7708160000 9.5512750000
C 18.3581130000 40.2831600000 9.6410360000
N 19.4804060000 40.3126660000 10.3559110000

H 20.5356530000 39.5202020000 6.2516680000
H 21.6512990000 38.6109730000 7.3078790000
H 21.5108750000 39.6645660000 9.8719120000
H 17.3828110000 40.6398140000 9.9574920000
H 17.9185470000 39.6182220000 7.6756640000
C 27.6858820000 32.8791140000 10.5420350000
C 26.6180750000 33.7973010000 9.9435880000
C 26.9508330000 35.2758350000 10.2158110000
C 25.7215400000 36.1712190000 10.1005080000
N 25.9479550000 37.5434740000 10.6729000000
H 27.4775180000 31.8136640000 10.3271090000
H 27.7390150000 32.9969450000 11.6414220000
H 25.6343830000 33.5530070000 10.3936040000
H 26.5151410000 33.6184320000 8.8550010000
H 27.3437570000 35.3625920000 11.2449780000
H 27.7528170000 35.6193070000 9.5335340000
H 25.3790340000 36.2828980000 9.0572320000
H 24.8916470000 35.7397430000 10.6849870000
H 26.5405140000 38.1062150000 10.0665610000
H 26.4183150000 37.4649190000 11.6429120000
H 25.0053010000 37.9838120000 10.7264210000
C 29.1670280000 39.2719580000 12.4010220000
C 29.2539310000 37.7492190000 12.2043830000
C 28.3658980000 37.0326270000 13.2352660000
O 27.0990840000 37.1086070000 13.0459130000
O 28.9190270000 36.4760330000 14.1999660000
H 28.1268020000 39.6336940000 12.2943660000
H 29.5220520000 39.5605000000 13.4085610000
H 28.9327380000 37.4798080000 11.1800680000
H 30.2962080000 37.4083840000 12.3256960000
C 23.2860860000 41.3878860000 11.0911610000
C 23.9512030000 40.8429920000 12.3283810000
N 23.6197940000 39.5936580000 12.8681730000
C 24.9282170000 41.3890730000 13.1419390000
C 24.3630090000 39.3892950000 13.9555260000
N 25.1674630000 40.4668210000 14.1607770000
H 23.6429180000 42.4110640000 10.8877760000
H 22.1887550000 41.4315990000 11.2037590000
H 25.4518180000 42.3382000000 13.0831230000
H 24.3501100000 38.5077980000 14.5881230000
H 25.8556450000 40.5601560000 14.9028470000
Cu 19.0653560000 37.1428590000 12.0876700000
Cu 20.8379930000 40.1585960000 14.8441650000
Cu 19.5130880000 40.5936760000 12.3703580000
Cu 22.2858700000 38.3991230000 12.0436630000
S 20.3558340000 38.6743640000 13.1652490000
H 13.8823520000 34.4589850000 13.7947810000
H 18.2078950000 43.4538230000 18.7141040000
H 29.7904720000 39.8117090000 11.6624870000
H 28.6893230000 33.1101600000 10.1336600000
H 15.4332960000 35.4573090000 7.2555400000
H 20.0962800000 37.8839350000 6.8101800000
H 19.2021600000 46.6208730000 11.9819550000
H 22.3234950000 44.3465260000 13.4912410000
H 23.5140760000 40.7648340000 10.2078750000
N 32.6137750000 21.5005580000 7.7918030000
N 31.8623760000 22.2746510000 7.9626680000
O 23.2441820000 38.0052810000 10.4987190000
H 22.9499240000 37.1658640000 10.1239230000