Quantum mechanical calculations suggest that lytic polysaccharide monooxygenases employ a copper-oxyl, oxygen-rebound mechanism

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Supporting Information

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Details of computational methods

The enzyme active site model (ASM) was taken from the recently solved *T. aurantiacus* LPMO structure (PDB 2YET) from Quinlan *et al.* (1). For the calculations presented in Figures 1-3 in the main text, we included the N-terminal N-methylation on the histidine residue.

To examine the hypothesized LPMO reaction mechanisms with DFT calculations, we employed a truncated model of the enzyme and polymeric cellulose substrate. The application of such cluster, or "theozyme", models has been successfully applied in the study of many biochemical transformations (2-11). In the LPMO ASM used here, the positions of α- and β-carbons of the active site amino acid residues were fixed during geometry optimizations to mimic the scaffold provided by the extended protein structure, while rest of the ASM is fully optimized.

To select the optimal ASM model, we examined smaller and larger models in terms of additional residues (including His1, Phe43, Trp82, His86, His164, Gln174, and Tyr175) using DFT geometry optimizations with a Cu(II) oxidation state. All DFT geometry optimized ASM models were superimposed with the experimental structure (2YET) to select the best ASM model based on the shape and electronic properties of the metal binding site (for example, bond distances, angles, dihedral angles, RMSD, Cu NPA charge, and coordination geometry). The results from this ASM screening process are shown in Fig. S1. The average RMSD values are well within the accepted range for theozyme models of 0.64 Å in terms of their ability to reproduce the crystal structure geometry (9).

For the initial O_2 binding to the ASM model, we initially constructed **[Cu(II)]-O-O·** complex by varying the O1W-Cu-O1-O2 dihedral angle in 30° increments for both end-on (η^1) and side-on (η^2) configurations. The initial and optimized structures are shown in Fig. S2. The results clearly predict that the initial conformation of O_2 is end-on (η^1).

The enzyme-substrate starting geometries were taken from molecular dynamics (MD) simulations of a similar fungal LPMO on cellulose and the perpendicular distance between the flat faces of the enzyme and substrate was kept fixed while moving the enzyme in the parallel plane for optimal oxidative attack geometries (12). Restraints were placed on selected carbons (C2 and C5 for both glucosyl units and C4 of non-reducing end and C1 of reducing end units, respectively) to maintain the cellobiose geometry to mimic the cellulose surface. We tested three enzyme-substrate complexes each for C1 and C4 oxidation by translating the **[Cu(II)]-O-O·** system along the cellulose chain at average separation distances from MD simulations wherein the oxygen could attack the C1 or C4 hydrogen. We applied the same procedure to two enzyme-substrate complexes for the **[Cu(II)]-O·** for both C1 and C4 attack. We chose only two conformations for the **[Cu(II)]-O·** system because this system did not exhibit as many configurations that would enable productive enzyme-substrate complexes.

All DFT calculations were performed with Gaussian09 (13). All geometry optimizations were conducted using the hybrid GGA B3LYP functional in the spin-unrestricted Kohn-Sham approach, with the 6-31G(d) basis set for all atoms. This functional is routinely used to study copper-oxygen complexes (14-17). Single point energies were computed with the 6-311++G(d,p) basis set and the B3LYP functional, which shows that the differences in the overall barriers between the mechanisms studied here are reasonably similar. Cu(I) complexes generate open shell singlet or triplet products due to the addition of triplet molecular oxygen, and therefore standard Kohn-Sham DFT is not directly applicable (18-21). We apply the Yamaguchi broken-spin-symmetry (BS) procedure (22, 23) to compute the energy of the spin-purified low-spin (LS) state (24) as:

$$ {}^{LS}E = \frac{{}^{BS}E({}^{HS}\langle S^2\rangle - {}^{LS}\langle S^2\rangle) - {}^{HS}E({}^{BS}\langle S^2\rangle - {}^{LS}\langle S^2\rangle)}{{}^{HS}\langle S^2\rangle - {}^{BS}\langle S^2\rangle} $$

$$ = \frac{E(UB3LYP_{singlet})({}^{HS}\langle S^2\rangle - 0) - E(UB3LYP_{triplet})({}^{BS}\langle S^2\rangle - 0)}{{}^{HS}\langle S^2\rangle - {}^{BS}\langle S^2\rangle} $$

where $^{HS}\langle S^2\rangle$ and $^{BS}\langle S^2\rangle$ are the total spin operator of high-spin coupled state (triplet for our case) and broken-spin-symmetry state (open shell singlet for our case), respectively. $^{LS}\langle S^2\rangle$ applied to 0 in this case assuming the closed shell singlet state.

We calculated two possible spin states (open-shell singlet and triplet) for all of the biradical species. The energy of spin-purified LS state and triplet state were compared and we report the lower energy species in the main text.

The local meta-GGA M06-L functional of Truhlar was also applied to the LPMO mechanisms. M06-L was chosen for its inclusion of medium-range correlation effects through the incorporation of a kinetic energy density term. We performed full geometry optimizations and compared these results against those obtained with the B3LYP functional. As can be seen in Fig S6, the computed activation barriers still clearly favor the second mechanism and so our conclusions remain unchanged regardless of the two functionals used.

Reported harmonic vibrational frequencies were calculated at the same level of theory as the geometry optimizations. A fine grid density was used for numerical integration in all DFT calculations. Harmonic vibrational frequencies were computed for all optimized structures to verify that they were either minima or transition structures, possessing zero imaginary frequencies or one imaginary frequency, respectively (see further details on how transition states were located directly below). A conductor-like polarizable continuum model (CPCM) (25, 26) with dielectric constant ε=4.3 was present in all our calculations to mimic the effect of the hydrophobic protein interior on electrostatic interactions. Liao and Thiel have recently shown such an approach yields acceptable results in the acetylene hydratase system (27). All reaction energetics were reported as changes in ΔE due to imposing Cartesian constraints. All the atomic charges were obtained from Natural Population Analysis (NPA) using NBO 6.0. Also, two- and three- body DFT-D3 corrections with zero-damping, developed by Grimme (28) have been included to compare the effects of dispersion on the energetics obtained with the uncorrected DFT results shown in Fig. S11.

All transition state structures were located as first order saddle points on the potential energy surface using the Berny algorithm within Gaussian09 (29). Preliminary adiabatic scans along interatomic coordinates were performed to obtain input structures with which to perform each transition state search. In computations with active site models (ASMs), Cartesian restraints are necessary to mimic the effect of the larger protein backbone and thus were applied to the Cα/β of the active site residues to fix these atoms in their crystallographic positions. The positions of remaining atoms were fully optimized to a transition state. Transition state structures were verified by the presence of an imaginary frequency corresponding to the reaction coordinate of interest.

In general it is not possible to follow the intrinsic reaction coordinate (IRC) for theozyme/active site model calculations since the Cartesian constraints required to maintain a realistic model of the active site are not tolerated by the implementation of IRC following in Gaussian09. We thus displaced each transition state by a small fraction (0.2) of the imaginary normal mode vibration and performed geometry optimizations (30, 31), which in each case confirmed the transition state connected the energy minima as depicted in each of the reaction coordinates shown.

To examine the effect of the *N*-methylated *N*-terminal histidine residue, we performed full DFT optimizations for both mechanisms without methylation of *N*-terminal histidine. The reaction coordinates obtained for both ASMs are within 1 kcal/mol of each other (the demethylated residue has a slightly higher barrier). However, this result lies within the uncertainty of the level of theory and so does not conclusively demonstrate a difference in catalytic proficiency.

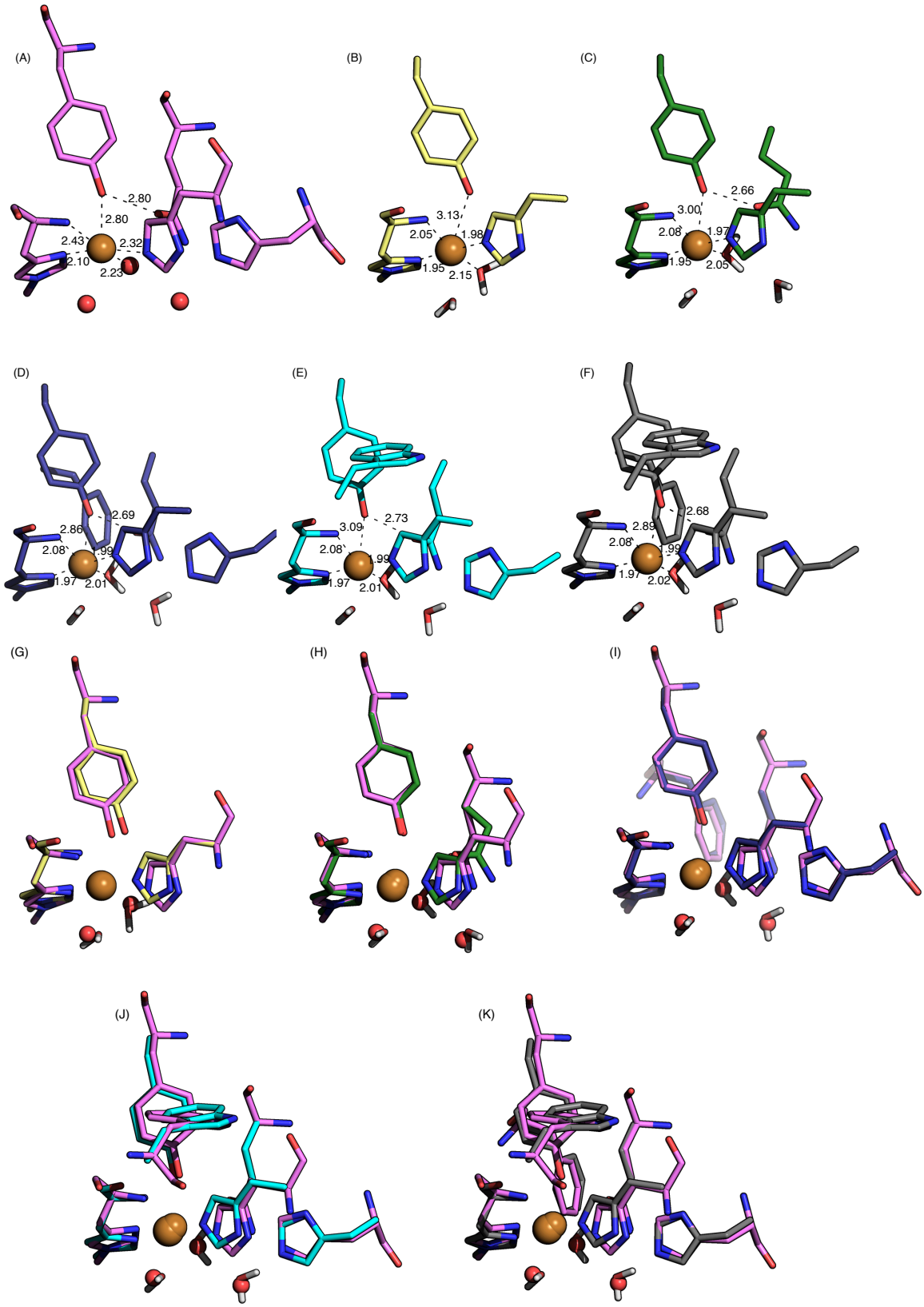


Figure S1. All tested ASM models (A) Detailed view of the LPMO active site (from 2YET crystal structure, pink stick). The DFT optimized structure of initial resting state (Cu(II)) with (B) model1: His1, His86, and Tyr175 in yellow stick, (C) model2: His1, His86, Tyr175, and Gln 173 in green stick, (D) model3: His1, His86,

Tyr175, Gln 173, His164 and Phe43 in purple stick, (E) model4: His1, His86, Tyr175, Gln 173, His164 and Trp82 in light blue stick, and (F) model5: His1, His86, Tyr175, Gln 173, His164, Phe43, and Trp82 in grey stick. Superimposed structures of experimental structure (2YET, pink stick) and the DFT optimized ASMs: (G) model1, (H) model2, (I) model3, (J) model4, (K) model5.

Table S1. Key bond distances, dihedral angle, Cu charge from NPA, and RMSD of the three different ASM models.

	2YET	**[Cu(II)]**[a]	**[Cu(II)]**-sm1[b]	**[Cu(II)]**-sm2[c]
Cu-Nδ (His1) (Å)	2.10	1.97	1.95	1.96
Cu-N (His1) (Å)	2.43	2.08	2.08	2.05
Cu-Nε (His86) (Å)	2.32	1.99	1.97	1.98
χ_3 (Gln173) (°)	7.1	5.4	-33.9	N/A
Cu-O(Tyr175) (Å)	2.80	3.08	3.00	3.13
Cu charge[d]	N/A	1.48	1.48	1.47
RMSD (Å)[e]	N/A	0.37	0.43	0.45

[a] His1, His86, Tyr175, Gln173, His164 (Fig. 1(C))
[b] model2: His1, His86, Tyr175, Gln173 (Fig. S1(C))
[c] model1: His1, His86, Tyr175 (Fig. S1(B))
[d] NPA charges (e)
[e] RMSD was calculated only with heavy atoms based on 2YET.

To find the optimal ASM model, we examined slightly smaller and larger models in terms of additional residues using DFT calculations. In Fig. S1, we show smaller and larger ASM models superimposed onto the experimental structure (2YET). The RMSD increases to 0.45 Å in the smaller system (model1) as shown in Fig. S1 (B) and S1 (G), showing Tyr175 moves more from Cu(II) center compared to the experimental structure. When we include Gln173 (model2, Fig. S1 (C) and S1 (H)), dihedral angle χ_3 of Gln173 is -33.9 ° (while 7.1° from 2YET) and results 0.43 Å RMSD. Bigger ASM models show RMSD 0.35 (model3), 0.51 (model4) and 0.53 (model5) Å while our target ASM model is 0.37 Å.

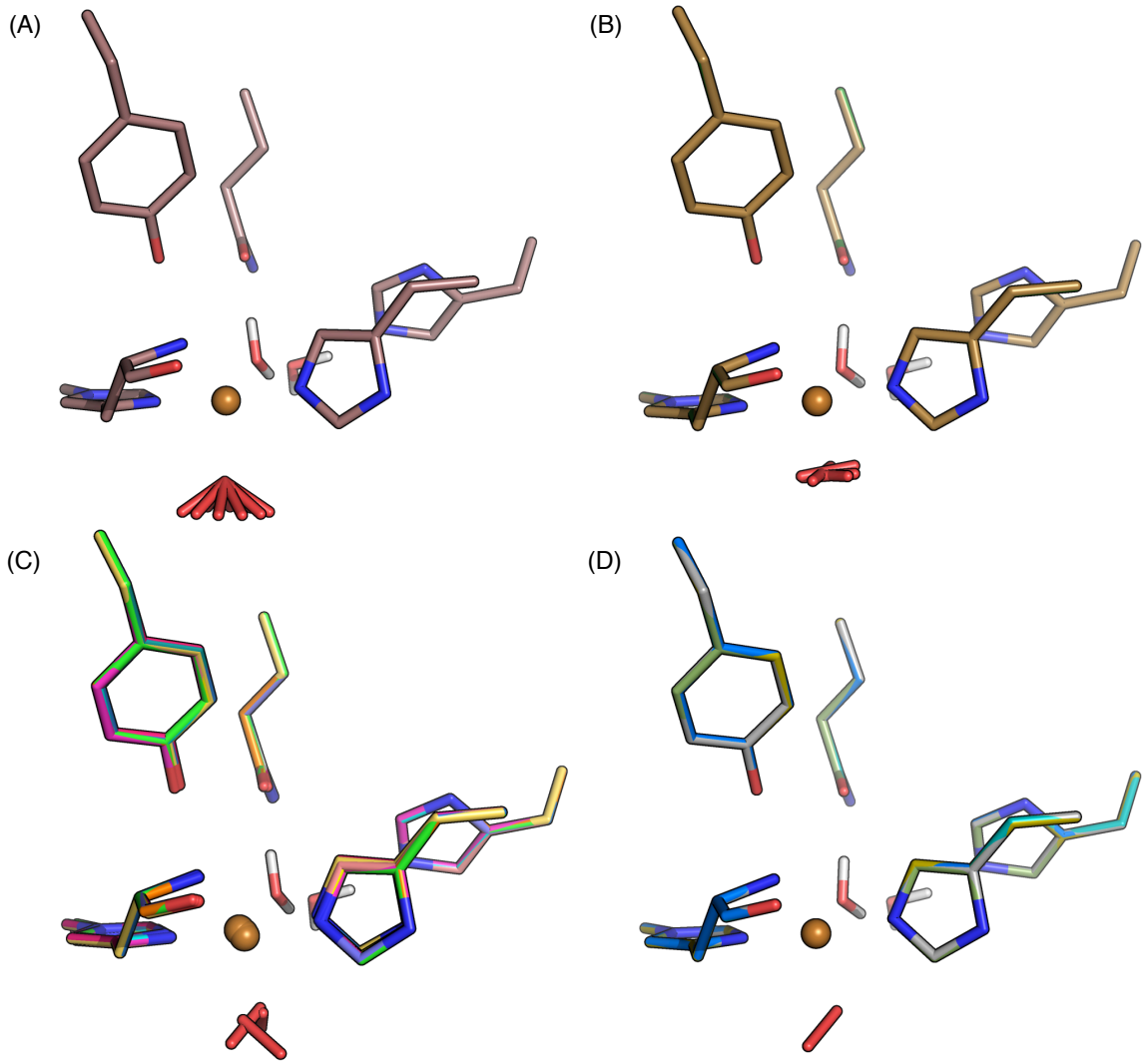


Figure S2. The initial and B3LYP optimized **[Cu(II)]-O-O·** end-on and side-on configurations. Superimposed (A) end-on initial structures, (B) side-on initial structures, (C) end-on B3LYP optimized configurations, and (D) side-on UB3LYP optimized configurations.

To build the initial O_2 enzyme-bound species, we examined O_2 binding to reduced state **[Cu(I)]** to form a (**[Cu(II)]-O-O·**) complex by rotating the O1W-Cu-O1-O2 dihedral angle in 30° increments for both end-on (η^1) and side-on (η^2) configurations and in both singlet and triplet states. All initial end-on/side-on configurations are shown in Fig. S2 (A) and Fig. S2 (B), respectively and the final end-on/side-on configurations that exhibit no steric clashes after the optimizations are shown in Fig. S2 (B) and Fig. S2 (D), respectively. All side-on configurations shifted to one end-on configuration after the DFT optimizations as shown in Fig. S2 (D). We selected the most stable optimized structure (Fig. 1(E)) among the 4 different optimized end-on configurations (Fig. S2 (B) and (D)) from both end-on and side-on initial configurations.

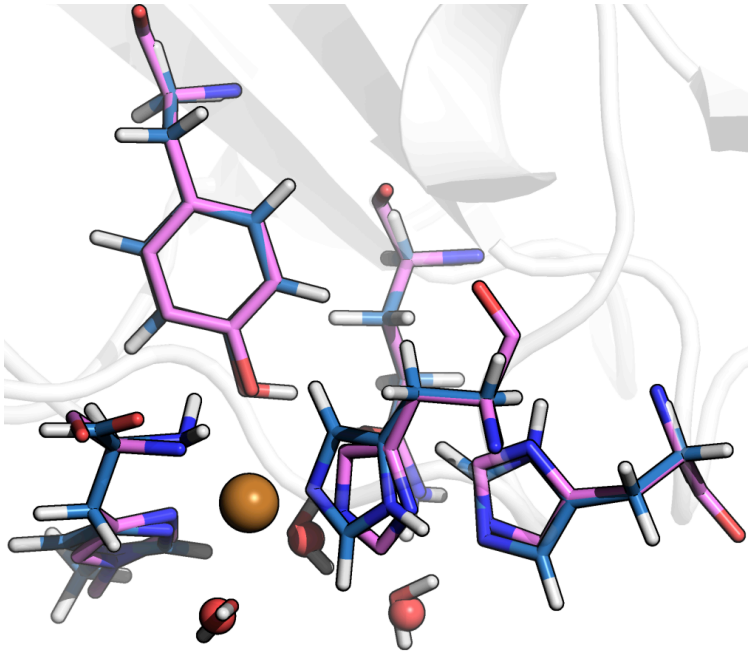


Figure S3. ASM with all hydrogen atoms shown.

Table S2. Calculated spin densities, NPA charges, and bond distances of singlet and triplet **[Cu(II)]-O-O·** complex.

	Spin density		Charge	
	Singlet	Triplet	Singlet	Triplet
Cu	0.66	0.60	1.33	1.38
O1	-0.27	0.59	-0.36	-0.40
O2	-0.54	0.67	-0.31	-0.27

Bond distances (Å)	Singlet	Triplet
Cu-O1	1.96	1.96
O1-O2	1.32	1.31

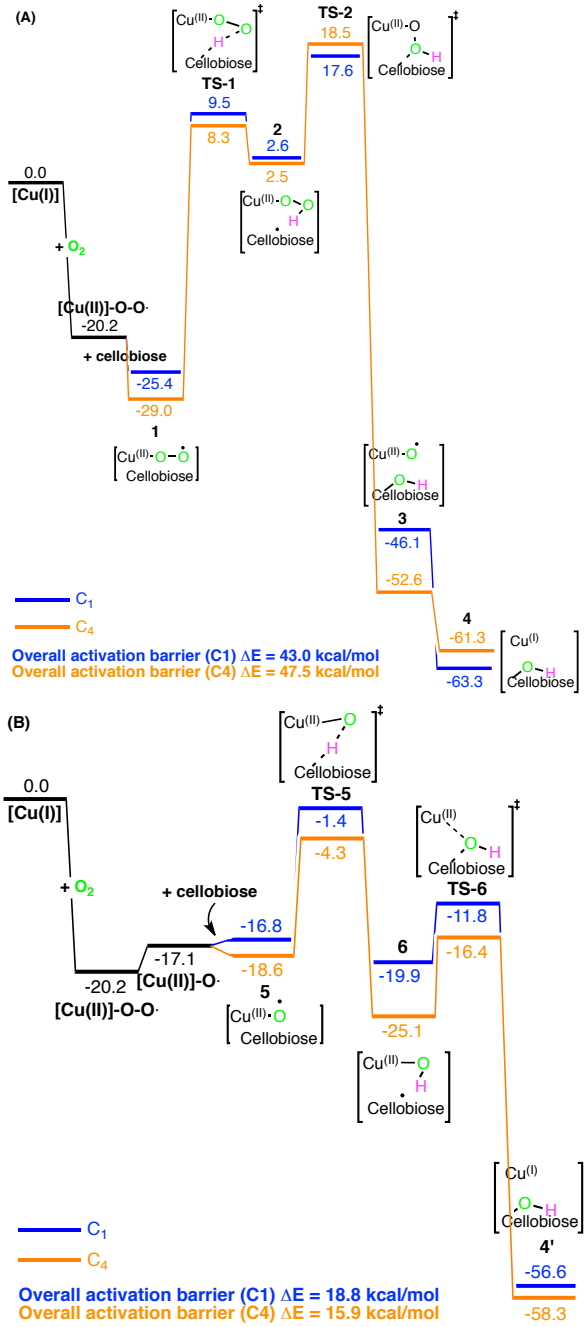


Figure S4. The energy diagram for the oxidative mechanism using (A) **[Cu(II)]-O-O·** ROS and (B) **[Cu(II)]-O·** ROS at C1 (in blue) and C4 (in orange) carbons. Energies are calculated with UB3LYP/6-31G(d) in kcal/mol.

We computed both oxidative mechanisms at the C1 and C4 carbons as shown in Fig. S4. Computed UB3LYP energy of rate-limiting is 43.0 and 47.5 kcal/mol using a **[Cu(II)]-O-O·** ROS, and 18.8 and 15.9 kcal/mol for the **[Cu(II)]-O·** at C1 and C4 carbons, respectively. The difference of energy barriers for C1 and C4 carbons lie within 4.5 and 2.0 kcal/mol for **[Cu(II)]-O-O·** and **[Cu(II)]-O·** ROS, respectively.

Table S3. UB3LYP/6-31G(d) energies (kcal/mol) of the oxidative mechanism using **[Cu(II)]-O-O·** ROS using 3 different substrate positions at C1 and C4 carbon positions.

C1	Test1	Test2	Test3
1	-25.4	-22.9	-21.7
TS-1	9.5	11.4	15.1
2	2.6	5.5	7.6
TS-2	17.6	19.5	20.7
3	-46.1	-38.7	-51.8
Overall barrier	43.0	42.4	42.4

C4	Test4	Test5	Test6
1	-29.0	-29.2	-22.1
TS-1	8.3	9.6	15.8
2	2.5	2.1	7.6
TS-2	18.5	18.6	24.1
3	-52.6	-45.6	-49.7
Overall barrier	47.5	47.8	46.2

Test1 (C1) and Test4 (C4) were selected for our present study.

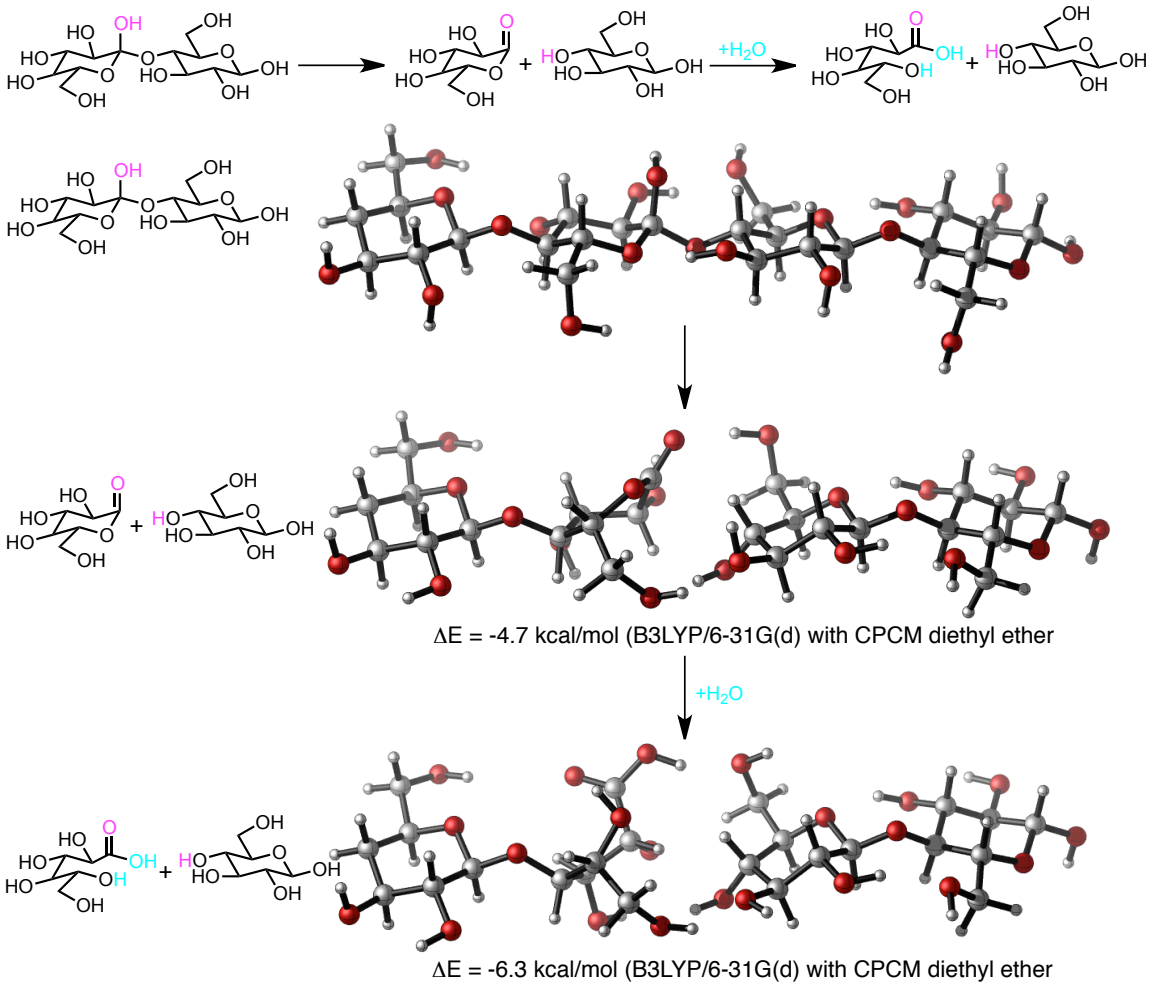


Figure S5. Cleavage of glycosidic bond from hydroxylated cellobiose via elimination and hydrolysis reactions.

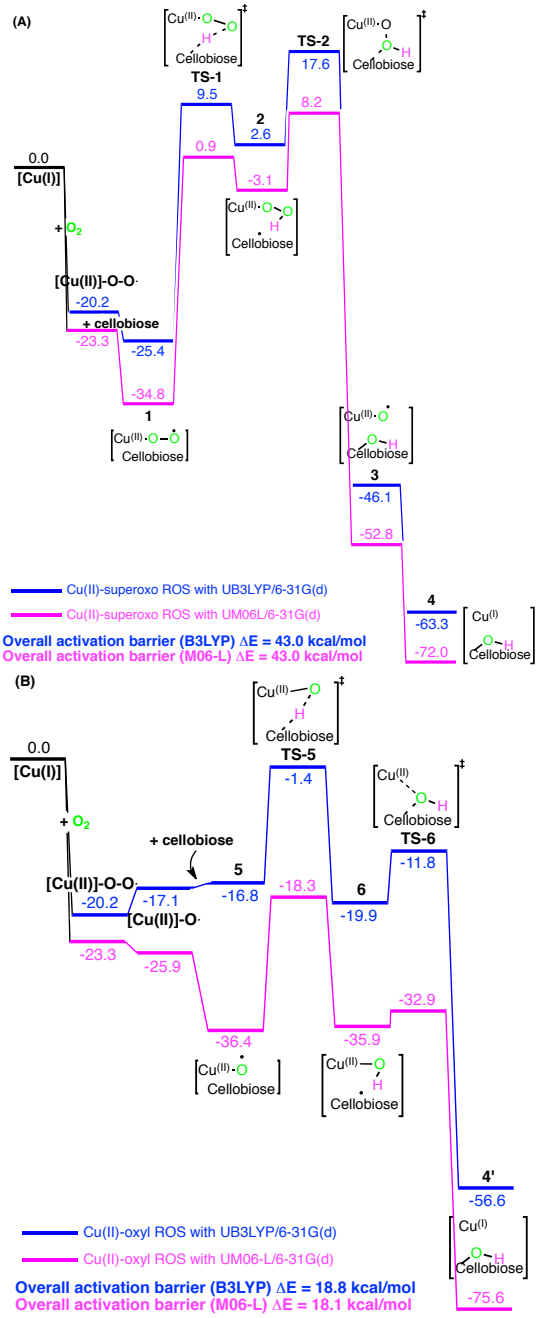


Figure S6. The energy diagram for the oxidative mechanism using (A) **[Cu(II)]-O-O·** ROS and (B) **[Cu(II)]-O·** ROS at C1 carbon using full optimizations of UB3LYP/6-31G(d) (in blue) and UM06-L/6-31G(d) (in pink) in kcal/mol.

We repeated the entire catalytic cycles with full optimizations of UM06-L functional to fully explore the effects that choice of functional has on the shape of the energy diagram for both mechanisms as described in Fig. S6. Overall, key rate limiting step (**TS-2**) to the overall rate and intermediates (**1**) are predicted same for both functionals in the **[Cu(II)]-O-O·** ROS mechanisms (shown in Figure S6 (A)). They have also same overall activation barrier (43.0 kcal/mol) for both UB3LYP and UM06-L functionals with the **[Cu(II)]-O-O·** ROS. The **[Cu(II)]-O·** ROS mechanism showed that C-H abstraction (**TS-5**) is rate-limiting

and shows 18.8 (UB3LYP) and 18.1 kcal/mol (UM06-L) above the relevant ROS, which is within 0.7 kcal/mol, so the barrier of the catalytic cycle is essentially unchanged.

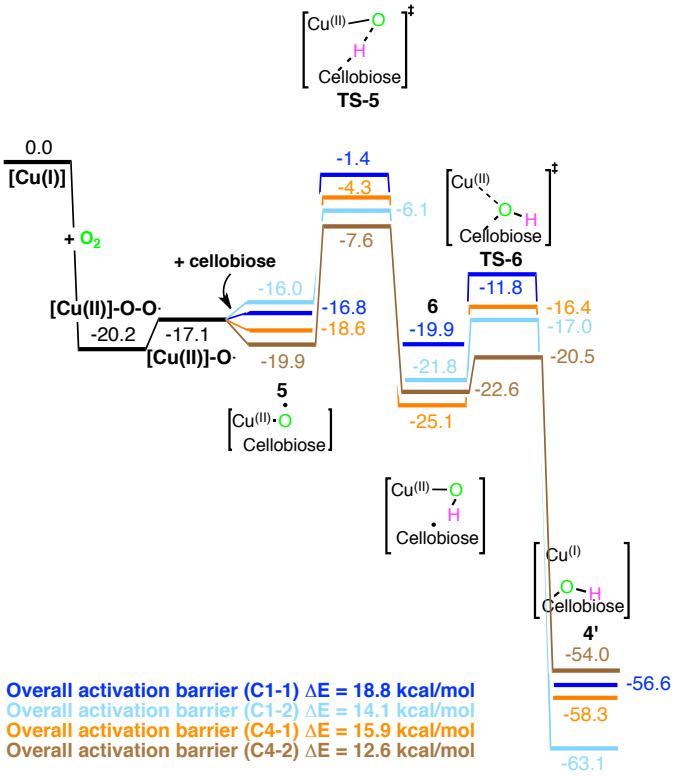


Figure S7. The energy diagram for the oxidative mechanism using **[Cu(II)]-O·** ROS using 2 different substrate positions at C1 and C4 carbon positions.

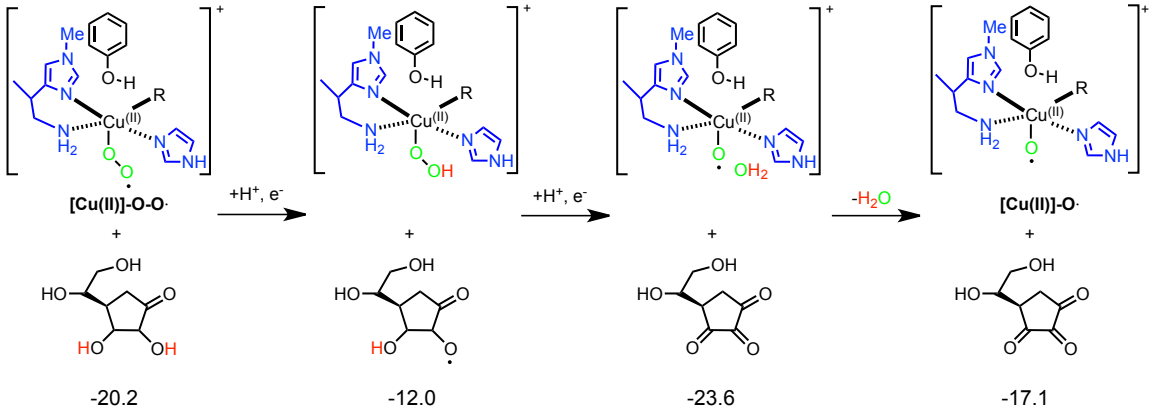


Figure S8. The computed thermodynamics of the hydrogen atom transfer from **[Cu(II)]-O-O·** ROS to **[Cu(II)]-O·** ROS using ascorbic acid. Energies are calculated with B3LYP/6-31G(d) in kcal/mol.

Table S4. Selected UB3LYP/6-31G(d) computed structural parameters and NPA charges and spin densities[a] for the reactants, intermediates, transition states and products for the **[Cu(II)]-O-O·** ROS mechanism.

Charges (spin densities)	^{1}**[Cu(II)]O-O·**	^{3}**[Cu(II)]O-O·**	^{1}**1**	^{3}**1**	^{1}**TS-1**	^{3}**TS-1**	^{1}**2**	^{3}**2**	^{1}**TS-2**	^{3}**TS-2**	^{1}**3**	^{3}**3**	^{1}**4**
Cu	1.326 (0.662)	1.376 (0.597)	1.343 (-0.682)	1.340 (0.636)	1.329 (-0.685)	1.433 (0.680)	1.324 (-0.708)	1.452 (0.707)	1.305 (-0.690)	1.442 (0.698)	1.443 (-0.678)	1.413 (0.685)	0.915
O1	-0.364 (-0.273)	-0.399 (0.594)	-0.362 (0.296)	-0.397 (0.591)	-0.508 (-0.042)	-0.597 (0.266)	-0.613 (-0.149)	-0.667 (0.146)	-0.723 (0.242)	-0.700 (0.579)	-0.837 (0.774)	-0.695 (1.133)	N/A
O2	-0.312 (-0.545)	-0.268 (0.671)	-0.321 (0.537)	-0.285 (0.637)	-0.427 (0.272)	-0.437 (0.310)	-0.526 (0.021)	-0.544 (0.028)	-0.657 (-0.128)	-0.634 (-0.150)	-0.795 (0.003)	-0.795 (0.001)	N/A
Nδ	-0.630 (0.052)	-0.643 (0.048)	-0.626 (-0.055)	-0.645 (0.054)	-0.625 (-0.052)	-0.641 (0.051)	-0.618 (-0.053)	-0.636 (0.053)	-0.625 (-0.049)	-0.642 (0.049)	-0.607 (-0.053)	-0.646 (0.069)	-0.659
N	-0.982 (0.048)	-0.990 (0.040)	-0.991 (-0.019)	-0.991 (0.012)	-0.982 (-0.015)	-0.984 (0.018)	-0.977 (-0.010)	-0.984 (0.010)	-0.972 (0.002)	-0.979 (0.007)	-0.970 (0.014)	-0.945 (-0.001)	-0.986
Nε	-0.634 (0.049)	-0.648 (0.048)	-0.629 (-0.053)	-0.647 (0.055)	-0.636 (-0.053)	-0.652 (-0.051)	-0.631 (-0.056)	-0.649 (0.056)	-0.622 (-0.058)	-0.641 (0.055)	-0.616 (-0.062)	-0.635 (0.076)	-0.656
Bond distances (Å)													
Cu-O1	1.96	1.96	1.97	1.97	1.94	1.95	1.91	1.91	1.90	1.90	1.84	1.81	N/A
O1-O2	1.32	1.31	1.32	1.32	1.42	1.41	1.47	1.47	1.70	1.70	N/A	N/A	N/A
Cu- Nδ (His1)	1.98	1.98	1.97	1.97	1.98	1.98	1.99	1.99	2.00	1.99	2.01	2.00	1.90
Cu-N (His1)	2.16	2.18	2.26	2.29	2.37	2.37	2.36	2.36	2.44	2.42	2.42	2.78	2.20
Cu- Nε (His86)	1.98	1.98	1.97	1.97	1.97	1.97	1.97	1.97	1.97	1.98	2.02	2.03	1.93
Cu-O1W	2.30	2.33	2.12	2.13	2.17	2.19	2.14	2.14	2.15	2.16	2.04	2.01	2.21
Cu-O (Tyr)	3.80	3.83	4.02	4.05	4.19	4.22	4.17	4.17	4.33	4.35	4.09	4.13	4.17
Coordination Geom./Num.	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	T/4

[a]The values in parentheses are spin densities

$^{1/3}$ superscript 1 and 3 refer singlet and triplet spin states, respectively

Table S5. Selected UB3LYP/6-31G(d) computed structural parameters and NPA charges and spin densities[a] for the reactants, intermediates, transition states and products for the **[Cu(II)]-O·** ROS mechanism.

Charges (spin densities)	^{1}**[Cu(II)]O·**	^{3}**[Cu(II)]O·**	^{1}**5**	^{3}**5**	^{1}**TS-5**	^{3}**TS-5**	^{1}**6**	^{3}**6**	^{1}**TS-6**	^{1}**4'**
Cu	1.443 (-0.695)	1.450 (0.729)	1.471 (0.692)	1.469 (0.735)	1.377 (-0.660)	1.460 (0.730)	1.326 (-0.732)	1.468 (0.732)	1.075 (-0.318)	0.918
O1	-0.888 (0.827)	-0.760 (1.091)	-0.911 (-0.790)	-0.754 (1.021)	-0.951 (0.421)	-0.974 (0.635)	-1.113 (-0.087)	-1.160 (0.118)	-0.945 (-0.124)	N/A
Nδ	-0.601 (-0.051)	-0.627 (0.061)	-0.618 (0.064)	-0.645 (0.068)	-0.641 (-0.045)	-0.660 (0.046)	-0.624 (-0.055)	-0.643 (0.055)	-0.667 (-0.024)	-0.678
N	-0.978 (-0.001)	-0.983 (0.022)	-0.983 (-0.002)	-0.979 (0.015)	-0.980 (-0.037)	-0.984 (0.059)	-0.978 (-0.004)	-0.983 (0.004)	-0.983 (-0.021)	-0.996
Nε	-0.607 (-0.056)	-0.634 (0.070)	-0.598 (0.057)	-0.637 (0.072)	-0.601 (-0.068)	-0.638 (0.078)	-0.621 (-0.065)	-0.641 (0.066)	-0.640 (-0.035)	-0.675
Bond distances (Å)										
Cu-O1	1.84	1.82	1.98	1.88	1.93	1.94	1.92	1.93	2.04	N/A
Cu- Nδ (His1)	2.00	2.01	2.00	1.99	1.99	1.99	2.00	2.00	1.95	1.88
Cu-N (His1)	2.41	2.29	2.33	2.33	2.31	2.23	2.30	2.30	2.24	2.16
Cu- Nε (His86)	2.01	2.00	1.98	1.99	1.92	1.93	1.99	1.99	1.91	1.88
Cu-O1W	2.06	2.12	2.05	2.08	2.26	2.41	2.07	2.07	3.46	3.43
Cu-O (Tyr)	4.57	4.49	4.52	4.43	4.20	4.14	4.58	4.58	4.03	4.11
Coordination Geom./Num.	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	TB/5	T/4

[a]The values in parentheses are spin densities

$^{1/3}$ superscript 1 and 3 refer singlet and triplet spin states, respectively

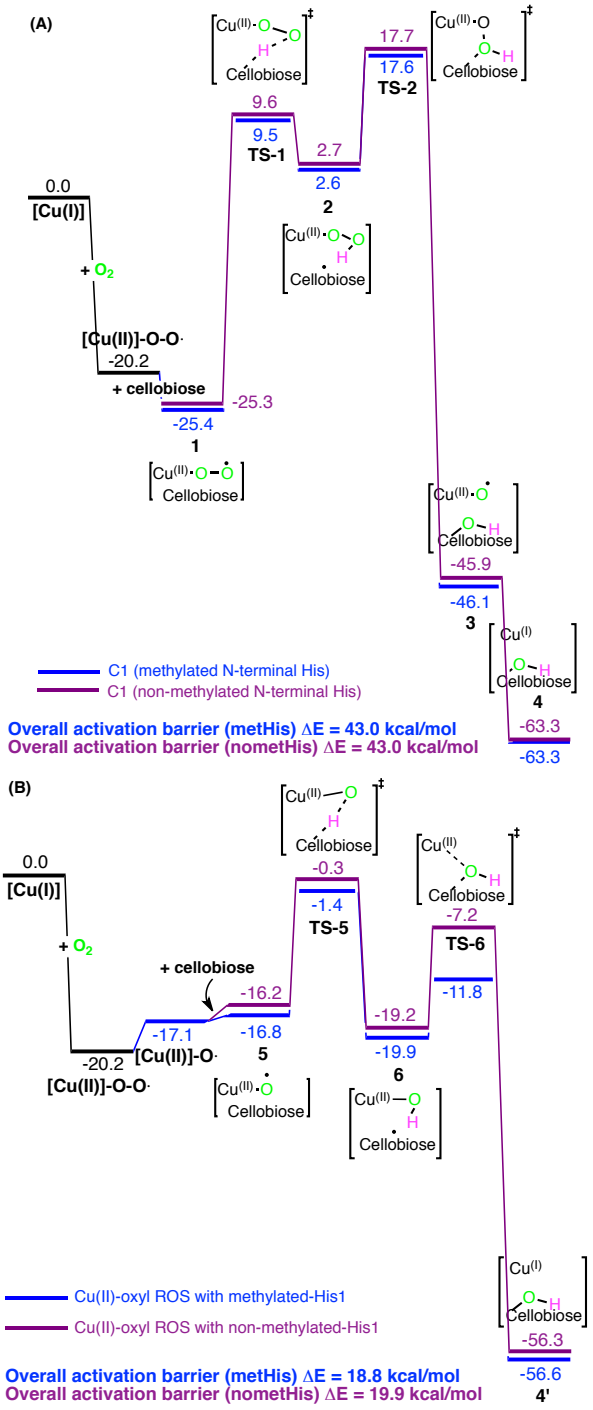
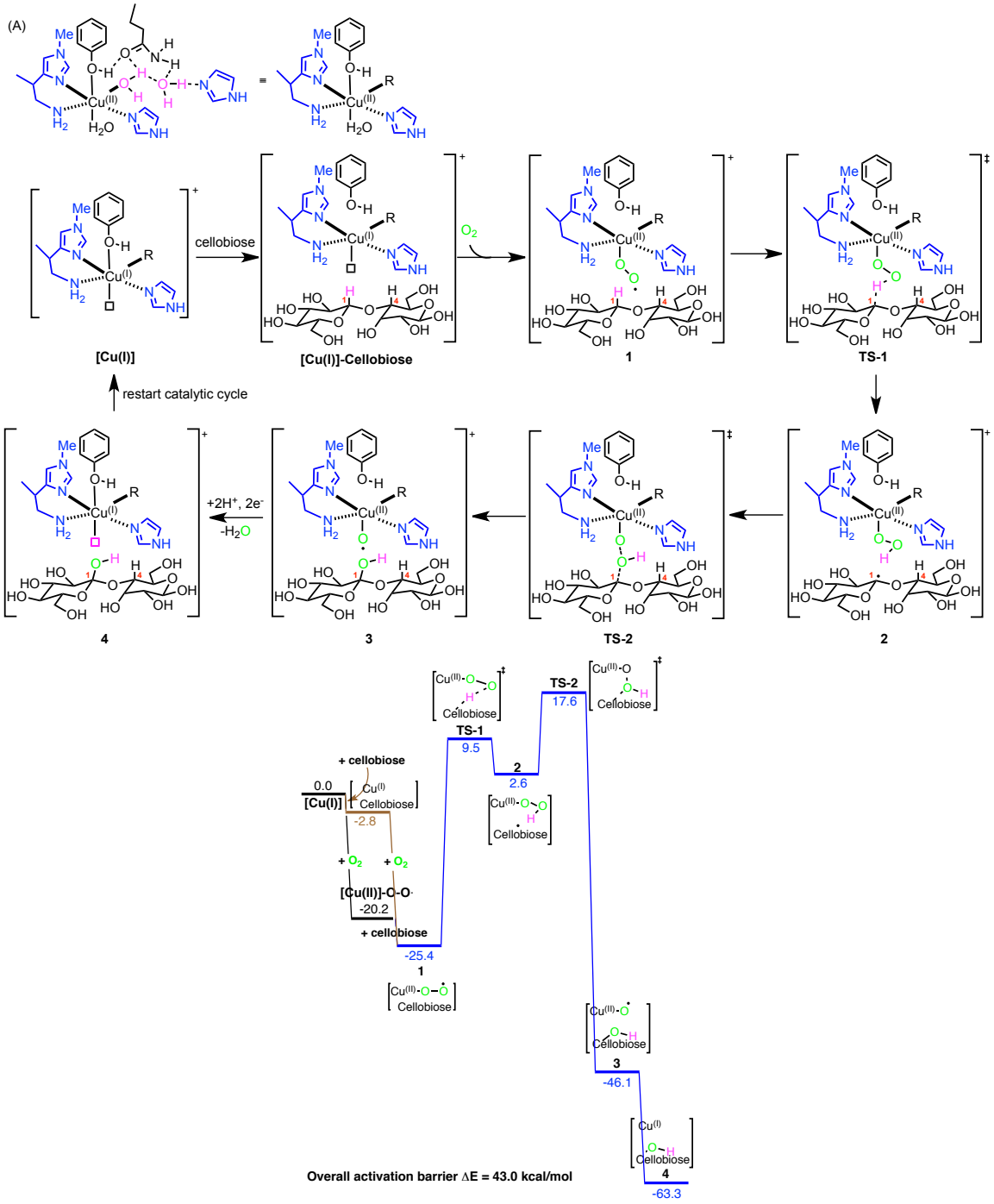


Figure S9. The full optimized energy diagram for the oxidative mechanism using (A) **[Cu(II)]-O-O·** ROS and (B) **[Cu(II)]-O·** ROS at C1 carbon with methylated-His1 (blue) and non-methylated-His1 (purple) using UB3LYP/6-31G(d) in kcal/mol.


(A)
cellobiose
O_2
[Cu(I)]
[Cu(I)]-Cellobiose
1
TS-1
2
TS-2
3
4
restart catalytic cycle
$+2H^+$, $2e^-$
$-H_2O$
+ cellobiose
0.0
[Cu(I)]
-2.8
+ O_2
+ O_2
[Cu(II)]-O-O·
-20.2
+ cellobiose
-25.4
1
TS-1
9.5
2
2.6
TS-2
17.6
3
-46.1
4
-63.3
Overall activation barrier ΔE = 43.0 kcal/mol

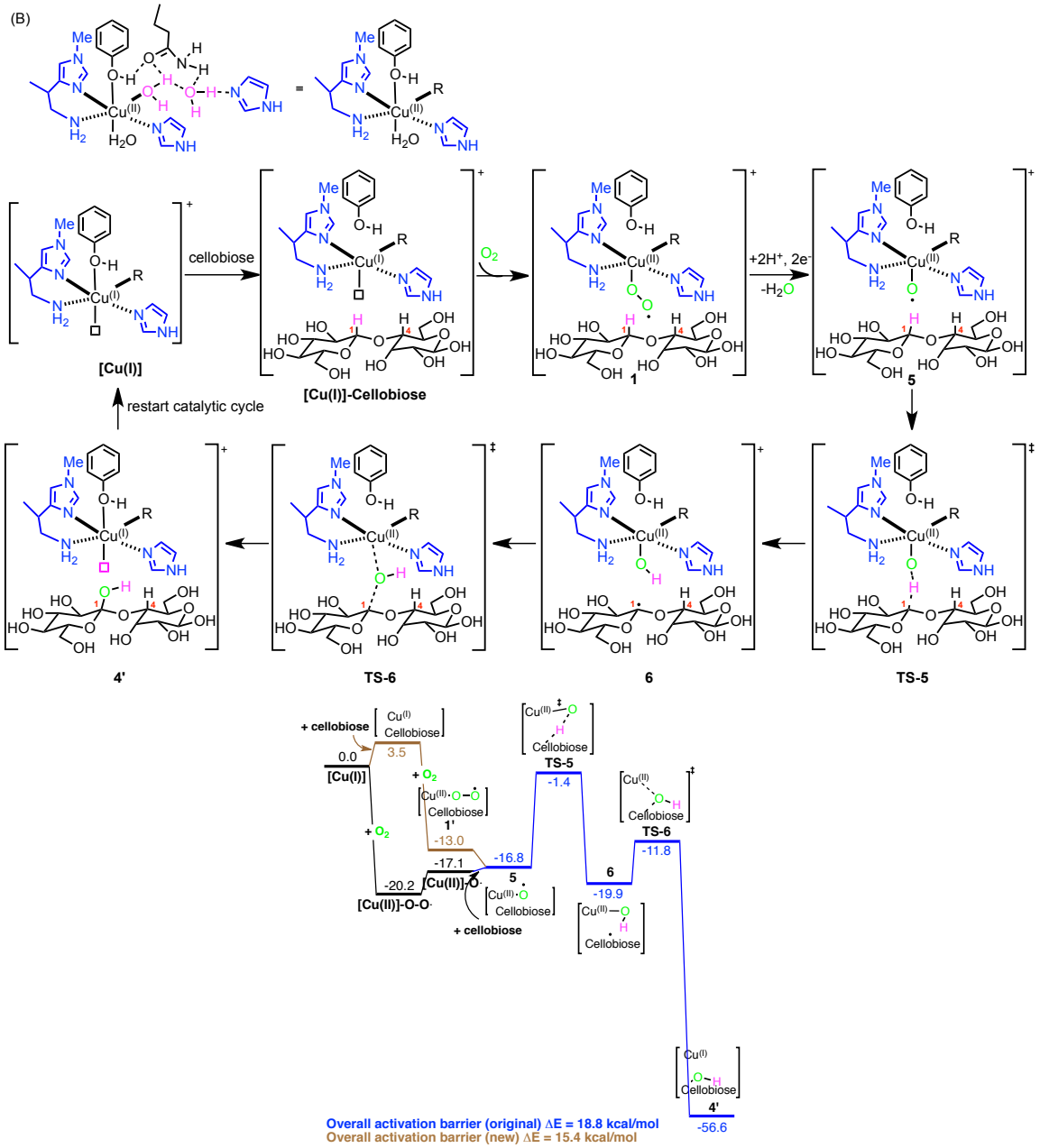


Figure S10. The mechanisms and energy diagrams (in brown color) for the oxidative mechanism using (A) **[Cu(II)]-O-O·** ROS and (B) **[Cu(II)]-O·** ROS at C1 carbons when cellobiose binds first before O_2 binds. Energies are calculated with UB3LYP/6-31G(d) in kcal/mol.

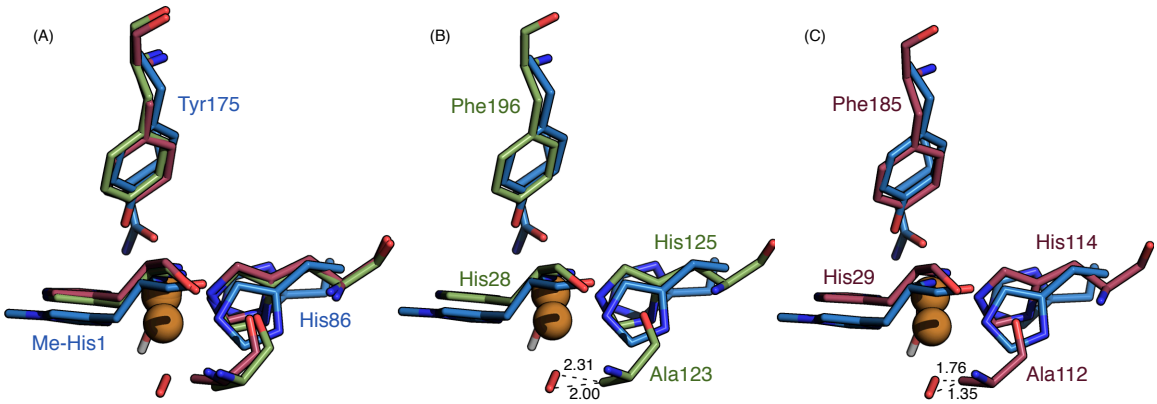
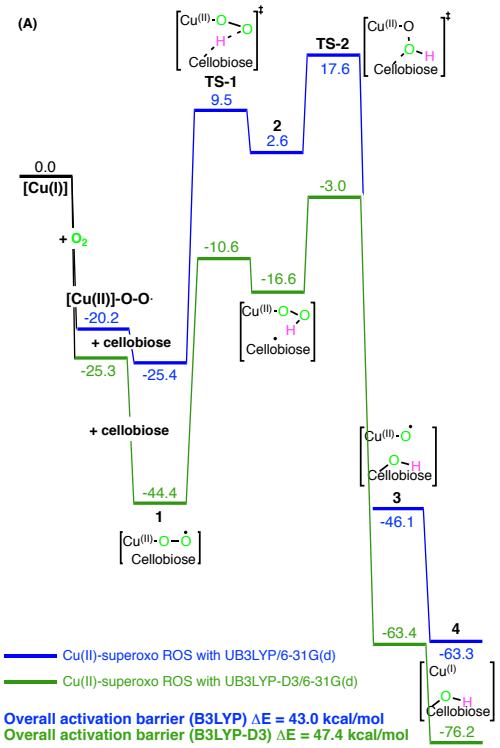


Figure S11. (A) Superimposed structures of CBM33 experimental structures (2YOX: green and 4ALT: purple sticks) and the DFT optimized **[Cu(II)]O-O·** complex structure (blue stick). Bond distances (Å) are shown between oxygen (O1 and O2) from **[Cu(II)]-O-O·** and Cβ from alanine residue of (B) 2YOX and (C) 4ALT.



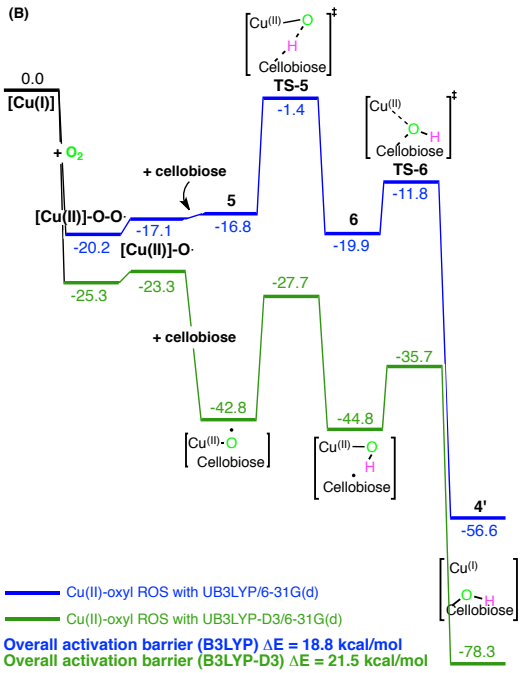


Figure S12. The energy diagram for the oxidative mechanism using (A) **[Cu(II)]-O-O·** ROS and (B) **[Cu(II)]-O·** ROS at C1 carbon using full optimizations of UB3LYP/6-31G(d) (in blue) and UB3LYP-D3/6-31G(d) (in green) in kcal/mol.

Complete Gaussian Reference:

(a) Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

(b) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

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Cartesian Coordinates and Absolute Energies

Unless noted otherwise, all reported values are for UB3LYP/6-31G(d)-optimized geometries as described in the main text. Molecular energies (harmonic) zero-point vibrational energies at 298K obtained with the B3LYP functional is quoted in Hartrees. Vibrational frequencies for all transition states are also reported.

[Cu(I)] singlet

N	1.81830	-1.90841	-1.55151
C	3.22810	-2.25820	-1.28603
C	3.95679	-2.66586	-2.56007
O	3.39595	-2.82439	-3.62451
C	3.34688	-3.37939	-0.26047
C	2.82763	-3.07195	1.10632
C	3.50605	-2.99402	2.29611
N	1.47817	-2.85377	1.33943
C	1.36204	-2.64653	2.64642
N	2.56449	-2.72350	3.26675
C	2.81597	-2.55446	4.69305
C	-4.34332	-0.00760	-4.01151
C	-2.84699	-0.25847	-3.78228
C	-2.40438	-1.31388	-2.82384
C	-1.56685	-1.18178	-1.75212
N	-2.58609	-2.68067	-2.95903
C	-1.86164	-3.30614	-1.99124
N	-1.22413	-2.42175	-1.23648
C	-7.98013	2.14852	-0.39078
C	-7.38993	0.76895	-0.68059
C	-6.09825	0.50047	0.03126
C	-5.77063	-0.33704	1.07055
N	-4.90983	1.14437	-0.27840
C	-3.94160	0.68004	0.55287
N	-4.43100	-0.21958	1.38694
C	-0.44920	5.74191	1.56350
C	-0.53819	4.21229	1.54106
C	-0.11405	3.61618	2.90481
C	-0.30203	2.11522	2.94064
O	0.52890	1.34493	2.40901
C	4.87585	5.65499	-2.31082
C	4.41184	4.35930	-2.98209
C	4.00724	3.32565	-1.94951
C	2.67026	3.16240	-1.56625
C	4.97459	2.57507	-1.26312
C	2.30934	2.31928	-0.51344
C	4.63472	1.73810	-0.20170
C	3.29781	1.63146	0.20329
O	3.00754	0.84752	1.28311
Cu	0.31943	-2.32048	-0.08194
O	-2.42162	-1.05082	3.03321
O	-0.62790	-0.65845	0.98620
H	-8.10150	-0.00737	-0.37839
H	-7.24887	0.64845	-1.76350
H	-6.42045	-1.01743	1.60345
H	-3.26695	-0.85361	2.52564
H	-2.90936	0.99583	0.50541
H	-8.92596	2.28200	-0.92685
H	0.10657	3.80920	0.75409
H	-1.56536	3.90135	1.31072
H	-0.69064	4.09138	3.70675
H	0.94497	3.82858	3.08449
H	0.57218	6.07441	1.78268
H	3.56656	4.57127	-3.64850
H	5.21984	3.96662	-3.61306

H	6.02096	2.66636	-1.54776
H	1.89263	3.71321	-2.09184
H	5.39644	1.18878	0.34440
H	1.26725	2.20109	-0.23078
H	2.13324	1.10752	1.65039
H	5.73850	5.47273	-1.65993
H	1.78771	-0.93530	-1.85952
H	3.73994	-1.37144	-0.88855
H	5.04691	-2.83770	-2.45448
H	2.81437	-4.25786	-0.65371
H	4.40045	-3.67152	-0.17449
H	4.55296	-3.10620	2.53452
H	0.44298	-2.43531	3.17173
H	1.87022	-2.34490	5.19479
H	3.50126	-1.71902	4.85813
H	3.24903	-3.46663	5.11194
H	-4.85292	0.25207	-3.07762
H	-2.38564	0.67416	-3.43696
H	-2.38467	-0.46490	-4.75915
H	-1.19282	-0.27416	-1.30790
H	-3.14797	-3.14661	-3.65875
H	-1.83566	-4.37869	-1.87109
H	-2.60179	-1.83133	3.57923
H	-0.11700	-0.00435	1.51423
H	-1.27131	-1.01997	1.63585
N	-1.41839	1.65343	3.52325
H	-1.67770	0.66157	3.49112
H	-2.08808	2.29800	3.91936
H	-4.78211	1.84168	-0.99944
H	-4.47369	0.81875	-4.71711
H	-4.84629	-0.88662	-4.43098
H	-7.30457	2.95246	-0.70543
H	-8.17454	2.27532	0.67964
H	-0.73869	6.16657	0.59593
H	-1.11130	6.16560	2.32767
H	5.16773	6.40602	-3.05486
H	4.07796	6.08300	-1.69296
H	1.53044	-2.43741	-2.37942

E = -3589.62537267

[Cu(II)]-O-O· singlet

N	2.14954	-1.13415	-1.26996
N	2.10426	-2.40434	1.25311
N	3.33847	-2.27669	3.06832
N	-2.34627	-2.27903	-2.92462
N	-0.71248	-1.99189	-1.48520
N	-4.88512	0.95691	-0.18082
N	-4.38271	-0.54687	1.34991
N	-1.70756	1.25636	3.76216
C	3.53449	-1.66521	-1.44786
C	3.75860	-2.04199	-2.90082
C	3.72788	-2.87440	-0.53926
C	3.41897	-2.60501	0.89320
C	4.20099	-2.52618	2.01579
C	2.08648	-2.20848	2.56256
C	3.71258	-2.12280	4.47042
C	-4.15734	0.24687	-4.09432
C	-2.65034	0.09288	-3.86015
C	-2.10135	-0.91656	-2.90414
C	-1.08559	-0.76378	-1.99440
C	-1.49922	-2.88836	-2.06168
C	-8.00103	1.73614	-0.35209
C	-7.29906	0.44316	-0.76643
C	-6.02696	0.18798	-0.02145
C	-5.68584	-0.73644	0.93517
C	-3.92727	0.48164	0.65646
C	-0.80742	5.69325	2.10533
C	-1.26649	4.23640	1.95214
C	-0.62219	3.31533	3.00600
C	-1.02422	1.87193	2.79519
C	4.55551	6.41334	-1.64717
C	4.20589	5.16073	-2.45286
C	3.56753	4.08474	-1.60466
C	2.17723	4.00851	-1.45578
C	4.35353	3.16309	-0.89840
C	1.58305	3.04940	-0.63504
C	3.77953	2.20369	-0.06764
C	2.38790	2.14752	0.06944
O	2.94658	-1.82808	-3.77709
O	-0.73809	1.29643	1.71223
O	1.86869	1.15989	0.86440
O	0.11408	-4.17289	0.06896
O	-2.67239	-1.43033	3.26520
O	-0.58314	-1.45331	1.51868
O	1.03559	-4.95634	-0.46618
Cu	0.72321	-2.32054	-0.15661
H	-7.96376	-0.41012	-0.59230
H	-7.10189	0.46124	-1.84734
H	-6.30194	-1.52440	1.34584
H	-3.40302	-1.21527	2.60661
H	-2.93288	0.90150	0.72336
H	-8.93023	1.86762	-0.91699
H	-1.01234	3.86761	0.95353
H	-2.35895	4.17877	2.04328
H	-0.88170	3.65234	4.01556
H	0.47019	3.36571	2.91468
H	0.27864	5.77843	1.98190
H	3.52849	5.43428	-3.27181
H	5.11691	4.76759	-2.92211
H	5.43634	3.19819	-0.99774
H	1.54253	4.70637	-1.99775
H	4.39363	1.49858	0.48570
H	0.50146	2.98901	-0.54901
H	0.91411	1.32513	1.05565

H	5.25747	6.17868	-0.83849
H	2.18376	-0.26403	-0.73616
H	4.27570	-0.89269	-1.19782
H	4.72622	-2.53358	-3.11830
H	3.06856	-3.68486	-0.87838
H	4.75824	-3.23754	-0.63326
H	5.26471	-2.63352	2.16378
H	1.20444	-2.00146	3.14680
H	2.81243	-1.92702	5.05449
H	4.40478	-1.28482	4.58482
H	4.18598	-3.03758	4.83586
H	-4.68844	0.49242	-3.16836
H	-2.24773	1.06016	-3.53651
H	-2.18200	-0.09469	-4.83846
H	-0.59603	0.15066	-1.69209
H	-3.03101	-2.75500	-3.49712
H	-1.48336	-3.94960	-1.86976
H	-3.05292	-2.04048	3.91565
H	-0.66551	-0.47628	1.57248
H	-1.30898	-1.77429	2.09767
H	-2.03410	0.28453	3.66131
H	-1.94652	1.75211	4.60964
H	-4.78229	1.74736	-0.80303
H	-4.32858	1.05312	-4.81343
H	-4.60713	-0.66482	-4.50440
H	-7.37295	2.61512	-0.53819
H	-8.24966	1.72288	0.71451
H	-1.28268	6.33257	1.35360
H	-1.06563	6.08957	3.09432
H	5.01813	7.17606	-2.28453
H	3.65960	6.85151	-1.19200
H	1.78449	-0.91085	-2.19930

E = -3739.97401565

[Cu(II)]-O-O· triplet

N	2.15319	-1.14650	-1.27137
N	2.08112	-2.42386	1.26049
N	3.30386	-2.27722	3.08331
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N	-1.71065	1.28781	3.75892
C	3.53919	-1.67562	-1.43180
C	3.78264	-2.05554	-2.88076
C	3.72615	-2.88256	-0.51911
C	3.40056	-2.61347	0.91012
C	4.17496	-2.52304	2.03720
C	2.05443	-2.22291	2.56903
C	3.66771	-2.11529	4.48713
C	-4.13772	0.25692	-4.10602
C	-2.63188	0.09838	-3.86684
C	-2.09374	-0.92017	-2.91446
C	-1.08558	-0.77982	-1.99440
C	-1.51160	-2.90038	-2.07876
C	-7.98721	1.76951	-0.37919
C	-7.28860	0.47293	-0.78790
C	-6.02318	0.21218	-0.03342
C	-5.69700	-0.70573	0.93467
C	-3.92499	0.49243	0.65484
C	-0.78704	5.70760	2.08961
C	-1.25082	4.25195	1.93874
C	-0.60440	3.33058	2.99129
C	-1.01736	1.88889	2.78965
C	4.58954	6.39912	-1.64875
C	4.23794	5.14548	-2.45209
C	3.59185	4.07372	-1.60396
C	2.20068	4.00317	-1.45990
C	4.37122	3.14939	-0.89377
C	1.59948	3.04713	-0.64054
C	3.79016	2.19303	-0.06437
C	2.39775	2.14221	0.06764
O	2.98283	-1.84334	-3.76866
O	-0.73216	1.30207	1.71277
O	1.87196	1.15747	0.86165
O	0.09373	-4.18711	0.07464
O	-2.70063	-1.39293	3.29301
O	-0.61882	-1.45914	1.52907
O	1.00623	-4.97754	-0.44071
Cu	0.71121	-2.34161	-0.16193
H	-7.95883	-0.37690	-0.61811
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H	-6.32325	-1.48355	1.34931
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H	3.56490	5.41951	-3.27448
H	5.14920	4.74744	-2.91672
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H	4.75883	-3.24219	-0.60071

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H	1.16687	-2.02056	3.14661
H	2.76347	-1.91534	5.06343
H	4.35941	-1.27690	4.60151
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H	-0.67964	-0.48087	1.58159
H	-1.34184	-1.76174	2.12078
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H	-7.35331	2.64521	-0.56088
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C	4.35508	-5.45080	-0.99882
C	4.92514	-2.75213	-0.61155
C	3.55857	-4.69563	-0.14091
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H	6.22543	-0.44945	3.97642
H	5.66568	-1.72657	2.89133
H	8.00793	-2.15830	1.91105
H	6.79174	-5.10104	-3.32727
H	5.75199	-6.49257	-3.05804
H	4.12429	-6.50352	-1.14725
H	6.55263	-3.06083	-1.97543
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H	3.43432	-1.75618	1.09752
H	7.04910	-7.06798	-0.97570
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H	4.61452	1.06166	4.48836
H	5.50134	3.83286	-0.78460
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C	-5.41447	-2.93602	1.16915
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C	-5.46193	-1.41780	1.40221
O	-4.24044	-1.06597	2.04474
C	-5.66319	-0.64835	0.09569
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H	-4.62616	-3.14130	2.90995
H	-4.16980	-0.09065	2.04471
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H	-7.57503	-3.21478	1.05688
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H	-7.80328	-0.93545	0.00526
H	-7.72500	-1.18941	-2.62059
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C	-4.75957	1.59513	0.01799
O	-5.81463	0.75280	0.37306
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C	-1.86186	2.66947	2.09552
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H	-5.26723	5.12527	-1.78859
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H	-3.95494	4.41883	1.37726
H	-2.29395	2.23507	0.05283
H	-1.88164	1.67879	2.55943
H	-0.84815	2.84188	1.71086
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C	-1.07959	-3.48465	2.00121
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C	1.90447	1.17820	-1.96924
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C	6.32570	6.92260	-0.30007
C	4.89082	6.59714	-0.71413
C	4.30520	5.42184	0.00499
C	3.30304	5.31377	0.93843
C	4.02625	3.30505	0.63284
C	8.21800	-1.09448	2.06456
C	6.93683	-0.26042	1.92373
C	5.86666	-0.65263	2.96418
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H	6.79430	-5.10547	-3.32421
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H	4.12767	-6.50764	-1.14258
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H	2.72164	-5.14406	0.38899
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H	3.43748	-1.75936	1.09966
H	7.05270	-7.07149	-0.97200
H	1.61465	-2.31120	-0.73874
H	0.50234	-4.19073	-1.23734
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O	-4.69365	5.22462	-1.00726
C	-3.32550	4.04522	0.55502
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C	4.40626	-5.43915	-0.99699
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C	3.58200	-4.68215	-0.16744
C	3.85359	-3.32356	0.02413
O	-0.03842	-2.87663	-3.84743
O	3.90411	-0.13424	1.55627
O	2.99664	-2.60287	0.81503
O	-2.12307	-0.16375	-0.64880
O	1.69220	2.40592	2.99344
O	1.30914	0.73690	0.90136
O	-2.82860	0.69278	-1.52817
Cu	-0.20124	-0.16685	-0.37477
H	4.23481	7.46351	-0.46447
H	4.85033	6.44936	-1.75605
H	2.71735	6.07740	1.41426
H	2.16218	3.11643	2.45059
H	4.18894	2.22043	0.65307
H	6.68209	7.82281	-0.79116
H	6.62467	-0.26891	0.92516
H	7.17372	0.81189	2.20079
H	6.12796	-0.67478	3.92913
H	5.63439	-1.80407	2.66287
H	8.08014	-2.11480	1.83837
H	6.87130	-5.08069	-3.28856
H	5.84047	-6.47877	-3.02523
H	4.18579	-6.49438	-1.14340
H	6.61323	-3.04247	-1.93486
H	2.73151	-5.12843	0.34024
H	5.14405	-1.67351	-0.48117
H	3.39970	-1.72726	1.02722
H	7.13326	-7.04827	-0.93888
H	1.61366	-2.20125	-0.77295
H	0.60961	-4.16349	-1.17479
H	-1.12746	-4.37998	-3.04133
H	-1.88345	-2.41495	-0.98025
H	-1.73806	-4.12363	-0.54705
H	-1.21590	-4.46458	2.24334
H	0.01629	-0.49456	2.94461
H	-0.18535	-1.92825	4.95857
H	0.21488	-3.63089	4.62594
H	-1.48785	-3.13195	4.81413
H	4.03605	4.18818	-3.08297
H	4.09186	1.66702	-3.28408
H	3.24329	1.77183	-4.80299
H	2.55132	0.63032	-1.43285
H	0.56081	3.04721	-4.22734
H	-1.20705	1.96379	-2.73451
H	1.13342	2.86751	3.63818
H	2.18744	0.35784	1.12769
H	1.14878	1.38373	1.62714
H	3.22775	1.36986	3.47767
H	4.61439	0.93952	4.45561
H	5.49877	3.84209	-0.79962
H	4.83289	3.61101	-4.56156
H	3.19844	4.28204	-4.63877
H	7.00734	6.11545	-0.46494
H	6.37576	7.15332	0.82243
H	9.03883	-0.67428	1.45492
H	8.63034	-1.04285	3.13855
H	8.18777	-6.98456	-2.36278
H	8.17311	-5.64159	-1.20482
H	1.18747	-1.84254	-2.32823
H	-3.74335	1.02423	-0.92330
H	-4.73095	-0.88664	-0.54410
C	-6.62431	-3.45255	0.44115
O	-6.48369	-4.77424	0.05767
C	-5.36173	-2.99375	1.17803
O	-5.25788	-3.68025	2.41519
C	-5.42466	-1.47786	1.41100
O	-4.22558	-1.12588	2.08967

C	-5.60440	-0.72563	0.09149
C	-6.87842	-1.21219	-0.61844
O	-6.75489	-2.65052	-0.77787
C	-7.12931	-0.55383	-1.97967
O	-5.96413	-0.08336	-2.65844
H	-4.58307	-3.19747	2.92301
H	-4.14335	-0.15358	2.08139
H	-5.37924	-0.83030	-2.86221
H	-7.51775	-3.28966	1.06433
H	-4.50187	-3.21857	0.52832
H	-6.29398	-1.25962	2.05362
H	-7.74687	-0.99826	0.02443
H	-7.69888	-1.25315	-2.60475
H	-7.73287	0.34204	-1.82391
C	-4.73742	1.55425	0.04903
O	-5.75735	0.68461	0.34711
C	-5.30473	2.86072	-0.49750
O	-6.01956	2.67850	-1.71180
C	-4.17523	3.88955	-0.68807
O	-4.68901	5.18250	-0.98206
C	-3.31636	4.00533	0.57270
C	-2.80714	2.63132	0.92507
O	-3.92554	1.74643	1.17152
C	-1.90440	2.62753	2.16126
O	-2.37795	3.42253	3.24122
H	-5.74544	1.83373	-2.12400
H	-5.24060	5.08783	-1.77713
H	-2.23723	4.34953	2.98816
H	-6.01499	3.25894	0.24288
H	-3.53051	3.54144	-1.51062
H	-3.95055	4.37532	1.39266
H	-2.23288	2.22387	0.08798
H	-1.83292	1.60164	2.53441
H	-0.90094	2.94618	1.85213
O	-2.19751	4.86300	0.38345
H	-7.33649	-5.07795	-0.29444
H	-2.55022	5.67734	-0.01477

E = -5037.82714051
Frequencies = -1815.8622

TS-1 triplet

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N	0.78900	2.41906	-3.48082
N	0.45676	1.07410	-1.77677
N	4.76999	4.11454	-0.16806
N	3.17364	3.96341	1.34412
N	4.09243	0.81224	3.59841
C	0.01921	-3.29202	-1.46046
C	-0.41649	-3.55785	-2.88817
C	-1.19852	-3.17146	-0.55125
C	-0.90130	-2.73342	0.84231
C	-0.95603	-3.40766	2.03474
C	-0.36499	-1.31824	2.40233
C	-0.54963	-2.75502	4.44970
C	3.88701	3.65500	-4.02952
C	3.34259	2.23888	-3.81077
C	2.05260	2.00456	-3.08074
C	1.81515	1.17340	-2.01800
C	-0.13777	1.83981	-2.67942
C	6.33118	6.93188	-0.24998
C	4.89943	6.59877	-0.66886
C	4.32351	5.41062	0.03636
C	3.33403	5.28607	0.98104
C	4.05384	3.28287	0.63105
C	8.25766	-1.07461	2.12298
C	6.97245	-0.24738	1.97749
C	5.82358	-0.76296	2.87281
C	4.52765	-0.00657	2.63779
C	7.54620	-6.39767	-1.68767
C	6.42985	-5.72260	-2.48682
C	5.51482	-4.88047	-1.62952
C	5.76910	-3.51864	-1.42682
C	4.40759	-5.44547	-0.98099
C	4.94985	-2.73826	-0.61213
C	3.58149	-4.68431	-0.15708
C	3.85287	-3.32487	0.02859
O	-0.03438	-2.90475	-3.83776
O	3.90393	-0.13415	1.55078
O	2.99394	-2.59980	0.81341
O	-2.12993	-0.22387	-0.79278
O	1.69747	2.40296	2.99418
O	1.29724	0.74244	0.89490
O	-2.83727	0.71008	-1.57880
Cu	-0.22337	-0.15932	-0.39462
H	4.24657	7.45443	-0.46430
H	4.86197	6.43964	-1.75544
H	2.72945	6.06994	1.41574
H	2.17099	3.11126	2.45143
H	4.19762	2.21163	0.65453
H	6.69407	7.81262	-0.79054
H	6.63951	-0.26363	0.93335
H	7.17642	0.80207	2.22654
H	6.11525	-0.70719	3.92733
H	5.62849	-1.81687	2.64109
H	8.08779	-2.11966	1.83871
H	6.87548	-5.09660	-3.27045
H	5.84289	-6.49266	-3.00403
H	4.18691	-6.50120	-1.12332
H	6.61812	-3.05408	-1.92395
H	2.72961	-5.12802	0.35053
H	5.14575	-1.67781	-0.48038
H	3.39768	-1.72368	1.02318

H	7.13466	-7.05903	-0.91626
H	1.61052	-2.19315	-0.76686
H	0.61995	-4.16366	-1.15431
H	-1.11818	-4.40512	-3.01902
H	-1.88835	-2.43794	-0.98582
H	-1.72285	-4.13431	-0.52018
H	-1.20743	-4.43051	2.27039
H	-0.05298	-0.43028	2.92889
H	-0.24117	-1.84136	4.95938
H	0.17753	-3.54465	4.65443
H	-1.53131	-3.05913	4.82139
H	4.03859	4.17857	-3.07939
H	4.09647	1.65655	-3.26801
H	3.26089	1.75390	-4.79493
H	2.53627	0.64109	-1.41867
H	0.57852	3.03822	-4.25259
H	-1.20560	1.97603	-2.76551
H	1.14390	2.86774	3.64113
H	2.17359	0.35898	1.11962
H	1.14416	1.39024	1.62113
H	3.23228	1.36256	3.47755
H	4.61525	0.92159	4.45637
H	5.50793	3.83217	-0.79933
H	4.84816	3.59625	-4.54906
H	3.21377	4.26524	-4.64242
H	7.01852	6.10521	-0.46376
H	6.38710	7.14371	0.82317
H	9.04825	-0.67400	1.47972
H	8.62573	-1.06193	3.15559
H	8.18910	-6.99975	-2.34040
H	8.17633	-5.65429	-1.18532
H	1.18464	-1.84840	-2.32523
H	-3.72626	1.01973	-0.94000
H	-4.72484	-0.89154	-0.53467
C	-6.62097	-3.45167	0.45093
O	-6.48114	-4.77400	0.06943
C	-5.35841	-2.99273	1.18776
O	-5.25517	-3.67831	2.42546
C	-5.42379	-1.47681	1.41951
O	-4.22724	-1.12172	2.10136
C	-5.59940	-0.72613	0.09863
C	-6.87287	-1.21270	-0.61210
O	-6.75038	-2.65135	-0.76921
C	-7.12193	-0.55608	-1.97452
O	-5.95588	-0.08697	-2.65252
H	-4.58283	-3.19346	2.93457
H	-4.15605	-0.14856	2.10576
H	-5.37203	-0.83447	-2.85710
H	-7.51446	-3.28726	1.07365
H	-4.49821	-3.21772	0.53862
H	-6.29506	-1.25906	2.05946
H	-7.74187	-0.99714	0.02950
H	-7.69123	-1.25589	-2.59931
H	-7.72523	0.34028	-1.82050
C	-4.72815	1.55289	0.05161
O	-5.74919	0.68456	0.35191
C	-5.29618	2.85921	-0.49642
O	-6.00997	2.67510	-1.71104
C	-4.16681	3.88804	-0.68734
O	-4.68002	5.18143	-0.98066
C	-3.30748	4.00390	0.57307
C	-2.79947	2.63004	0.92773
O	-3.91657	1.74665	1.17620
C	-1.89295	2.62699	2.16117
O	-2.36516	3.42035	3.24253
H	-5.73567	1.82947	-2.12136
H	-5.23112	5.08762	-1.77617
H	-2.22492	4.34776	2.99064
H	-6.00714	3.25869	0.24277
H	-3.52231	3.54046	-1.51029
H	-3.94117	4.37466	1.39308
H	-2.22628	2.22331	0.08811
H	-1.81941	1.60064	2.53314
H	-0.89086	2.94724	1.84954
O	-2.18812	4.86058	0.38298
H	-7.33390	-5.07753	-0.28293
H	-2.54005	5.67424	-0.01737

E = -5037.8271462
Frequencies = -1825.9975

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N	0.84257	-2.07196	-1.38261
N	-0.48423	-1.50060	1.11478
N	-0.62738	-2.62863	3.00081
N	0.80538	2.49564	-3.35920
N	0.51573	1.06678	-1.71833
N	4.74661	4.12294	-0.15817
N	3.13696	3.97752	1.34088
N	4.07836	0.85047	3.62384
C	-0.01649	-3.26980	-1.50078
C	-0.45804	-3.45224	-2.94003
C	-1.23352	-3.15136	-0.59024
C	-0.91926	-2.77848	0.81985
C	-1.01008	-3.48913	1.98897
C	-0.31649	-1.44521	2.42792
C	-0.57739	-2.94029	4.42533
C	3.86442	3.68183	-4.03736
C	3.31711	2.26567	-3.82532
C	2.07119	2.03053	-3.03814
C	1.86340	1.15045	-2.01038
C	-0.09826	1.89467	-2.55013
C	6.31763	6.93460	-0.24290
C	4.88494	6.60658	-0.66262
C	4.30246	5.42062	0.04164

C	3.30480	5.29953	0.97828
C	4.02104	3.29412	0.63546
C	8.22865	-1.08768	2.08891
C	6.94507	-0.25705	1.94827
C	5.84294	-0.70340	2.93308
C	4.53092	0.01634	2.68476
C	7.50380	-6.39012	-1.74789
C	6.38842	-5.70873	-2.54300
C	5.47830	-4.87707	-1.67026
C	5.73433	-3.51813	-1.45169
C	4.38309	-5.45339	-1.01126
C	4.93181	-2.75288	-0.60661
C	3.57370	-4.70738	-0.15754
C	3.85092	-3.35209	0.04946
O	-0.03342	-2.78563	-3.86194
O	3.91057	-0.15974	1.60318
O	3.01223	-2.64409	0.87018
O	-2.01869	-0.13749	-0.62051
O	1.66516	2.40606	2.98943
O	1.34907	0.67651	0.93709
O	-2.54441	0.51290	-1.83020
Cu	-0.13391	-0.19274	-0.34374
H	4.23517	7.46478	-0.45880
H	4.84779	6.44749	-1.74923
H	2.69908	6.08557	1.40746
H	2.12959	3.11945	2.44650
H	4.16109	2.22251	0.65985
H	6.68387	7.81386	-0.78358
H	6.56013	-0.34257	0.92623
H	7.16711	0.80486	2.11510
H	6.17671	-0.55683	3.96604
H	5.65118	-1.77519	2.79943
H	8.03622	-2.14670	1.88114
H	6.83332	-5.07434	-3.32017
H	5.80060	-6.47367	-3.06673
H	4.16037	-6.50686	-1.16681
H	6.57341	-3.04460	-1.95718
H	2.73139	-5.15978	0.35827
H	5.13004	-1.69483	-0.46035
H	3.41624	-1.76959	1.08193
H	7.09077	-7.05724	-0.98232
H	1.61579	-2.27327	-0.74767
H	0.54206	-4.18415	-1.23913
H	-1.20555	-4.25272	-3.10762
H	-1.89524	-2.37041	-0.98271
H	-1.78567	-4.09847	-0.60132
H	-1.31261	-4.50558	2.18985
H	0.03506	-0.59044	2.98432
H	-0.23036	-2.05926	4.96677
H	0.11331	-3.76808	4.60438
H	-1.57268	-3.21317	4.78507
H	4.07113	4.17974	-3.08382
H	4.09441	1.66253	-3.34111
H	3.17859	1.80829	-4.81665
H	2.59721	0.56880	-1.47459
H	0.57748	3.15586	-4.09057
H	-1.16628	2.03641	-2.59372
H	1.07647	2.86213	3.61115
H	2.23252	0.31347	1.17277
H	1.17259	1.33694	1.64678
H	3.20734	1.38049	3.49287
H	4.60349	0.99761	4.47469
H	5.48882	3.83752	-0.78304
H	4.79601	3.62931	-4.60878
H	3.16588	4.31398	-4.59781
H	7.00227	6.10552	-0.45608
H	6.37377	7.14660	0.83022
H	8.99324	-0.73963	1.38627
H	8.64381	-1.01304	3.10087
H	8.14831	-6.98728	-2.40370
H	8.13265	-5.65033	-1.23875
H	1.23622	-1.86949	-2.30266
H	-4.76707	-0.78196	-0.48934
C	-6.65601	-3.42504	0.41374
O	-6.52363	-4.74483	0.02491
C	-5.39192	-2.97248	1.15201
O	-5.26876	-3.68637	2.37160
C	-5.47429	-1.46372	1.42567
O	-4.27601	-1.11842	2.11111
C	-5.66014	-0.67527	0.13020
C	-6.90159	-1.18040	-0.63806
O	-6.76252	-2.61312	-0.80335
C	-7.08235	-0.51070	-2.00251
O	-5.86957	-0.10807	-2.64392
H	-4.59486	-3.20788	2.88473
H	-4.20120	-0.14615	2.12864
H	-5.34856	-0.89420	-2.87366
H	-7.55346	-3.25508	1.02869
H	-4.53568	-3.17086	0.48940
H	-6.34413	-1.27494	2.07645
H	-7.80074	-0.97242	-0.03664
H	-7.67059	-1.17531	-2.64725
H	-7.63774	0.41764	-1.85893
C	-4.85422	1.61932	0.15771
O	-5.84898	0.73106	0.44200
C	-5.33230	2.89566	-0.49115
O	-6.01814	2.66888	-1.71718
C	-4.17325	3.89293	-0.69575
O	-4.65774	5.18450	-1.03346
C	-3.32674	4.02283	0.57109
C	-2.82534	2.64206	0.91864
O	-3.96670	1.77710	1.20369
C	-1.89044	2.62756	2.12932
O	-2.28402	3.48804	3.19054
H	-5.67587	1.85017	-2.12841
H	-5.20329	5.07975	-1.83150

H	-2.12279	4.39563	2.88300
H	-6.06332	3.37886	0.17817
H	-3.52622	3.50851	-1.50083
H	-3.96274	4.39209	1.38926
H	-2.28873	2.19648	0.07593
H	-1.86190	1.61324	2.53751
H	-0.88142	2.87815	1.77836
O	-2.20356	4.87447	0.38681
H	-7.37733	-5.04206	-0.33055
H	-2.54739	5.68834	-0.02029
H	-3.39575	0.83641	-1.47138

E = -5037.83802748

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N	0.84257	-2.07196	-1.38261
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N	4.74661	4.12294	-0.15817
N	3.13696	3.97752	1.34088
N	4.07836	0.85047	3.62384
C	-0.01649	-3.26980	-1.50078
C	-0.45804	-3.45224	-2.94003
C	-1.23352	-3.15136	-0.59024
C	-0.91926	-2.77848	0.81985
C	-1.01008	-3.48913	1.98897
C	-0.31649	-1.44521	2.42792
C	-0.57739	-2.94029	4.42533
C	3.86442	3.68183	-4.03736
C	3.31711	2.26567	-3.82532
C	2.07119	2.03053	-3.03814
C	1.86340	1.15045	-2.01038
C	-0.09826	1.89467	-2.55013
C	6.31763	6.93460	-0.24290
C	4.88494	6.60658	-0.66262
C	4.30246	5.42062	0.04164
C	3.30480	5.29953	0.97828
C	4.02104	3.29412	0.63546
C	8.22865	-1.08768	2.08891
C	6.94507	-0.25705	1.94827
C	5.84294	-0.70340	2.93308
C	4.53092	0.01634	2.68476
C	7.50380	-6.39012	-1.74789
C	6.38842	-5.70873	-2.54300
C	5.47830	-4.87707	-1.67026
C	5.73433	-3.51813	-1.45169
C	4.38309	-5.45339	-1.01126
C	4.93181	-2.75288	-0.60661
C	3.57370	-4.70738	-0.15754
C	3.85092	-3.35209	0.04946
O	-0.03342	-2.78563	-3.86194
O	3.91057	-0.15974	1.60318
O	3.01223	-2.64409	0.87018
O	-2.01869	-0.13749	-0.62051
O	1.66516	2.40606	2.98943
O	1.34907	0.67651	0.93709
O	-2.54441	0.51290	-1.83020
Cu	-0.13391	-0.19274	-0.34374
H	4.23517	7.46478	-0.45880
H	4.84779	6.44749	-1.74923
H	2.69908	6.08557	1.40746
H	2.12959	3.11945	2.44650
H	4.16109	2.22251	0.65985
H	6.68387	7.81386	-0.78358
H	6.56013	-0.34257	0.92623
H	7.16711	0.80486	2.11510
H	6.17671	-0.55683	3.96604
H	5.65118	-1.77519	2.79943
H	8.03622	-2.14670	1.88114
H	6.83332	-5.07434	-3.32017
H	5.80060	-6.47367	-3.06673
H	4.16037	-6.50686	-1.16681
H	6.57341	-3.04460	-1.95718
H	2.73139	-5.15978	0.35827
H	5.13004	-1.69483	-0.46035
H	3.41624	-1.76959	1.08193
H	7.09077	-7.05724	-0.98232
H	1.61579	-2.27327	-0.74767
H	0.54206	-4.18415	-1.23913
H	-1.20555	-4.25272	-3.10762
H	-1.89524	-2.37041	-0.98271
H	-1.78567	-4.09847	-0.60132
H	-1.31261	-4.50558	2.18985
H	0.03506	-0.59044	2.98432
H	-0.23036	-2.05926	4.96677
H	0.11331	-3.76808	4.60438
H	-1.57268	-3.21317	4.78507
H	4.07113	4.17974	-3.08382
H	4.09441	1.66253	-3.34111
H	3.17859	1.80829	-4.81665
H	2.59721	0.56880	-1.47459
H	0.57748	3.15586	-4.09057
H	-1.16628	2.03641	-2.59372
H	1.07647	2.86213	3.61115
H	2.23252	0.31347	1.17277
H	1.17259	1.33694	1.64678
H	3.20734	1.38049	3.49287
H	4.60349	0.99761	4.47469
H	5.48882	3.83752	-0.78304
H	4.79601	3.62931	-4.60878
H	3.16588	4.31398	-4.59781
H	7.00227	6.10552	-0.45608
H	6.37377	7.14660	0.83022

H	8.99324	-0.73963	1.38627
H	8.64381	-1.01304	3.10087
H	8.14831	-6.98728	-2.40370
H	8.13265	-5.65033	-1.23875
H	1.23622	-1.86949	-2.30266
H	-4.76707	-0.78196	-0.48934
C	-6.65601	-3.42504	0.41374
O	-6.52363	-4.74483	0.02491
C	-5.39192	-2.97248	1.15201
O	-5.26876	-3.68637	2.37160
C	-5.47429	-1.46372	1.42567
O	-4.27601	-1.11842	2.11111
C	-5.66014	-0.67527	0.13020
C	-6.90159	-1.18040	-0.63806
O	-6.76252	-2.61312	-0.80335
C	-7.08235	-0.51070	-2.00251
O	-5.86957	-0.10807	-2.64392
H	-4.59486	-3.20788	2.88473
H	-4.20120	-0.14615	2.12864
H	-5.34856	-0.89420	-2.87366
H	-7.55346	-3.25508	1.02869
H	-4.53568	-3.17086	0.48940
H	-6.34413	-1.27494	2.07645
H	-7.80074	-0.97242	-0.03664
H	-7.67059	-1.17531	-2.64725
H	-7.63774	0.41764	-1.85893
C	-4.85422	1.61932	0.15771
O	-5.84898	0.73106	0.44200
C	-5.33230	2.89566	-0.49115
O	-6.01814	2.66888	-1.71718
C	-4.17325	3.89293	-0.69575
O	-4.65774	5.18450	-1.03346
C	-3.32674	4.02283	0.57109
C	-2.82534	2.64206	0.91864
O	-3.96670	1.77710	1.20369
C	-1.89044	2.62756	2.12932
O	-2.28402	3.48804	3.19054
H	-5.67587	1.85017	-2.12841
H	-5.20329	5.07975	-1.83150
H	-2.12279	4.39563	2.88300
H	-6.06332	3.37886	0.17817
H	-3.52622	3.50851	-1.50083
H	-3.96274	4.39209	1.38926
H	-2.28873	2.19648	0.07593
H	-1.86190	1.61324	2.53751
H	-0.88142	2.87815	1.77836
O	-2.20356	4.87447	0.38681
H	-7.37733	-5.04206	-0.33055
H	-2.54739	5.68834	-0.02029
H	-3.39575	0.83641	-1.47138

E = -5037.83802491

TS-2 singlet

N	-0.81864	-2.05493	1.37107
N	0.67264	-1.34310	-1.09069
N	0.73160	-2.38371	-3.03359
N	-0.82569	2.34204	3.55118
N	-0.49384	1.13632	1.74934
N	-4.83209	4.08452	0.17557
N	-3.21194	3.93324	-1.31076
N	-4.09182	0.80021	-3.57542
C	-0.01020	-3.28904	1.43114
C	0.42435	-3.56487	2.85649
C	1.20959	-3.15413	0.52667
C	0.95310	-2.67614	-0.85945
C	0.99253	-3.33206	-2.06312
C	0.54268	-1.20468	-2.40283
C	0.69334	-2.61033	-4.47422
C	-3.93920	3.61360	4.02679
C	-3.38330	2.20286	3.80173
C	-2.08849	2.00159	3.08497
C	-1.85060	1.26036	1.95985
C	0.10255	1.79617	2.72839
C	-6.39585	6.89331	0.25779
C	-4.96299	6.56869	0.67955
C	-4.37996	5.38018	-0.01930
C	-3.37551	5.25549	-0.94796
C	-4.10492	3.25298	-0.61356
C	-8.25349	-1.11390	-2.16705
C	-6.97509	-0.27780	-2.01254
C	-5.80187	-0.80743	-2.86933
C	-4.51086	-0.04181	-2.62720
C	-7.51401	-6.45308	1.61564
C	-6.40546	-5.77412	2.42232
C	-5.48474	-4.93422	1.56901
C	-5.73516	-3.57189	1.36583
C	-4.37742	-5.50190	0.92282
C	-4.91337	-2.79409	0.55141
C	-3.54851	-4.74332	0.09932
C	-3.81740	-3.38367	-0.08875
O	0.00700	-2.95002	3.81695
O	-3.87433	-0.18198	-1.54927
O	-2.96088	-2.66105	-0.87804
O	1.88804	-0.26772	1.42315
O	-1.69614	2.38636	-2.92944
O	-1.23664	0.68898	-0.87887
O	3.23423	0.72516	1.12764
Cu	0.28169	-0.09923	0.42383
H	-4.31365	7.42630	0.47207
H	-4.92638	6.41459	1.76692
H	-2.76263	6.03896	-1.37156
H	-2.18611	3.08770	-2.39060
H	-4.25097	2.18218	-0.64327
H	-6.76303	7.77484	0.79410

H	-6.66662	-0.26816	-0.96048
H	-7.17786	0.76468	-2.29018
H	-6.07087	-0.77546	-3.93097
H	-5.60815	-1.85497	-2.61059
H	-8.08611	-2.15124	-1.85460
H	-6.85833	-5.14582	3.19990
H	-5.82221	-6.54187	2.94719
H	-4.15912	-6.55801	1.06632
H	-6.58371	-3.10506	1.86167
H	-2.69646	-5.18914	-0.40606
H	-5.10661	-1.73344	0.41819
H	-3.36298	-1.78113	-1.07490
H	-7.09489	-7.11598	0.84966
H	-1.59355	-2.19757	0.72252
H	-0.60094	-4.16857	1.12278
H	1.15702	-4.38767	2.97700
H	1.88461	-2.42167	0.98865
H	1.73312	-4.11731	0.48387
H	1.18481	-4.36457	-2.31218
H	0.29065	-0.29360	-2.92211
H	0.41454	-1.67982	-4.97050
H	-0.04530	-3.37971	-4.71192
H	1.67624	-2.92727	-4.83235
H	-4.08024	4.14332	3.07836
H	-4.12618	1.62315	3.24127
H	-3.31092	1.70589	4.78055
H	-2.56941	0.80120	1.30099
H	-0.61980	2.88480	4.37946
H	1.17030	1.87324	2.86035
H	-1.14311	2.86048	-3.57017
H	-2.09781	0.27349	-1.10191
H	-1.12287	1.36543	-1.58801
H	-3.23425	1.35238	-3.44830
H	-4.61989	0.92029	-4.42868
H	-5.57909	3.80208	0.79608
H	-4.90716	3.54835	4.53324
H	-3.27598	4.22201	4.65239
H	-7.07992	6.06480	0.47491
H	-6.45200	7.10005	-0.81636
H	-9.05931	-0.70137	-1.55083
H	-8.59857	-1.12685	-3.20756
H	-8.16184	-7.05429	2.26435
H	-8.14070	-5.71193	1.10572
H	-1.21287	-1.88106	2.29647
H	4.73293	-0.82692	0.44814
C	6.63728	-3.38730	-0.45907
O	6.49644	-4.70972	-0.07385
C	5.37365	-2.93381	-1.19745
O	5.25507	-3.65094	-2.41534
C	5.45620	-1.42437	-1.46894
O	4.25330	-1.07038	-2.14389
C	5.62380	-0.67014	-0.15599
C	6.86852	-1.15265	0.61760
O	6.77318	-2.59056	0.75180
C	6.92411	-0.57188	2.02594
O	5.67809	-0.68361	2.72066
H	4.57392	-3.18200	-2.92742
H	4.17713	-0.09796	-2.14397
H	5.46769	-1.63128	2.77485
H	7.52850	-3.22941	-1.08661
H	4.51527	-3.13123	-0.53722
H	6.32370	-1.22931	-2.12055
H	7.78377	-0.87715	0.07172
H	7.72888	-1.06636	2.58542
H	7.13830	0.49621	1.96224
C	4.76433	1.62694	-0.12296
O	5.76752	0.75270	-0.39967
C	5.26122	2.90800	0.52014
O	5.93094	2.68692	1.75795
C	4.12035	3.92496	0.70909
O	4.62201	5.21877	1.01542
C	3.26751	4.04347	-0.54976
C	2.77114	2.66776	-0.91401
O	3.91827	1.81204	-1.19192
C	1.86373	2.67055	-2.14588
O	2.28960	3.53073	-3.19441
H	5.33034	2.16345	2.31840
H	5.17666	5.12620	1.80843
H	2.11789	4.43864	-2.89415
H	6.01904	3.35347	-0.13995
H	3.47450	3.56146	1.52355
H	3.89913	4.42211	-1.36740
H	2.22671	2.22000	-0.07965
H	1.83868	1.65855	-2.56052
H	0.84857	2.92777	-1.81872
O	2.14049	4.89030	-0.35945
H	7.35123	-5.01550	0.27147
H	2.48350	5.70988	0.03644
H	3.78098	0.29087	1.81271

E = -5037.81253258
Frequencies = -698.2735

TS-2 triplet

N	0.81700	-2.05600	-1.36533
N	-0.72813	-1.30751	1.07520
N	-0.78924	-2.31623	3.03464
N	0.83517	2.33176	-3.57130
N	0.48638	1.15369	-1.75362
N	4.84604	4.07505	-0.17668
N	3.22120	3.92193	1.30435
N	4.08737	0.79398	3.58027
C	0.01364	-3.29491	-1.41908
C	-0.41902	-3.58116	-2.84290
C	-1.20670	-3.15733	-0.51575

C	-0.97084	-2.65122	0.86354
C	-1.01211	-3.28728	2.07759
C	-0.62181	-1.14370	2.38657
C	-0.77544	-2.51532	4.47987
C	3.95096	3.59967	-4.02353
C	3.39358	2.18982	-3.79649
C	2.09336	1.99837	-3.08805
C	1.84513	1.27560	-1.95352
C	-0.10037	1.79810	-2.74905
C	6.40782	6.88353	-0.25829
C	4.97497	6.55951	-0.68057
C	4.39163	5.37017	0.01658
C	3.38428	5.24430	0.94192
C	4.11731	3.24271	0.61023
C	8.25625	-1.12125	2.18157
C	6.97874	-0.28423	2.02468
C	5.80811	-0.80832	2.88800
C	4.51516	-0.04951	2.63732
C	7.51466	-6.46618	-1.59257
C	6.40734	-5.78758	-2.40124
C	5.48457	-4.94719	-1.55063
C	5.73659	-3.58544	-1.34526
C	4.37312	-5.51321	-0.91017
C	4.91218	-2.80659	-0.53466
C	3.54148	-4.75348	-0.09029
C	3.81183	-3.39445	0.09957
O	-0.00275	-2.97049	-3.80637
O	3.88553	-0.19689	1.55645
O	2.95274	-2.66969	0.88459
O	-1.87408	-0.26741	-1.50369
O	1.69707	2.37511	2.91578
O	1.25259	0.65932	0.86551
O	-3.22595	0.69961	-1.14125
Cu	-0.29806	-0.10855	-0.45276
H	4.32561	7.41686	-0.47208
H	4.93856	6.40688	-1.76817
H	2.76904	6.02705	1.36341
H	2.18977	3.07559	2.37869
H	4.26495	2.17215	0.64115
H	6.77501	7.76578	-0.79341
H	6.66743	-0.28134	0.97346
H	7.18306	0.75979	2.29520
H	6.07758	-0.76472	3.94909
H	5.61757	-1.85908	2.63998
H	8.08643	-2.16017	1.87577
H	6.86161	-5.15962	-3.17831
H	5.82520	-6.55561	-2.92692
H	4.15362	-6.56884	-1.05526
H	6.58845	-3.11991	-1.83664
H	2.68655	-5.19835	0.41108
H	5.10663	-1.74644	-0.39961
H	3.36015	-1.79375	1.08801
H	7.09443	-7.12902	-0.82714
H	1.59221	-2.19361	-0.71577
H	0.60869	-4.16903	-1.10437
H	-1.14867	-4.40721	-2.95903
H	-1.89033	-2.44440	-0.99444
H	-1.71954	-4.12553	-0.45863
H	-1.18355	-4.31967	2.34173
H	-0.39951	-0.21870	2.89452
H	-0.49813	-1.57737	4.96277
H	-0.04529	-3.28437	4.74294
H	-1.76578	-2.81954	4.82859
H	4.08514	4.13286	-3.07607
H	4.13139	1.61246	-3.22705
H	3.32751	1.68785	-4.77313
H	2.55702	0.82765	-1.28010
H	0.63701	2.86221	-4.40937
H	-1.16648	1.86961	-2.89519
H	1.13989	2.85073	3.55179
H	2.11296	0.24667	1.09535
H	1.13938	1.34252	1.56729
H	3.22893	1.34335	3.44610
H	4.61101	0.92000	4.43540
H	5.59513	3.79343	-0.79504
H	4.92241	3.53351	-4.52324
H	3.29145	4.20526	-4.65578
H	7.09194	6.05535	-0.47654
H	6.46397	7.08883	0.81613
H	9.06164	-0.71394	1.56130
H	8.60345	-1.12853	3.22144
H	8.16359	-7.06738	-2.24018
H	8.14046	-5.72487	-1.08179
H	1.21229	-1.88688	-2.29126
H	-4.72992	-0.82718	-0.43616
C	-6.63534	-3.38381	0.46633
O	-6.49528	-4.70695	0.08306
C	-5.37183	-2.93024	1.20488
O	-5.25255	-3.64848	2.42211
C	-5.45602	-1.42110	1.47762
O	-4.25329	-1.06620	2.15298
C	-5.62223	-0.66691	0.16449
C	-6.86370	-1.15080	-0.61432
O	-6.76945	-2.58893	-0.74563
C	-6.90866	-0.57418	-2.02468
O	-5.65839	-0.69585	-2.71092
H	-4.57311	-3.17840	2.93536
H	-4.17482	-0.09391	2.14749
H	-5.45402	-1.64515	-2.76054
H	-7.52689	-3.22439	1.09298
H	-4.51340	-3.12647	0.54440
H	-6.32379	-1.22710	2.12916
H	-7.78188	-0.87266	-0.07482
H	-7.71192	-1.06657	-2.58799
H	-7.11737	0.49528	-1.96633
C	-4.75619	1.62710	0.12271

O	-5.76320	0.75597	0.40647
C	-5.25273	2.90853	-0.52257
O	-5.91801	2.68444	-1.76259
C	-4.11059	3.92440	-0.71223
O	-4.61050	5.21823	-1.02162
C	-3.25876	4.04399	0.54689
C	-2.76394	2.66844	0.91385
O	-3.91136	1.81602	1.19541
C	-1.85255	2.67799	2.14373
O	-2.25200	3.57428	3.17212
H	-5.31327	2.16179	-2.31937
H	-5.16547	5.12429	-1.81425
H	-2.07059	4.46978	2.84099
H	-6.01228	3.35597	0.13405
H	-3.46442	3.55884	-1.52565
H	-3.89056	4.42352	1.36377
H	-2.22202	2.21851	0.07863
H	-1.85275	1.67651	2.58324
H	-0.83192	2.90108	1.80872
O	-2.13054	4.89018	0.35809
H	-7.35005	-5.01246	-0.26258
H	-2.47219	5.71055	-0.03737
H	-3.79404	0.25171	-1.79924

E = -5037.81416124
Frequencies = -690.8038

3 singlet

N	0.92633	-2.13617	-1.34455
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N	0.82532	2.44942	-3.18327
N	0.75683	1.13146	-1.42838
N	4.78119	4.16979	-0.14465
N	3.14358	4.00381	1.31959
N	4.11788	0.91672	3.62457
C	-0.03772	-3.22444	-1.58653
C	-0.48140	-3.21253	-3.03642
C	-1.25040	-3.11475	-0.66919
C	-0.92548	-2.90098	0.77019
C	-1.06288	-3.71678	1.86412
C	-0.25356	-1.76886	2.49919
C	-0.61459	-3.43209	4.34306
C	3.82949	3.75086	-4.07859
C	3.28355	2.33264	-3.87667
C	2.14006	2.07875	-2.94335
C	2.06827	1.26735	-1.83774
C	0.02932	1.85516	-2.26380
C	6.29992	6.96985	-0.26652
C	4.86535	6.64525	-0.68239
C	4.29365	5.45617	0.02111
C	3.27865	5.32312	0.93622
C	4.06436	3.33420	0.64872
C	8.22384	-1.07263	1.98357
C	6.93951	-0.24114	1.85655
C	5.87694	-0.63038	2.90405
C	4.57102	0.10101	2.67130
C	7.48208	-6.34038	-1.89752
C	6.36275	-5.65216	-2.68111
C	5.48143	-4.81837	-1.78014
C	5.71603	-3.45013	-1.60215
C	4.45250	-5.41040	-1.03317
C	4.96323	-2.69302	-0.70444
C	3.69480	-4.67324	-0.12694
C	3.95795	-3.30993	0.04804
O	0.03632	-2.52506	-3.89316
O	3.95580	-0.05217	1.58147
O	3.17944	-2.61951	0.93807
O	-1.58592	-0.33581	-0.97751
O	1.70953	2.47977	3.01069
O	1.29452	0.45959	1.31480
O	-3.97604	1.07729	-1.20640
Cu	0.03985	-0.23453	-0.13138
H	4.21538	7.50134	-0.47096
H	4.82394	6.49164	-1.76975
H	2.64046	6.09799	1.33759
H	2.16021	3.17799	2.43456
H	4.23834	2.26859	0.70001
H	6.66428	7.85349	-0.80131
H	6.51300	-0.37135	0.85673
H	7.17449	0.82580	1.96421
H	6.25261	-0.44708	3.91640
H	5.66222	-1.70360	2.82312
H	8.01805	-2.13893	1.83379
H	6.79905	-5.01865	-3.46348
H	5.75970	-6.41221	-3.19468
H	4.24493	-6.47113	-1.15759
H	6.50198	-2.96357	-2.17596
H	2.90499	-5.13815	0.45620
H	5.14627	-1.62829	-0.58869
H	3.54508	-1.71480	1.07427
H	7.07212	-7.00171	-1.12548
H	1.66434	-2.45392	-0.71889
H	0.43280	-4.21126	-1.43132
H	-1.32129	-3.89385	-3.27880
H	-1.85709	-2.25569	-0.99347
H	-1.86371	-4.01774	-0.77582
H	-1.42467	-4.72877	1.96519
H	0.14618	-0.99091	3.13001
H	-0.21376	-2.63162	4.96637
H	0.01996	-4.31647	4.44221
H	-1.62720	-3.67320	4.67669
H	4.17153	4.18559	-3.13320
H	4.10398	1.69430	-3.52766
H	3.00610	1.92940	-4.86151

H	2.87266	0.75371	-1.33208
H	0.50008	3.03677	-3.93987
H	-1.04654	1.93703	-2.24650
H	1.15867	2.95016	3.65532
H	2.26401	0.28123	1.36286
H	1.16820	1.28185	1.84700
H	3.24826	1.45274	3.50405
H	4.63943	1.04024	4.48143
H	5.54554	3.89604	-0.74752
H	4.67689	3.71966	-4.77021
H	3.07669	4.42557	-4.50229
H	6.98425	6.14321	-0.49005
H	6.36106	7.17279	0.80807
H	8.96033	-0.76316	1.23440
H	8.68116	-0.95372	2.97288
H	8.11539	-6.94501	-2.55769
H	8.12153	-5.60349	-1.39765
H	1.35668	-1.88457	-2.23505
H	-4.78778	-0.90579	-0.56045
C	-6.66794	-3.39894	0.35798
O	-6.52090	-4.71338	-0.05260
C	-5.40058	-2.95272	1.09438
O	-5.28104	-3.67859	2.30719
C	-5.46508	-1.44110	1.37245
O	-4.24179	-1.09209	2.01028
C	-5.65758	-0.68931	0.05973
C	-6.92317	-1.14487	-0.67227
O	-6.83430	-2.58301	-0.84033
C	-7.04759	-0.51044	-2.05330
O	-5.80111	-0.46559	-2.76715
H	-4.58323	-3.22696	2.81233
H	-4.14305	-0.12085	1.96575
H	-5.50436	-1.38139	-2.90427
H	-7.55247	-3.26100	0.99965
H	-4.54535	-3.15173	0.43036
H	-6.31417	-1.23915	2.04584
H	-7.81637	-0.88738	-0.08254
H	-7.80334	-1.04933	-2.63630
H	-7.35277	0.53100	-1.94303
C	-4.72921	1.56304	-0.13877
O	-5.77599	0.72514	0.26406
C	-5.32219	2.91474	-0.52052
O	-6.09858	2.85524	-1.71575
C	-4.21824	3.97212	-0.67661
O	-4.77067	5.26433	-0.89397
C	-3.33977	4.04821	0.56688
C	-2.82849	2.67247	0.89961
O	-3.91080	1.72922	1.00859
C	-2.03226	2.61402	2.20542
O	-2.71887	3.14379	3.33268
H	-5.50999	2.53496	-2.42226
H	-5.41442	5.17089	-1.61718
H	-2.65558	4.11052	3.28739
H	-6.01587	3.22986	0.26421
H	-3.58024	3.68399	-1.52789
H	-3.96809	4.40905	1.39685
H	-2.15321	2.33437	0.10154
H	-1.82433	1.56342	2.43189
H	-1.07209	3.12163	2.04639
O	-2.22170	4.90639	0.37722
H	-7.37768	-5.01998	-0.39220
H	-2.58101	5.74536	0.04228
H	-4.55377	0.56585	-1.82232

E = -5037.90717255

3 triplet

N	-0.59359	-2.04044	1.75819
N	0.45444	-1.65834	-1.19352
N	0.86669	-2.92768	-2.95393
N	-1.40138	2.90476	2.45525
N	-1.16422	1.21590	1.07158
N	-4.76545	4.05245	0.30041
N	-3.14473	3.99540	-1.18977
N	-4.24829	1.03678	-3.65909
C	0.13810	-3.29314	1.59503
C	0.57188	-3.91633	2.92093
C	1.34614	-3.14343	0.67695
C	1.03602	-2.83816	-0.75328
C	1.29180	-3.62916	-1.84376
C	0.37182	-1.75290	-2.51753
C	0.94021	-3.37464	-4.34079
C	-3.84089	3.56009	4.24413
C	-3.27188	2.15605	4.01109
C	-2.37434	1.98931	2.81828
C	-2.21032	0.94722	1.93707
C	-0.69855	2.40973	1.41208
C	-6.37836	6.81532	0.50757
C	-4.93712	6.50703	0.91252
C	-4.33342	5.36196	0.16505
C	-3.32797	5.29692	-0.76747
C	-4.02715	3.26887	-0.52572
C	-8.17010	-1.21013	-1.90647
C	-6.90011	-0.35923	-1.76559
C	-5.91131	-0.60246	-2.92107
C	-4.62679	0.16875	-2.71838
C	-7.32579	-6.54472	1.86052
C	-6.21611	-5.85386	2.65544
C	-5.37498	-4.96004	1.76446
C	-5.59687	-3.57995	1.68920
C	-4.40498	-5.50730	0.90942
C	-4.90527	-2.77481	0.78030
C	-3.71161	-4.72271	-0.00870
C	-3.97572	-3.34914	-0.09544
O	0.28602	-3.45958	4.00784

O	-3.95908	-0.00480	-1.66400
O	-3.30506	-2.63143	-1.04326
O	1.21444	0.08489	0.95858
O	-1.83466	2.63402	-3.09667
O	-1.31120	0.40539	-1.75771
O	4.01417	1.04975	1.27590
Cu	-0.19199	-0.06779	-0.16351
H	-4.30808	7.38678	0.73755
H	-4.89348	6.31109	1.99301
H	-2.72915	6.10885	-1.15620
H	-2.23717	3.27305	-2.42320
H	-4.15799	2.19855	-0.60630
H	-6.76351	7.66736	1.07783
H	-6.40304	-0.58800	-0.81823
H	-7.16615	0.70550	-1.73701
H	-6.37299	-0.35106	-3.88194
H	-5.64388	-1.66674	-2.95308
H	-7.92836	-2.27939	-1.90153
H	-6.65650	-5.26087	3.46647
H	-5.58188	-6.61377	3.13055
H	-4.19875	-6.57499	0.95134
H	-6.33159	-3.11977	2.34684
H	-2.97773	-5.16083	-0.67919
H	-5.09033	-1.70406	0.74460
H	-3.65077	-1.71257	-1.09660
H	-6.90773	-7.16279	1.05776
H	-1.25964	-2.15221	2.52264
H	-0.53969	-4.03935	1.14483
H	1.15868	-4.85702	2.83360
H	1.99366	-2.35463	1.08235
H	1.92725	-4.07269	0.70161
H	1.73548	-4.61003	-1.92327
H	-0.06067	-1.00808	-3.16488
H	0.52446	-2.59793	-4.98386
H	0.36467	-4.29474	-4.46915
H	1.98098	-3.55480	-4.62169
H	-4.41762	3.90963	3.38139
H	-4.09166	1.43687	3.90608
H	-2.71998	1.84884	4.91099
H	-2.75956	0.01934	1.88065
H	-1.23324	3.79953	2.89528
H	0.11712	2.94171	0.94584
H	-1.29959	3.15743	-3.71302
H	-2.28689	0.25113	-1.66774
H	-1.25491	1.29934	-2.18479
H	-3.39401	1.59929	-3.56285
H	-4.81192	1.16769	-4.48767
H	-5.51131	3.73055	0.90268
H	-4.50239	3.55236	5.11565
H	-3.05227	4.29536	4.44274
H	-7.04283	5.96393	0.69532
H	-6.44296	7.06095	-0.55783
H	-8.86086	-1.01761	-1.07859
H	-8.69763	-0.98880	-2.84177
H	-7.93159	-7.19397	2.50422
H	-7.99366	-5.80835	1.39862
H	0.06733	-1.31567	2.04667
H	4.85194	-0.86227	0.59701
C	6.76445	-3.31198	-0.37066
O	6.64337	-4.63739	0.01058
C	5.48727	-2.87242	-1.09397
O	5.37038	-3.57831	-2.31894
C	5.53127	-1.35596	-1.34521
O	4.30010	-1.00960	-1.97043
C	5.71713	-0.62351	-0.02100
C	6.98386	-1.07607	0.70632
O	6.91329	-2.51859	0.84597
C	7.11033	-0.46494	2.09732
O	5.87037	-0.44245	2.82249
H	4.67392	-3.11831	-2.81833
H	4.20124	-0.03849	-1.92347
H	5.58175	-1.36241	2.94830
H	7.64589	-3.14136	-1.00864
H	4.63825	-3.09485	-0.42936
H	6.37441	-1.13117	-2.01865
H	7.87493	-0.79890	0.12167
H	7.87577	-1.00694	2.66461
H	7.40580	0.58091	2.00297
C	4.74785	1.60020	0.22666
O	5.81249	0.79527	-0.20527
C	5.31263	2.95754	0.64442
O	6.09422	2.88568	1.83584
C	4.18808	3.98740	0.82736
O	4.71187	5.28472	1.08154
C	3.30765	4.07916	-0.41318
C	2.81957	2.70214	-0.77397
O	3.92186	1.78057	-0.91078
C	2.03364	2.66361	-2.08777
O	2.71477	3.24561	-3.19280
H	5.51059	2.56727	2.54709
H	5.35767	5.18648	1.80226
H	2.62038	4.20827	-3.12290
H	5.99852	3.30378	-0.13402
H	3.55447	3.66101	1.66840
H	3.91873	4.48200	-1.23536
H	2.15986	2.31832	0.01434
H	1.85703	1.61590	-2.35036
H	1.05830	3.14076	-1.92523
O	2.16370	4.89905	-0.18976
H	7.50578	-4.93457	0.34429
H	2.49547	5.72777	0.19588
H	4.62808	0.59828	1.90473

E = -5037.91562941

4 singlet (for mechanism 1)

N	0.58905	-2.01130	-1.67519
N	-0.64651	-1.26966	1.01526
N	-0.78077	-2.22866	3.00741
N	0.75690	2.29832	-3.56863
N	0.46966	1.07007	-1.75405
N	4.74043	4.07693	-0.30419
N	3.17621	4.04024	1.24910
N	4.17104	1.02193	3.65119
C	-0.06666	-3.31309	-1.42311
C	-0.50404	-3.98200	-2.71891
C	-1.27413	-3.15671	-0.50569
C	-1.00288	-2.59696	0.84823
C	-1.09100	-3.19873	2.07777
C	-0.52082	-1.08844	2.32548
C	-0.77116	-2.38968	4.45641
C	3.85887	3.52468	-4.19024
C	3.29972	2.12062	-3.93303
C	2.02975	1.92873	-3.16201
C	1.82246	1.17600	-2.03787
C	-0.14525	1.76277	-2.70271
C	6.37766	6.85909	-0.51128
C	4.93810	6.53365	-0.90904
C	4.34122	5.39439	-0.14309
C	3.37166	5.34093	0.82877
C	4.01577	3.30306	0.54410
C	8.23130	-1.11248	2.03113
C	6.95466	-0.27342	1.87812
C	5.96965	-0.52600	3.03673
C	4.62712	0.12108	2.77638
C	7.42047	-6.51418	-1.64678
C	6.30458	-5.84446	-2.45119
C	5.40733	-4.98778	-1.58011
C	5.63632	-3.61441	-1.42835
C	4.36150	-5.55620	-0.83673
C	4.87406	-2.83621	-0.55520
C	3.59421	-4.79784	0.04581
C	3.86005	-3.43126	0.20736
O	-0.42052	-3.44613	-3.80470
O	3.98692	-0.18435	1.73948
O	3.10728	-2.73141	1.10594
O	1.74469	2.52570	2.99944
O	1.55171	0.71059	0.92635
O	-3.90021	1.10436	-1.18663
Cu	0.10446	-0.27320	-0.42332
H	4.30348	7.41175	-0.74610
H	4.89313	6.32081	-1.98608
H	2.80410	6.16188	1.24476
H	2.19240	3.22210	2.42702
H	4.12061	2.22918	0.60435
H	6.75565	7.70515	-1.09528
H	6.46026	-0.52004	0.93362
H	7.20548	0.79441	1.84025
H	6.39715	-0.18577	3.98619
H	5.78990	-1.60511	3.12713
H	7.99744	-2.18346	2.02537
H	6.74554	-5.22760	-3.24430
H	5.70708	-6.61683	-2.95285
H	4.15045	-6.61877	-0.93954
H	6.43042	-3.13921	-2.00088
H	2.80299	-5.25400	0.63437
H	5.06515	-1.77122	-0.45540
H	3.50597	-1.84457	1.26009
H	7.00753	-7.16049	-0.86365
H	1.59426	-2.16878	-1.75524
H	0.65183	-3.98674	-0.93683
H	-0.93607	-4.99695	-2.61186
H	-2.00384	-2.50758	-1.01176
H	-1.76011	-4.13357	-0.39141
H	-1.34382	-4.20734	2.36793
H	-0.21684	-0.17331	2.80833
H	-0.41241	-1.46514	4.91100
H	-0.10484	-3.20884	4.73785
H	-1.77980	-2.60050	4.82226
H	4.03907	4.06166	-3.25255
H	4.05996	1.53784	-3.39957
H	3.18378	1.61907	-4.90537
H	2.56458	0.71000	-1.41010
H	0.52417	2.85927	-4.37727
H	-1.21184	1.90582	-2.79111
H	1.21361	3.00405	3.65484
H	2.40088	0.35601	1.27287
H	1.30886	1.39609	1.58200
H	3.28094	1.51605	3.50202
H	4.72384	1.27150	4.45931
H	5.45256	3.74440	-0.94059
H	4.80704	3.44599	-4.73087
H	3.17871	4.13398	-4.79654
H	7.04793	6.00950	-0.68595
H	6.44136	7.12198	0.55007
H	8.92959	-0.91598	1.21030
H	8.74832	-0.88639	2.97125
H	8.05796	-7.13087	-2.29152
H	8.05618	-5.76631	-1.15855
H	0.30623	-1.71324	-2.61297
H	-4.80340	-0.91865	-0.60677
C	-6.68976	-3.34765	0.55277
O	-6.54243	-4.67646	0.18255
C	-5.41489	-2.88697	1.26696
O	-5.33588	-3.52091	2.53295
C	-5.41131	-1.36263	1.42336
O	-4.16566	-1.01979	2.02110
C	-5.61861	-0.67241	0.07649
C	-6.92706	-1.13128	-0.56019
O	-6.88900	-2.57786	-0.65384
C	-7.13530	-0.65004	-1.99226

O	-6.13195	-1.15299	-2.86437
H	-4.62503	-3.05938	3.01011
H	-4.11200	-0.04630	2.06198
H	-6.12096	-2.11458	-2.71734
H	-7.56047	-3.19910	1.21146
H	-4.56292	-3.17411	0.63025
H	-6.24046	-1.07722	2.09120
H	-7.77372	-0.80754	0.06439
H	-8.13852	-0.95988	-2.32069
H	-7.08050	0.44064	-2.02172
C	-4.67446	1.58282	-0.12098
O	-5.71751	0.74403	0.26316
C	-5.28519	2.91480	-0.56717
O	-6.05424	2.79545	-1.75901
C	-4.18393	3.97008	-0.76058
O	-4.73865	5.25880	-0.98920
C	-3.28699	4.06818	0.46922
C	-2.78780	2.70070	0.85122
O	-3.88320	1.78687	1.03802
C	-1.95997	2.70567	2.14144
O	-2.57035	3.39712	3.22335
H	-5.49130	2.35419	-2.41971
H	-5.35589	5.16704	-1.73510
H	-2.42715	4.34554	3.07747
H	-5.97778	3.24163	0.21246
H	-3.56104	3.66746	-1.61708
H	-3.90094	4.46101	1.29492
H	-2.13220	2.31992	0.05601
H	-1.83322	1.66864	2.46611
H	-0.96689	3.11329	1.91673
O	-2.15933	4.90454	0.24517
H	-7.40555	-5.00097	-0.12255
H	-2.50926	5.74125	-0.10515
H	-3.24396	0.46604	-0.85158

E = -4962.75498342

[Cu(II)]-O· singlet

N	-1.81344	-1.49337	1.38104
N	-1.74348	-2.61247	-1.34968
N	-3.10366	-2.44257	-3.07517
N	2.85267	-2.46487	2.74947
N	1.31348	-2.22031	1.20193
N	4.97725	1.32996	0.09631
N	4.35966	-0.09863	-1.46484
N	1.23570	1.66145	-3.54054
C	-3.13320	-2.14678	1.49021
C	-3.35251	-2.66055	2.90385
C	-3.28856	-3.29665	0.50045
C	-3.02348	-2.91644	-0.92100
C	-3.87527	-2.81139	-1.99030
C	-1.82916	-2.33163	-2.64186
C	-3.57975	-2.21208	-4.43507
C	4.53426	0.16868	3.87249
C	3.03184	-0.08737	3.70573
C	2.55211	-1.11108	2.72720
C	1.59697	-0.98720	1.75254
C	2.08927	-3.09408	1.82354
C	8.02803	2.23820	0.06372
C	7.45082	0.86475	0.40944
C	6.11691	0.60786	-0.22249
C	5.70380	-0.27004	-1.19536
C	3.95292	0.87278	-0.66775
C	0.42323	5.78238	-1.68929
C	0.51624	4.25168	-1.63104
C	-0.10969	3.58114	-2.87777
C	0.14643	2.08700	-2.88570
C	-4.74905	5.78627	2.38710
C	-4.25828	4.50854	3.07006
C	-3.90985	3.44536	2.04916
C	-2.59741	3.28316	1.59067
C	-4.90999	2.66518	1.44790
C	-2.29197	2.40960	0.54583
C	-4.62641	1.79497	0.39724
C	-3.31471	1.68612	-0.08264
O	-2.57058	-2.47168	3.81325
O	-0.59920	1.29289	-2.26625
O	-3.07781	0.86172	-1.14578
O	-0.15483	-4.33797	0.17158
O	2.33398	-0.99946	-3.01756
O	0.52284	-0.85580	-1.04564
Cu	-0.19972	-2.51942	-0.07955
H	8.13557	0.07798	0.07494
H	7.37338	0.76125	1.50053
H	6.29466	-1.01248	-1.71353
H	3.18578	-0.76765	-2.52716
H	2.94661	1.26078	-0.60515
H	9.00535	2.37561	0.53867
H	0.01229	3.88098	-0.73240
H	1.56976	3.95282	-1.55260
H	0.30300	4.03739	-3.78505
H	-1.19206	3.74257	-2.88460
H	-0.61956	6.11353	-1.75756
H	-3.38023	4.73415	3.68792
H	-5.03533	4.13793	3.75125
H	-5.93776	2.75757	1.79312
H	-1.79603	3.85940	2.04888
H	-5.41267	1.21795	-0.08117
H	-1.26907	2.29725	0.19893
H	-2.21279	1.09851	-1.55038
H	-5.64206	5.59040	1.78265
H	-1.93510	-0.53684	1.05323
H	-3.93921	-1.41920	1.30576
H	-4.28548	-3.23651	3.06074
H	-2.58095	-4.09053	0.77054

H	-4.29982	-3.71115	0.58150
H	-4.93984	-2.96705	-2.07691
H	-1.00907	-2.04603	-3.28321
H	-2.73179	-1.93459	-5.06261
H	-4.31302	-1.40183	-4.44263
H	-4.03790	-3.12150	-4.83172
H	4.99624	0.47361	2.92743
H	2.54312	0.85253	3.42382
H	2.61953	-0.34159	4.69363
H	1.09583	-0.09451	1.41339
H	3.51810	-2.92130	3.35945
H	2.11821	-4.15590	1.63157
H	2.51637	-1.79315	-3.54413
H	-0.02478	-0.16522	-1.48804
H	1.21252	-1.08397	-1.72167
H	1.54178	0.68365	-3.50366
H	1.83608	2.32227	-4.01388
H	4.91727	2.07637	0.77595
H	4.68986	0.96612	4.60543
H	5.06556	-0.72027	4.23166
H	7.37624	3.04943	0.40807
H	8.15648	2.34878	-1.01832
H	0.86017	6.23231	-0.79132
H	0.95926	6.17783	-2.55989
H	-5.00339	6.55843	3.12324
H	-3.98022	6.19464	1.72090
H	-1.42257	-1.42970	2.32378

E = -3664.78079186

[Cu(II)]-O· triplet

N	-1.79057	-1.51634	1.34245
N	-1.80012	-2.52166	-1.36593
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N	2.77841	-2.51973	2.74915
N	1.23287	-2.20804	1.22291
N	4.99776	1.28092	0.09585
N	4.38009	-0.12926	-1.48230
N	1.25588	1.68064	-3.52423
C	-3.11855	-2.16225	1.47818
C	-3.30503	-2.68085	2.89468
C	-3.28090	-3.30262	0.47860
C	-3.06059	-2.88906	-0.94016
C	-3.92803	-2.78664	-1.99708
C	-1.90620	-2.20414	-2.64629
C	-3.67644	-2.09721	-4.42251
C	4.56395	0.10268	3.86060
C	3.06013	-0.14616	3.69557
C	2.54825	-1.15198	2.71766
C	1.58824	-0.98672	1.75429
C	1.96875	-3.11715	1.84108
C	8.05555	2.19291	0.06117
C	7.47402	0.81863	0.39615
C	6.13924	0.56793	-0.23682
C	5.72596	-0.29834	-1.22011
C	3.97237	0.82935	-0.67048
C	0.45977	5.78148	-1.63982
C	0.54708	4.24997	-1.59550
C	-0.07915	3.60421	-2.85544
C	0.15554	2.10741	-2.88851
C	-4.70172	5.76854	2.45022
C	-4.21403	4.48290	3.12042
C	-3.87313	3.42643	2.08986
C	-2.56565	3.27427	1.61352
C	-4.87607	2.64223	1.49874
C	-2.26837	2.40589	0.56212
C	-4.60055	1.77689	0.44169
C	-3.29442	1.67750	-0.05489
O	-2.49347	-2.50686	3.78037
O	-0.61825	1.31076	-2.30863
O	-3.06486	0.85454	-1.12122
O	0.00511	-4.29606	-0.08180
O	2.33384	-0.99174	-3.03850
O	0.52451	-0.80494	-1.04735
Cu	-0.27470	-2.49606	-0.05981
H	8.15703	0.03281	0.05581
H	7.39656	0.70694	1.48643
H	6.31797	-1.03146	-1.75016
H	3.19113	-0.77891	-2.55181
H	2.96394	1.21006	-0.59791
H	9.03298	2.32367	0.53780
H	0.03694	3.87159	-0.70368
H	1.59851	3.94442	-1.51712
H	0.34557	4.06950	-3.75259
H	-1.15907	3.78070	-2.86669
H	-0.58168	6.11630	-1.71038
H	-3.33308	4.69986	3.73729
H	-4.99023	4.10942	3.80094
H	-5.89988	2.72729	1.85728
H	-1.76200	3.85400	2.06324
H	-5.38935	1.19672	-0.02870
H	-1.24941	2.30057	0.20163
H	-2.21128	1.10211	-1.54320
H	-5.59732	5.58149	1.84679
H	-1.91329	-0.56060	1.01075
H	-3.92001	-1.42836	1.30724
H	-4.24090	-3.24420	3.07495
H	-2.56182	-4.09497	0.72591
H	-4.28218	-3.73642	0.58122
H	-4.98638	-2.98143	-2.08091
H	-1.10361	-1.86491	-3.28358
H	-2.84369	-1.77381	-5.04843
H	-4.43514	-1.31092	-4.39960
H	-4.10885	-3.00843	-4.84319
H	5.02532	0.41517	2.91767

H	2.57901	0.80180	3.42686
H	2.65243	-0.40188	4.68533
H	1.12863	-0.07218	1.41409
H	3.42621	-3.00390	3.35663
H	1.92310	-4.17795	1.65155
H	2.49806	-1.78834	-3.56650
H	-0.01977	-0.12588	-1.50897
H	1.20873	-1.05282	-1.71887
H	1.54980	0.69855	-3.50027
H	1.87775	2.34368	-3.96570
H	4.93723	2.01735	0.78621
H	4.72260	0.89286	4.60067
H	5.09324	-0.79150	4.20972
H	7.40581	3.00340	0.41119
H	8.18504	2.31131	-1.01993
H	0.89362	6.22286	-0.73606
H	1.00122	6.18258	-2.50442
H	-4.95070	6.53506	3.19401
H	-3.93334	6.17983	1.78531
H	-1.38414	-1.44953	2.27906

E =-3664.78460514

5 singlet

N	-1.42534	-1.74128	1.72561
N	-0.27517	-2.14875	-0.85052
N	-1.01545	-3.34622	-2.54373
N	0.93662	2.08127	3.39836
N	0.37130	0.83645	1.68396
N	-1.47934	5.57331	0.07541
N	-0.26686	4.45734	-1.38866
N	-2.79257	1.99842	-3.66544
C	-1.30985	-3.20942	1.86425
C	-1.08286	-3.57106	3.32534
C	-0.19427	-3.80465	1.01115
C	-0.45937	-3.44896	-0.41520
C	-0.92870	-4.19733	-1.46152
C	-0.60995	-2.12683	-2.13383
C	-1.40167	-3.72325	-3.89758
C	-0.93932	4.86395	3.98890
C	-1.22753	3.36519	3.84901
C	-0.34270	2.47865	3.04578
C	-0.66750	1.69422	1.97178
C	1.32857	1.09003	2.56583
C	-1.18715	8.71888	-0.02036
C	-0.16043	7.70018	0.47737
C	-0.35405	6.35140	-0.14818
C	0.38016	5.63437	-1.06182
C	-1.38354	4.45244	-0.68318
C	-7.03005	2.83308	-2.18597
C	-5.58402	2.37158	-1.95357
C	-5.07354	1.41184	-3.05379
C	-3.57828	1.22130	-2.91330
C	-9.33895	-1.83198	1.84833
C	-8.04789	-1.80723	2.67542
C	-6.82994	-1.87765	1.77941
C	-6.13599	-0.72223	1.40412
C	-6.42750	-3.09413	1.20529
C	-5.10808	-0.76206	0.46026
C	-5.41134	-3.15333	0.25480
C	-4.76566	-1.97694	-0.14967
O	-1.04056	-2.75172	4.22105
O	-3.10175	0.41833	-2.07281
O	-3.81519	-2.06329	-1.12443
O	-0.03161	2.24374	-2.94818
O	-0.67308	0.64792	-0.87233
Cu	0.19582	-0.68553	0.42463
H	0.85276	8.04055	0.23910
H	-0.21280	7.62130	1.57166
H	1.33313	5.89681	-1.49962
H	-0.01347	3.12783	-2.46053
H	-2.13314	3.67448	-0.68684
H	-1.01458	9.69824	0.43908
H	-5.50153	1.87593	-0.98086
H	-4.92939	3.25256	-1.91711
H	-5.31158	1.82006	-4.04260
H	-5.56471	0.43798	-2.96439
H	-7.71932	1.98115	-2.21769
H	-8.01456	-0.89284	3.28046
H	-8.05136	-2.65045	3.37840
H	-6.93689	-4.01243	1.49048
H	-6.41125	0.23362	1.84548
H	-5.12693	-4.09554	-0.20494
H	-4.58575	0.14552	0.17272
H	-3.61468	-1.16069	-1.46406
H	-9.40678	-2.75069	1.25474
H	-2.34189	-1.51069	1.34540
H	-2.25365	-3.69388	1.57394
H	-0.94069	-4.65000	3.53000
H	0.77269	-3.40229	1.32441
H	-0.17595	-4.89325	1.12643
H	-1.17246	-5.24551	-1.53936
H	-0.58032	-1.26499	-2.78095
H	-1.43150	-2.82803	-4.52046
H	-2.39133	-4.18576	-3.88677
H	-0.67069	-4.42598	-4.30592
H	-0.90992	5.35929	3.01258
H	-2.23143	3.24939	3.42315
H	-1.29803	2.93902	4.86085
H	-1.58275	1.68140	1.40163
H	1.48365	2.43963	4.17032
H	2.27051	0.57056	2.63523
H	0.64228	2.29367	-3.64338
H	-1.54724	0.48606	-1.30680
H	-0.15087	1.12822	-1.55808

H	-1.77520	2.03188	-3.51616
H	-3.20179	2.66384	-4.30660
H	-2.24960	5.80453	0.68859
H	-1.72691	5.33022	4.58847
H	0.01781	5.05574	4.48745
H	-2.21089	8.41472	0.22594
H	-1.12513	8.83710	-1.10732
H	-7.35677	3.49949	-1.38054
H	-7.12354	3.37665	-3.13322
H	-10.22494	-1.78085	2.49267
H	-9.37509	-0.98414	1.15463
H	-1.40067	-1.34719	2.66958
C	3.19632	-5.12930	-0.94766
O	2.26775	-6.12984	-0.67500
C	2.47623	-3.94159	-1.59616
O	2.00174	-4.31477	-2.88374
C	3.46922	-2.75515	-1.72246
O	2.78397	-1.70207	-2.39498
C	3.93443	-2.35379	-0.32605
C	4.60246	-3.54214	0.36081
O	3.75570	-4.70832	0.30333
C	4.82517	-3.28932	1.85890
O	3.63525	-3.11014	2.60150
H	1.85698	-3.47781	-3.35761
H	3.30440	-0.88316	-2.27601
H	3.06353	-2.42844	2.18421
H	4.00038	-5.49525	-1.60824
H	1.66050	-3.64758	-0.94237
H	4.33541	-3.07510	-2.32617
H	3.03450	-2.06236	0.23681
H	5.57315	-3.73935	-0.12180
H	5.33018	-4.16094	2.28727
H	5.50557	-2.43084	1.95545
C	4.40313	-0.00018	0.08828
O	4.87925	-1.26384	-0.29398
C	5.48065	0.75363	0.90573
O	5.54427	0.28457	2.25107
C	5.21889	2.26349	0.99090
O	6.35952	2.95585	1.48238
C	4.86456	2.83814	-0.37663
C	3.68715	2.05052	-0.89720
O	4.11395	0.70191	-1.12731
C	3.16416	2.63384	-2.21667
O	4.18737	3.08466	-3.09262
H	6.12927	-0.48797	2.27943
H	6.56249	2.57632	2.35391
H	4.54283	3.89827	-2.69646
H	6.44278	0.60984	0.39543
H	4.36214	2.43176	1.66321
H	5.71010	2.69065	-1.06194
H	2.86283	2.05788	-0.16749
H	2.61829	1.84831	-2.74533
H	2.46280	3.44308	-1.98045
O	4.51165	4.21560	-0.30457
H	2.75447	-6.89707	-0.33101
H	5.22367	4.65306	0.19314
O	1.75305	-1.39013	1.23662
H	3.48149	-0.10578	0.67443

E= -4962.67742836

5 triplet

N	-1.47015	-1.77104	1.65956
N	-0.22643	-2.15816	-0.84932
N	-0.96935	-3.34493	-2.54814
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N	0.36441	0.84946	1.67473
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N	-0.30763	4.45293	-1.39542
N	-2.80958	1.97353	-3.67652
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C	-1.01636	-3.50187	3.33176
C	-0.16539	-3.81042	1.00960
C	-0.42551	-3.45743	-0.41746
C	-0.89577	-4.19947	-1.46745
C	-0.55436	-2.13004	-2.13427
C	-1.34625	-3.71711	-3.90602
C	-0.98924	4.85159	3.98573
C	-1.26425	3.35037	3.84564
C	-0.36823	2.47740	3.04256
C	-0.67845	1.70263	1.95762
C	1.31094	1.09805	2.56886
C	-1.26589	8.70392	-0.02414
C	-0.23093	7.69422	0.47488
C	-0.41210	6.34435	-0.15212
C	0.32905	5.63486	-1.06606
C	-1.42507	4.43776	-0.69137
C	-7.05488	2.76740	-2.19607
C	-5.60515	2.31850	-1.96194
C	-5.08581	1.36760	-3.06555
C	-3.58928	1.18921	-2.92547
C	-9.32784	-1.91726	1.83594
C	-8.03801	-1.88123	2.66453
C	-6.81569	-1.93205	1.77519
C	-6.15267	-0.76211	1.38856
C	-6.37293	-3.14544	1.22595
C	-5.11081	-0.78786	0.46097
C	-5.34114	-3.19059	0.29136
C	-4.72202	-2.00285	-0.11890
O	-1.03921	-2.64465	4.19228
O	-3.10617	0.38956	-2.08597
O	-3.73875	-2.07701	-1.06367
O	-0.05084	2.24259	-2.95998
O	-0.68132	0.63406	-0.87840
Cu	0.19824	-0.70329	0.44216

H	0.77962	8.04353	0.23834
H	-0.28437	7.61419	1.56901
H	1.28024	5.90599	-1.50245
H	-0.04206	3.12523	-2.47037
H	-2.16821	3.65365	-0.69717
H	-1.10307	9.68459	0.43607
H	-5.52040	1.82010	-0.99096
H	-4.95836	3.20499	-1.92125
H	-5.32731	1.77765	-4.05275
H	-5.56873	0.38926	-2.98005
H	-7.73584	1.90905	-2.23342
H	-8.01820	-0.96976	3.27465
H	-8.03289	-2.72777	3.36347
H	-6.86005	-4.07294	1.51993
H	-6.46124	0.19185	1.81150
H	-5.02126	-4.13123	-0.14779
H	-4.60608	0.12810	0.16901
H	-3.57842	-1.17906	-1.43646
H	-9.38395	-2.83352	1.23728
H	-2.34092	-1.61099	1.15650
H	-2.21534	-3.76560	1.61977
H	-0.78461	-4.55590	3.57986
H	0.79789	-3.40044	1.32278
H	-0.13902	-4.89839	1.12829
H	-1.14896	-5.24512	-1.54899
H	-0.51329	-1.26710	-2.77907
H	-1.37891	-2.81878	-4.52427
H	-2.33294	-4.18594	-3.90236
H	-0.60888	-4.41320	-4.31432
H	-0.96284	5.34650	3.00908
H	-2.26623	3.22564	3.41779
H	-1.33217	2.92273	4.85697
H	-1.58761	1.69148	1.37780
H	1.44575	2.43498	4.18653
H	2.25319	0.57967	2.64520
H	0.61933	2.30456	-3.65786
H	-1.55050	0.47102	-1.32085
H	-0.15776	1.12156	-1.55647
H	-1.79257	2.01549	-3.52597
H	-3.22393	2.63630	-4.31712
H	-2.30384	5.78032	0.68187
H	-1.78098	5.31227	4.58428
H	-0.03403	5.05133	4.48489
H	-2.28728	8.39038	0.22016
H	-1.20301	8.82323	-1.11093
H	-7.39033	3.42724	-1.38882
H	-7.15090	3.31407	-3.14130
H	-10.21468	-1.88027	2.47994
H	-9.37391	-1.06616	1.14672
H	-1.57900	-1.34741	2.58384
C	3.23888	-5.10570	-0.94515
O	2.31971	-6.11547	-0.67541
C	2.50924	-3.92435	-1.59459
O	2.04058	-4.30040	-2.88366
C	3.49328	-2.72990	-1.71919
O	2.80025	-1.68240	-2.39299
C	3.95225	-2.32338	-0.32224
C	4.62964	-3.50628	0.36482
O	3.78923	-4.67779	0.30826
C	4.85864	-3.25491	1.86095
O	3.67106	-3.08537	2.61008
H	1.89863	-3.46447	-3.36021
H	3.31485	-0.85967	-2.27541
H	3.08789	-2.41951	2.18588
H	4.04934	-5.46332	-1.60240
H	1.69042	-3.63887	-0.94181
H	4.36243	-3.04337	-2.32196
H	3.05321	-2.03992	0.23991
H	5.59969	-3.69848	-0.12134
H	5.37214	-4.12336	2.28564
H	5.53342	-2.39173	1.95564
C	4.40043	0.03339	0.09134
O	4.88887	-1.22529	-0.29053
C	5.46982	0.79701	0.91041
O	5.53523	0.32829	2.25570
C	5.19492	2.30454	0.99515
O	6.32918	3.00679	1.48742
C	4.83712	2.87599	-0.37285
C	3.66721	2.07812	-0.89472
O	4.10558	0.73289	-1.12398
C	3.13973	2.65603	-2.21456
O	4.15982	3.11117	-3.09206
H	6.12545	-0.44025	2.28465
H	6.53351	2.63086	2.36017
H	4.50989	3.92836	-2.69857
H	6.43372	0.66137	0.40127
H	4.33615	2.46559	1.66665
H	5.68477	2.73586	-1.05718
H	2.84219	2.07829	-0.16570
H	2.59750	1.86673	-2.74132
H	2.43398	3.46163	-1.97905
O	4.47208	4.25019	-0.30118
H	2.81306	-6.87798	-0.33037
H	5.17946	4.69372	0.19779
O	1.73205	-1.39464	1.27432
H	3.47976	-0.07919	0.67787

E = -4962.68085167

TS-5 singlet

N	-1.29497	-1.91175	1.62388
N	0.06096	-2.09110	-0.79167
N	-0.69085	-3.10071	-2.59867
N	0.72964	2.10693	3.51395
N	0.30011	0.65687	1.93682

N	-1.84479	5.34335	0.11347
N	-0.58847	4.40977	-1.43926
N	-2.83710	1.70691	-3.84310
C	-1.17413	-3.38649	1.76322
C	-0.99095	-3.75031	3.22626
C	-0.00756	-3.89388	0.92183
C	-0.19995	-3.41366	-0.47793
C	-0.67468	-4.04623	-1.59410
C	-0.23573	-1.94330	-2.07653
C	-1.05504	-3.33980	-3.98996
C	-1.38516	4.66513	3.98981
C	-1.56894	3.15229	3.82727
C	-0.57851	2.32357	3.12832
C	-0.82366	1.41282	2.14392
C	1.23069	1.09388	2.77379
C	-1.83003	8.54639	0.02318
C	-0.74469	7.59297	0.52582
C	-0.82252	6.24726	-0.13283
C	-0.05968	5.64153	-1.10212
C	-1.66227	4.26030	-0.68473
C	-7.22576	2.30803	-2.30955
C	-5.75562	1.94240	-2.05870
C	-5.09340	1.07755	-3.15063
C	-3.59182	1.08570	-2.93308
C	-9.27690	-2.55444	1.62977
C	-8.00382	-2.45322	2.47847
C	-6.75350	-2.29348	1.64765
C	-6.20752	-1.02804	1.40356
C	-6.12961	-3.40356	1.06023
C	-5.08289	-0.86622	0.59588
C	-5.01196	-3.26022	0.24072
C	-4.49165	-1.98485	-0.00252
O	-1.05286	-2.94181	4.13001
O	-3.08968	0.58842	-1.89335
O	-3.37486	-1.87758	-0.78986
O	-0.13889	2.27601	-3.08949
O	-0.51222	0.75189	-0.81398
Cu	0.41044	-0.73059	0.61255
H	0.24603	8.01249	0.32100
H	-0.81668	7.48483	1.61622
H	0.83643	6.02017	-1.57382
H	-0.22620	3.13961	-2.57738
H	-2.31613	3.39990	-0.67651
H	-1.74511	9.52293	0.51244
H	-5.66502	1.42051	-1.10148
H	-5.18192	2.87423	-1.95752
H	-5.33862	1.45978	-4.14768
H	-5.45675	0.04546	-3.09086
H	-7.85413	1.41335	-2.39447
H	-8.09641	-1.60525	3.16864
H	-7.92013	-3.35230	3.10312
H	-6.52992	-4.39880	1.24164
H	-6.66423	-0.15217	1.85959
H	-4.54074	-4.12127	-0.22474
H	-4.65485	0.11799	0.42993
H	-3.33408	-0.96809	-1.17335
H	-9.23008	-3.41289	0.94969
H	-2.08221	-1.71181	1.00589
H	-2.09433	-3.88750	1.42868
H	-0.79259	-4.82139	3.42542
H	0.94167	-3.51825	1.32390
H	0.03934	-4.98734	0.94593
H	-0.96831	-5.06952	-1.76866
H	-0.14440	-1.03302	-2.64515
H	-1.02630	-2.39318	-4.53135
H	-2.06425	-3.75439	-4.04484
H	-0.34629	-4.03923	-4.44110
H	-1.28396	5.16496	3.02044
H	-2.52291	2.98021	3.31398
H	-1.71507	2.73043	4.83425
H	-1.73402	1.25544	1.58743
H	1.22934	2.59932	4.24222
H	2.23013	0.70113	2.84395
H	0.50104	2.44577	-3.79827
H	-1.41915	0.64953	-1.18332
H	-0.03694	1.21141	-1.53848
H	-1.83443	1.86590	-3.66917
H	-3.26413	2.14948	-4.64472
H	-2.60590	5.47056	0.76732
H	-2.25427	5.08418	4.50558
H	-0.49647	4.91118	4.58281
H	-2.83415	8.15835	0.22905
H	-1.74530	8.69856	-1.05800
H	-7.61248	2.91291	-1.48269
H	-7.34022	2.88648	-3.23385
H	-10.16309	-2.67418	2.26383
H	-9.41591	-1.65422	1.01973
H	-1.51232	-1.52736	2.54558
C	3.49564	-4.96086	-0.99580
O	2.63240	-6.02731	-0.75016
C	2.70710	-3.81616	-1.64202
O	2.21996	-4.22339	-2.91454
C	3.68267	-2.61739	-1.80722
O	2.98401	-1.60091	-2.52423
C	4.07487	-2.18013	-0.40532
C	4.77012	-3.29951	0.35477
O	3.99613	-4.51742	0.27117
C	4.87411	-2.99808	1.85672
O	3.63539	-2.74686	2.48591
H	2.10139	-3.40112	-3.42036
H	3.44441	-0.75437	-2.37215
H	3.18728	-1.97106	2.05784
H	4.33458	-5.26486	-1.64421
H	1.90158	-3.54022	-0.97290
H	4.55745	-2.94307	-2.39471
H	3.14707	-1.92851	0.10601

H	5.78211	-3.46583	-0.05050
H	5.31194	-3.87243	2.35008
H	5.58250	-2.16486	1.98328
C	4.36106	0.20300	0.07076
O	4.93014	-1.00188	-0.32712
C	5.34454	1.03830	0.96742
O	5.41316	0.55855	2.30246
C	4.97178	2.52269	1.06532
O	6.05175	3.28299	1.59070
C	4.61103	3.09295	-0.30212
C	3.49809	2.23647	-0.85160
O	4.00783	0.91103	-1.09267
C	2.96061	2.79404	-2.17457
O	3.97240	3.28779	-3.04120
H	6.00477	-0.20953	2.32589
H	6.25937	2.91077	2.46428
H	4.27433	4.12811	-2.65735
H	6.32720	0.97036	0.47726
H	4.09054	2.61864	1.71934
H	5.47936	3.01204	-0.97047
H	2.66617	2.17338	-0.13648
H	2.45026	1.98894	-2.70783
H	2.22389	3.57182	-1.94160
O	4.16139	4.43912	-0.22127
H	3.16281	-6.75587	-0.38725
H	4.82995	4.91805	0.29818
O	2.26958	-0.75581	1.13491
H	3.28202	-0.08754	0.69254

E = -4962.65545893
Frequencies = =1575.2511

TS-5 triplet

N	-1.24464	-1.93971	1.60688
N	0.09731	-2.07939	-0.79311
N	-0.64760	-3.04363	-2.62602
N	0.68991	2.08946	3.54469
N	0.28683	0.61191	1.98568
N	-1.85990	5.27432	0.14951
N	-0.62213	4.44507	-1.47560
N	-2.86137	1.70291	-3.86339
C	-1.14306	-3.42379	1.72287
C	-0.97406	-3.81080	3.18145
C	0.03095	-3.90862	0.87853
C	-0.16115	-3.40915	-0.51423
C	-0.63242	-4.01550	-1.64605
C	-0.19718	-1.89798	-2.07344
C	-1.00680	-3.24747	-4.02442
C	-1.46486	4.60621	4.01338
C	-1.62801	3.09236	3.83861
C	-0.61924	2.28041	3.15099
C	-0.84729	1.35395	2.17767
C	1.20769	1.07413	2.81949
C	-1.95897	8.51265	0.07742
C	-0.86123	7.57001	0.57344
C	-0.89810	6.23738	-0.11517
C	-0.14588	5.69573	-1.12998
C	-1.65369	4.22074	-0.68170
C	-7.26787	2.22071	-2.30997
C	-5.79313	1.87300	-2.06069
C	-5.10340	1.03748	-3.15754
C	-3.60161	1.08848	-2.93644
C	-9.25624	-2.70037	1.58855
C	-7.98534	-2.58872	2.43922
C	-6.73509	-2.37301	1.62122
C	-6.22392	-1.08675	1.41153
C	-6.06848	-3.45173	1.02283
C	-5.08790	-0.87543	0.63158
C	-4.93911	-3.25843	0.22988
C	-4.45017	-1.96415	0.02671
O	-1.02611	-3.01253	4.09460
O	-3.08751	0.63159	-1.88447
O	-3.31239	-1.80943	-0.72396
O	-0.16274	2.33491	-3.15781
O	-0.45077	0.80409	-0.84118
Cu	0.44764	-0.81443	0.69702
H	0.12244	8.01683	0.39319
H	-0.94549	7.43489	1.65977
H	0.70823	6.13278	-1.62844
H	-0.25398	3.19493	-2.64250
H	-2.25700	3.32428	-0.66608
H	-1.89869	9.48005	0.58816
H	-5.69837	1.33968	-1.11023
H	-5.23694	2.81323	-1.94064
H	-5.35677	1.41923	-4.15275
H	-5.43589	-0.00573	-3.10774
H	-7.88406	1.31901	-2.40963
H	-8.10186	-1.76343	3.15296
H	-7.87856	-3.50197	3.03928
H	-6.44196	-4.46188	1.17677
H	-6.71482	-0.23439	1.87641
H	-4.43322	-4.09526	-0.24341
H	-4.68439	0.12392	0.49688
H	-3.29877	-0.90192	-1.11657
H	-9.18861	-3.53901	0.88582
H	-2.02322	-1.72078	0.98158
H	-2.06478	-3.90461	1.36691
H	-0.79601	-4.88759	3.36680
H	0.97550	-3.53291	1.29133
H	0.08770	-5.00198	0.88735
H	-0.92256	-5.03467	-1.84828
H	-0.10805	-0.97151	-2.61475
H	-0.98505	-2.28597	-4.53919
H	-2.01222	-3.66908	-4.09324
H	-0.29141	-3.92830	-4.49323

H	-1.35136	5.11372	3.04934
H	-2.57269	2.91238	3.31090
H	-1.78427	2.66366	4.84132
H	-1.75455	1.17602	1.62189
H	1.17960	2.59916	4.26780
H	2.21345	0.69835	2.89549
H	0.46466	2.51658	-3.87487
H	-1.36658	0.70248	-1.18204
H	-0.00836	1.27433	-1.57781
H	-1.86120	1.88567	-3.69786
H	-3.29890	2.11500	-4.67546
H	-2.59665	5.34308	0.83886
H	-2.34765	5.01254	4.51589
H	-0.58989	4.85915	4.62365
H	-2.95768	8.10071	0.26219
H	-1.86368	8.68943	-0.99911
H	-7.66399	2.80757	-1.47466
H	-7.38901	2.81152	-3.22561
H	-10.13762	-2.85972	2.22043
H	-9.41969	-1.78820	1.00279
H	-1.46530	-1.56810	2.53345
C	3.54984	-4.91277	-1.04430
O	2.70122	-5.99316	-0.81066
C	2.74641	-3.77371	-1.68210
O	2.27174	-4.17388	-2.96166
C	3.69911	-2.55547	-1.82705
O	2.98422	-1.54340	-2.53354
C	4.08072	-2.12894	-0.41879
C	4.80061	-3.24517	0.32065
O	4.03903	-4.47150	0.22925
C	4.93771	-2.96987	1.82363
O	3.71309	-2.74999	2.48911
H	2.14348	-3.34788	-3.45902
H	3.43448	-0.69197	-2.37838
H	3.24924	-1.97158	2.08272
H	4.39617	-5.19848	-1.69124
H	1.93218	-3.52281	-1.01393
H	4.58261	-2.85675	-2.41451
H	3.15197	-1.90348	0.10084
H	5.80655	-3.39414	-0.10662
H	5.40221	-3.84666	2.28755
H	5.63722	-2.12840	1.94719
C	4.33466	0.25465	0.07456
O	4.91840	-0.94068	-0.32785
C	5.31578	1.09499	0.96840
O	5.40336	0.60770	2.29942
C	4.92368	2.57342	1.07825
O	5.99371	3.34348	1.60961
C	4.55557	3.14960	-0.28539
C	3.45477	2.28256	-0.84271
O	3.97118	0.96111	-1.08463
C	2.91721	2.83887	-2.16609
O	3.92992	3.32958	-3.03405
H	5.99992	-0.15689	2.31071
H	6.20988	2.96281	2.47751
H	4.22584	4.17584	-2.65914
H	6.29453	1.04261	0.46831
H	4.04103	2.65247	1.73281
H	5.42621	3.08602	-0.95288
H	2.62006	2.21300	-0.13106
H	2.40475	2.03480	-2.69886
H	2.18180	3.61794	-1.93392
O	4.08688	4.48808	-0.19431
H	3.24084	-6.71798	-0.45383
H	4.74849	4.97221	0.32916
O	2.30814	-0.77282	1.22645
H	3.25646	-0.07429	0.72619

E = -4962.65535708

Frequencies = -1761.4579

6 singlet

N	-1.42460	-1.72717	1.75944
N	-0.27731	-2.12421	-0.82535
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N	0.94786	2.09416	3.43666
N	0.43105	0.90112	1.66880
N	-1.43918	5.58412	0.05606
N	-0.22570	4.46401	-1.40418
N	-2.77652	2.01317	-3.65578
C	-1.32068	-3.19931	1.86909
C	-1.11691	-3.59396	3.32617
C	-0.20730	-3.80166	1.01836
C	-0.46036	-3.42940	-0.40602
C	-0.93178	-4.16707	-1.45880
C	-0.61455	-2.08943	-2.10764
C	-1.42198	-3.66389	-3.88499
C	-0.90953	4.87470	3.98387
C	-1.20562	3.37735	3.84555
C	-0.31034	2.51304	3.04593
C	-0.60286	1.76879	1.93771
C	1.35432	1.11712	2.59799
C	-1.13113	8.72573	-0.03067
C	-0.11060	7.70214	0.46978
C	-0.30789	6.35562	-0.15943
C	0.42677	5.63628	-1.07097
C	-1.34632	4.46474	-0.70492
C	-7.00281	2.86870	-2.19660
C	-5.55955	2.39982	-1.96173
C	-5.06395	1.43545	-3.06514
C	-3.57224	1.22116	-2.92951
C	-9.34226	-1.77862	1.84055
C	-8.05224	-1.75967	2.66933
C	-6.83715	-1.85118	1.76993
C	-6.12706	-0.70824	1.38688

C	-6.45921	-3.07475	1.19368
C	-5.11005	-0.76565	0.43151
C	-5.45477	-3.15144	0.23212
C	-4.79578	-1.98596	-0.18329
O	-1.06911	-2.79301	4.23786
O	-3.10607	0.38499	-2.11657
O	-3.86556	-2.08855	-1.17519
O	-0.01629	2.22480	-2.93126
O	-0.73204	0.67349	-0.82811
Cu	0.16088	-0.66651	0.47553
H	0.90502	8.03867	0.23640
H	-0.16809	7.62140	1.56365
H	1.38345	5.89437	-1.50329
H	0.01601	3.11763	-2.46161
H	-2.10054	3.69138	-0.71455
H	-0.95668	9.70370	0.43101
H	-5.47958	1.90342	-0.98903
H	-4.89820	3.27563	-1.92760
H	-5.29802	1.85089	-4.05197
H	-5.56971	0.46906	-2.97772
H	-7.69589	2.01993	-2.22825
H	-8.00851	-0.84006	3.26557
H	-8.06416	-2.59671	3.37959
H	-6.98050	-3.98449	1.48482
H	-6.38222	0.25277	1.82917
H	-5.19149	-4.09870	-0.22982
H	-4.57785	0.13369	0.13622
H	-3.64733	-1.18907	-1.51188
H	-9.41881	-2.70217	1.25575
H	-2.35676	-1.48294	1.42802
H	-2.26633	-3.66597	1.55746
H	-0.99665	-4.67907	3.51138
H	0.76923	-3.43151	1.34263
H	-0.20892	-4.89133	1.12352
H	-1.17592	-5.21428	-1.54733
H	-0.58936	-1.22056	-2.74548
H	-1.42648	-2.76551	-4.50402
H	-2.42523	-4.09651	-3.87367
H	-0.71380	-4.38637	-4.29887
H	-0.87452	5.36587	3.00555
H	-2.20700	3.26489	3.41301
H	-1.28170	2.94932	4.85601
H	-1.49350	1.78525	1.33091
H	1.46575	2.42024	4.24225
H	2.28613	0.58910	2.71582
H	0.65026	2.25368	-3.63462
H	-1.58727	0.48923	-1.28909
H	-0.19058	1.13678	-1.50893
H	-1.75927	2.03198	-3.50347
H	-3.17752	2.70384	-4.27509
H	-2.21090	5.81829	0.66633
H	-1.69354	5.35106	4.58054
H	0.04876	5.06044	4.48267
H	-2.15707	8.42525	0.21088
H	-1.06408	8.84536	-1.11718
H	-7.32842	3.53814	-1.39318
H	-7.09163	3.41099	-3.14503
H	-10.22900	-1.71174	2.48250
H	-9.36793	-0.93715	1.13865
H	-1.35864	-1.35445	2.71055
C	3.17879	-5.14710	-0.93419
O	2.24676	-6.14485	-0.65795
C	2.46599	-3.95636	-1.58519
O	1.94850	-4.34030	-2.85224
C	3.50809	-2.81710	-1.76570
O	2.84758	-1.76743	-2.47288
C	3.96772	-2.38858	-0.37910
C	4.59170	-3.56585	0.37414
O	3.73467	-4.72380	0.31459
C	4.75438	-3.28041	1.87386
O	3.54196	-3.10789	2.57597
H	1.82558	-3.50839	-3.34116
H	3.38699	-0.96046	-2.38433
H	2.94663	-2.46883	2.11271
H	3.98120	-5.51908	-1.59369
H	1.68107	-3.61766	-0.91568
H	4.35177	-3.19146	-2.36943
H	3.07723	-2.05630	0.14818
H	5.58005	-3.79481	-0.05781
H	5.26290	-4.13502	2.33331
H	5.42168	-2.41084	1.97500
C	4.54723	-0.03288	-0.02218
O	4.94931	-1.29576	-0.37121
C	5.48839	0.72616	0.91880
O	5.41826	0.24694	2.26402
C	5.21437	2.23554	0.99983
O	6.33493	2.93420	1.52267
C	4.88925	2.81196	-0.37118
C	3.70856	2.03404	-0.89234
O	4.10890	0.66600	-1.13448
C	3.18833	2.61117	-2.21331
O	4.21577	3.02565	-3.10074
H	6.00581	-0.51979	2.34836
H	6.49567	2.58518	2.41534
H	4.57993	3.84814	-2.73231
H	6.51533	0.60453	0.53535
H	4.33859	2.38885	1.64918
H	5.74203	2.65655	-1.04693
H	2.88869	2.03402	-0.16203
H	2.61867	1.83290	-2.72672
H	2.50775	3.43795	-1.97838
O	4.53831	4.18751	-0.30962
H	2.73084	-6.90639	-0.29788
H	5.23541	4.62222	0.21144
O	1.77137	-1.38495	1.24884
H	2.41133	-0.66355	1.12332

E = -4962.68583737

6 triplet

N	-1.42572	-1.72747	1.75874
N	-0.27454	-2.12381	-0.82517
N	-1.02004	-3.30194	-2.53157
N	0.95460	2.10937	3.42615
N	0.43681	0.90619	1.66521
N	-1.44070	5.58353	0.05661
N	-0.22706	4.46272	-1.40298
N	-2.77701	2.01327	-3.65356
C	-1.32127	-3.19966	1.86848
C	-1.11737	-3.59404	3.32555
C	-0.20783	-3.80189	1.01775
C	-0.46031	-3.42882	-0.40642
C	-0.93285	-4.16514	-1.45963
C	-0.61135	-2.08789	-2.10756
C	-1.42154	-3.66000	-3.88573
C	-0.91092	4.87439	3.98326
C	-1.20686	3.37701	3.84494
C	-0.31038	2.51518	3.04335
C	-0.60352	1.76473	1.93943
C	1.36436	1.13389	2.58709
C	-1.13289	8.72540	-0.03128
C	-0.11226	7.70191	0.46917
C	-0.30958	6.35513	-0.15946
C	0.42523	5.63530	-1.07048
C	-1.34764	4.46366	-0.70364
C	-7.00399	2.86778	-2.19721
C	-5.56069	2.39905	-1.96234
C	-5.06410	1.43310	-3.06389
C	-3.57209	1.22060	-2.92734
C	-9.34299	-1.77976	1.83994
C	-8.05297	-1.76068	2.66872
C	-6.83783	-1.85208	1.76931
C	-6.12764	-0.70911	1.38656
C	-6.45996	-3.07553	1.19273
C	-5.11072	-0.76631	0.43108
C	-5.45554	-3.15204	0.23113
C	-4.79656	-1.98648	-0.18410
O	-1.07155	-2.79317	4.23743
O	-3.10506	0.38548	-2.11376
O	-3.86684	-2.08879	-1.17648
O	-0.01619	2.22336	-2.92991
O	-0.72875	0.67103	-0.82668
Cu	0.16553	-0.66692	0.47704
H	0.90327	8.03840	0.23534
H	-0.16937	7.62155	1.56309
H	1.38185	5.89329	-1.50298
H	0.01531	3.11613	-2.46009
H	-2.10170	3.69014	-0.71267
H	-0.95822	9.70350	0.43003
H	-5.48056	1.90424	-0.98883
H	-4.89949	3.27504	-1.92940
H	-5.29814	1.84658	-4.05155
H	-5.56894	0.46637	-2.97498
H	-7.69729	2.01914	-2.22729
H	-8.00929	-0.84106	3.26493
H	-8.06479	-2.59772	3.37898
H	-6.98124	-3.98535	1.48367
H	-6.38268	0.25181	1.82913
H	-5.19232	-4.09922	-0.23100
H	-4.57855	0.13311	0.13598
H	-3.64696	-1.18893	-1.51116
H	-9.41946	-2.70332	1.25514
H	-2.35732	-1.48368	1.42543
H	-2.26689	-3.66667	1.55715
H	-0.99538	-4.67897	3.51070
H	0.76856	-3.43207	1.34223
H	-0.21030	-4.89165	1.12231
H	-1.17909	-5.21183	-1.54866
H	-0.58393	-1.21897	-2.74523
H	-1.42282	-2.76157	-4.50471
H	-2.42617	-4.08941	-3.87497
H	-0.71540	-4.38466	-4.29928
H	-0.87750	5.36584	3.00503
H	-2.20844	3.26354	3.41321
H	-1.28103	2.94827	4.85523
H	-1.49855	1.77133	1.33888
H	1.47533	2.44259	4.22700
H	2.30279	0.61644	2.70063
H	0.64583	2.25540	-3.63744
H	-1.58428	0.48717	-1.28739
H	-0.18716	1.13380	-1.50770
H	-1.75980	2.03265	-3.50102
H	-3.17842	2.70291	-4.27374
H	-2.21250	5.81797	0.66666
H	-1.69400	5.35055	4.58131
H	0.04806	5.06024	4.48069
H	-2.15879	8.42510	0.21070
H	-1.06619	8.84468	-1.11785
H	-7.32895	3.53841	-1.39452
H	-7.09323	3.40877	-3.14635
H	-10.22974	-1.71295	2.48187
H	-9.36872	-0.93829	1.13803
H	-1.36192	-1.35493	2.71007
C	3.17839	-5.14700	-0.93480
O	2.24657	-6.14491	-0.65888
C	2.46548	-3.95633	-1.58580
O	1.95002	-4.33976	-2.85386
C	3.50574	-2.81525	-1.76381
O	2.84428	-1.76593	-2.47047
C	3.96523	-2.38721	-0.37684
C	4.59115	-3.56561	0.37353

O	3.73395	-4.72348	0.31419
C	4.75842	-3.28335	1.87327
O	3.54826	-3.11821	2.58100
H	1.82698	-3.50760	-3.34232
H	3.38405	-0.95901	-2.38344
H	2.94564	-2.48490	2.11964
H	3.98117	-5.51867	-1.59403
H	1.67919	-3.61951	-0.91702
H	4.35069	-3.18758	-2.36706
H	3.07527	-2.05560	0.15194
H	5.57825	-3.79337	-0.06182
H	5.27271	-4.13672	2.32853
H	5.42221	-2.41100	1.97389
C	4.54584	-0.03189	-0.02250
O	4.94756	-1.29534	-0.37033
C	5.48742	0.72648	0.91819
O	5.41531	0.24798	2.26371
C	5.21461	2.23609	0.99881
O	6.33610	2.93459	1.51994
C	4.88807	2.81222	-0.37179
C	3.70745	2.03419	-0.89296
O	4.10820	0.66641	-1.13539
C	3.18692	2.61166	-2.21355
O	4.21420	3.02464	-3.10190
H	5.99956	-0.52126	2.34843
H	6.49700	2.58713	2.41318
H	4.57917	3.84720	-2.73445
H	6.51454	0.60354	0.53572
H	4.33974	2.39042	1.64909
H	5.74053	2.65720	-1.04807
H	2.88778	2.03370	-0.16246
H	2.61566	1.83415	-2.72628
H	2.50761	3.43934	-1.97821
O	4.53692	4.18773	-0.30977
H	2.73071	-6.90659	-0.29920
H	5.23441	4.62241	0.21082
O	1.76239	-1.39896	1.26650
H	2.40792	-0.68115	1.15067

E = -4962.68573107

TS-6 singlet

N	-1.05404	-2.23519	1.71121
N	0.20185	-2.06941	-0.78654
N	-0.53598	-2.88841	-2.69437
N	0.59963	1.94516	3.60952
N	0.30644	0.42235	2.05988
N	-1.87519	4.98627	0.29030
N	-0.71561	4.73394	-1.56663
N	-3.03736	2.04198	-3.98621
C	-0.97513	-3.70297	1.57316
C	-0.86196	-4.34919	2.94469
C	0.22110	-4.07363	0.70348
C	0.00546	-3.43360	-0.63289
C	-0.46182	-3.94893	-1.81151
C	-0.12362	-1.78049	-2.04015
C	-0.90938	-2.97336	-4.10095
C	-1.73515	4.15365	4.31616
C	-1.81489	2.64573	4.05549
C	-0.74909	1.94735	3.31450
C	-0.90678	0.99447	2.34882
C	1.20429	1.01734	2.82823
C	-2.45458	8.24398	0.60818
C	-1.30515	7.33696	1.05053
C	-1.15011	6.15676	0.14068
C	-0.44113	5.97276	-1.02203
C	-1.58098	4.16227	-0.74737
C	-7.41282	1.81337	-2.13609
C	-5.92150	1.53436	-1.90622
C	-5.16041	1.15714	-3.19008
C	-3.66456	1.35715	-3.01979
C	-9.11516	-3.42340	1.47622
C	-7.85307	-3.29038	2.33055
C	-6.64670	-2.76612	1.57886
C	-6.31962	-1.40375	1.58674
C	-5.81804	-3.62992	0.84758
C	-5.20418	-0.91448	0.90327
C	-4.70969	-3.15645	0.14706
C	-4.39659	-1.79267	0.17174
O	-0.92993	-3.72846	3.98604
O	-3.06239	0.92461	-2.00905
O	-3.25304	-1.38725	-0.47363
O	2.38828	-0.12419	0.52076
O	-0.35275	3.14673	-3.75987
O	-0.23788	1.21524	-1.77353
Cu	0.55069	-0.97520	0.78334
H	-0.36666	7.90249	1.05242
H	-1.46541	7.00006	2.08265
H	0.24657	6.65886	-1.49684
H	-0.39713	3.86619	-3.06257
H	-1.99741	3.17132	-0.85447
H	-2.55450	9.10404	1.28012
H	-5.80165	0.73669	-1.16806
H	-5.46203	2.43075	-1.46927
H	-5.52140	1.75224	-4.03648
H	-5.34265	0.10428	-3.44134
H	-7.92440	0.94171	-2.56211
H	-8.06373	-2.62716	3.17920
H	-7.61054	-4.27074	2.76111
H	-6.04267	-4.69422	0.82585
H	-6.93518	-0.71044	2.15596
H	-4.07939	-3.82986	-0.42711
H	-4.94681	0.14023	0.95415
H	-3.34477	-0.48630	-0.86351
H	-8.95435	-4.10835	0.63540

H	-1.85221	-1.89044	1.17519
H	-1.88405	-4.11552	1.11223
H	-0.70457	-5.44558	2.93940
H	1.14807	-3.71271	1.16318
H	0.30792	-5.15960	0.59373
H	-0.70952	-4.95662	-2.10749
H	-0.08411	-0.78640	-2.46376
H	-0.94414	-1.96632	-4.51869
H	-1.89362	-3.43747	-4.20010
H	-0.17089	-3.56770	-4.64624
H	-1.64739	4.72256	3.38369
H	-2.74810	2.43445	3.51954
H	-1.93415	2.15144	5.03263
H	-1.81908	0.68302	1.86175
H	1.06240	2.52123	4.29973
H	2.26386	0.82037	2.82572
H	0.36243	3.38701	-4.36852
H	-1.20477	1.05702	-1.80296
H	-0.09316	1.84726	-2.51046
H	-2.04965	2.30922	-3.92719
H	-3.56602	2.41917	-4.75990
H	-2.52052	4.77990	1.04091
H	-2.63843	4.48417	4.83712
H	-0.87548	4.41754	4.94338
H	-3.40903	7.70542	0.60801
H	-2.28310	8.62196	-0.40505
H	-7.90853	2.06259	-1.19170
H	-7.55690	2.65452	-2.82449
H	-9.94979	-3.81077	2.07172
H	-9.41665	-2.45423	1.06166
H	-1.22941	-2.02231	2.69574
C	3.78558	-4.77043	-1.27117
O	3.02237	-5.92063	-1.13724
C	2.91879	-3.64322	-1.84375
O	2.51434	-3.95796	-3.17004
C	3.74986	-2.33597	-1.84214
O	2.94441	-1.32716	-2.45553
C	4.13509	-1.98844	-0.40944
C	4.94570	-3.11633	0.18709
O	4.18399	-4.34816	0.06314
C	5.29571	-2.91303	1.66680
O	4.25954	-2.33583	2.44701
H	2.31510	-3.10172	-3.58740
H	3.47279	-0.50974	-2.49761
H	4.35467	-1.36713	2.36483
H	4.68599	-4.93805	-1.88369
H	2.06395	-3.53130	-1.18630
H	4.65565	-2.49313	-2.44982
H	3.24223	-1.83352	0.18523
H	5.89362	-3.23419	-0.36603
H	5.52631	-3.89550	2.09200
H	6.20498	-2.30096	1.71940
C	4.35884	0.41379	0.05272
O	4.93243	-0.76657	-0.31540
C	5.22173	1.20184	1.08084
O	5.18324	0.48849	2.32646
C	4.76128	2.65321	1.27359
O	5.79124	3.46731	1.83108
C	4.34564	3.27923	-0.05473
C	3.29326	2.38547	-0.66113
O	3.98533	1.16223	-1.04326
C	2.64241	2.99053	-1.90497
O	3.54690	3.70524	-2.73993
H	6.08171	0.44061	2.68736
H	5.83843	3.28717	2.78320
H	3.77066	4.51828	-2.25592
H	6.24722	1.21038	0.68402
H	3.88257	2.65161	1.93282
H	5.20904	3.31304	-0.73396
H	2.51806	2.11676	0.05987
H	2.22322	2.18145	-2.50792
H	1.81406	3.63054	-1.58027
O	3.80911	4.58399	0.13150
H	3.60926	-6.63464	-0.83800
H	4.45497	5.06068	0.68165
H	2.29258	-0.12615	-0.44786

E = -4962.66586565
Frequencies = -500.7567

4' singlet (mechanism 2)

N	-1.01313	-2.22535	1.94250
N	0.07454	-2.04146	-0.78330
N	-0.62094	-2.88033	-2.69881
N	0.64899	1.71937	3.74372
N	0.36608	0.49858	1.93485
N	-1.63546	5.05499	0.33419
N	-0.49255	4.81329	-1.53479
N	-3.03551	2.27809	-3.92370
C	-1.06012	-3.65771	1.59202
C	-1.06694	-4.52369	2.84890
C	0.11454	-4.05623	0.70517
C	-0.09946	-3.40990	-0.62778
C	-0.54161	-3.93565	-1.81098
C	-0.23844	-1.76277	-2.04561
C	-0.98349	-2.97727	-4.10741
C	-1.53117	4.20891	4.37362
C	-1.66200	2.70536	4.10810
C	-0.64016	1.97304	3.31857
C	-0.79449	1.21085	2.19280
C	1.21979	0.83200	2.89858
C	-2.16865	8.33805	0.69156
C	-1.04291	7.39320	1.11526
C	-0.90918	6.22482	0.18681
C	-0.21084	6.04760	-0.98360

C	-1.35222	4.23795	-0.71194
C	-7.36333	2.07953	-2.01281
C	-5.87873	1.75236	-1.80362
C	-5.15360	1.39554	-3.11517
C	-3.65160	1.55802	-2.97607
C	-9.18369	-3.11652	1.60084
C	-7.90701	-3.02722	2.43907
C	-6.70017	-2.60151	1.62088
C	-6.22514	-1.28431	1.63901
C	-6.04900	-3.50880	0.76907
C	-5.16204	-0.87264	0.82827
C	-4.99803	-3.11410	-0.05585
C	-4.55924	-1.78184	-0.05101
O	-0.92895	-4.07489	3.96806
O	-3.03741	1.06238	-2.00173
O	-3.54148	-1.45000	-0.90001
O	3.12864	0.02899	1.01636
O	-0.29761	3.27222	-3.78529
O	-0.21187	1.25710	-1.89232
Cu	0.20415	-0.92641	0.71839
H	-0.09158	7.93683	1.13108
H	-1.21300	7.04055	2.14054
H	0.47505	6.73525	-1.45880
H	-0.26415	3.97022	-3.06690
H	-1.77270	3.24933	-0.82394
H	-2.24681	9.18577	1.38173
H	-5.77432	0.92796	-1.09349
H	-5.38788	2.62124	-1.34603
H	-5.52283	2.02106	-3.93559
H	-5.36372	0.35391	-3.38996
H	-7.90036	1.23633	-2.46396
H	-8.05831	-2.31776	3.26201
H	-7.71206	-4.00351	2.90241
H	-6.38076	-4.54473	0.73867
H	-6.69214	-0.55742	2.30039
H	-4.51952	-3.82013	-0.72884
H	-4.80628	0.15361	0.87337
H	-3.49744	-0.48322	-1.08191
H	-9.07095	-3.83971	0.78493
H	-1.96823	-1.86922	1.99191
H	-1.98720	-3.87377	1.04799
H	-1.17700	-5.61285	2.67730
H	1.06168	-3.74267	1.15967
H	0.15597	-5.14374	0.58518
H	-0.76336	-4.94915	-2.10724
H	-0.19304	-0.77227	-2.47820
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H	-2.27382	4.84449	1.08953
H	-2.40552	4.55789	4.93069
H	-0.64003	4.44711	4.96567
H	-3.13650	7.82405	0.67956
H	-1.98690	8.73323	-0.31332
H	-7.84782	2.31098	-1.05803
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H	-10.03593	-3.43200	2.21419
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H	-0.66886	-2.16711	2.90582
C	3.63114	-4.85891	-1.32079
O	2.82357	-5.97791	-1.16623
C	2.79107	-3.70426	-1.87945
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O	2.85671	-1.38877	-2.46409
C	4.03589	-2.10347	-0.42371
C	4.86383	-3.25074	0.12861
O	4.09982	-4.47628	-0.00295
C	5.20600	-3.08223	1.61382
O	4.12612	-2.61261	2.41062
H	2.18729	-3.14567	-3.61863
H	3.31032	-0.53611	-2.32377
H	4.06704	-1.64898	2.28507
H	4.49871	-5.06350	-1.96859
H	1.93695	-3.57640	-1.22275
H	4.55223	-2.57655	-2.46647
H	3.13009	-2.01971	0.17678
H	5.80477	-3.33911	-0.43822
H	5.49398	-4.06165	2.00709
H	6.07618	-2.41861	1.69665
C	4.22326	0.26163	0.19588
O	4.83087	-0.91347	-0.28128
C	5.25207	1.04971	1.04216
O	5.43651	0.45598	2.32716
C	4.85153	2.51686	1.24995
O	5.92818	3.26166	1.80432
C	4.46178	3.16565	-0.08003
C	3.37188	2.31233	-0.67804
O	3.88136	0.99832	-0.95870
C	2.81594	2.89726	-1.98138
O	3.81946	3.38066	-2.86789
H	6.24088	-0.08399	2.30018
H	6.13958	2.85562	2.66156
H	4.12010	4.23130	-2.50884
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H	3.97957	2.55418	1.92031
H	5.33255	3.15742	-0.75151
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H	2.27706	2.10799	-2.51103
H	2.09741	3.68450	-1.72716
O	3.96949	4.48618	0.09286
H	3.38975	-6.71859	-0.89316
H	4.63129	4.95406	0.63031
H	2.30598	-0.20118	0.51972

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