Supporting information

Spectroscopic and Theoretical Study of Cu^{I} Binding to His111 in the Human Prion Protein Fragment 106-115

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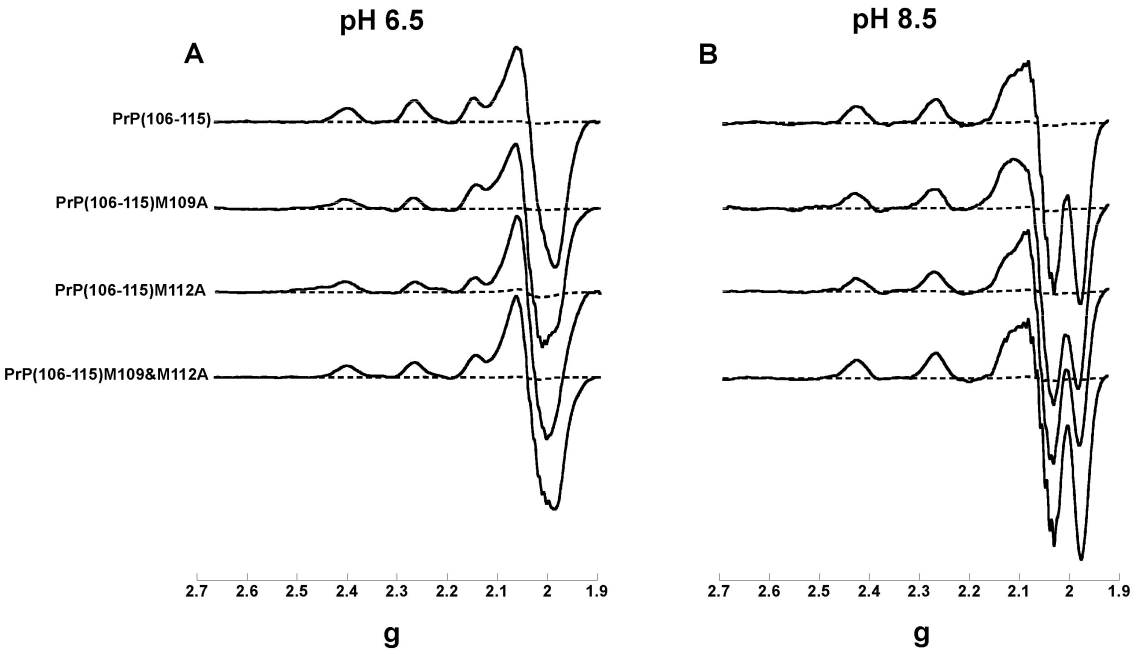

Figure S1. EPR spectra of the Cu(II)-peptide (solid lines) and after adding 100 Eq of ascorbic acid in anaerobic conditions (dashed lines) at pH 6.5 (A) and 8.5 (B). In all cases residual Cu(II) was less than 3 %.

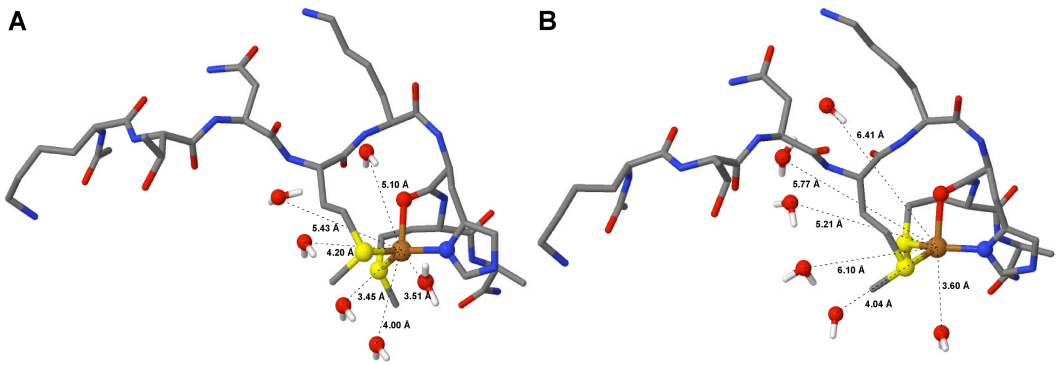

Figure S2. Representative distribution of explicit H_2O molecules. In the 1N1O2Sa1 model at the beginning of optimization (A), water molecules are located between 3.5 and 5.5 Å. At the end of the optimization (B) with deMon2k, OPBE/TZVP/GEN-A2, water molecules are found around 3.5 and 6.5 Å. For clarity, most H atoms are not shown

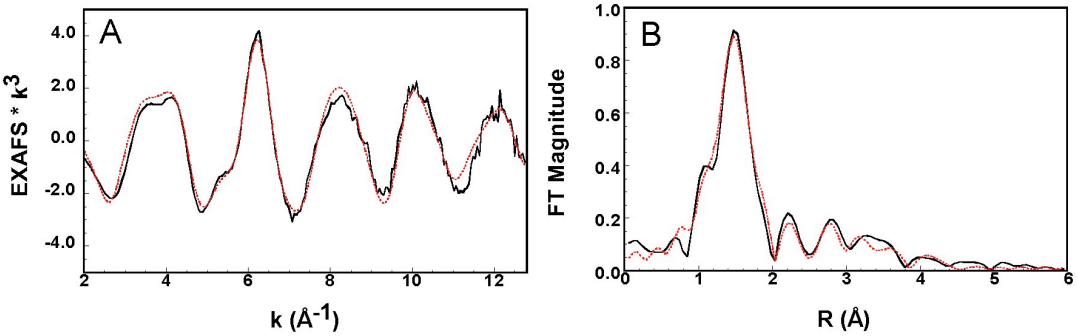

Figure S3. Representative EXAFS (A) and its Fourier transform (B) (solid black line) for Cu(II)-PrP(106-115) at pH 6.5. The best fit with parameters listed in Table 1, is shown in dotted red line.

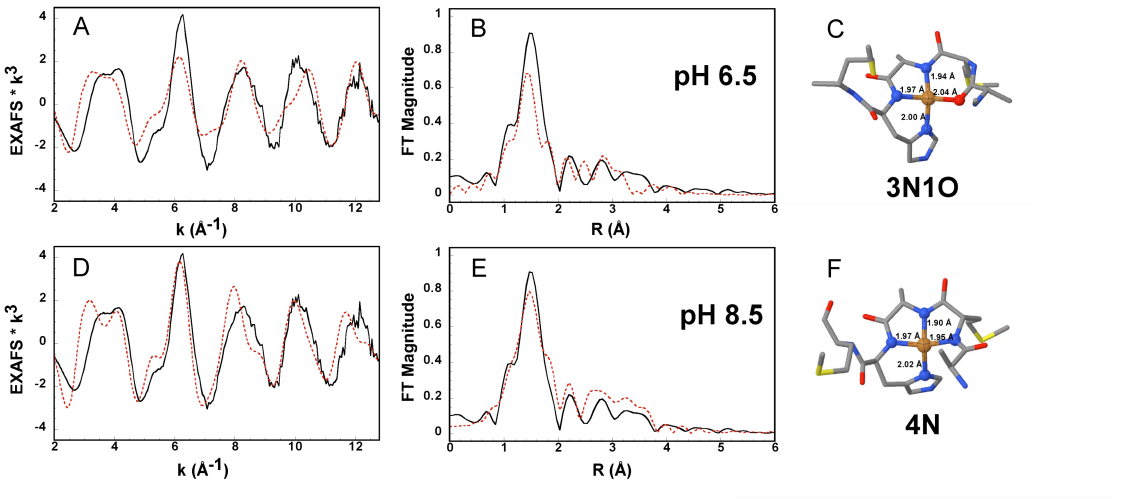

Figure S4. EXAFS data and Fourier transforms of Cu(II)-PrP(106-115) at pH 6.5 (A, B) and 8.5 (D, E) (solid black line) and their simulations (dashed red line) using reoptimized structures Cu(II)-3N1O (C) and Cu(II)-4N (F). The average of the bond distances between the four ligands is 1.99 and 1.96 Å in the 3N1O and 4N models, respectively.

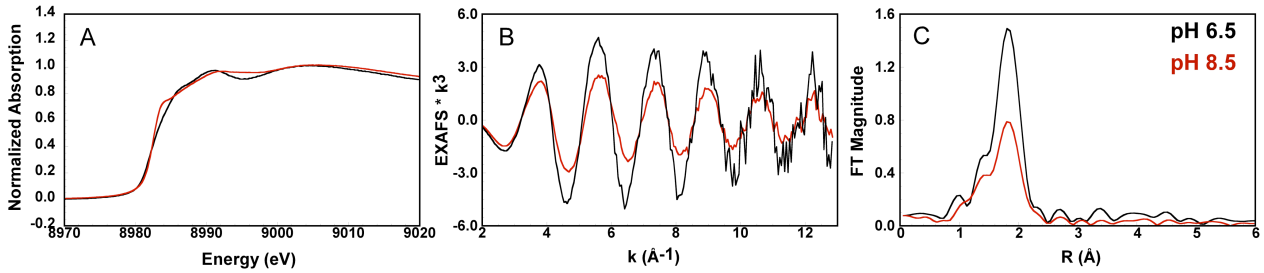

Figure S5. XANES (A), EXAFS (B) and Fourier transforms (C) of Cu(I)-PrP(106-115) at pH 6.5 (black line) and 8.5 (red line). At low pH, the spectrum exhibits a higher EXAFS data intensity as compared to that for pH 8.5.

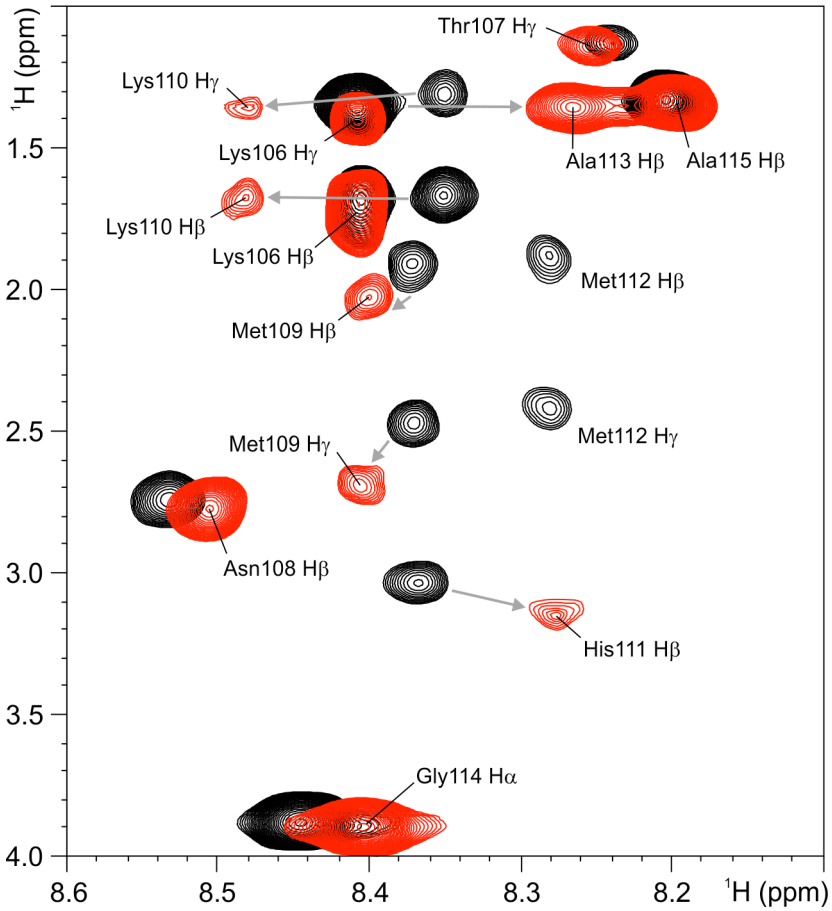

Figure S6. TOCSY ^{1}H-^{1}H of PrP(106-115) (black) and Cu(I)-PrP(106-115) (red) at pH 6.5. The most affected signals, in the presence of Cu(I), are those corresponding to Met109, Met112, His111 and Lys110.

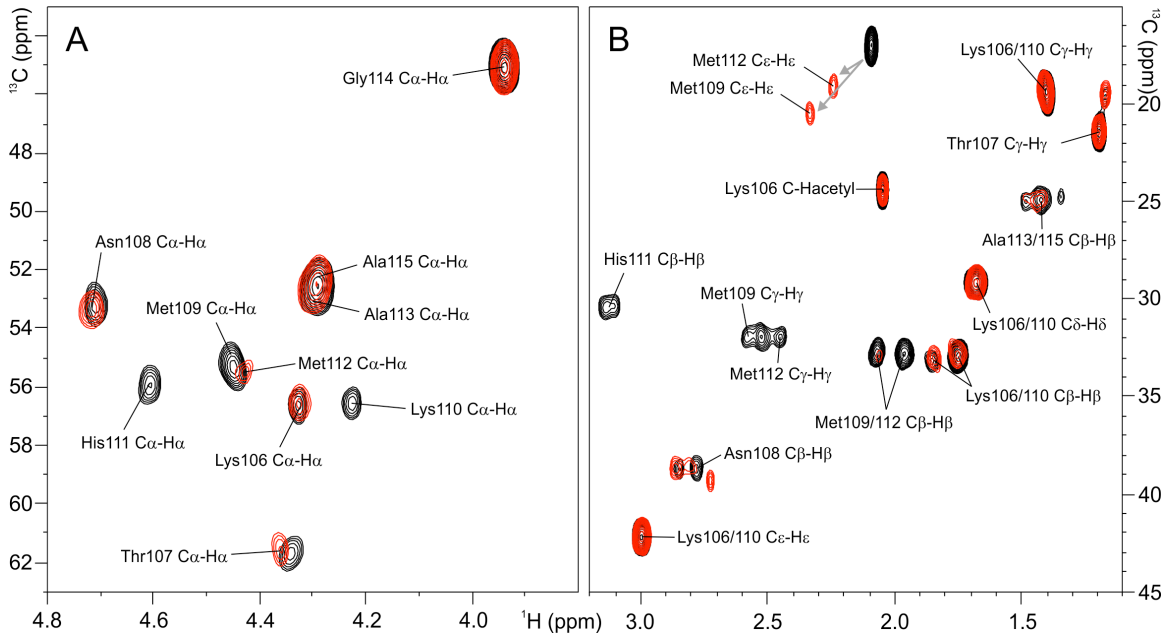

Figure S7. HSQC ^{1}H-^{13}C of PrP(106-115) (black) and Cu(I)-PrP(106-115) (red) at pH 6.5. Cα (A), Cβ, Cγ, Cδ and Cε (B). The most affected Cα signals correspond to His111 and Lys110, while the most affected Cβ, Cγ, Cδ and Cε correspond to His111, Met109 and Met112.

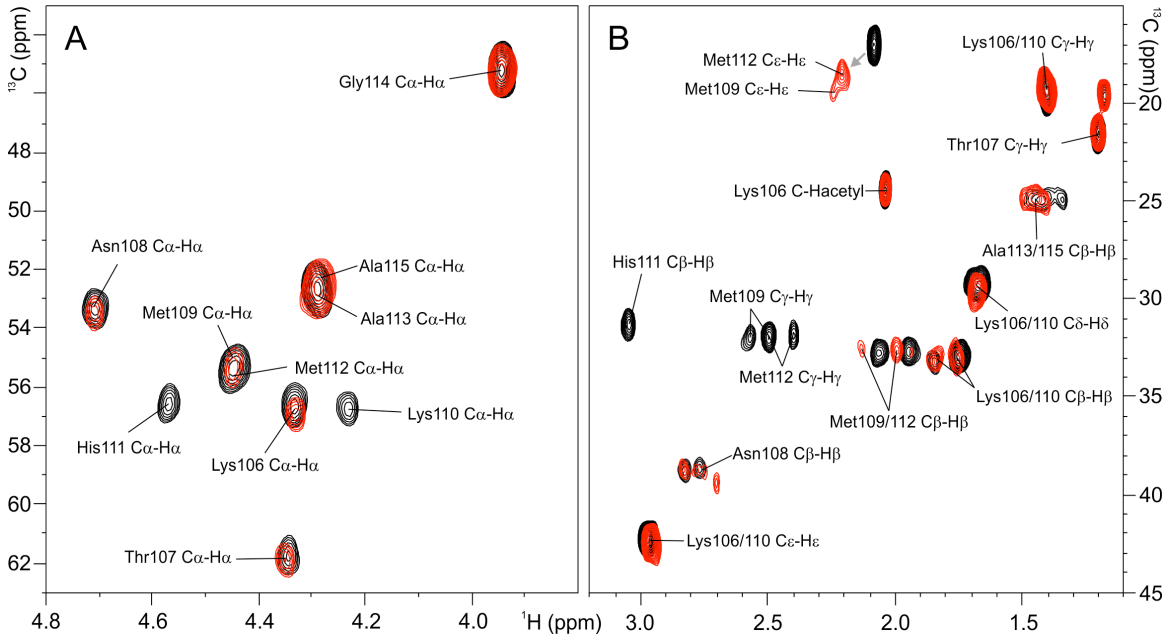

Figure S8. HSQC ^{1}H-^{13}C of PrP(106-115) (black) and Cu(I)-PrP(106-115) (red) at pH 8.5. Cα (A), Cβ, Cγ, Cδ and Cε (B). The most affected Cα signals correspond to His111 and Lys110, while the most affected Cβ, Cγ, Cδ and Cε correspond to His111, Met109 and Met112.

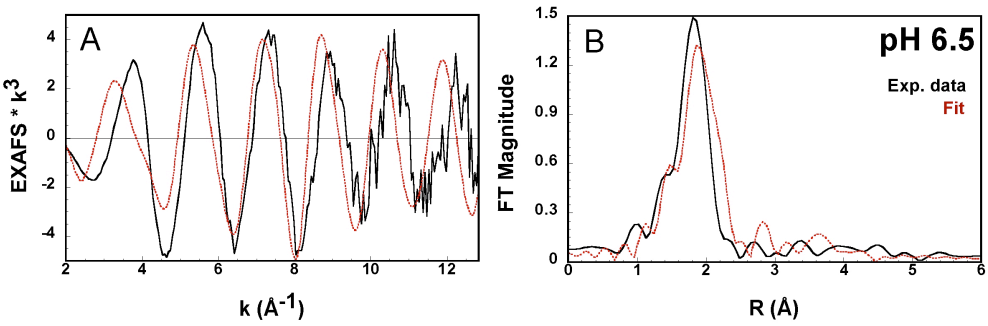

Figure S9. EXAFS (A) and Fourier transform (B) of Cu(I)-PrP(106-115) at pH 6.5 (solid black line) and the corresponding simulation (dashed red line) using the optimized structure 1N1O2Sc1, as listed in Table S2.

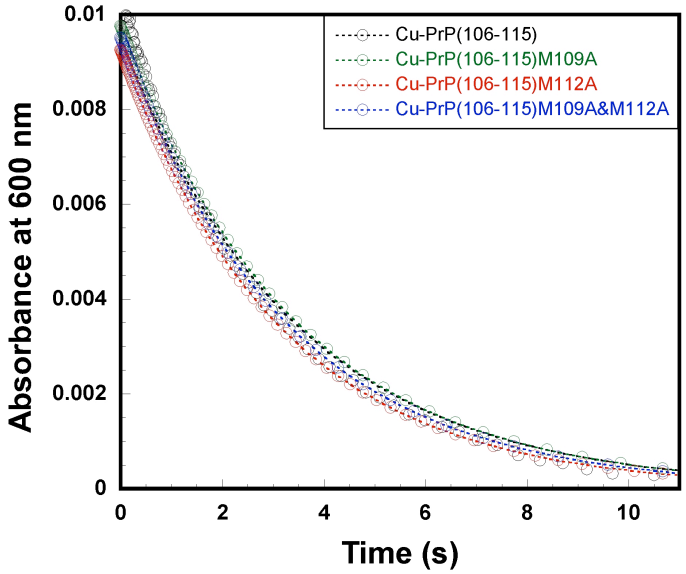

Figure S10. Stopped-flow absorption data and their fits of reduction of Cu(II)-PrP(106-115), (black) Cu(II)-PrP(106-115)M109A, (green) Cu(II)-PrP(106-115)M112A, (red) and Cu(II)-PrP(106-115)M109&M112A (blue) complexes at pH 6.5 with 20 equiv. of ascorbate.

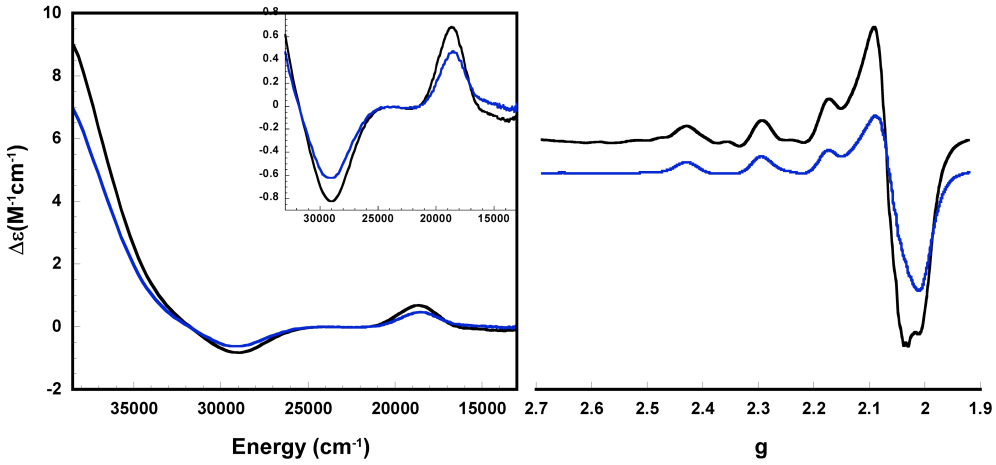

Figure S11. Representative CD and EPR spectra of Cu(II)-PrP(106-115) (black line) and in the end point of reoxidation kinetics (blue line), the signals associated with the Cu(II)-3N1O complex are recovered after reoxidation.

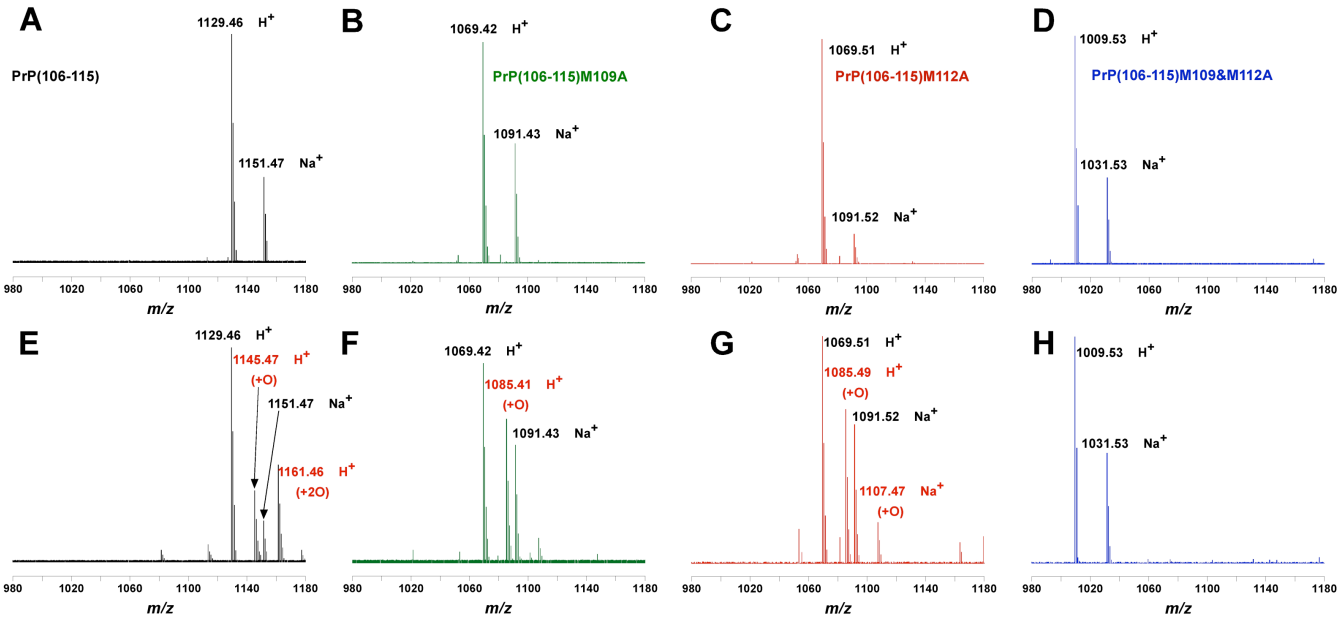

Figure S12. MALDI-TOF/TOF analysis of the PrP(106-115) (black), PrP(106-115)M109A (green), PrP(106-115)M112A (red) and PrP(106-115)M109&M112A (blue) peptides, before (A, B, C, D) and after a redox cycle with ascorbate and oxygen (E, F, G, H).

Table S1. Lowest Harmonic Frequencies of the Selected Optimized Cu(I)-PrP(106-115) Structures with the OPBE Functional.

Models	**Frequency cm^{-1}**
3N1O	2.1
4N	9.3
1N1O2Sa	11.5
$2N1O1S_{M109}a$	6.8
$2N1O1S_{M112}a$	7.6

Table S2. Copper-ligand Distances (Å) for Selected Geometry-Optimized Models for the Cu(I)-PrP(106-115) Complexes: Effects of Implicit and Explicit Solvation.

	Model	Without Solvation	Implicit Solvation (ORCA)	Explicit Solvation (4 H_2O)	Explicit Solvation (6 H_2O)
Models at pH 6.5	1N1O2Sa	2S – 2.300 1N1O – 2.140	2S – 2.345 1N1O – 2.120	2S – 2.340 1N1O – 2.160	2S – 2.350 1N1O – 2.170
	1N1O2Sc1	2S – 2.340 1N1O – 2.155	2S – 2.365 1N1O – 2.170	2S – 2.345 1N1O – 2.145	2S – 2.360 1N1O – 2.160
Models at pH 8.5	2N1O1S$_{M109}$a	1S – 2.280 1N – 2.020 1N1O – 2.200	1S – 2.300 1N – 2.030 1N1O – 2.180	1S – 2.310 1N – 2.020 1N1O – 2.180	1S – 2.320 1N – 2.020 1N1O – 2.150
	2N1O1S$_{M112}$a	1S – 2.360 1N – 2.010 1N1O – 2.140	1S – 2.420 1N – 2.010 1N1O – 2.200	1S – 2.350 1N – 2.000 1N1O – 2.180	1S – 2.340 1N – 2.000 1N1O – 2.170

Table S3. Initial Models of the Coordination of Cu(I)-PrP(106-113) at pH 6.5 and 8.5. In Group 1 the Ligands Include His111 Imidazole Nitrogen, Sulfur Atoms from Met109 and Met112, in the Groups 2 and 3 the Ligands Include His111 Imidazole Nitrogen and Only one Sulfur Atom from Either Met109 or Met112, Respectively. [+, #, *]

Group 1		Group 2A			Group 2B		
Model	Fourth Ligand	Model	Third Ligand	Fourth Ligand	Model	Third Ligand	Fourth Ligand
2N2Sa*	N^-_{H111}	3N1S$_{M109}$a*	N^-_{H111}	N^-_{K110}	3N1S$_{M112}$a*	N^-_{H111}	N^-_{K110}
2N2Sb*	N^-_{K110}	3N1S$_{M109}$b	N^-_{H111}	N^-_{M109}	3N1S$_{M112}$b	N^-_{H111}	N^-_{M109}
2N2Sa1	N_{H111}	3N1S$_{M109}$c*	N^-_{K110}	N^-_{M109}	3N1S$_{M112}$c*	N^-_{K110}	N^-_{M109}
2N2Sb1	N_{K110}	3N1S$_{M109}$a1	N_{H111}	N^-_{K110}	3N1S$_{M112}$a1	N_{H111}	N^-_{K110}
1N1O2Sa*	O_{H111}	3N1S$_{M109}$a2	N^-_{H111}	N_{K110}	3N1S$_{M112}$a2	N^-_{H111}	N_{K110}
1N1O2Sb*	O_{K110}	3N1S$_{M109}$a3	N_{H111}	N_{K110}	3N1S$_{M112}$a3	N_{H111}	N_{K110}
1N1O2Sc	O_{N108}	3N1S$_{M109}$b1	N_{H111}	N^-_{M109}	3N1S$_{M112}$c1	N_{K110}	N^-_{M109}
1N1O2Sa1	$O_{w/H111}$	3N1S$_{M109}$b2	N^-_{H111}	N_{M109}	3N1S$_{M112}$c2	N^-_{K110}	N_{M109}
1N1O2Sb1	$O_{w/K110}$	3N1S$_{M109}$b3	N_{H111}	N_{M109}	3N1S$_{M112}$c3	N_{K110}	N_{M109}
1N1O2Sc1*	$O_{w/N108}$	3N1S$_{M109}$c1	N_{K110}	N^-_{M109}	2N1O1S$_{M112}$a*	N^-_{K110}	O_{H111}
		3N1S$_{M109}$c2	N^-_{K110}	N_{M109}	2N1O1S$_{M112}$a1	N_{K110}	O_{H111}
		3N1S$_{M109}$c3	N_{K110}	N_{M109}	2N1O1S$_{M112}$b	N^-_{H111}	O_{M109}
		2N1O1S$_{M109}$a*	N^-_{K110}	O_{H111}	2N1O1S$_{M112}$c	N^-_{M109}	O_{H111}
		2N1O1S$_{M109}$a1	N_{K110}	O_{H111}	2N1O1S$_{M112}$c1	N_{M109}	O_{H111}
		2N1O1S$_{M109}$b*	N^-_{H111}	O_{M109}	2N1O1S$_{M112}$d*	N^-_{M109}	O_{K110}
		2N1O1S$_{M109}$c*	N^-_{A113}	O_{A113}	2N1O1S$_{M112}$d1	N^-_{M109}	$O_{w/K110}$
		2N1O1S$_{M109}$a2	N^-_{K110}	$O_{w/H111}$	2N1O1S$_{M112}$a2	N^-_{K110}	$O_{w/H111}$
		1N2O1S$_{M109}$a	O_{K110}	O_{H111}	1N2O1S$_{M112}$a	O_{H111}	O_{M109}
					1N2O1S$_{M112}$b	O_{H111}	O_{K110}
					1N2O1S$_{M112}$c	O_{M109}	O_{K110}

[+] In the table

N^- is nitrogen belonging to deprotonated amide of backbone

N is nitrogen belonging to protonated amide of backbone

O is oxygen belonging to the carbonyl of backbone

O_w is oxygen belonging to a H_2O molecule

[#] Models with O_w, oxygen atom belonging to the carbonyl of backbone were replaced in the same place for an oxygen atom belonging to a water molecule.

[*] After optimization, only these models retain their tetracoordinated structure.

Table S4. Structural and Energetic Parameters of the Optimized Models in Group 1. (OPBE/TZVP, With and Without 6 Explicit Water Molecules). * ΔE is the Relative Energy in kcal/mol. Experimental EXAFS Bond Distances at pH 6.5 for 2 Cu-S and 2 Cu-N/O are 2.37 and 2.17 Å, Respectively, (Table 2).

	Model	Ligands	Average BD (OPBE)	Average BD (Explicit Solvation, 6 H_2O)	ΔE (Explicit Solvation)
Bond (Å)	2N2Sb	S_{M109} S_{M112} N_{Im} N^-_{K110}	Cu-2S 2.34 Cu-2N 2.09	Cu-2S 2.36 Cu-2N 2.09	0.00
	2N2Sa	S_{M109} S_{M112} N_{Im} N^-_{H111}	Cu-2S 2.32 Cu-2N 2.10	Cu-2S 2.34 Cu-2N 2.10	8.41
	1N1O2Sa	S_{M109} S_{M112} N_{Im} O_{H111}	Cu-2S 2.30 Cu-1N1O 2.14	Cu-2S 2.35 Cu-1N1O 2.17	0.00
	1N1O2Sc1	S_{M109} S_{M112} N_{Im} O_w	Cu-2S 2.34 Cu-1N1O 2.15	Cu-2S 2.36 Cu-1N1O 2.16	4.20
	1N1O2Sb	S_{M109} S_{M112} N_{Im} O_{K110}	Cu-2S 2.32 Cu-1N1O 2.16	Cu-2S 2.34 Cu-1N1O 2.14	13.32

* In the table

N^- is nitrogen belonging to deprotonated amide of backbone

N_{Im} is nitrogen belonging to imidazol of His111

O is oxygen belonging to the carbonyl of backbone

O_w is oxygen belonging to a H_2O molecule

Table S5. Structural and Energetic Parameters of the Optimized Geometries for the Group 2A. (OPBE/TZVP, With and Without 6 Explicit Water Molecules). * ΔE is the Relative Energy in kcal/mol. Experimental EXAFS Bond Distances at pH 8.5 for 1 Cu-S, 1 Cu-N/O and 2 Cu-N/O are 2.35, 1.97 and 2.15 Å, Respectively, (Table 2).

	Model	Ligands	Average BD in OPBE	Average BD (Explicit Solvation, 6 H_2O)	ΔE (Explicit Solvation)
Bond (Å)	3N1S$_{M109}$a	S_{M109} N_{Im} N^-_{H111} N^-_{K110}	Cu-1S 2.27 Cu-1N 2.04 Cu-2N 2.10	Cu-1S 2.28 Cu-3N 2.10	0.00
	3N1S$_{M109}$c	S_{M109} N_{Im} N^-_{K110} N^-_{M109}	Cu-1S 2.31 Cu-1N 2.04 Cu-2N 2.15	Cu-1S 2.36 Cu-1N 2.04 Cu-2N 2.13	14.67
	2N1O1S$_{M109}$a	S_{M109} N_{Im} N^-_{K110} O_{H111}	Cu-1S 2.28 Cu-1N 2.02 Cu-1N1O 2.20	Cu-1S 2.32 Cu-1N 2.02 Cu-1N1O 2.15	0.00
	2N1O1S$_{M109}$b	S_{M109} N_{Im} N^-_{H111} O_{M109}	Cu-1S 2.27 Cu-1O 2.36 Cu-2N 2.02	Cu-1S 2.28 Cu-1O 2.45 Cu-2N 2.03	9.45
	2N1O1S$_{M109}$c	S_{M109} N_{Im} N^-_{A113} O_{A113}	Cu-1S 2.22 Cu-1O 2.30 Cu-2N 2.01	Cu-1S 2.30 Cu-1O 2.43 Cu-2N 2.04	11.28

* In the table

N^- is nitrogen belonging to deprotonated amide of backbone

N_{Im} is nitrogen belonging to imidazol of His111

O is oxygen belonging to the carbonyl of backbone

Table S6. Structural and Energetic Parameters of the Optimized Geometries for the Group 2B. (OPBE/TZVP, With and Without 6 Explicit Water Molecules). * ΔE is the Relative Energy in kcal/mol. Experimental EXAFS Bond Distances at pH 8.5 for 1 Cu-S, 1 Cu-N/O and 2 Cu-N/O are 2.35, 1.97 and 2.15 Å, Respectively, (Table 2). *

	Model	Ligands	Average BD in OPBE		Average BD (Explicit Solvation, 6 H_2O)		ΔE (Explicit Solvation)
Bond (Å)	$3N1S_{M112}a$	S_{M112} N_{Im} N^-_{H111} N^-_{K110}	Cu-1S Cu-3N	2.30 2.04	Cu-1S Cu-3N	2.28 2.03	0.00
	$3N1S_{M112}c$	S_{M112} N_{Im} N^-_{K110} N^-_{M109}	Cu-1S Cu-3N	2.29 2.06	Cu-1S Cu-3N	2.30 2.04	6.63
	$2N1O1S_{M112}a$	S_{M112} N_{Im} N^-_{K110} O_{H111}	Cu-1S Cu-1N Cu-1N1O	2.36 2.01 2.14	Cu-1S Cu-1N Cu-1N1O	2.34 2.00 2.17	0.00
	$2N1O1S_{M112}d$	S_{M112} N_{Im} N^-_{M109} O_{K110}	Cu-1S Cu-1N Cu-1N1O	2.36 2.04 2.20	Cu-1S Cu-1O Cu-2N	2.35 3.39 2.02	9.56

* In the table

N^- is nitrogen belonging to deprotonated amide of backbone

N_{Im} is nitrogen belonging to imidazol of His111

O is oxygen belonging to the carbonyl of backbone

Table S7. Calculated Reorganization Energies (λ_i) for the Pairs Cu(II)-3N1O/Cu(I)-1N1O2S and Cu(II)-4N/Cu(I)-2N1O1S Models at pH 6.5 and 8.5.

	ID	Structure	Energy (a. u.)	λ_i (a. u.)	λ_i (eV)
pH 6.5	$E_{ox}(Red_{geom})$	Cu(II)-1N1O2Sa	-5941.968973	0.065875	1.79
	$E_{ox}(Ox_{geom})$	Cu(II)-3N1O	-5942.132491		
	$E_{red}(Ox_{geom})$	Cu(I)-3N1O	-5942.271824		
	$E_{red}(Red_{geom})$	Cu(I)-1N1O2Sa	-5942.240056		
	$E_{ox}(Red_{geom})$	Cu(II)-1N1O2Sc1	-5941.986104	0.079190	2.15
	$E_{ox}(Ox_{geom})$	Cu(II)-3N1O	-5942.132491		
	$E_{red}(Ox_{geom})$	Cu(I)-3N1O	-5942.271824		
	$E_{red}(Red_{geom})$	Cu(I)-1N1O2Sc1	-5942.283818		
pH 8.5	$E_{ox}(Red_{geom})$	Cu(II)-2N1O1S$_{M109}$a	-5941.661874	0.058984	1.60
	$E_{ox}(Ox_{geom})$	Cu(II)-4N	-5941.906563		
	$E_{red}(Ox_{geom})$	Cu(I)-4N	-5942.015464		
	$E_{red}(Red_{geom})$	Cu(I)-2N1O1S$_{M109}$a	-5941.888744		
	$E_{ox}(Red_{geom})$	Cu(II)-2N1O1S$_{M112}$a	-5941.587744	0.061087	1.66
	$E_{ox}(Ox_{geom})$	Cu(II)-4N	-5941.906563		
	$E_{red}(Ox_{geom})$	Cu(I)-4N	-5942.015464		
	$E_{red}(Red_{geom})$	Cu(I)-2N1O1S$_{M112}$a	-5941.818821		

Estimation of E°$_{(Cu(II/I)-PrP(106-115))}$ at pH 6.5 and 8.5 by Reductive Titrations

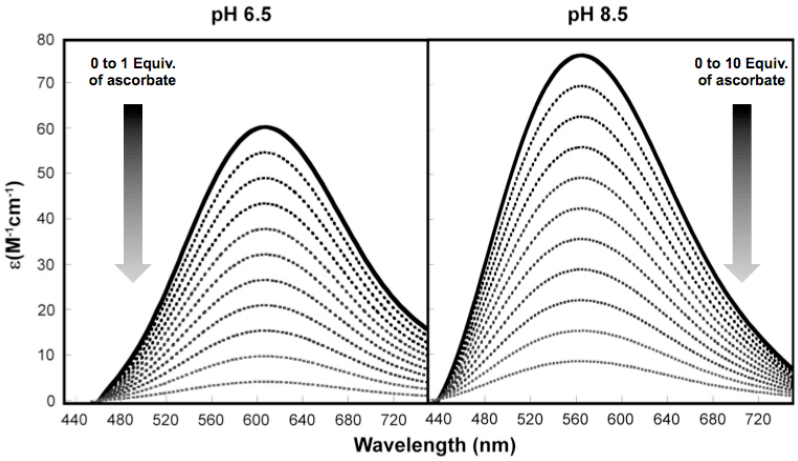

Figure S13. Representative anaerobic titration with ascorbate of the complex Cu(II)-PrP(106-115), followed by the loss in the d-d band (dotted lines). At pH 6.5 the titration was to 1 equiv. of ascorbate, whereas titration at pH 8.5 was to 10 equiv.

E°$_{(Cu(II/I)-PrP(106-115))}$ value was estimated by $\Delta G^{\circ} = -nF\Delta E^{\circ}$, where ΔE° = E°$_{(Cu(II/I)-PrP(106-115))}$ - E°$_{(AA/DA)}$, E°$_{(AA/DA)}$ = 0.052 V vs. NHE, and $\Delta G^{\circ} = -RT\ln K_{eq}$.

Considering:

$$2Cu(II) - L + AA \underset{K_{eq}}{\rightleftharpoons} 2Cu(I) - L + DA \quad \text{and} \quad K_{eq} = \frac{\left[\frac{x}{2}\right][x]^2}{\left[\frac{C_i - x}{2}\right][C_i - x]^2}$$

Where C_i is the [Cu(II)-L] at the starting point of the titration and x is the [Cu(I)-L] obtained by the percent of reduction in the titration followed by UV-Vis of Cu(II)-PrP(106-115) with 1 or 10 equiv. of ascorbate.

At pH 6.5 ΔG° = -4.62 kcal/mol ΔE° = 0.1002 V and E°$_{(Cu(II/I)-PrP(106-115))}$ = 152 mV.

At pH 8.5 ΔG° = - 1.09 kcal/mol, ΔE° = 0.0238 V and E°$_{(Cu(II/I)-PrP(106-115))}$ = 75.8 mV.

ΔΔG° = (ΔG°$_{(3N1O)}$- ΔG°$_{(4N)}$) = - 3.52 kcal/mol

Calculation of $k_{ET(3N1O)}/k_{ET(4N)}$ using Marcus Equation

Assuming that the term H_{AB} is comparable for both reduction processes (i.e. $H^2_{AB(3N1O)} = H^2_{AB(4N)}$), the ratio of the reduction rates for the Cu(II)-3N1O and Cu(II)-4N complexes take the form:

$$\frac{k_{ET(3N1O)}}{k_{ET(4N)}} = \frac{\lambda^{\frac{1}{2}}_{(4N)}}{\lambda^{\frac{1}{2}}_{(3N1O)}} e^{\frac{(\Delta G^{\circ}_{(4N)}+\lambda_{(4N)})^2}{4\lambda_{(4N)}k_B T} - \frac{(\Delta G^{\circ}_{(3N1O)}+\lambda_{(3N1O)})^2}{4\lambda_{(3N1O)}k_B T}}$$

Where:

$\lambda_{(3N1O)} = 1.79 eV$ and $\lambda_{(4N)} = 1.6 eV$ are the calculated values for the reorganization energies (Table S7).

Using the value of $\Delta G^{\circ}_{(3N1O)} = -4.62\ kcal/mol$ and $\Delta G^{\circ}_{(4N)} = -1.09\ kcal/mol$, which are derived from the reductive titration (vide supra), we obtain $k_{ET(3N1O)}/k_{ET(4N)} = 2.3$. The ratio of experimental reduction rates for the Cu(II)-3N1O and Cu(II)-4N species is 2.14.

Calculation of Outer-Sphere Electron Transfer Rate

The rate of outer-sphere reduction of O_2 by Cu(I)-PrP(106-115) complexes was obtained as follows:

$$k_{et} = Ze^{(\frac{-\Delta G^{\neq}}{RT})}$$

Where:

$$\Delta G^{\neq} = (\frac{\lambda}{4})(\frac{\lambda + \Delta G^{\circ}}{\lambda})^2$$

Z (frequency factor) = $10^{11} M^{-1}s^{-1}$

λ (total reorganization energy) = $(\lambda_{Cu\text{-}PrP,\ donor} + \lambda_{O2,\ acceptor})/2$ = 1.84 eV

$\lambda_{O2,\ acceptor}$ = 1.89 eV (experimental value)

$\lambda_{Cu\text{-}PrP,\ donor}$ = 1.79 eV (calculated value for Cu(II)-3N1O and Cu(I)-1N1O2Sa in this work). *

$\Delta G^{\circ} = -nF\Delta E^{\circ}$ = 0.31 eV

ΔE° = - 0.16 V ($O_2/O_2^{\cdot -}$) – 0.152 V (Cu(I/II)-PrP(106-115)) = - 0.31 V

Using these values the second ET rate is estimated to be 3.79 $M^{-1}s^{-1}$, which, accounting for $[O_2]$ = 0.0741 mM results in a first order rate constant of 2.81×10^{-4} s^{-1}

* If use the calculated λ value for the pair Cu(II)-3N1O/Cu(I)-1N1O2Sc1 (2.15 eV) the first order ET rate constant is estimated to be $4.49 \times 10^{-5} s^{-1}$

Experimental Details

Electron Paramagnetic Resonance (EPR) Spectroscopy. Cu(II) and Cu(I) samples for EPR spectroscopy were acquired either using the same samples prepared to K-Edge X-Ray Absorption Measurements or the end point in the re-oxidation experiments. X-band EPR spectra were collected using a Bruker EMX spectrometer, ER 041 XG microwave bridge, and ER 4102ST cavity. The following conditions were used: microwave frequency, 9.4 GHz; temperature, 77 K; microwave power, 10 mW; modulation amplitude, 5 G; modulation frequency, 100 kHz; time constant, 327 ms; conversion time, 83 ms; and averaging over 12 scans. EPR spectra were baseline- corrected using KaleidaGraph 4.1.3.

Circular Dichroism (CD) Spectroscopy. CD spectra were recorded using a Jasco J-815 CD spectropolarimeter. Spectra were recorded in quartz cells with 1 cm path lengths at the end point of reoxidation experiments.

Electronic Structure Calculations of reoptimized Cu(II) models. In the calculations of the model 4N, reported models 4Na and 4Nb (Rivillas-Acevedo L. et al. Inorg. Chem 2011, 50, 1956-1972) were used, calculations were performed using the deMon2k code with the functional OPBE; TZVP and GEN-A2 were used as orbital and auxiliary basis sets, respectively. In calculations of the model 3N1O, was built a smaller model from 3Nb1 model (Rivillas-Acevedo L. et al. Inorg. Chem 2011, 50, 1956 -1972) with the sequence CH_3-TAMAHM-CH_3. The optimizations were carried out using the ORCA program with

the functional B3LYP and BP86, TZVP basis set was used to the Cu(II) ion, nitrogen and oxygen atoms. Implicit solvation model COSMO was included in these calculations.

Matrix-Assisted Laser Desorption/Ionization time of flight/time of flight (MALDI-TOF/TOF) Mass Spectrometry. Molecular masses of native and modified peptides were determined in a 4800 MALDI-TOF/TOF plus instrument (AB Sciex, Framingham, MA). Briefly, in the reoxidation kinetics experiments, Cu(II)-peptide samples were taken before reduction (aerobic conditions) and after re-oxidation by oxygen (Cu(I)-complex with ~ 0.5 equiv of O2). In order to remove the metal ion, the samples were treated 15 equiv of ethylenediaminetetraacetic acid (EDTA), loaded into C-18 micro-columns (C18 ZipTip Agilent Technologies, Santa Clara, CA), and eluted with 0.1 % trifluoroacetic acid (TFA) in 50 % acetonitrile (ACN). The eluted peptides were concentrated in a volume of 2 μL and mixed in the matrix solution (α-cyano-4-hydroxycinnamic acid in 50 % aqueous acetonitrile containing 0.1 % TFA). Cumulative 1000 scans were collected on a mass rage of 850-4000 Da and analyzed by Data Explorer software v. 4.9 (AB Sciex, Framingham, MA). External calibration was performed with a mixture of peptide standards.

Cartesian Coordinates for Optimized Structures

2N2Sb Model

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.241000
N	1.149300	0.000000	-0.716600
H	2.005700	-0.250100	-0.230700
H	1.182200	-0.097100	-1.734000
C	-1.278200	0.003300	-0.837500
C	-2.450700	0.764900	-0.154700
N	-3.736300	0.203300	-0.620900
C	-4.907400	0.467000	0.015500
O	-4.961600	1.276600	0.950100
H	-3.694000	-0.521600	-1.334100
C	-2.289200	2.269800	-0.430200
O	-1.334300	2.864400	0.118700
N	-3.152300	2.852000	-1.265800
H	-3.849000	2.238700	-1.686600
C	-3.172800	4.271300	-1.715600
C	-3.049000	5.279900	-0.548500
O	-3.839200	5.159700	0.444000
N	-2.147227	6.238468	-0.745917
C	-2.091800	7.225600	0.360600
H	-2.324800	4.438300	-2.408200
C	-1.343800	8.560300	0.124200
O	-1.982200	9.609700	0.311900
N	0.018600	8.637400	-0.027400
C	0.871400	7.744100	-0.829700
H	0.352300	9.600100	0.030000
H	0.247500	6.917700	-1.180500
C	2.081700	7.226500	-0.032300
O	2.716700	7.987800	0.699300
N	2.553400	5.943300	-0.214600
H	3.472800	5.862300	0.224800
C	2.138700	4.685900	-0.877300
C	0.917700	4.652700	-1.838100
C	1.202400	5.181400	-3.264100
H	1.710900	6.161300	-3.283900
H	0.049800	5.172600	-1.386900
H	-2.377700	0.638300	0.942100
C	-6.144000	-0.320400	-0.509700
N	-7.343900	0.105400	0.195200
C	-7.707700	-0.404200	1.413000
O	-7.079500	-1.303800	1.976100
H	-7.914800	0.815400	-0.243200

C	-8.961000	0.280800	1.984900
N	-9.452900	-0.465500	3.141000
C	-10.777100	-0.413000	3.497500
O	-11.578100	0.319900	2.908500
H	-8.823300	-1.139100	3.560900
C	-11.159400	-1.298900	4.662000
C	-6.345700	-0.172900	-2.042600
O	-6.645300	1.225300	-2.243500
H	-6.983600	1.322800	-3.149700
C	-7.446400	-1.100800	-2.579700
H	-8.429800	-0.874100	-2.135800
H	-10.314200	-1.857300	5.101700
H	-11.927900	-2.017200	4.324000
H	-11.636300	-0.686800	5.450000
C	-4.534000	4.461100	-2.445200
C	-4.936700	5.942900	-2.671400
H	-4.993600	6.494900	-1.711500
H	-7.192900	-2.158000	-2.356200
H	-1.103300	0.366100	-1.873600
H	-7.524100	-1.002900	-3.683500
H	1.803600	4.453800	-3.848900
H	0.586500	3.593300	-1.915800
C	3.394400	4.110700	-1.617000
O	4.287500	4.820000	-2.074900
N	3.374800	2.748400	-1.710700
C	4.321100	2.005800	-2.553600
H	2.566600	2.225700	-1.374400
C	3.528900	1.257200	-3.635800
O	2.519400	0.590600	-3.356100
N	4.019200	1.338200	-4.889100
H	3.598600	0.765000	-5.616800
H	4.875800	1.844800	-5.108100
C	5.175100	1.014500	-1.719600
H	4.532300	0.325000	-1.143100
H	5.803100	1.595200	-1.017400
H	5.845100	0.429500	-2.380100
H	5.010400	2.754200	-2.996300
H	-4.539200	3.886200	-3.398000
H	-3.120800	7.582400	0.595300
C	-8.711900	1.782900	2.334500
C	-7.583900	2.031000	3.365500
H	-7.886200	1.534800	4.309200
H	-9.673200	2.162100	2.736100
C	-7.351100	3.553100	3.620500
C	-6.095400	4.129900	2.930600
N	-6.102400	3.866800	1.451900

H	-6.944000	4.286700	1.045900
H	-6.082000	2.848600	1.243200
H	-5.274700	4.312300	0.939000
H	-5.173600	3.679700	3.344200
H	-6.033300	5.230700	3.059800
H	-6.647300	1.531100	3.040800
H	-7.199800	3.734300	4.706400
H	-8.249700	4.139500	3.328500
H	1.839900	3.980600	-0.064800
H	-9.755900	0.274600	1.205400
H	-5.406400	-0.423900	-2.585200
H	-8.553600	2.346800	1.386900
H	-5.339500	4.035100	-1.799500
S	-3.829600	6.968600	-3.688800
H	-5.968000	-1.393600	-0.255400
H	-5.947700	5.986900	-3.144200
C	1.473800	8.580500	-2.002900
C	0.410100	9.209800	-2.878600
C	0.508000	10.425500	-3.516100
N	-0.695700	10.645300	-4.133800
C	-1.500900	9.600300	-3.849000
N	-0.865900	8.693900	-3.103900
H	-0.966600	11.478800	-4.675300
H	-2.522800	9.544500	-4.200300
H	1.327800	11.139400	-3.556500
H	2.177300	7.954200	-2.595500
H	2.094100	9.394800	-1.559700
H	-1.570000	-1.074800	-0.902500
C	-3.927500	6.130000	-5.306300
H	-3.333900	5.201600	-5.299300
H	-3.559300	6.849000	-6.062500
H	-4.987700	5.906400	-5.542200
C	-1.570500	6.655400	1.738500
C	-0.420500	5.607800	1.691700
H	0.530900	6.092000	1.409500
H	-2.451900	6.210300	2.237600
H	-1.228700	7.530500	2.331200
H	-0.665100	4.826400	0.946400
C	-0.231900	4.981000	3.105900
C	0.769100	3.803800	3.121600
N	0.124800	2.544000	2.583500
H	-0.576800	2.191700	3.246800
H	0.795900	1.770600	2.445800
H	-0.362500	2.687400	1.661200
H	1.659000	4.029000	2.498900
H	1.103000	3.586400	4.151500

H	0.155100	5.743100	3.814000
H	-1.202200	4.616800	3.503600
S	-0.405800	5.395800	-4.123900
C	0.107100	6.322600	-5.595500
H	0.386300	7.349800	-5.312300
H	-0.737100	6.334200	-6.309700
H	0.963400	5.805200	-6.071100
Cu	-1.713700	6.825300	-2.715100
O	-2.324700	2.010600	-4.375000
H	-2.184400	1.563500	-5.226000
H	-1.723800	2.778600	-4.403100
O	-4.047300	10.931800	-5.601600
H	-4.417200	10.413500	-6.339000
H	-4.755400	10.968200	-4.922600
O	-6.019500	10.781200	-3.400700
H	-5.595700	10.507900	-2.560200
H	-6.548600	11.557200	-3.161600
H	-4.067600	9.494700	-8.799600
O	-4.568900	9.086600	-8.075000
H	-5.446100	8.926300	-8.460600
H	-3.945600	9.846100	-0.326300
O	-4.882700	9.822500	-0.616800
H	-5.349500	10.302400	0.085400
H	-2.667600	12.276500	-5.990800
O	-1.744900	12.602900	-6.079600
H	-1.810600	13.568900	-6.105300

2N2Sa model

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.254500
N	1.126900	0.000000	-0.722800
C	2.479900	0.098000	-0.164400
H	1.084900	-0.095000	-1.739600
C	-1.294500	0.025800	-0.846200
N	-2.443900	0.096600	0.068500
C	-3.576700	-0.675100	-0.018200
O	-4.232600	-0.921800	1.008900
H	-2.267700	0.525800	0.969900
C	-3.953600	-1.086600	-1.457600
N	-3.211899	-2.297281	-1.936654
C	-3.892600	-3.533100	-1.783400
O	-5.041400	-3.822900	-2.176800
C	3.346700	0.772200	-1.246800
O	3.152000	0.544500	-2.446500
N	4.334100	1.578300	-0.802400

H	4.481300	1.797100	0.180200
H	4.950400	2.008800	-1.487000
C	3.066400	-1.297100	0.177100
C	-5.481600	-0.935100	-1.722400
C	-5.649100	-0.347300	-3.100800
C	-6.680000	0.400800	-3.617300
N	-6.333400	0.689600	-4.919000
C	-5.121600	0.138400	-5.163900
N	-4.684900	-0.513200	-4.091200
H	-6.881800	1.247300	-5.568900
H	-4.606100	0.232200	-6.114200
H	-7.611400	0.744600	-3.173900
C	-3.133800	-4.728900	-1.097100
N	-3.074900	-6.001800	-1.883300
C	-2.268000	-6.429900	-2.863200
O	-2.258300	-7.635600	-3.212800
H	-3.712700	-6.718400	-1.541000
C	-1.330500	-5.424900	-3.544100
N	0.023500	-5.962300	-3.309900
C	1.178400	-5.291000	-3.547100
O	1.234600	-4.114800	-3.926700
H	0.090200	-6.979000	-3.221400
C	-1.800000	-4.431400	-0.351600
C	-2.109800	-3.898500	1.071500
C	-0.848500	-3.615400	1.929100
C	-1.230200	-2.893300	3.238600
N	-1.769500	-1.501100	2.973900
H	-1.088600	-0.931900	2.412700
H	-1.924400	-1.014300	3.868600
C	2.427900	-6.165200	-3.238800
N	2.795600	-6.987900	-4.413800
C	2.274900	-8.214100	-4.649300
O	1.334800	-8.677500	-3.979200
H	3.562600	-6.653100	-4.989100
H	2.176300	-6.865700	-2.424000
C	2.973000	-8.974700	-5.816600
N	2.735600	-10.406300	-5.706700
C	3.307200	-11.156100	-4.717600
O	4.224600	-10.745100	-4.001700
H	1.953900	-10.778900	-6.234800
C	2.613200	-12.515600	-4.541900
N	3.388800	-13.392400	-3.670500
C	3.462300	-14.744700	-3.907300
O	2.782800	-15.292700	-4.780000
H	4.025300	-12.938300	-3.023200
C	4.415000	-15.485000	-2.995600

C	2.504800	-8.458700	-7.204800
O	1.160800	-8.958900	-7.366900
H	0.927000	-8.844700	-8.302900
C	3.446800	-8.926000	-8.325900
H	-3.877300	-5.002800	-0.318600
C	3.641900	-5.310800	-2.800900
C	4.457000	-6.027600	-1.722000
O	3.914500	-6.623600	-0.788300
N	5.804100	-5.908100	-1.830100
H	6.390300	-6.361000	-1.134600
H	6.263400	-5.468100	-2.621500
C	-1.676200	-5.340000	-5.061900
C	-3.176500	-4.974000	-5.288300
H	-3.825800	-5.185600	-4.413400
H	-3.501800	-0.281400	-2.071500
H	-0.996200	-4.587800	-5.502900
H	2.484000	-1.749200	1.001500
H	3.477700	-10.026300	-8.397000
H	-2.017900	-3.448300	3.785600
H	5.187700	-15.976500	-3.614200
H	-0.350500	-2.778000	3.900400
H	3.872300	-16.298500	-2.478700
H	4.913100	-14.848300	-2.241200
H	-1.398200	-4.413800	-3.103800
H	3.024700	-1.948500	-0.712400
H	-1.213000	-5.376300	-0.278900
H	4.117800	-1.198300	0.512300
H	-5.938500	-0.262300	-0.966000
H	3.125300	-8.511300	-9.305400
H	4.262900	-4.991900	-3.669500
H	-2.719800	-2.981800	0.960000
H	3.275400	-4.362800	-2.354300
H	4.068800	-8.804800	-5.695900
H	4.478500	-8.561100	-8.135500
H	-0.396000	-4.586500	2.241300
H	-1.361700	-0.951000	-1.362100
H	-2.721200	-4.659100	1.608200
H	-3.602300	-5.563000	-6.134100
H	-6.003900	-1.908800	-1.671800
H	-1.474400	-6.322200	-5.540000
C	1.192900	-12.149400	-3.982200
C	0.457000	-13.217800	-3.140300
C	-1.031000	-12.848200	-2.909000
C	-1.326800	-11.434300	-2.361100
N	-1.261200	-10.345500	-3.417900
H	-1.768000	-10.644100	-4.261300

H	-0.290500	-10.100900	-3.699400
H	-1.721400	-9.461300	-3.102300
H	-0.635700	-11.143400	-1.545900
H	-2.362600	-11.407700	-1.968900
H	0.496500	-14.187500	-3.673700
H	-1.444500	-13.543300	-2.143800
H	1.322400	-11.240100	-3.365100
H	0.993200	-13.343400	-2.177500
H	2.479800	-13.034100	-5.514300
C	-1.334700	1.186100	-1.893400
C	-0.681700	0.898600	-3.279400
H	-2.400800	1.434600	-2.057400
H	-1.160900	1.544000	-4.045100
H	0.401300	1.135600	-3.290500
H	-0.861100	2.112500	-1.500800
H	-0.083300	-3.037600	1.374700
H	0.559300	-11.912100	-4.866000
H	2.433500	0.700200	0.766100
H	-1.193400	-3.700400	-0.913500
H	-1.624500	-13.031000	-3.832800
H	2.479200	-7.345000	-7.196500
H	-2.677400	-1.505100	2.460200
S	-3.547776	-3.247724	-5.653195
C	-2.666476	-2.964024	-7.217595
H	-1.571176	-2.987724	-7.092595
H	-2.989876	-1.978524	-7.597695
H	-2.970676	-3.738924	-7.948095
S	-0.820900	-0.862400	-3.771000
C	0.161500	-0.863100	-5.293700
H	0.333800	-1.923100	-5.540600
Cu	-2.989700	-1.764300	-3.945300
H	-0.355300	-0.326200	-6.113000
H	1.130800	-0.375400	-5.079400
O	-7.022373	-3.744180	-7.267703
H	-6.062373	-3.744180	-7.267703
H	-7.342828	-2.839244	-7.267703
O	-2.220951	-6.054721	-8.186730
H	-1.296676	-6.314174	-8.186730
O	-8.099032	-5.844430	-0.865522
H	-8.401014	-4.978694	-1.149965
O	0.284886	-7.003986	2.011218
H	1.186186	-7.086804	1.691218
O	-5.986398	-8.562586	-2.788799
H	-5.030863	-8.652491	-2.810478
H	-6.222241	-7.633732	-2.845440
O	-5.223331	-6.282555	-9.495495

H	-2.775010	-6.838696	-8.186730
H	-5.745703	-7.021695	-9.815495
H	-5.223331	-6.282555	-8.535495
H	-8.251904	-5.942893	0.077100
H	0.284886	-7.003986	2.971218

1N1O2Sa Model

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.241700
N	1.134800	0.000000	-0.725000
H	2.027400	0.062000	-0.242000
H	1.137900	0.023700	-1.742800
C	-1.317800	0.041700	-0.787200
N	-2.291700	-0.776400	-0.046800
C	-3.368300	-1.348900	-0.629400
O	-3.677300	-1.178600	-1.818100
H	-2.118200	-0.870800	0.951500
C	-1.791900	1.514800	-0.930400
H	-2.041600	1.929100	0.061200
H	-2.671500	1.546800	-1.599000
H	-0.990200	2.128200	-1.387500
H	-1.209100	-0.389400	-1.803800
C	-4.216500	-2.260600	0.302600
N	-5.569900	-2.246800	-0.305600
C	-6.722700	-2.439600	0.362300
O	-6.829100	-3.052000	1.445000
H	-5.580300	-1.755600	-1.204300
C	-7.903600	-1.658900	-0.209800
N	-9.115200	-2.368100	-0.664700
C	-9.539200	-3.654400	-0.901900
O	-10.685300	-3.810700	-1.339200
H	-9.838200	-1.726900	-0.989200
C	-8.646700	-4.859100	-0.583100
N	-8.976500	-5.267900	0.794300
C	-8.132700	-5.996100	1.548500
O	-7.044700	-6.442700	1.135100
H	-9.868300	-4.948900	1.184800
C	-8.595200	-6.227500	2.996600
N	-8.531900	-7.682200	3.269200
C	-9.663000	-8.385300	3.547000
O	-10.755800	-7.891800	3.840100
H	-7.690600	-8.181500	2.979200
C	-7.719300	-5.395700	3.985900
C	-9.530200	-9.911900	3.344900
N	-10.117700	-10.660200	4.461300

C	-9.396200	-11.061400	5.554000
O	-8.194700	-10.839800	5.712100
H	-11.133000	-10.647500	4.537100
C	-10.276600	-11.813300	6.575000
N	-9.598000	-12.988900	7.109400
C	-9.214000	-14.032200	6.342800
O	-9.394500	-14.086400	5.114700
H	-9.279800	-12.917300	8.073100
C	-3.568200	-3.660100	0.446300
C	-8.525100	-15.232400	7.046200
N	-7.250200	-15.439100	6.317500
C	-5.961700	-15.412700	6.720000
O	-5.562100	-15.190600	7.885200
H	-7.399700	-15.603900	5.327200
C	-4.973000	-15.666300	5.608100
C	-8.457500	-15.164700	8.592200
H	-7.724800	-14.407700	8.918000
C	-8.185100	-16.558800	9.220100
C	-8.436100	-4.047700	4.269800
H	-4.257000	-16.437200	5.943200
H	-7.568100	-4.573700	-0.623100
H	-4.389200	-14.742200	5.440700
H	-5.420600	-15.985000	4.648700
C	-4.022600	-4.473100	1.691700
H	-5.046200	-4.860200	1.547800
H	-7.623400	-5.979000	4.922000
H	-4.311800	-1.796600	1.301000
H	-2.466300	-3.540100	0.465900
H	-7.373500	-17.074600	8.668400
H	-8.474900	-10.232800	3.250700
H	-6.716000	-5.214200	3.554700
H	-8.836900	-3.588700	3.347800
H	-7.555600	-1.026600	-1.057100
H	-11.190100	-12.158400	6.045100
H	-3.811300	-4.270700	-0.448700
H	-9.101500	-17.172100	9.080000
H	-9.660300	-5.951500	3.129400
H	-3.344200	-5.348400	1.811400
H	-9.279600	-4.232100	4.982100
C	-7.873100	-16.487100	10.748900
C	-6.409900	-16.799500	11.108200
N	-5.458400	-15.741100	10.591300
H	-5.705200	-14.819500	10.978400
H	-4.495000	-15.950700	10.899200
H	-5.458400	-15.660400	9.534900
H	-6.088800	-17.766700	10.678700

H	-6.282300	-16.844500	12.205900
H	-8.161800	-15.501000	11.171000
H	-8.478900	-17.238400	11.300300
C	-10.308800	-10.228200	2.028200
C	-10.171300	-11.612100	1.398600
O	-10.304400	-11.737100	0.156200
N	-9.963300	-12.693300	2.157800
H	-9.916000	-13.597800	1.693900
H	-9.884700	-12.687700	3.177700
H	-11.394300	-10.043500	2.191800
H	-9.981400	-9.510100	1.247600
C	-8.781000	-6.027300	-1.622300
C	-10.122400	-6.810000	-1.637200
C	-9.895100	-8.265000	-2.134100
C	-11.223100	-9.046000	-2.106800
N	-10.958100	-10.534900	-2.211400
H	-10.232700	-10.725900	-2.918800
H	-11.811600	-11.046200	-2.487300
H	-10.637400	-10.930200	-1.274100
H	-11.782600	-8.878500	-1.166800
H	-10.579900	-6.843600	-0.627000
H	-7.942600	-6.718900	-1.401700
H	-9.128900	-8.776100	-1.511600
H	-11.871400	-8.747400	-2.958100
H	-10.845100	-6.282100	-2.295800
H	-9.173100	-16.096600	6.773700
C	-8.335900	-0.700800	0.961100
C	-7.233500	0.164800	1.531700
C	-7.065800	1.509300	1.310200
N	-6.023500	1.911800	2.109800
C	-5.562800	0.828400	2.775700
N	-6.271200	-0.254000	2.461000
H	-5.633900	2.848000	2.168700
H	-4.754600	0.872000	3.503800
H	-7.629400	2.199400	0.685400
H	-8.803200	-1.302000	1.764600
H	-9.114200	-0.011900	0.561800
H	-8.573000	-5.599500	-2.631500
H	-9.478500	-14.873300	8.941300
H	-9.528100	-8.227800	-3.189200
C	-10.703200	-10.859200	7.757000
O	-9.728000	-10.884600	8.818400
C	-12.055600	-11.277000	8.343500
H	-8.969700	-10.359100	8.511900
H	-12.023900	-12.302400	8.752500
H	-12.847900	-11.222800	7.570900

H	-10.801500	-9.829000	7.359300
H	-12.322800	-10.587700	9.170300
S	-4.054338	-3.641830	3.307949
C	-2.355638	-3.032630	3.564549
H	-2.068238	-2.237130	2.858749
H	-2.316838	-2.638330	4.594849
H	-1.658938	-3.892130	3.461449
S	-7.402750	-2.729820	4.983767
C	-6.556350	-3.529620	6.377467
H	-5.820250	-4.264620	6.010867
H	-7.312650	-3.989320	7.043767
H	-6.023550	-2.717120	6.901367
Cu	-5.905187	-2.178033	3.272499
O	-0.573600	0.050800	4.217300
H	-0.241900	0.144000	3.302800
H	0.219300	0.052000	4.774000
H	-2.203400	0.878200	4.824500
O	-3.113600	1.105200	5.126200
H	-3.027900	1.971900	5.550900
H	-11.603000	-3.537600	2.702800
O	-11.617200	-4.377900	2.205100
H	-12.443000	-4.358800	1.700000
O	-3.721300	-1.495600	6.630500
H	-3.320000	-1.481000	7.513100
H	-3.566100	-0.596500	6.277500
H	-10.761300	-1.568200	4.516400
O	-11.053000	-1.629500	3.592000
H	-11.638300	-0.866100	3.467800
O	-6.890400	-9.523500	1.034800
H	-6.057500	-9.975600	0.829300
H	-6.695000	-8.575300	0.896900

1N1O2Sc1

C	0.010971	-0.004242	-0.009208
O	0.010971	-0.004242	1.230392
N	1.144371	-0.004242	-0.735908
H	1.171771	0.025858	-1.752108
H	2.027471	0.026658	-0.234208
C	-1.317829	-0.003842	-0.800508
N	-2.351629	-0.189442	0.232592
C	-3.583129	-0.669342	0.031992
O	-4.068229	-0.882642	-1.102108
C	-1.527029	1.300558	-1.608208
C	-4.431529	-0.964142	1.295392
N	-3.707029	-1.891742	2.198992

C	-4.042329	-3.165442	2.526492
O	-3.295129	-3.870842	3.214692
H	-2.803229	-1.610342	2.580792
C	-4.879529	0.328358	2.025692
C	-5.845229	1.160258	1.132892
H	-1.939229	-0.081442	1.167892
C	-5.442529	-3.740542	2.125192
N	-5.236229	-5.205342	2.111092
C	-5.877829	-6.220642	1.509392
O	-5.357129	-7.364242	1.523592
C	-7.281329	-6.061842	0.898492
N	-7.348029	-6.806042	-0.375708
C	-7.811329	-6.465542	-1.607408
O	-7.988429	-7.368142	-2.445008
H	-7.110229	-7.793142	-0.324908
C	-8.091329	-4.985142	-1.998408
N	-7.923929	-4.931042	-3.455808
C	-7.412129	-3.882042	-4.141508
O	-6.918229	-2.874142	-3.607108
H	-8.300129	-5.721942	-3.981408
H	-4.345429	-5.452142	2.559492
C	-7.403629	-4.086242	-5.679208
N	-8.742629	-4.400742	-6.214708
C	-9.214929	-5.653042	-6.339408
O	-8.567629	-6.634642	-5.913908
C	-6.775229	-2.897942	-6.444508
C	-7.666429	-1.664242	-6.587108
O	-8.847829	-1.622542	-6.203208
N	-7.074229	-0.607842	-7.183508
H	-6.126229	-0.645442	-7.549008
H	-7.633229	0.220658	-7.377808
H	-9.296829	-3.588542	-6.481708
C	-10.585129	-5.742542	-7.050308
N	-10.858029	-7.102942	-7.496208
C	-10.380629	-7.591642	-8.680808
O	-9.641529	-6.935542	-9.420708
H	-11.508829	-7.647842	-6.946408
C	-10.820829	-9.042942	-8.943708
N	-10.508829	-9.424542	-10.318508
C	-11.222029	-10.417242	-10.945608
O	-12.084729	-11.066542	-10.346608
C	-10.853529	-10.655842	-12.391408
H	-9.876129	-8.825542	-10.836208
C	-11.721429	-5.253942	-6.109308
O	-11.865129	-6.292642	-5.131508
H	-12.611429	-6.062142	-4.535208

C	-13.007929	-4.972442	-6.897908
C	-10.177529	-10.024842	-7.915908
C	-8.631729	-9.962442	-7.866508
C	-8.044229	-10.871542	-6.743608
C	-7.504929	-10.098042	-5.526108
N	-8.567729	-9.222142	-4.903208
H	-9.367829	-9.799242	-4.617108
H	-8.225529	-8.750242	-4.040908
C	-6.381629	-3.256442	3.281292
C	-7.877729	-3.328642	3.107192
C	-8.774229	-3.842142	4.014992
N	-10.023729	-3.620842	3.485392
C	-9.871029	-2.976242	2.305492
N	-8.579829	-2.780742	2.034592
H	-10.910229	-3.840742	3.933892
H	-8.897129	-8.452342	-5.540608
C	-9.546229	-4.584842	-1.591808
C	-10.003429	-3.198042	-2.169708
C	-8.330829	-6.641542	1.919692
C	-8.318229	-8.185342	2.194992
C	-8.204529	-8.562842	3.698092
C	-6.854929	-8.294142	4.391392
N	-5.709429	-9.029542	3.724992
H	-4.860429	-8.976942	4.312592
H	-5.938029	-10.028842	3.597592
H	-8.599729	-4.345542	4.968192
H	-10.688229	-2.654342	1.664292
H	-10.023129	-10.026842	-12.757308
H	-13.379029	-5.879042	-7.409308
H	-1.484329	2.184558	-0.949808
H	-11.079429	-3.243242	-2.454708
H	-11.745129	-10.474942	-13.018308
H	-10.590729	-11.720642	-12.531708
H	-2.506229	1.267858	-2.120708
H	-0.749129	1.409858	-2.387708
H	-9.409329	-2.893142	-3.045308
H	-6.665029	-9.438742	-5.814708
H	-13.807229	-4.606642	-6.221608
H	-5.912829	2.210358	1.491392
H	-12.816629	-4.190442	-7.663408
H	-5.341929	-1.479342	0.949792
H	-5.839729	-2.589542	-5.931008
H	-7.159129	-10.791142	-4.732508
H	-6.912529	-8.636242	5.442392
H	-9.337429	-6.362742	1.541392
H	-5.489629	-8.579642	2.799592

H	-8.256029	-10.299542	-8.853108
H	-7.542429	-8.710242	1.606792
H	-7.180129	-11.447542	-7.138308
H	-5.502029	1.208958	0.080892
H	-9.286129	-8.610842	1.841592
H	-7.568129	-5.007442	0.750392
H	-5.350929	0.059858	2.994192
H	-7.316229	-4.334242	-1.543308
H	-8.959329	-8.001642	4.286492
H	-6.154129	-2.185642	3.466392
H	-8.211029	-6.074642	2.866492
H	-10.265329	-5.332542	-1.994908
H	-9.660829	-4.580042	-0.488708
H	-6.588129	-7.220842	4.407092
H	-10.497329	-11.044142	-8.215808
H	-6.506629	-3.250542	-7.465608
H	-6.771829	-4.980342	-5.867108
H	-6.100129	-3.801842	4.206392
H	-8.466229	-9.638242	3.825392
H	-4.011929	0.981958	2.270392
H	-5.768629	-3.409142	1.120292
H	-8.792329	-11.626442	-6.416608
H	-1.350629	-0.867442	-1.498008
H	-10.641829	-9.857342	-6.916608
H	-10.524829	-5.095742	-7.955208
H	-11.922429	-9.117042	-8.804308
H	-8.283429	-8.912842	-7.755908
H	-11.407129	-4.309942	-5.605608
S	-7.594429	0.600258	0.995692
C	-8.211929	0.845458	2.691392
H	-7.759629	1.768158	3.104992
H	-7.986929	-0.021242	3.328192
H	-9.304029	1.011858	2.619992
S	-9.918929	-1.823842	-0.948308
C	-10.147229	-0.414342	-2.065908
H	-9.349329	-0.407942	-2.826908
H	-11.133829	-0.508842	-2.556408
H	-10.113729	0.505558	-1.456008
Cu	-7.946858	-1.641716	0.335189
O	-6.352405	-2.287050	-1.004088
H	-6.636905	-2.445350	-1.936888
H	-5.516005	-1.751150	-1.097088
O	-13.860800	-5.767300	-2.970700
H	-14.672900	-6.295900	-2.927200
H	-14.161800	-4.838000	-2.902500
O	-14.368300	-2.741100	-2.850900

H	-14.917400	-2.375900	-2.137900
H	-14.734900	-2.339800	-3.656700
O	-7.891000	-5.860600	6.786400
H	-8.610300	-6.174800	7.359800
H	-7.281900	-5.428500	7.407000
O	-12.873945	-4.742629	0.843963
H	-11.913945	-4.742629	0.843963
H	-13.194399	-3.837693	0.843963
O	-13.354508	-4.632216	3.870892
H	-13.876880	-5.371356	3.550892
H	-13.354508	-4.632216	4.830892

1N1O2Sb

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.234600
N	1.121000	0.000000	-0.762600
C	2.472300	-0.038100	-0.179400
H	1.061200	-0.070500	-1.776400
C	3.440200	0.581900	-1.191600
O	3.346100	0.332700	-2.406600
N	4.406200	1.369500	-0.682400
H	5.124800	1.736700	-1.301100
H	4.495900	1.552500	0.315100
C	-1.337800	0.045800	-0.787600
N	-2.265000	-0.877400	-0.086800
C	-3.282700	-1.590700	-0.632400
O	-3.815400	-2.552800	-0.067000
H	-1.996500	-1.114200	0.870200
C	2.911500	-1.493500	0.142800
C	-3.812300	-1.149000	-2.010200
N	-3.768100	-2.318400	-2.904900
C	-3.606719	-2.104314	-4.226238
O	-3.412953	-0.834826	-4.673960
H	-3.964700	-3.226800	-2.495200
C	-3.709300	-3.263500	-5.244800
N	-2.398000	-3.540600	-5.864000
C	-1.471300	-2.888100	-6.650300
O	-0.579900	-3.608200	-7.121000
H	-2.085200	-4.506400	-5.761400
C	-1.441800	-1.354300	-6.956400
N	-0.073800	-1.151300	-7.496700
C	0.671200	-0.039400	-7.328400
O	0.261800	1.008200	-6.801100
H	0.347900	-1.980900	-7.914200
C	2.098300	-0.122900	-7.916700

N	2.124900	0.788500	-9.077900
C	2.678400	0.439100	-10.273800
O	3.187300	-0.673000	-10.475300
H	1.831300	1.747700	-8.921100
C	3.166900	0.247600	-6.828800
C	4.062300	-0.927200	-6.448100
O	4.519800	-1.728000	-7.286900
N	4.368700	-1.011200	-5.142200
H	4.993800	-1.748300	-4.828100
H	3.988800	-0.381600	-4.430400
C	2.616500	1.565500	-11.348900
N	3.721500	1.399700	-12.285800
C	4.972600	1.859800	-11.987900
O	5.198400	2.681800	-11.091900
H	3.599800	0.713500	-13.024400
C	6.077000	1.147500	-12.778600
N	7.308500	1.932900	-12.791500
C	8.115000	1.973100	-13.907100
O	7.909100	1.251400	-14.885600
C	9.264900	2.950000	-13.802400
H	7.417200	2.611100	-12.041900
C	-4.281200	-4.608200	-4.687900
C	-4.833300	-5.544100	-5.811500
C	-5.017900	-6.990500	-5.275200
C	-5.597400	-8.017200	-6.268100
N	-7.054200	-7.719900	-6.637200
H	-7.123900	-7.032900	-7.403300
H	-7.578000	-7.357100	-5.822600
H	-7.525600	-8.584600	-6.956500
C	-1.904100	1.490900	-0.805100
C	-1.178300	2.450700	-1.776300
C	1.257500	1.586600	-12.095200
O	1.200400	0.360600	-12.842000
H	0.521400	0.473700	-13.527600
C	1.136900	2.830500	-12.995000
C	6.227700	-0.219100	-12.028000
C	7.477100	-1.066500	-12.348800
C	7.378600	-2.473900	-11.699800
C	7.091300	-2.459300	-10.180200
N	5.601600	-2.466700	-9.879300
H	5.195400	-3.367500	-10.163000
H	5.388600	-2.331400	-8.864000
H	5.076200	-1.724300	-10.380300
C	-2.493400	-0.880200	-8.020800
C	-3.791700	-0.136000	-7.580500
C	-5.289400	-0.617200	-1.916100

C	-5.472500	0.870800	-2.116900
C	-6.365300	1.651900	-1.425700
N	-6.272600	2.914400	-1.957000
C	-5.341300	2.890900	-2.934200
N	-4.828400	1.669700	-3.069600
H	-6.815100	3.722700	-1.665300
H	-5.086500	3.765100	-3.524000
H	-7.033600	1.409800	-0.602400
H	-4.459200	-0.758300	-6.965900
H	1.913800	2.834600	-13.776200
H	10.221400	2.398100	-13.863700
H	9.263900	3.564500	-12.882800
H	9.238200	3.617600	-14.681700
H	2.285200	-1.883100	0.966300
H	-5.588600	-9.022100	-5.802600
H	-1.947600	-0.246800	-8.745100
H	-2.966100	1.472500	-1.106600
H	-1.859100	1.920300	0.214900
H	1.238100	3.759800	-12.394600
H	7.506700	-3.354800	-9.676800
H	3.965200	-1.504400	0.486800
H	-1.678600	3.442000	-1.770000
H	-5.890900	-1.129400	-2.695600
H	-5.031800	-8.055300	-7.218100
H	-0.122700	2.616000	-1.483100
H	0.139300	2.858600	-13.480500
H	7.527000	-1.565300	-9.695200
H	8.347600	-2.999500	-11.841800
H	-5.735200	-0.907200	-0.941200
H	7.565100	-1.180700	-13.448000
H	-4.351100	0.110800	-8.514400
H	8.384700	-0.535800	-11.995400
H	3.831200	1.042500	-7.232400
H	2.813400	-2.133600	-0.750300
H	-4.016600	-7.398300	-5.012700
H	-2.851900	-1.747100	-8.622900
H	-5.136600	-4.368500	-4.016600
H	-4.415300	-2.868800	-6.007000
H	6.234300	0.036600	-10.948000
H	-1.164700	-0.326400	-1.817100
H	-4.143700	-5.558300	-6.683800
H	2.759200	2.544800	-10.838900
H	-5.613400	-7.005100	-4.334100
H	2.682800	0.702200	-5.937500
H	-3.501400	-5.122200	-4.088200
H	5.319900	-0.813700	-12.268500

H	6.610600	-3.081100	-12.228500
H	2.449000	0.530200	0.773400
H	-1.537700	-0.756500	-6.036000
H	-5.804400	-5.099200	-6.134100
H	-3.193300	-0.366000	-2.464800
H	5.790600	0.934100	-13.828400
H	0.438700	1.616700	-11.337600
H	2.336300	-1.121000	-8.319100
S	-3.752385	1.439019	-6.629883
C	-2.678285	2.527819	-7.614383
H	-1.631885	2.207619	-7.531483
H	-2.810785	3.550919	-7.210683
H	-3.022185	2.528419	-8.670183
S	-1.112198	1.824491	-3.486958
C	-0.407598	3.254091	-4.362658
Cu	-3.217200	1.340000	-4.333500
H	-0.108398	2.884391	-5.355358
H	-1.148298	4.072491	-4.438958
H	0.479602	3.606391	-3.803458
O	0.983404	3.741630	-9.040324
H	1.943404	3.741630	-9.040324
H	0.662949	4.646566	-9.040324
O	1.731628	-4.628745	-5.770722
H	2.632928	-4.711563	-6.090722
O	1.286875	-3.611319	-9.943339
H	0.907947	-2.789362	-10.263339
O	-2.423893	0.610865	-11.991824
O	6.376276	1.465420	-7.508910
H	7.277576	1.382602	-7.828910
O	0.448881	-4.853343	-2.388378
H	0.069953	-4.031385	-2.708378
H	1.286875	-3.611319	-8.983339
H	1.731628	-4.628745	-4.810722
H	0.448881	-4.853343	-1.428378
H	5.853904	0.726280	-7.828910
H	-3.130520	0.997143	-12.514382
H	-2.511734	-0.345108	-11.991824

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.234200
N	1.147000	0.000000	-0.727300
H	1.155900	-0.025100	-1.742600
H	2.033200	0.017700	-0.230500
C	-1.298400	0.051600	-0.818900

N	-2.273600	-0.837500	-0.188700
C	-3.276300	-1.435100	-0.879200
O	-3.475400	-1.265000	-2.090600
H	-2.206000	-0.966400	0.821200
C	-4.166000	-2.358400	0.006200
N	-5.115400	-1.544700	0.791700
C	-4.806600	-1.023800	2.005400
O	-3.683100	-1.127600	2.518700
H	-6.059900	-1.421800	0.435900
C	-4.935600	-3.386800	-0.846200
C	-5.971900	-0.324100	2.742300
N	-6.224008	-1.130092	3.933001
C	-7.178400	-1.989800	3.974200
O	-7.981800	-2.263600	2.940500
H	-8.658700	-2.993300	3.218800
C	-7.406500	-2.765500	5.266900
N	-6.264634	-2.574667	6.179720
C	-5.507200	-3.648700	6.388300
O	-5.748600	-4.850900	6.055700
C	-5.496300	-4.564600	-0.011400
C	-1.810200	1.518400	-0.889100
H	-2.093200	1.864600	0.120700
H	-2.681700	1.555600	-1.567700
H	-6.154000	-4.204500	0.806500
H	-3.511700	-2.877400	0.738100
H	-4.275700	-3.738200	-1.663600
C	-4.163500	-3.287100	7.062700
N	-3.702900	-4.270900	8.065900
C	-3.045700	-5.453200	7.894400
O	-2.512800	-5.868900	6.865500
H	-4.064600	-4.086000	9.001900
C	-3.116800	-2.930900	5.958300
C	-2.264100	-1.727900	6.398600
H	-2.473500	-3.799800	5.726000
C	-3.022900	-6.281700	9.218500
N	-4.418900	-6.518800	9.633000
C	-4.866300	-6.301600	10.885400
O	-4.140100	-5.919200	11.823500
H	-5.071100	-6.853400	8.915100
C	-6.396400	-6.474400	11.032000
N	-6.718300	-6.852000	12.418100
C	-6.451900	-8.115400	12.847400
O	-6.253800	-9.057200	12.073600
H	-6.816300	-6.081600	13.079100
H	-2.565500	-5.669300	10.019300
C	-6.412900	-8.282100	14.394100

N	-6.091900	-9.680400	14.717400
C	-4.988400	-10.370200	14.339100
O	-3.934500	-9.848900	13.924600
H	-6.891500	-10.243700	14.988500
C	-5.100800	-11.865800	14.492100
H	-4.201700	-12.241200	15.010500
H	-6.002000	-12.210700	15.031900
H	-5.105500	-12.312900	13.479500
H	-4.374900	-2.376600	7.651800
H	-3.644200	-2.648600	5.025300
H	-1.017800	2.177700	-1.298300
C	-2.252200	-7.618400	9.029700
C	-2.064300	-8.313800	10.359200
O	-1.243800	-7.918600	11.210600
N	-2.873400	-9.377700	10.558100
H	-3.629200	-9.571100	9.904700
H	-2.915700	-9.848800	11.460600
H	-1.134100	-0.306900	-1.857600
H	-6.745200	-7.293300	10.366800
C	-5.543700	1.127500	3.157600
C	-6.387200	1.699400	4.262300
C	-7.288700	2.737000	4.222400
N	-7.802100	2.846600	5.497100
C	-7.233400	1.883900	6.263000
N	-6.356800	1.183800	5.556800
H	-8.533400	3.485400	5.794100
H	-7.502400	1.723400	7.302400
H	-7.588300	3.397200	3.411100
H	-4.483000	1.095000	3.473700
H	-1.255300	-7.376800	8.602300
H	-2.794100	-8.238700	8.280600
H	-7.455700	-3.833900	4.986800
H	-1.746500	-1.905000	7.363000
H	-5.785400	-2.886100	-1.365300
H	-7.448500	-8.116400	14.767900
H	-6.111500	-5.227000	-0.661700
H	-5.630300	1.779200	2.254700
H	-6.875800	-0.254400	2.096600
H	-1.511100	-1.458600	5.627300
C	-7.107200	-5.149900	10.620200
O	-6.917900	-4.230200	11.717700
H	-7.231900	-3.366100	11.391800
C	-8.600200	-5.372500	10.309300
H	-9.118000	-5.801300	11.189100
H	-9.083400	-4.408900	10.044400
H	-8.720100	-6.065000	9.446000

H	-6.582400	-4.757800	9.724100
C	-8.739000	-2.269400	5.917600
H	-8.472400	-1.443500	6.606500
H	-9.420700	-1.819100	5.165000
C	-9.502000	-3.409000	6.670600
C	-10.609200	-4.107900	5.823500
C	-10.152900	-5.007800	4.645500
N	-9.774300	-4.270600	3.403000
H	-10.633900	-3.951600	2.941200
H	-9.338500	-4.955400	2.770800
H	-8.783800	-4.172100	7.042800
H	-9.280100	-5.614900	4.956700
H	-11.330000	-3.346500	5.460200
H	-10.979400	-5.719300	4.432700
H	-10.024900	-2.971200	7.547900
H	-11.175100	-4.782100	6.505700
S	-3.326294	-0.230316	6.635216
S	-4.251500	-5.591200	0.845200
C	-3.263200	-6.261800	-0.524900
H	-2.666900	-5.472900	-1.008600
H	-3.916300	-6.769900	-1.260400
H	-2.573200	-7.003800	-0.076500
C	-2.497894	0.975584	5.552316
H	-2.381494	0.533584	4.548416
H	-3.159694	1.858584	5.502016
H	-1.522794	1.254784	5.994816
C	-5.498200	-7.149700	15.016300
H	-4.998900	-6.643800	14.172400
H	-6.176400	-6.396300	15.464100
C	-4.443600	-7.496800	16.119400
H	-4.148800	-8.559300	16.072800
C	-3.208300	-6.559800	15.984200
C	-2.046600	-7.093200	15.113400
N	-2.476900	-7.454500	13.714900
H	-2.994100	-6.698300	13.230600
H	-1.673800	-7.672200	13.088600
H	-3.058100	-8.320800	13.742500
H	-1.592400	-8.001100	15.549600
H	-1.257900	-6.318500	15.036400
H	-4.909800	-7.336000	17.114400
H	-3.525300	-5.569400	15.593000
H	-2.756300	-6.364500	16.981400
Cu	-5.412451	-0.684912	5.817992
H	-6.210500	-6.693400	3.077300
O	-6.853900	-6.490400	3.778000
H	-6.352900	-5.933200	4.407800

O	-4.328600	-1.007600	10.040400
H	-4.024200	-0.589300	10.859800
H	-3.913600	-0.484100	9.327600
O	-11.521100	-0.432200	7.275600
H	-10.832100	-0.102400	7.885500
H	-12.322800	0.042200	7.545400
H	-6.339900	-6.316300	7.059000
O	-6.605600	-7.077900	7.635400
H	-6.815900	-7.783100	7.003800
O	-7.253000	-1.762500	9.672900
H	-7.297300	-2.176100	8.787500
H	-6.318000	-1.476400	9.747400
H	-8.499700	-0.104600	9.411900
O	-9.072800	0.655400	9.173100
H	-9.261700	1.093500	10.015600

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.241100
N	1.115700	0.000000	-0.769700
C	2.441300	-0.180200	-0.178700
H	1.021300	0.065100	-1.785400
C	-1.317600	0.068600	-0.785200
N	-2.315100	-0.645000	0.017300
C	-3.381200	-1.290000	-0.525000
O	-3.627000	-1.283900	-1.737900
H	-2.189600	-0.580400	1.026500
C	3.369200	1.015800	-0.459600
O	3.324300	1.698200	-1.479900
N	4.275400	1.256800	0.556800
H	4.433100	0.505900	1.241200
H	5.093800	1.791600	0.273100
C	-4.233800	-2.154900	0.431000
N	-3.463200	-3.383100	0.692700
C	-4.067800	-4.540800	1.057600
O	-5.294300	-4.637400	1.213700
H	-2.452500	-3.323800	0.720500
C	-3.081700	-5.711900	1.299200
N	-2.231777	-5.318306	2.453455
C	-1.201400	-6.016500	2.796900
O	-0.699400	-7.114800	2.231600
H	-1.148900	-7.428400	1.381300
C	-0.407000	-5.608800	4.032600
N	-0.228187	-4.145110	4.159327
C	0.755413	-3.708310	3.351627

O	1.290313	-4.334610	2.391427
C	-3.847100	-7.035900	1.551100
C	3.088300	-1.490100	-0.708800
H	4.118600	-1.613700	-0.321900
H	2.482500	-2.351900	-0.360100
H	-5.110700	-2.456700	-0.179300
C	-1.011300	-6.216300	5.332500
C	-2.528400	-6.076500	5.569000
H	-3.106000	-6.574900	4.765700
H	-0.447500	-5.790700	6.188300
H	-3.172200	-7.798500	1.985500
H	-4.630800	-6.849900	2.316700
H	-1.217900	-0.467800	-1.751600
H	2.270100	-0.269300	0.912800
H	-2.813900	-6.553600	6.531300
H	-0.786100	-7.305700	5.333900
C	-4.565200	-7.623200	0.300600
C	-3.697900	-7.977200	-0.933500
C	-2.579400	-9.017000	-0.672000
N	-1.330700	-8.392400	-0.154900
H	-0.870100	-7.901700	-0.926300
H	-0.688800	-9.149600	0.108800
H	-5.363200	-6.918000	-0.004200
H	-3.256700	-7.081200	-1.410900
H	-2.385000	-9.570400	-1.614100
H	-2.931200	-9.760300	0.074600
H	-5.095900	-8.547700	0.629900
H	3.122700	-1.496500	-1.818300
H	-2.424200	-5.789900	0.402500
H	0.573500	-6.114700	3.899500
H	-4.387400	-8.403400	-1.700700
C	-1.705200	1.553500	-1.102300
C	-2.062300	1.706600	-2.600000
H	-2.582600	1.840900	-0.489600
H	-2.791000	0.927700	-2.899000
H	-0.889200	2.249500	-0.822400
H	-2.530700	2.699200	-2.799100
C	1.392213	-2.312910	3.696027
N	1.155313	-1.922810	5.112527
C	1.165713	-0.655110	5.566427
O	1.194813	0.373890	4.852427
H	1.149213	-2.697910	5.772327
H	0.961313	-1.528810	3.041527
C	0.936413	-0.522210	7.098827
N	1.703513	0.617790	7.624327
C	3.040413	0.666690	7.846927

O	3.775413	-0.318710	7.934327
H	1.199813	1.498490	7.552327
C	3.563713	2.130290	8.016727
N	5.029413	2.130790	8.001927
C	5.819013	1.812790	6.951427
O	5.379913	1.617890	5.799427
H	5.479913	2.251790	8.901727
C	7.288013	1.700990	7.267927
H	7.859113	2.345390	6.574927
H	7.603913	0.660090	7.069127
H	7.559513	1.958790	8.308827
H	1.223013	-1.463810	7.618127
H	3.265013	2.464090	9.036927
C	-0.582987	-0.203910	7.332727
O	-0.884987	1.112890	6.789027
H	-0.419887	1.147390	5.927427
C	-0.969387	-0.220110	8.816727
H	-0.405087	0.533290	9.397227
H	-2.052087	-0.010610	8.911127
H	-1.199487	-0.963210	6.814027
H	-0.760087	-1.226510	9.241927
C	-4.832500	-1.485700	1.710000
C	-3.903300	-0.980100	2.786000
C	-4.059500	0.178800	3.508700
N	-3.000400	0.238400	4.380200
C	-2.214200	-0.831200	4.152800
N	-2.743583	-1.618285	3.220393
H	-2.854900	0.922600	5.119800
H	-1.274900	-1.025900	4.658600
H	-4.829800	0.949600	3.470200
H	-5.545500	-2.204500	2.156900
H	-5.449000	-0.629100	1.352800
C	2.929413	-2.489410	3.413427
C	3.774913	-1.301710	3.802027
O	3.995213	-0.351710	3.012027
N	4.267713	-1.344410	5.048327
H	3.963313	-2.069110	5.700727
H	4.721313	-0.523510	5.454327
H	3.022913	-2.681510	2.330927
H	3.284813	-3.396710	3.945627
S	-0.664300	1.497700	-3.757800
C	0.280200	3.035200	-3.517400
H	0.725300	3.077200	-2.511100
H	-0.377400	3.904800	-3.707900
H	1.096200	3.019200	-4.265000
C	2.839513	3.065390	6.969527

H	2.440413	2.405190	6.184327
C	3.594713	4.250090	6.291327
H	4.652513	3.997290	6.106827
C	2.850813	4.601590	4.972027
C	3.436013	3.986290	3.683327
N	3.533013	2.478890	3.688527
H	2.665113	1.988790	3.958727
H	3.752513	2.135590	2.729927
H	4.300013	2.147190	4.304227
H	4.457513	4.359890	3.484327
H	2.794513	4.274890	2.828027
H	1.778913	4.322590	5.054527
H	3.581313	5.129090	6.969727
H	2.860513	5.698990	4.788127
H	1.974413	3.530590	7.489627
S	-3.220700	-4.387400	5.577100
C	-2.333200	-3.614000	6.969700
H	-1.320600	-3.332000	6.639900
H	-2.925900	-2.735800	7.292500
H	-2.300900	-4.334300	7.816600
Cu	-2.210200	-3.546800	3.617800
O	3.145200	-6.476800	6.134600
H	3.837000	-7.072300	6.460100
H	3.251900	-6.488800	5.156500
H	2.714100	-5.678200	2.758400
O	3.403000	-6.276600	3.130200
H	3.361700	-7.069100	2.574600
O	-4.474300	-0.091500	7.452600
H	-4.975900	0.360800	8.149700
H	-5.119200	-0.738000	7.091500
O	-6.265100	-2.308300	6.449200
H	-5.792900	-3.151700	6.565600
H	-6.668100	-2.415900	5.567800
H	3.406100	-3.545600	7.850700
O	3.033500	-3.680500	6.965700
H	3.136300	-4.643600	6.786300
O	-7.311600	-3.765500	3.556800
H	-8.212700	-4.077800	3.387100
H	-6.787600	-4.134200	2.820100

$2N1O1S_{M109}a$

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.240200
N	1.101000	0.000000	-0.779300
C	2.478200	0.104700	-0.239600

H	1.025000	0.124400	-1.790400
C	3.142786	1.265152	-0.973724
O	2.861286	1.438353	-2.207824
N	3.956494	2.002009	-0.240701
C	4.799544	3.134571	-0.672427
C	3.875800	4.366100	-0.632000
O	3.311000	4.892900	-1.615100
N	3.653300	4.966700	0.578900
C	3.840500	4.599300	2.010600
H	3.081300	5.805500	0.462500
C	5.309000	4.246600	2.369600
O	5.712393	2.945776	2.166946
N	5.988800	5.282100	2.893300
C	7.394800	5.191900	3.303800
H	5.563000	6.198200	3.015300
C	7.654100	6.349600	4.300500
O	6.935700	7.361900	4.322500
N	8.722300	6.149200	5.094400
C	9.271600	7.151600	6.015600
H	9.288700	5.302300	5.014100
C	8.642500	7.014500	7.427400
C	10.788900	6.898800	6.071900
O	11.252300	5.764500	5.910700
N	11.565200	7.973600	6.336600
H	11.192700	8.910000	6.475600
H	12.564500	7.829500	6.450900
C	8.360900	5.240500	2.083700
C	8.383000	6.601600	1.356600
C	3.247700	-1.236500	-0.473800
C	3.868300	-1.833400	0.812400
C	-1.336200	0.048700	-0.777900
N	-2.317200	-0.745600	-0.019200
C	-3.209900	-1.600900	-0.564800
O	-3.280800	-1.850900	-1.783000
C	-4.100500	-2.316600	0.476800
N	-5.432600	-2.536900	-0.086200
C	-6.319600	-1.515400	-0.222600
O	-6.161700	-0.421900	0.327800
H	-5.574100	-3.426300	-0.559900
H	-2.271500	-0.637100	0.992100
C	-7.537800	-1.843300	-1.130400
N	-8.383300	-0.648600	-1.255600
C	-8.027300	0.553500	-1.758600
O	-6.983400	0.761200	-2.413900
C	-9.008400	1.663900	-1.493100
H	-9.247300	-0.677800	-0.723800

C	2.722200	3.593900	2.442300
C	3.061585	2.781221	3.626437
C	2.844885	3.003421	4.962537
N	3.401085	1.925821	5.615837
C	3.933885	1.092921	4.687937
N	3.744185	1.585321	3.471037
H	3.395485	1.769021	6.618037
C	-1.790800	1.539700	-0.886500
C	-2.997700	1.677100	-1.803400
O	-2.922500	1.465800	-3.027400
N	-4.131600	2.053600	-1.181400
H	-4.185500	2.045700	-0.165000
H	-5.020600	2.062000	-1.679100
C	5.664444	2.783271	-1.934427
C	6.411944	3.921671	-2.688727
C	5.642744	4.701471	-3.785427
C	4.697744	3.877971	-4.680927
N	3.406244	3.537771	-3.975927
H	2.636744	3.498071	-4.659027
H	3.203944	4.264371	-3.244927
C	-3.457100	-3.678700	0.918500
O	-3.718200	-4.703500	-0.059300
H	-3.145700	-4.517400	-0.822700
C	-4.033700	-4.140300	2.260500
H	2.364285	3.826021	5.488437
H	4.429385	0.159021	4.931137
C	-7.023600	-2.530900	-2.462200
C	-7.589600	-2.099000	-3.855400
C	-6.474400	-2.209700	-4.935700
C	-5.659800	-0.924300	-5.204600
N	-4.970700	-0.385000	-3.970900
H	-4.386300	-1.084500	-3.483700
H	-4.326800	0.396000	-4.192800
H	-5.686600	0.007200	-3.315400
H	-9.981500	1.333400	-1.085900
H	-9.180300	2.223500	-2.428800
H	5.144144	2.113271	-2.637027
H	-3.576200	-5.109600	2.539800
H	-0.981900	2.136900	-1.353700
H	6.855144	4.651071	-1.973027
H	-3.799500	-3.394500	3.047200
H	8.756000	5.978200	7.788400
H	5.155944	2.947271	-5.061027
H	4.434744	4.503271	-5.556827
H	7.570300	7.279900	7.368400
H	2.385500	0.293400	0.849400

H	-5.127400	-4.275200	2.207600
H	9.130700	7.704800	8.142900
H	-4.880200	-1.133200	-5.964100
H	-8.417600	-2.787000	-4.126400
H	-6.913900	-2.477800	-5.921400
H	1.801700	4.197800	2.604600
H	8.046900	4.443000	1.378800
H	-5.924000	-2.435800	-2.465700
H	-8.549200	2.367300	-0.771600
H	5.077544	5.549071	-3.355927
H	-1.978800	1.938200	0.135700
H	-8.016800	-1.082000	-3.825400
H	3.398244	2.637671	-3.422427
H	-6.300000	-0.108600	-5.585900
H	4.202000	-2.881300	0.635400
H	3.134600	-1.864000	1.646000
H	-7.234100	-3.616000	-2.369800
H	6.471744	2.156371	-1.487827
H	7.368600	7.019600	1.205100
H	8.994500	7.338200	1.917400
S	9.143200	6.357500	-0.293700
C	9.344700	8.077100	-0.839600
H	9.794600	8.052300	-1.848700
H	10.017300	8.616400	-0.150400
H	8.366000	8.584500	-0.890100
H	2.525900	-1.983900	-0.865400
H	-8.157100	-2.592800	-0.589000
H	3.614300	5.549600	2.542900
H	9.391000	4.985400	2.410500
H	2.530600	2.872500	1.624600
H	-5.777400	-3.037300	-4.683100
H	-4.213300	-1.665000	1.367700
H	7.554900	4.216100	3.808300
H	4.012000	-1.128600	-1.273100
H	-1.248900	-0.394100	-1.787700
H	6.396644	5.152071	-4.467327
S	5.326818	-0.981223	1.507491
C	6.518618	-1.060323	0.139991
H	7.501818	-0.766123	0.555591
Cu	4.536900	1.195200	1.654500
H	6.595718	-2.104123	-0.224309
H	6.211018	-0.373823	-0.663209
H	-2.362700	-3.528500	1.043000
H	9.035400	8.161700	5.622200
H	7.280944	3.433571	-3.189227
H	5.560444	3.312771	0.106773

O	8.706665	2.031655	3.953649
H	8.327737	2.853612	3.633649
O	6.640095	-0.661695	6.639879
H	7.541394	-0.744513	6.319879
O	3.541894	-2.260566	5.123679
H	3.162966	-1.438609	4.803679
O	0.926173	-2.123464	2.696648
H	1.827473	-2.206282	2.376648
O	4.874502	8.026476	0.308934
H	5.775802	7.943658	-0.011066
H	4.495574	8.848433	-0.011066
O	0.473182	5.001014	-1.865051
H	0.094255	5.822971	-2.185051
H	8.706665	2.031655	4.913649
H	6.117722	-1.400835	6.319879
H	3.541894	-2.260566	6.083679
H	0.926173	-2.123464	3.656648
H	-0.049190	4.261874	-2.185051

2N1O1S$_{M109}$b

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.234917
N	1.138811	0.000000	-0.729637
H	2.024175	0.076114	-0.236123
H	1.149018	0.032815	-1.746354
C	-1.320835	0.028235	-0.796579
N	-2.308173	-0.669407	0.034235
C	-3.377058	-1.338979	-0.424936
O	-3.691661	-1.381500	-1.630393
H	-2.099863	-0.643210	1.032552
C	-4.111360	-2.124206	0.686815
N	-5.504700	-2.414131	0.337162
C	-6.457136	-1.447742	0.321863
O	-6.188871	-0.244153	0.480041
H	-5.809095	-3.379231	0.217706
C	-7.906548	-1.913034	0.119105
N	-8.020461	-3.171521	-0.664487
C	-8.519965	-2.992644	-1.889611
O	-8.785813	-1.892863	-2.482855
C	-8.764733	-4.311236	-2.661214
N	-10.187891	-4.727512	-2.569304
C	-11.019253	-4.713720	-1.501644
O	-10.815144	-4.137315	-0.419527
H	-10.582095	-5.109210	-3.426290
C	-12.261240	-5.612738	-1.639821

N	-12.888619	-5.522914	-2.970481
C	-13.664555	-4.444994	-3.299963
O	-13.836434	-3.495786	-2.535715
H	-12.886588	-6.340397	-3.573673
C	-1.756882	1.489335	-1.080213
C	-11.861658	-7.083142	-1.340876
C	-11.087025	-7.329594	-0.015620
H	-1.938827	2.017844	-0.128531
C	-14.275436	-4.406612	-4.730432
N	-13.940218	-3.085237	-5.280597
C	-14.851599	-2.237419	-5.812232
O	-16.061001	-2.506822	-5.928590
H	-12.976243	-2.766667	-5.179108
C	-14.291950	-0.851303	-6.191174
N	-14.931046	-0.395552	-7.428399
C	-14.614034	-0.922983	-8.637625
O	-13.617081	-1.630734	-8.817886
H	-15.773900	0.163153	-7.301412
H	-15.372625	-4.430705	-4.604667
C	-15.616415	-0.554638	-9.769758
N	-15.238604	-1.258654	-11.002104
C	-15.162874	-2.593871	-11.183799
O	-15.621825	-3.436766	-10.382567
H	-14.813414	-0.676679	-11.716230
C	-14.492479	-3.022725	-12.460649
H	-15.119984	-3.782928	-12.957426
H	-14.286143	-2.202585	-13.172581
C	-3.338687	-3.433591	1.028999
C	-2.726033	-4.163414	-0.193288
H	-2.686940	1.481848	-1.680677
H	-13.533169	-3.512639	-12.203353
H	-0.974170	2.026109	-1.652672
H	-11.517048	-6.744467	0.822007
H	-13.198357	-0.918717	-6.362421
H	-3.472175	-4.350379	-0.993651
H	-1.220307	-0.510521	-1.762011
H	-8.420380	-1.089833	-0.420347
H	-12.983065	-5.246810	-0.880737
H	-4.039505	-4.116756	1.551773
H	-12.812763	-7.649926	-1.224302
H	-1.890344	-3.563038	-0.613139
H	-11.316397	-7.533819	-2.199528
H	-2.522158	-3.204091	1.746650
H	-11.207753	-8.402644	0.255028
C	-8.396256	-4.250371	-4.175371
H	-8.760958	-3.298605	-4.605253

C	-6.890340	-4.519566	-4.474202
C	-5.858227	-3.570548	-3.820890
C	-5.868618	-2.107652	-4.350161
N	-6.110007	-1.148692	-3.213263
H	-6.012371	-0.159792	-3.491413
H	-5.404361	-1.316533	-2.462674
H	-7.086853	-1.276914	-2.854028
H	-4.890407	-1.847596	-4.796996
H	-6.654163	-1.916776	-5.107988
H	-6.646980	-5.542032	-4.120937
H	-5.971459	-3.572473	-2.715879
H	-6.745000	-4.517386	-5.576540
H	-8.142002	-5.085917	-2.160623
H	-15.475577	0.527676	-9.986505
C	-13.821867	-5.553653	-5.690844
C	-14.599962	-5.486746	-7.002067
O	-15.778479	-5.872806	-7.069359
N	-13.909442	-5.003950	-8.053747
H	-13.034073	-4.504150	-7.902152
H	-14.382285	-4.809733	-8.936339
H	-14.112599	-6.532188	-5.254397
H	-4.845824	-3.993375	-4.011423
H	-12.721068	-5.502441	-5.857823
H	-4.110968	-1.476325	1.593200
C	-8.616188	-1.987138	1.511191
C	-8.086622	-2.996642	2.491050
C	-7.595252	-2.822032	3.758875
N	-7.323514	-4.083451	4.241057
C	-7.626044	-4.983194	3.275931
N	-8.090073	-4.357687	2.200336
H	-6.944909	-4.305082	5.156113
H	-7.439601	-1.923216	4.346117
H	-7.460294	-6.052632	3.377792
H	-9.679737	-2.234013	1.313986
H	-8.566614	-0.970670	1.960949
H	-8.939797	-5.068080	-4.710080
C	-14.577396	0.173930	-5.031608
O	-15.937990	0.653879	-5.097809
H	-16.503879	-0.066001	-4.770074
C	-13.640248	1.381443	-5.139763
H	-13.753667	1.898239	-6.109269
H	-12.588389	1.053171	-5.022384
H	-13.883691	2.101142	-4.331429
H	-14.402784	-0.330893	-4.058078
S	-2.040782	-5.754130	0.390280
C	-1.121918	-6.315189	-1.071855

H	-0.301106	-5.608894	-1.284282
H	-1.789087	-6.396585	-1.948846
H	-0.698788	-7.308390	-0.834136
C	-17.099146	-0.736269	-9.240728
H	-17.031633	-1.253860	-8.268903
H	-17.491862	0.277430	-9.019252
C	-18.183932	-1.433071	-10.126771
H	-17.728781	-2.099065	-10.879709
C	-19.185511	-2.208532	-9.221389
C	-18.870022	-3.702688	-8.986097
N	-17.510608	-3.933287	-8.363159
H	-17.357415	-3.394726	-7.494885
H	-17.365235	-4.924448	-8.098532
H	-16.763248	-3.709316	-9.058756
H	-18.881831	-4.276142	-9.930697
H	-19.630056	-4.139859	-8.308501
H	-18.739263	-0.650517	-10.684318
H	-19.289532	-1.698491	-8.239817
H	-20.202605	-2.201374	-9.671280
S	-9.267119	-7.044260	0.046837
C	-8.664267	-7.875186	-1.454677
H	-8.906278	-7.305674	-2.365997
H	-7.569712	-7.963211	-1.343923
H	-9.106032	-8.894838	-1.514010
Cu	-8.603337	-4.881556	0.325328
H	-7.499071	-8.659982	2.107449
O	-6.655746	-8.377813	2.501721
H	-6.338162	-9.149839	2.994497
O	-6.198192	1.626442	-2.227213
H	-6.330209	2.584428	-2.272881
H	-6.289261	1.396290	-1.282976
H	-4.374747	-6.635306	0.276213
O	-5.343769	-6.691478	0.151250
H	-5.654605	-7.261607	0.879783
H	-10.519270	-1.603282	-3.605312
O	-11.409216	-1.570667	-4.015434
H	-12.008199	-1.642025	-3.251716
H	-5.255811	-7.207674	-1.832807
O	-5.256475	-7.290015	-2.810025
H	-4.756451	-8.100241	-2.993549
H	-12.331137	-4.401773	1.371091
O	-12.878203	-5.090157	1.788888
H	-13.327873	-4.652425	2.527599

2N1O1S$_{M109}$c

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.234500
N	1.100800	0.000000	-0.799600
C	2.495400	0.301500	-0.362200
H	0.936000	0.247700	-1.776600
C	3.138000	-0.752400	0.598800
O	3.875700	-0.329800	1.519700
N	2.930100	-2.041700	0.282300
C	3.667300	-2.981000	1.135700
C	3.814900	-4.331100	0.435500
O	2.862518	-4.771085	-0.289786
N	5.008100	-4.951400	0.623000
H	5.107800	-5.915700	0.314500
H	5.715300	-4.563100	1.241300
C	2.983900	-3.224800	2.517300
C	2.628000	1.761000	0.170800
C	4.030100	2.370300	-0.087400
C	-1.353900	-0.158400	-0.764100
N	-1.444100	0.890600	-1.824600
C	-2.116800	1.102200	-3.001700
O	-2.238500	2.261000	-3.418500
H	-1.158800	1.808300	-1.467900
C	-1.493700	-1.635600	-1.226400
C	-1.290000	-2.655600	-0.131100
C	-2.041600	-3.045700	0.948700
N	-1.366800	-4.107200	1.513500
C	-0.240400	-4.325900	0.794200
N	-0.164600	-3.462600	-0.214200
H	-1.645900	-4.608700	2.349300
C	-2.737600	-0.001000	-3.895400
N	-1.722000	-1.025000	-4.244100
C	-1.937900	-2.141000	-4.951100
O	-3.064300	-2.473800	-5.392300
C	-0.738700	-3.116200	-5.127200
N	-1.099600	-3.984200	-6.270500
C	-0.823300	-5.304900	-6.341500
O	-0.119400	-5.933700	-5.543400
H	-1.768900	-3.585400	-6.926600
H	-0.764100	-0.702700	-4.096800
C	-1.473900	-6.030100	-7.542500
N	-0.392600	-6.592800	-8.369000
C	-0.377200	-6.545900	-9.723700
O	-1.240800	-5.958300	-10.401600
H	0.331500	-7.109500	-7.879200

C	0.858500	-7.217800	-10.360800
N	0.478600	-7.835200	-11.630600
C	-0.233100	-8.992200	-11.670500
O	-0.410900	-9.695300	-10.671200
H	0.609600	-7.263500	-12.461500
C	-4.090200	-0.512400	-3.301600
C	-5.260500	-0.291700	-4.301300
C	-6.556300	-1.049400	-3.885700
C	-6.878300	-2.219400	-4.831200
N	-5.757100	-3.226200	-4.832800
H	-5.645500	-3.618200	-3.891900
H	-5.951800	-4.038100	-5.470300
H	-4.839700	-2.820100	-5.129100
C	-2.411100	-7.147400	-6.976900
C	-3.298500	-7.706300	-8.071100
O	-4.273000	-7.056400	-8.524900
N	-2.944300	-8.909100	-8.540800
H	-2.096800	-9.372100	-8.217300
H	-3.444200	-9.355700	-9.308200
C	-0.801100	-9.342600	-13.073500
N	-1.605300	-10.568400	-12.983300
C	-2.707500	-10.773100	-12.233100
O	-3.341300	-9.863700	-11.650900
C	-3.157600	-12.205600	-12.148300
H	-1.177100	-11.391600	-13.394300
C	0.680500	-2.493000	-5.327900
C	1.832900	-3.268900	-4.625600
H	-2.944500	-2.617200	1.383700
Cu	1.594268	-2.837809	-1.037376
C	2.013200	-6.176500	-10.582600
O	1.767000	-5.400200	-11.768700
H	1.057200	-4.771100	-11.555000
C	3.359400	-6.888100	-10.745200
H	0.498200	-5.096500	0.988000
C	-1.481300	-8.053000	-13.696800
C	-2.882100	-8.138500	-14.389700
C	-3.682100	-6.830500	-14.123100
C	-4.630600	-6.851500	-12.904600
N	-3.923100	-7.154200	-11.598300
H	-3.114700	-6.537800	-11.411100
H	-3.622700	-8.160000	-11.591900
H	-4.561200	-7.031700	-10.792900
S	2.393161	-2.442904	-3.157711
H	-4.239300	-12.257800	-12.363600
H	-2.622900	-12.900000	-12.821600
H	1.958300	-3.598600	2.350800

H	3.354300	-7.582200	-11.602300
H	4.151200	-6.132600	-10.915200
H	2.955300	-2.266600	3.063700
H	3.602400	-7.455500	-9.823600
H	-1.515000	-7.291500	-12.898600
H	4.131400	3.324700	0.471300
H	2.445600	1.767900	1.263800
H	-3.084800	-6.683700	-6.225500
H	-7.799800	-2.748600	-4.519700
H	-3.020100	-12.556300	-11.106600
H	-3.449100	-9.027600	-14.064600
H	1.579700	-4.331700	-4.453100
H	-5.418000	-7.619100	-13.014000
H	0.888800	-2.471000	-6.417100
H	-5.122800	-5.863600	-12.801500
H	-2.725500	-8.242500	-15.483400
H	-4.340500	-6.593500	-14.987500
H	-1.789700	-7.915900	-6.465900
H	-7.010000	-1.863100	-5.870100
H	3.562100	-3.957500	3.121100
H	-5.467300	0.796400	-4.365400
H	2.737900	-3.235100	-5.270500
H	-0.741000	-1.881100	-2.002100
H	-7.439300	-0.376200	-3.915000
C	4.120061	-3.042004	-3.099511
H	4.096661	-4.147304	-3.100811
H	4.663661	-2.635104	-3.972511
H	4.543161	-2.690304	-2.142811
H	0.067900	-9.601600	-13.719200
H	-0.784300	-7.655800	-14.462600
H	1.223200	-8.022400	-9.688800
H	4.831900	1.678400	0.223900
H	-4.925800	-0.593500	-5.316000
H	0.726900	-1.431700	-5.007500
H	-2.987000	-5.968600	-14.031100
H	1.868400	2.403700	-0.322400
H	-6.484800	-1.424900	-2.841800
H	-2.989000	0.582100	-4.810800
H	-2.045100	-5.332000	-8.184200
S	4.228800	2.762500	-1.870100
C	5.819700	3.631500	-1.895700
H	6.039900	3.889600	-2.947000
H	5.763200	4.552000	-1.288900
H	6.615900	2.973000	-1.506500
H	-4.014500	-1.576300	-2.997400
H	-2.142300	0.063800	-0.013800

H	2.073300	-5.521200	-9.684700
H	3.091000	0.221100	-1.291300
H	-0.745800	-3.753100	-4.214000
H	-4.315400	0.039300	-2.362400
H	-2.503600	-1.802200	-1.636300
H	4.680300	-2.569100	1.351100
O	1.112500	0.766300	-4.192800
H	2.043900	0.516600	-4.087500
H	1.067700	1.701600	-3.890200
H	-5.467300	-6.028200	-7.237700
O	-6.090500	-5.639600	-6.582900
H	-6.912900	-6.136300	-6.700500
H	1.850400	3.687300	-2.643700
O	0.953200	3.376700	-2.877000
H	0.476000	4.145800	-3.223700
H	-3.204300	0.509200	3.176100
O	-2.952800	-0.025200	2.408200
H	-1.981600	0.057500	2.347700
O	0.411800	-6.393800	-2.110600
H	1.371800	-6.393800	-2.110600
H	0.091300	-5.488900	-2.110600
O	-3.923000	-3.559400	-1.046400
H	-2.963000	-3.559400	-1.046400
H	-4.243500	-2.654500	-1.046400

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.239800
N	1.128900	0.000000	-0.741800
H	2.023800	-0.106100	-0.269600
H	1.082600	-0.240700	-1.729400
C	-1.316200	0.001000	-0.804800
N	-2.031400	-1.247400	-0.532900
C	-1.666000	-2.423400	-1.127000
O	-0.806200	-2.491300	-2.013900
H	-2.735200	-1.258300	0.202200
C	-2.360200	-3.670600	-0.551500
N	-2.846200	-4.519200	-1.648600
C	-4.127600	-4.875300	-1.914200
O	-4.358500	-5.634800	-2.878000
H	-2.164800	-4.900200	-2.301600
C	-1.337600	-4.440800	0.330500
C	-5.326000	-4.353900	-1.072600
N	-5.437000	-4.767900	0.323400
C	-5.371500	-6.022500	0.729300

O	-4.911700	-7.056900	0.108300
C	-1.197000	-3.728000	1.706200
C	-5.984200	-6.282300	2.130500
N	-5.792900	-5.103800	2.993000
C	-5.911600	-5.111700	4.308100
O	-5.637700	-4.087400	5.026500
C	-2.185300	1.226800	-0.452700
H	-2.383800	1.262600	0.634600
H	-3.217200	-3.401200	0.094800
H	-3.128700	1.172100	-1.029300
H	-1.648100	2.148000	-0.750500
H	-1.088300	-2.629300	1.607000
H	-6.185800	-4.784700	-1.630000
H	-1.680000	-5.489900	0.464900
H	-1.089900	0.026400	-1.892100
H	-0.310100	-4.095800	2.272700
C	-6.383800	-6.347800	5.128600
N	-5.348900	-6.505900	6.165500
C	-4.802300	-7.649100	6.625200
O	-5.121000	-8.801000	6.302400
H	-5.033500	-5.612800	6.537000
C	-3.649300	-7.339600	7.623200
N	-4.246800	-7.057200	8.945100
C	-3.934700	-5.966300	9.682700
O	-3.124400	-5.100600	9.310300
H	-4.866800	-7.757400	9.338200
C	-4.726900	-5.834200	10.997600
N	-3.919600	-5.085600	11.963100
C	-2.863100	-5.674400	12.581700
O	-2.699900	-6.899000	12.600200
H	-4.012200	-4.072900	11.911700
H	-3.166000	-6.394400	7.305300
C	-1.871800	-4.687400	13.264800
N	-0.730800	-5.451700	13.789700
C	0.121700	-6.223500	13.076900
O	0.229100	-6.191900	11.834600
H	-0.748100	-5.610700	14.791400
C	0.985400	-7.138400	13.908200
H	2.027900	-7.069300	13.552400
H	0.960100	-6.936300	14.995000
H	0.647300	-8.178700	13.738200
C	-7.760400	-6.032200	5.786900
C	-8.408300	-7.318500	6.381700
H	-7.670900	-7.917000	6.949900
H	-7.623000	-5.259800	6.568600
H	-6.430200	-7.293500	4.551200

H	-4.905500	-6.846300	11.415600
H	-8.451100	-5.612800	5.022500
C	-2.598500	-8.479600	7.690600
C	-1.325300	-7.945100	8.323300
O	-0.620400	-7.082000	7.761400
N	-1.038600	-8.442900	9.543500
H	-0.276400	-8.057000	10.098200
H	-1.701500	-9.047300	10.023300
H	-2.367900	-8.803000	6.654000
H	-3.026900	-9.359200	8.226800
H	-2.387300	-4.265300	14.156200
H	-8.816300	-7.958400	5.564600
H	-5.476400	-7.183200	2.541400
H	-0.342500	-4.476200	-0.168900
C	-6.115100	-5.129400	10.755900
O	-5.938700	-3.713400	10.651300
H	-5.850200	-3.501400	9.698200
C	-7.066800	-5.416800	11.919300
H	-6.686800	-4.979700	12.859900
H	-8.053900	-4.965300	11.702800
H	-7.197900	-6.509400	12.060600
H	-6.546900	-5.546100	9.814700
S	-9.785200	-6.836400	7.478300
C	-10.454000	-8.451600	7.961000
H	-10.771800	-9.015400	7.066400
H	-9.705600	-9.037000	8.525800
H	-11.334000	-8.260800	8.602700
C	-7.509200	-6.606100	1.892100
H	-7.951900	-6.894600	2.864300
H	-8.011800	-5.675100	1.563000
C	-7.776700	-7.770700	0.882900
C	-8.081700	-7.252500	-0.554000
C	-7.573900	-8.170300	-1.693600
N	-6.117200	-7.913900	-1.989100
H	-5.660700	-8.751900	-2.374900
H	-5.954800	-7.140000	-2.654300
H	-8.163400	-8.005600	-2.611700
H	-7.664400	-6.240300	-0.693000
H	-7.684200	-9.228700	-1.386300
H	-8.661900	-8.347200	1.224000
H	-6.915700	-8.472200	0.890700
H	-9.182100	-7.144000	-0.671200
C	-1.559200	-3.486300	12.284000
H	-1.973100	-3.761600	11.299700
H	-2.153200	-2.619300	12.637600
C	-0.094000	-2.964900	12.111500

H	0.646100	-3.742200	12.367400
C	0.106200	-2.447700	10.656300
C	0.677100	-3.461000	9.638000
N	-0.193500	-4.686400	9.473300
H	-1.183600	-4.460800	9.274200
H	0.116900	-5.284700	8.686100
H	-0.127800	-5.277000	10.330400
H	1.679600	-3.823000	9.932300
H	0.750200	-2.972800	8.647900
H	0.062900	-2.121500	12.817100
H	-0.853100	-2.056800	10.257200
H	0.823200	-1.597400	10.642300
C	-5.530500	-2.787000	-1.230400
C	-6.192100	-2.062100	-0.077200
C	-7.343900	-1.315900	-0.137500
N	-7.576400	-0.852500	1.143300
C	-6.573200	-1.305000	1.936200
N	-5.724900	-2.049500	1.236200
H	-8.320400	-0.213200	1.412000
H	-6.499000	-1.096000	2.998200
H	-7.992700	-1.076100	-0.979300
H	-4.586200	-2.253000	-1.452500
H	-6.172900	-2.643200	-2.132800
S	-2.673800	-4.071800	2.735600
C	-2.397100	-2.975000	4.156300
H	-3.279000	-3.136000	4.803300
H	-2.307700	-1.911300	3.851600
H	-1.459000	-3.295400	4.656800
H	-5.586400	-7.604800	-1.068800
Cu	-4.781225	-3.707855	1.929191
H	0.515800	-0.787300	3.252200
O	0.697100	-1.144300	4.144800
H	1.469100	-0.637900	4.441200
H	-1.405400	-6.465600	3.809900
O	-1.068300	-7.322100	4.130800
H	-1.005600	-7.213800	5.095500
H	-3.017600	-7.895100	0.652000
O	-2.070200	-8.129900	0.680400
H	-1.893500	-8.334400	1.614000
O	-5.446200	-2.856100	7.756500
H	-5.636400	-3.202700	6.855300
H	-4.505500	-2.613700	7.728900
O	-9.833100	-4.103500	-0.337900
H	-10.601700	-3.524900	-0.218000
H	-9.064300	-3.519400	-0.210600
O	-1.679200	-1.899000	7.517900

H	-1.800200	-2.118900	6.576900
H	-1.509100	-0.943500	7.510600

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.238400
N	1.144800	0.000000	-0.720400
H	1.155900	-0.018300	-1.736900
H	2.031300	0.027000	-0.224000
C	-1.299500	0.057300	-0.815900
N	-2.274700	-0.856300	-0.217900
C	-3.154400	-1.567100	-0.967000
O	-3.185000	-1.536100	-2.204200
H	-2.342800	-0.867400	0.796100
C	-1.837400	1.514200	-0.864200
H	-2.193300	1.829600	0.131700
H	-2.668500	1.562600	-1.593200
C	-4.106300	-2.499300	-0.165900
N	-5.451000	-2.292100	-0.736700
C	-6.718800	-2.171000	-0.280200
O	-7.620900	-2.214300	-1.152300
H	-5.458100	-2.336100	-1.755600
C	-3.680400	-3.988200	-0.405100
C	-2.828900	-4.629700	0.733300
H	-2.361100	-3.884800	1.404000
H	-4.601900	-4.599000	-0.509900
H	-1.041400	2.206400	-1.204500
H	-4.066100	-2.264700	0.914000
H	-2.024300	-5.272600	0.315700
H	-1.132200	-0.279300	-1.860800
H	-3.147000	-4.077200	-1.372800
C	-7.245700	-1.865600	1.165400
N	-8.507900	-2.633800	1.311300
C	-8.728600	-3.966700	1.516400
O	-9.926200	-4.343500	1.592900
H	-9.339500	-2.063500	1.376800
C	-7.515700	-4.903000	1.553800
N	-7.036029	-4.984086	2.969532
C	-7.506200	-5.929800	3.820000
O	-8.276800	-6.902400	3.626900
C	-6.912300	-5.730300	5.242500
N	-5.446314	-5.582674	5.134673
C	-4.747314	-6.017674	6.165173
O	-5.189514	-6.461774	7.284673
C	-3.215014	-5.943274	5.945973

N	-2.638914	-4.991074	6.917173
C	-1.631714	-4.152474	6.636073
O	-1.007914	-4.147474	5.544973
H	-3.065114	-4.956374	7.843873
H	-3.076914	-5.502374	4.949773
C	-7.738600	-6.222500	0.772300
C	-1.232814	-3.210174	7.800273
N	-0.223214	-3.924774	8.611373
C	-0.596314	-4.676074	9.680873
O	-1.760714	-4.756574	10.087373
H	0.752486	-3.861674	8.321073
C	-0.726914	-1.843574	7.261473
O	0.454386	-2.018474	6.438573
H	0.184686	-2.744874	5.825873
C	-0.404514	-0.855574	8.386773
C	0.574086	-5.447174	10.352373
N	0.201686	-5.790674	11.740473
C	-0.640614	-6.770874	12.165573
O	-0.981814	-7.769974	11.504673
H	0.301686	-5.013374	12.391673
C	-1.134614	-6.568574	13.578273
H	-1.127214	-7.538574	14.103973
H	0.426186	-1.225174	9.020573
H	-8.552400	-6.810600	1.236000
H	-0.557214	-5.829874	14.165973
H	-2.186514	-6.231574	13.514673
H	-0.095414	0.117026	7.953273
H	-1.303714	-0.697374	9.017973
H	-6.790300	-6.785800	0.886500
H	-2.095914	-3.026874	8.467773
H	-7.589800	-0.817800	1.024100
H	-6.672200	-4.382900	1.051500
C	0.950686	-6.636574	9.421173
H	0.021186	-7.145974	9.109773
C	2.009786	-7.611774	10.006073
H	1.768386	-7.882474	11.054673
C	2.146086	-8.876874	9.109873
C	1.307886	-10.091474	9.560273
N	-0.170814	-9.806074	9.645473
H	-0.666714	-10.684074	9.841173
H	-0.395614	-9.146974	10.423273
H	1.437986	-10.913574	8.830973
H	1.637386	-10.453574	10.552873
H	1.892786	-8.631474	8.057973
H	1.396486	-6.201174	8.507673
H	3.197486	-9.238974	9.108773

H	-7.175400	-6.625500	5.855200
H	2.993386	-7.095074	10.031073
H	-1.557914	-1.424374	6.655873
H	1.455886	-4.770774	10.431673
C	-7.509700	-4.474500	5.953600
C	-9.058200	-4.529200	5.958900
H	-9.471300	-4.653400	4.940800
H	-7.149200	-4.497700	7.003800
H	-7.155600	-3.563200	5.436400
H	-9.385100	-5.378100	6.603100
C	-7.999400	-5.975500	-0.754700
C	-9.496600	-6.190400	-1.142100
C	-10.157100	-5.049500	-1.932200
N	-10.178400	-3.770500	-1.126900
H	-10.882900	-3.124600	-1.506600
H	-9.256500	-3.271000	-1.137600
H	-10.403700	-3.969800	-0.115300
H	-9.631300	-4.838300	-2.882000
H	-11.208500	-5.322000	-2.147300
H	-10.097600	-6.390500	-0.231900
H	-7.629900	-4.973000	-1.062800
H	-9.584200	-7.095700	-1.781400
H	-7.387800	-6.699000	-1.345900
H	-0.577514	-9.400374	8.722373
C	-6.581700	-1.949200	2.581800
C	-5.146100	-1.639700	2.869900
C	-4.438700	-0.465200	2.925500
N	-3.196000	-0.792000	3.412200
C	-3.192100	-2.120800	3.699000
N	-4.354200	-2.671100	3.361000
H	-2.440500	-0.145900	3.664100
H	-2.343700	-2.643400	4.146000
H	-4.762700	0.556000	2.720900
H	-6.763400	-2.957800	3.012500
H	-7.178800	-1.237700	3.186300
C	-2.498814	-7.345274	5.943573
C	-2.226814	-8.033474	7.270773
O	-1.147914	-8.684974	7.410973
N	-3.156314	-7.892474	8.206773
H	-3.003314	-8.277774	9.139273
H	-4.052514	-7.351974	7.993873
H	-3.145714	-8.026774	5.349073
H	-1.520814	-7.253474	5.421573
S	-9.726900	-2.982700	6.671500
C	-11.503200	-3.185300	6.372000
H	-11.872400	-4.076100	6.910700

H	-12.019800	-2.288200	6.762100
H	-11.703500	-3.293600	5.289900
S	-3.932312	-5.715659	1.754376
C	-2.736212	-7.005759	2.228576
H	-3.304612	-7.727559	2.836976
H	-2.362512	-7.495859	1.306976
H	-1.908112	-6.559359	2.808776
Cu	-5.072381	-4.580147	3.397805
O	3.150000	-4.403200	7.932300
H	2.973600	-4.477000	6.978900
H	3.622800	-3.556700	8.000200
O	-0.500300	0.432000	4.282600
H	-0.082800	0.291300	3.413300
H	-0.046300	-0.178300	4.890300
O	-5.683500	-9.029000	3.399000
H	-6.102900	-9.778900	2.952200
H	-6.426400	-8.415400	3.569200
O	-7.826700	1.371100	2.644400
H	-8.265500	2.233000	2.585500
H	-7.998400	1.063600	3.557900
H	-8.416400	0.650100	6.234400
O	-8.095700	0.108400	5.497400
H	-8.541800	-0.755200	5.632500
H	-4.697700	-0.811100	7.434000
O	-4.201000	-1.446900	7.977300
H	-4.889500	-2.059600	8.284800

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.236700
N	1.136000	0.000000	-0.733100
H	2.026300	0.035500	-0.243800
H	1.143300	-0.022200	-1.749400
C	-1.320700	0.035000	-0.786400
N	-2.301400	-0.692300	0.025800
C	-3.425900	-1.237700	-0.472700
O	-3.723400	-1.220100	-1.679000
H	-2.090200	-0.701600	1.022700
C	-1.768500	1.505900	-1.012700
H	-1.985900	1.983800	-0.041900
H	-2.665900	1.512500	-1.658800
H	-0.969200	2.075800	-1.527000
H	-1.229900	-0.467400	-1.771800
C	-4.412000	-1.866800	0.560000
N	-5.241600	-2.781200	-0.247500

C	-6.140100	-3.678900	0.197100
O	-6.202080	-4.152258	1.366156
H	-5.278500	-2.468200	-1.220400
C	-7.243200	-3.985500	-0.825300
N	-8.032800	-5.182900	-0.503300
C	-9.013900	-5.561400	0.366300
O	-9.509200	-6.690900	0.134600
H	-7.843000	-5.953200	-1.138400
C	-9.676900	-4.790500	1.531500
N	-8.921492	-4.354616	2.675647
C	-9.193292	-4.986216	3.823747
O	-10.072392	-5.896516	4.037047
H	-10.222300	-5.619000	2.008300
C	-8.303492	-4.592116	5.022247
N	-9.127892	-4.476916	6.253147
C	-9.206492	-3.353216	6.991347
O	-8.672892	-2.263116	6.724747
H	-9.603092	-5.320716	6.582747
H	-7.837792	-3.609116	4.863047
C	-10.076492	-3.477116	8.267247
N	-9.307892	-2.853916	9.358947
C	-9.156292	-3.373616	10.596547
O	-9.645992	-4.458716	10.963547
H	-8.848192	-1.977616	9.122747
C	-8.236792	-2.541316	11.515347
N	-8.721092	-2.611216	12.893247
C	-9.829292	-1.929316	13.287447
O	-10.334192	-1.033316	12.604747
H	-8.320992	-3.352016	13.465047
C	-10.402992	-2.379816	14.660547
N	-11.636392	-1.631716	14.937347
C	-12.763492	-1.612916	14.192347
O	-13.013792	-2.421616	13.273447
H	-11.546492	-0.904316	15.639147
C	-13.745892	-0.534116	14.563247
H	-14.751292	-0.980216	14.655447
H	-13.506192	0.010784	15.494747
H	-10.280792	-4.526116	8.556247
H	-13.789092	0.197084	13.732847
C	-3.786200	-2.479300	1.846200
C	-4.172800	-1.695600	3.115800
H	-4.097600	-3.530700	1.952500
H	-8.267692	-1.478616	11.197647
C	-11.425492	-2.726716	8.031847
C	-12.371492	-2.955116	9.200647
O	-12.862492	-4.074016	9.439447

N	-12.629592	-1.857016	9.936847
H	-12.086292	-1.007116	9.800947
H	-13.153392	-1.924716	10.808247
H	-11.921792	-3.157416	7.138247
H	-2.676300	-2.528700	1.798800
H	-3.442600	-1.902600	3.927000
C	-7.190292	-5.669916	5.206247
H	-6.550992	-5.674516	4.306947
C	-6.326092	-5.369416	6.468947
H	-7.659592	-6.672416	5.302847
H	-6.044592	-4.296116	6.500047
H	-11.212992	-1.652216	7.835447
H	-9.675192	-2.058916	15.439047
C	-10.747000	-3.768600	1.018900
H	-10.467400	-2.753500	1.368800
C	-12.175600	-4.152600	1.520300
H	-12.113800	-4.459900	2.583700
H	-12.824800	-3.252100	1.499300
H	-10.790600	-3.734900	-0.091600
H	-4.189700	-0.592100	2.964400
H	-6.910292	-5.618616	7.384647
H	-5.097700	-1.041900	0.861500
H	-6.741000	-4.256600	-1.784100
C	-12.849900	-5.267000	0.650200
C	-13.101900	-6.619100	1.345600
N	-11.850600	-7.337800	1.762600
H	-11.138700	-7.353100	0.999600
H	-12.085900	-8.327800	2.030100
H	-11.377200	-6.875100	2.561600
H	-12.284500	-5.443300	-0.285000
H	-13.736500	-6.496600	2.243800
H	-13.632300	-7.294200	0.644800
H	-13.861700	-4.926500	0.336500
C	-6.755492	-3.059316	11.425147
O	-6.564592	-4.194016	12.290547
H	-6.964292	-4.958716	11.842547
C	-5.775192	-1.964716	11.848047
H	-5.962792	-1.631716	12.883047
H	-4.741192	-2.359716	11.792547
H	-5.863492	-1.095116	11.164647
H	-6.541792	-3.338916	10.366947
S	-4.723092	-6.235416	6.550747
C	-5.173292	-7.983216	6.344347
H	-5.554492	-8.169516	5.326147
H	-5.912792	-8.272416	7.115047
H	-4.240092	-8.559416	6.497447

C	-8.113200	-2.704600	-1.135300
C	-7.963000	-1.431000	-0.336200
C	-7.811800	-0.169200	-0.857100
N	-7.858700	0.700100	0.204300
C	-8.039200	-0.029300	1.327500
N	-8.086600	-1.330400	1.046500
H	-7.819900	1.722800	0.169200
H	-8.135400	0.411500	2.314900
H	-7.677400	0.166900	-1.882800
H	-9.171100	-2.998400	-1.024000
H	-7.999500	-2.431600	-2.204700
C	-10.470192	-3.962516	14.706647
H	-10.243292	-4.322416	13.688147
H	-9.629292	-4.305016	15.343547
C	-11.744992	-4.694616	15.242147
H	-12.637892	-4.048416	15.191647
C	-11.963692	-6.020716	14.456647
C	-12.909992	-5.940416	13.237647
N	-12.461692	-4.938116	12.198147
H	-11.485792	-5.073316	11.884747
H	-13.029292	-4.990616	11.332247
H	-12.590592	-3.968516	12.571447
H	-13.932792	-5.646116	13.534347
H	-12.966492	-6.933216	12.748147
H	-11.585892	-4.937516	16.313547
H	-10.986892	-6.440116	14.133247
H	-12.416892	-6.792616	15.116647
S	-5.842067	-2.126291	3.826430
C	-6.155267	-0.528091	4.648230
H	-7.009967	-0.663991	5.334030
H	-6.343367	0.264309	3.901630
H	-5.252767	-0.273491	5.236430
Cu	-7.569802	-2.736860	2.371185
O	-12.773200	-9.955400	2.571000
H	-12.367400	-10.796100	2.310000
H	-12.779100	-9.965800	3.555700
O	-12.617000	-9.644200	5.457200
H	-12.578500	-10.394400	6.069400
H	-11.945000	-9.010700	5.782500
O	-7.738900	3.597200	1.138700
H	-8.504400	4.193600	1.117800
H	-6.976700	4.189200	1.034200
O	-10.946000	-7.209000	6.312000
H	-11.750600	-6.722800	6.559500
H	-10.629200	-6.755400	5.488200
H	-3.022800	-5.064500	4.684800

O	-2.400600	-4.540000	4.142100
H	-1.534500	-4.939000	4.318400
H	-6.358300	-6.502700	1.940600
O	-6.377800	-7.412900	2.293400
H	-5.883400	-7.933600	1.642900

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.234800
N	1.189700	0.000000	-0.669200
C	1.645100	0.213500	-2.048500
C	-1.395600	-0.091300	-0.690500
N	-2.285000	0.901100	-0.061100
C	-1.960431	2.177230	0.168825
O	-0.733750	2.477513	0.100302
H	-2.972000	0.534300	0.588400
C	-3.048400	3.199500	0.578800
N	-4.425700	3.233800	-0.009800
C	-4.942400	4.381100	-0.594100
O	-6.048400	4.796600	-0.200700
H	-5.125800	2.856000	0.634700
C	-4.297300	5.135000	-1.770700
N	-2.843500	5.016300	-2.013100
C	-2.113400	5.965700	-1.443700
O	-2.480500	6.803300	-0.534800
C	-0.643200	6.116200	-1.892200
N	-0.495600	7.533300	-2.318200
C	0.129900	7.976600	-3.429500
O	0.641900	7.241300	-4.294400
H	-0.880100	8.220800	-1.673100
C	0.111800	9.518900	-3.583600
N	1.371800	9.958500	-4.181900
C	2.522100	10.009700	-3.459900
O	2.534800	9.918000	-2.228600
H	1.380600	10.038500	-5.195400
H	-4.579600	6.194000	-1.564000
H	1.981100	-0.003000	-0.023900
C	-1.433200	-0.068900	-2.252700
H	-1.077300	-1.073800	-2.579100
H	-0.772600	0.712100	-2.649800
C	3.184300	-0.022500	-2.017400
O	3.843800	-0.058500	-0.972300
N	3.722500	-0.149500	-3.253400
C	5.167200	-0.214800	-3.489300
C	5.652500	-1.687900	-3.473600

H	3.163100	-0.004500	-4.089300
C	5.460600	0.509900	-4.815900
O	4.574900	1.057300	-5.487000
N	6.755000	0.503500	-5.200700
H	7.003300	0.948200	-6.077700
H	7.488500	0.031200	-4.678600
C	3.805700	10.208700	-4.313100
N	4.984000	10.187400	-3.436200
C	5.384200	9.186500	-2.621400
O	4.927900	8.024300	-2.656400
C	6.471200	9.561300	-1.649800
H	5.423300	11.090300	-3.289600
C	-3.109900	2.927400	2.109300
C	-3.781700	4.071300	2.919300
C	-2.908600	5.353900	3.020900
C	-3.689300	6.668100	2.839500
N	-4.268700	6.842100	1.454300
H	-4.680900	7.783800	1.382800
C	0.313900	5.838800	-0.691100
C	1.773800	5.851400	-1.131500
O	2.236000	4.986600	-1.900900
N	2.519100	6.843800	-0.607600
H	2.069300	7.632800	-0.146700
H	3.469700	7.001800	-0.938700
C	-4.997500	4.817100	-3.145200
C	-6.500300	4.441500	-3.105100
C	1.388900	1.675800	-2.572200
H	0.679200	2.177400	-1.896300
H	2.324200	2.265500	-2.489900
C	0.869800	1.750300	-4.043800
H	-5.024300	6.164500	1.244600
C	-1.105300	9.973600	-4.463800
O	-0.819400	9.788400	-5.862700
H	-0.852800	8.831900	-6.032700
C	-1.419100	11.457100	-4.237500
H	-3.529100	6.768300	0.668400
C	3.783000	9.223300	-5.558300
C	5.017100	8.320400	-5.897900
C	4.537400	6.934000	-6.417800
C	4.431300	5.814000	-5.358200
N	3.514200	6.172500	-4.212300
H	2.571300	6.472000	-4.511500
H	3.959700	6.911900	-3.622000
H	3.345700	5.365400	-3.581000
H	6.916300	10.559700	-1.813100
H	7.269000	8.799800	-1.694400

H	5.144100	-2.276600	-4.258600
H	-2.283800	11.747900	-4.865300
H	-0.561500	12.094600	-4.511800
H	5.403200	-2.129200	-2.490300
H	-7.107400	5.309500	-2.761500
H	-1.673300	11.633800	-3.172600
H	-4.895200	5.746300	-3.738700
H	6.749200	-1.777900	-3.602000
H	2.894500	8.579000	-5.444500
H	-3.011500	7.525700	3.011200
H	0.124000	4.821500	-0.300000
H	6.050800	9.529000	-0.625900
H	5.690900	8.210000	-5.031200
H	-4.524000	6.721400	3.565400
H	5.414400	5.582300	-4.910700
H	4.034900	4.890500	-5.826700
H	-2.487900	5.412200	4.048900
H	5.605300	8.819900	-6.695300
H	-2.560300	4.172100	0.400300
H	0.100500	6.584200	0.114000
H	5.243300	6.540200	-7.182700
H	-3.656200	1.986100	2.336800
H	-3.967200	3.683800	3.942900
H	-2.026400	5.321000	2.346300
H	3.592200	9.842400	-6.457800
H	-2.070600	2.784200	2.479700
H	1.703200	1.899300	-4.761700
H	3.758700	11.243400	-4.720900
H	0.029100	9.996200	-2.585500
H	0.285700	0.864100	-4.376000
H	-1.781000	-1.079300	-0.361200
H	-4.429400	4.018200	-3.653700
H	-6.693100	3.589900	-2.426600
H	-0.429700	5.461200	-2.752400
H	3.559700	7.034400	-6.936100
H	-4.795000	4.278800	2.513200
H	-1.996200	9.379300	-4.163300
H	5.673100	0.331000	-2.664900
S	-6.979000	3.986200	-4.810800
C	-8.722800	3.546500	-4.596700
H	-9.279300	4.409300	-4.191100
H	-8.834800	2.674200	-3.929600
H	-9.125600	3.307300	-5.598600
H	1.203400	-0.519400	-2.754500
S	-0.386402	3.226798	-4.146322
Cu	-2.315325	3.222879	-2.804031

N	-3.228500	1.460200	-3.194400
C	-4.431800	1.293000	-3.741000
N	-4.764200	-0.016600	-3.769400
C	-3.742300	-0.734300	-3.197500
C	-2.781700	0.183000	-2.856500
C	-1.188902	2.878698	-5.737922
H	-5.633400	-0.389400	-4.137600
H	-3.745600	-1.818700	-3.115000
H	-5.103200	2.054700	-4.128000
H	-2.119102	2.316998	-5.562522
H	-1.396102	3.838098	-6.247422
H	-0.513602	2.295598	-6.395322
O	-1.515372	3.828084	-9.642561
H	-0.614072	3.745266	-9.962561
O	-2.058489	-1.117360	-7.717817
H	-2.437417	-0.295403	-8.037817
O	-2.878347	-4.864027	-5.320364
H	-1.977047	-4.946845	-5.640364
O	1.379887	0.062627	2.590676
H	2.281187	-0.020191	2.270676
O	3.301311	6.081125	2.185662
H	4.202611	5.998308	1.865662
H	2.922384	6.903083	1.865662
O	8.115201	4.422624	-4.384505
H	7.736274	5.244581	-4.704505
H	-2.058489	-1.117360	-6.757817
H	-3.400719	-5.603167	-5.640364
H	0.857515	-0.676512	2.270676
H	-2.037744	3.088944	-9.962561
H	8.115201	4.422624	-3.424505