Supporting information for:

Phenol-Induced O–O Bond Cleavage in a Low-Spin Heme-Peroxo-Copper Complex: Implications for O_2 Reduction in Heme-Copper Oxidases

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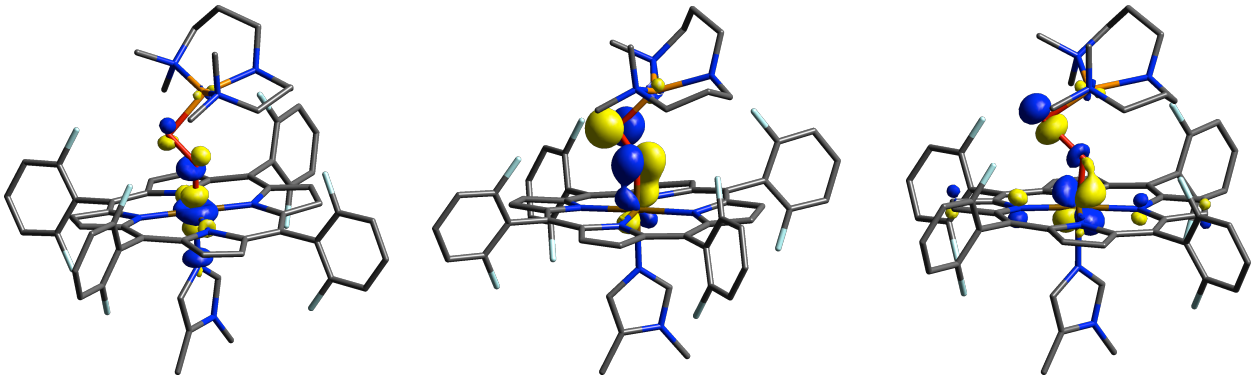
1. Orbital Overlap of Fe^{III} with the peroxo in **1**



O_2^{2-} (π^*_σ) → Fe (d_{z2}) O_2^{2-} (π^*_v) → Fe (d_{xz}) Fe (d_{yz}) → O_2^{2-} (σ^*)

Figure S1. MO contour plots showing interaction of Fe d-orbitals with peroxide π* and σ*, shown in order (left to right) of increasing population on Fe in **1**. Note that the docked reactant **D** exhibits nearly identical overlap, but the phenol has been omitted here for clarity. All MOs shown are β-spin.

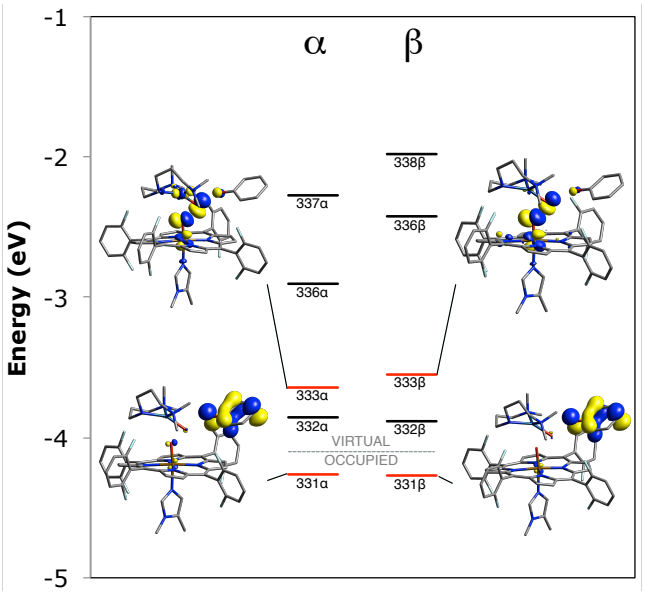


Figure S2. FMOs at the TS, showing Fe d_{yz} overlap with σ*, and fully occupied phenolate α/β HOMOs.

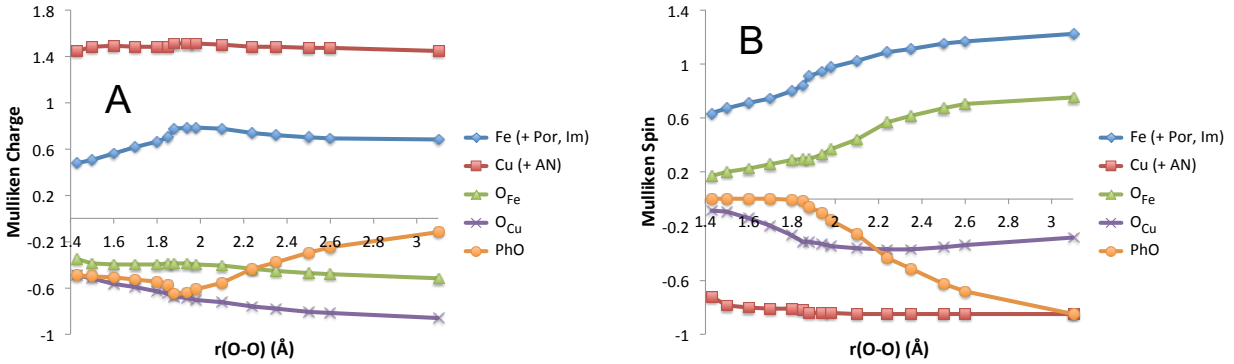


Figure S3. (A) Mulliken Charge, and (B) Mulliken Spin for the Fe and Cu fragments (including non-peroxo ligands), peroxo O atoms, and PhO over the PI reaction coordinate defined by the IRC. The increasing charge and spin on Fe indicate β ET, while the increasing charge/decreasing spin on phenolate indicate α ET. The increase in negative charge on the phenolate in $\mathbf{TS_{PI}}$ compared to **D** is a result of the O_{Cu}–H bond formation (and the O_{Ph}–H weakening).

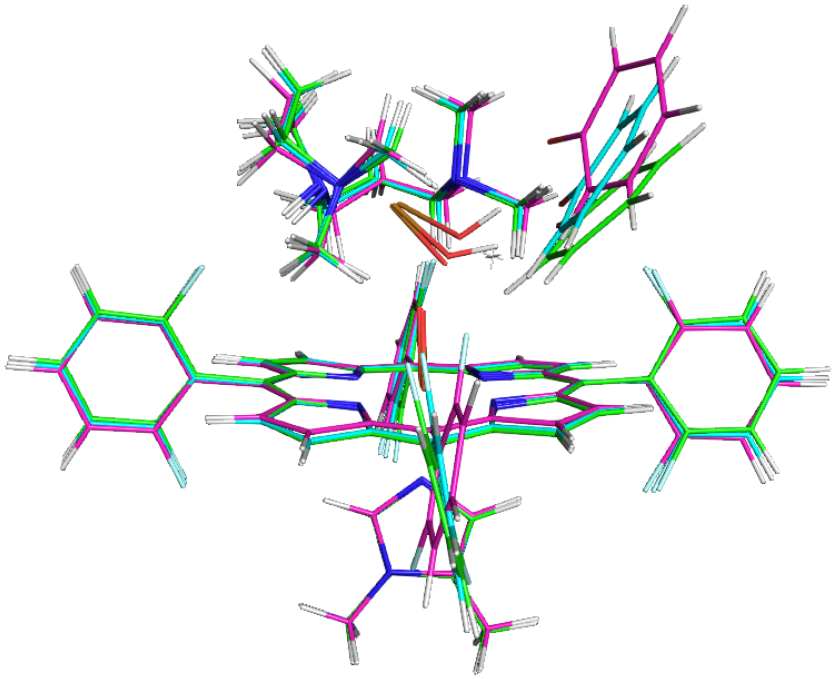


Figure S4. Overlayed structures along the PI reaction pathway after the transition state. taken at *r*(O–O) = 2.0 Å (green), 2.2 Å (blue), 2.6 Å (pink), showing rotation of the phenolate ring as the out-of-plane O_{Ph} *p*-orbital is directed toward the σ^*_{O-O} orbital.

2. Geometric comparison of TS_{PT} and TS_{HB}

Table S1. Bond distances for TS_{PT} and TS_{HB}, obtained from transition state optimizations using BP86 and B3LYP

	BP86		**B3LYP**	
Bond/vector	**TS_{PT} (Å)**	**TS_{HB} (Å)**	**TS_{PT} (Å)**	**TS_{HB} (Å)**
$Fe–O_{Fe}$	1.679	1.662	1.672	1.682
$Fe–O_{Cu}$	3.166	3.590	3.164	3.259
$O_{Fe}–O_{Cu}$	1.882	2.301	1.905	1.953
$Cu–O_{Cu}$	1.901	1.839	1.924	1.877
$Cu–O_{Fe}$	2.51	2.431	2.465	2.368
$O_{Cu}–O_{Ph}$	2.447	2.571	2.600[a]	2.659
$O_{Cu}–H$	1.116	1.543	1.044	1.670
$O_{Ph}–H$	1.349	1.039	1.583	1.005

[a] Note that this geometric parameter was constrained in the optimization (see main text, Figure 13 caption).

3. Analysis of electron transfer over the PI reaction pathway

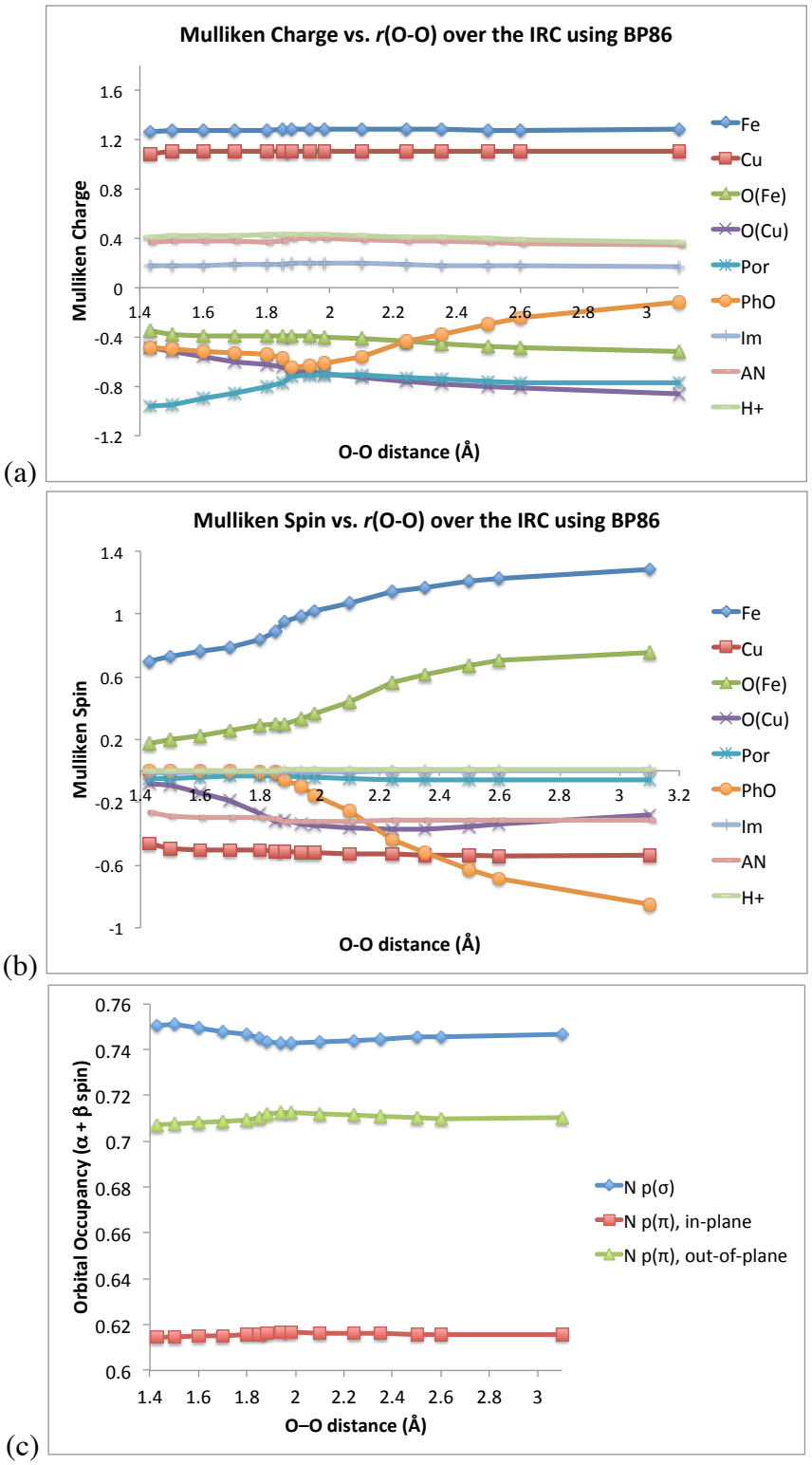


Figure S5. Mulliken (a) charge and (b) spin over the PT pathway IRC, itemized by metal and ligand fragments. (c) Population densities of the porphyrin N-atom p-orbitals vs. O–O distance over the IRC, designated by bonding symmetry to Fe and the porphyrin plane. Note that while

the porphyrin charge shown in (c) increases before the TS_{PT} but the Fe charge remains nearly constant, the Mulliken spin (b) and orbital occupancies (Figure 9) indicate that the β e^- donated into the O–O σ* derives purely from Fe. Furthermore, the charge increase on the porphyrin ring is due to polarization of the Fe–N σ bonds toward Fe, as clearly demonstrated by a population analysis of the p-orbitals on the porphyrin N-atoms (c), showing that only the p_σ (i.e. lone pair directed toward Fe) decreases in occupation. The MOs of interest involving the N *p*-orbitals are shown in Figure S6.

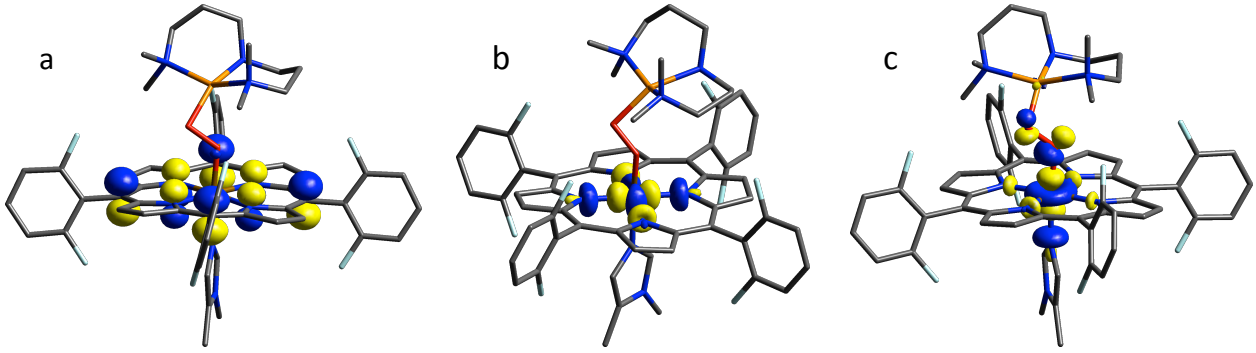


Figure S6. MO contour plots for the key orbitals pertinent to charge transfer out the N *p*-orbitals in **1**. Note that the porphyrin a_{2u} orbital (a) is occupied, while the Fe-centered d(x^2-y^2) and d(z^2) are unoccupied throughout the reaction coordinate. The N *p*(π) orbital corresponds to the "p(π), out-of-plane" in Figure S5. The in-plane N *p*(π) orbitals are predominantly involved in σ bonding of the porphyrin framework and do not contribute to the FMOs.

4. Electronic structure of Cu-oxyl formed in HB reaction pathway

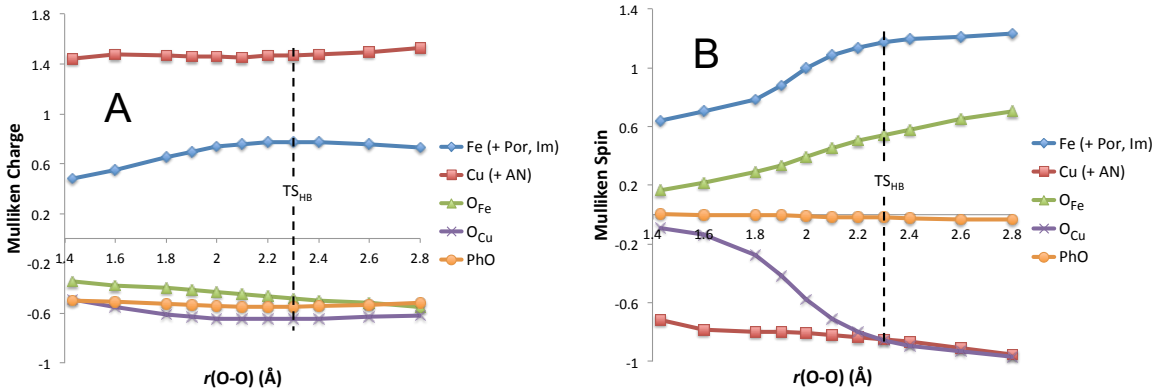
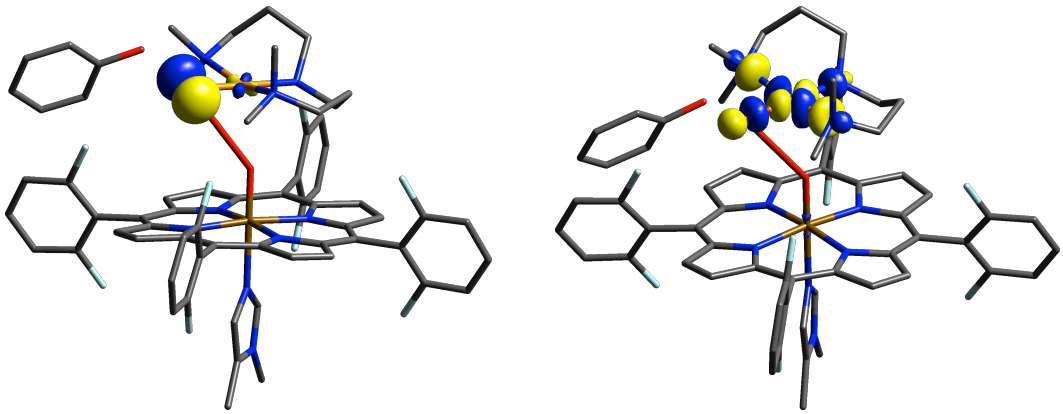


Figure S7. (A) Mulliken Charge and (B) Spin along the HB reaction coordinate, without proton transfer from phenol.



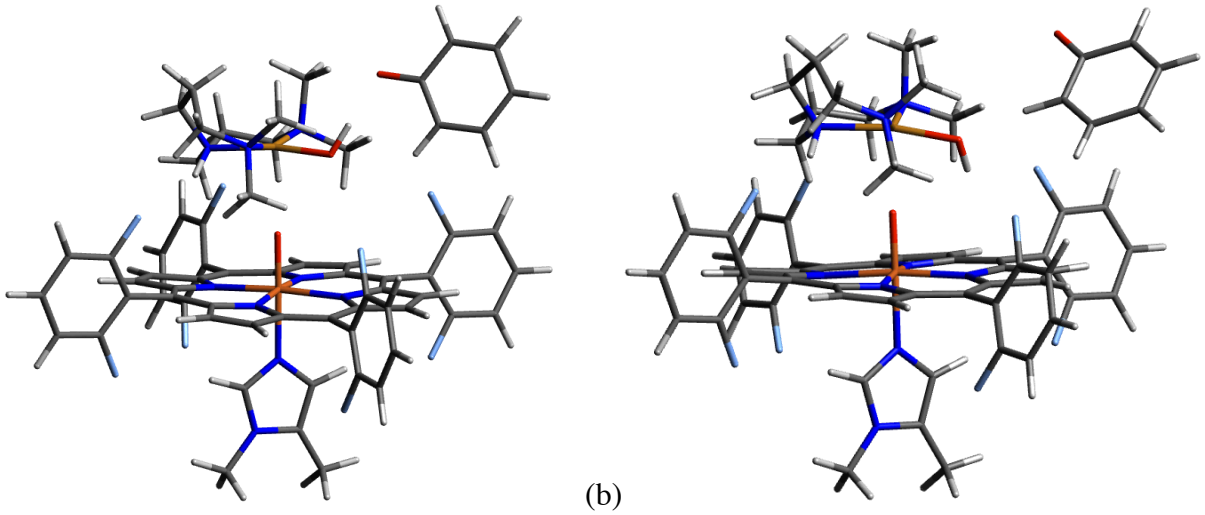
332α (LUMO) 333α (LUMO +1)

Figure S8. MO contours for the α-spin LUMOs of the Cu fragment in TS_{HB}, showing the orthogonality of the singly-occupied orbitals in the triplet Cu-oxyl species.

5. Comparison of {1 + PhOH} calculated in B3LYP vs. BP86

Table S2. Comparison of Mayer Bond Orders and Mulliken charges obtained for **1** using BP86 and B3LYP, focusing on metals and atoms directly bound to metals.

	BP86	**B3LYP**
Mayer Bond Order		
Fe–O	.67	.63
Fe–N_{Por}	.47	.41
O–O	.89	.85
Cu–O	.34	.35
Cu–N_{AN}	.27	.24
Mulliken Charge		
Fe	1.25	1.37
Cu	1.06	1.16
O_{Fe}	-.34	-.44
O_{Cu}	-.42	-.50
N_{Por} (average)	-1.06	-1.03
N_{AN} (average)	-.71	-0.76



(a) (b)

Figure S9. Optimized product structures for **1•PhOH** using BP86 (a) and B3LYP (b), consisting of a fully cleaved Fe^{IV}=O / Cu^{II}–OH and a phenoxy radical. Note that the structure calculated in B3LYP differs from that in BP86 because the Cu^{II}–OH product has a more negatively charged -OH ligand (and a consequently less positively charged H) in the less covalent B3LYP, making the Cu^{II}–OH a weaker H-bond donor and resulting in the PhO• dissociating (whereas it remains bound in BP86).

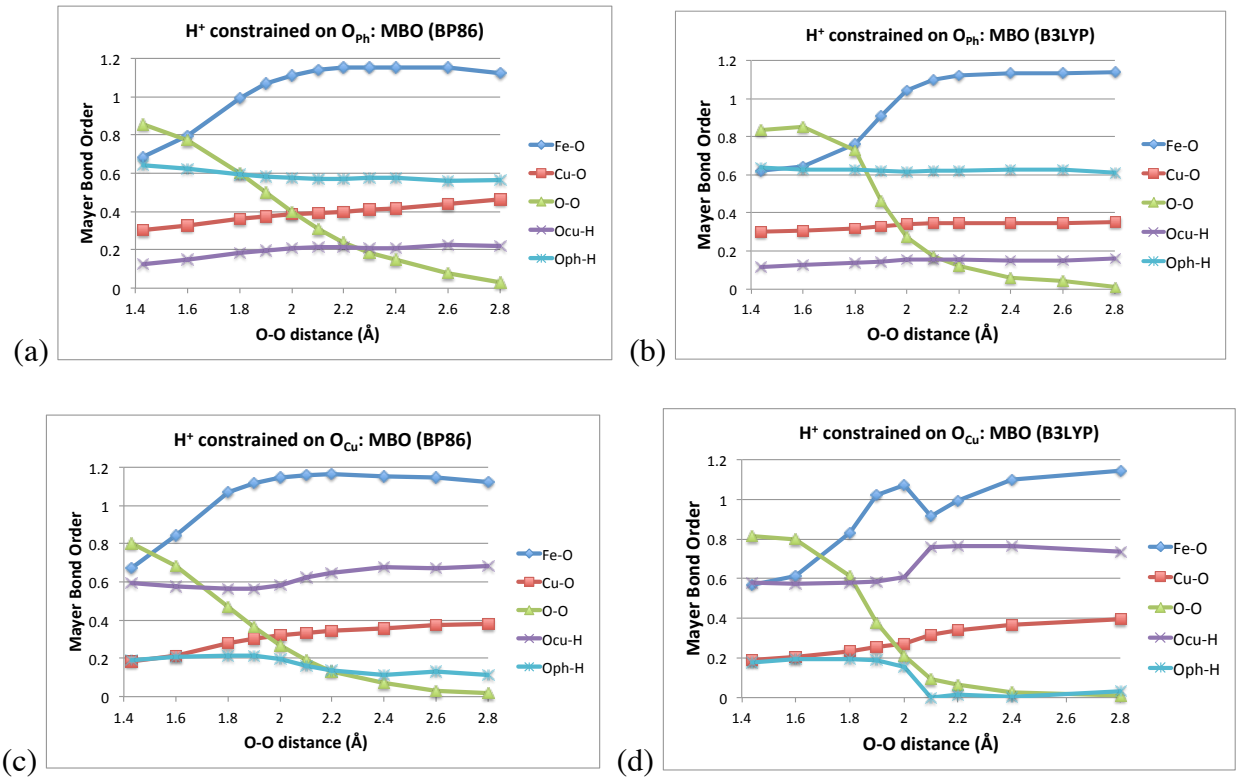
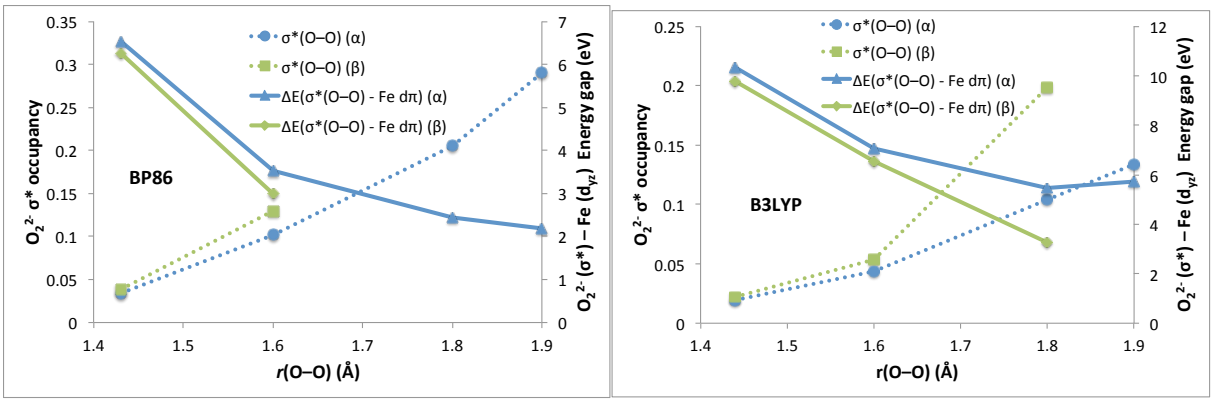
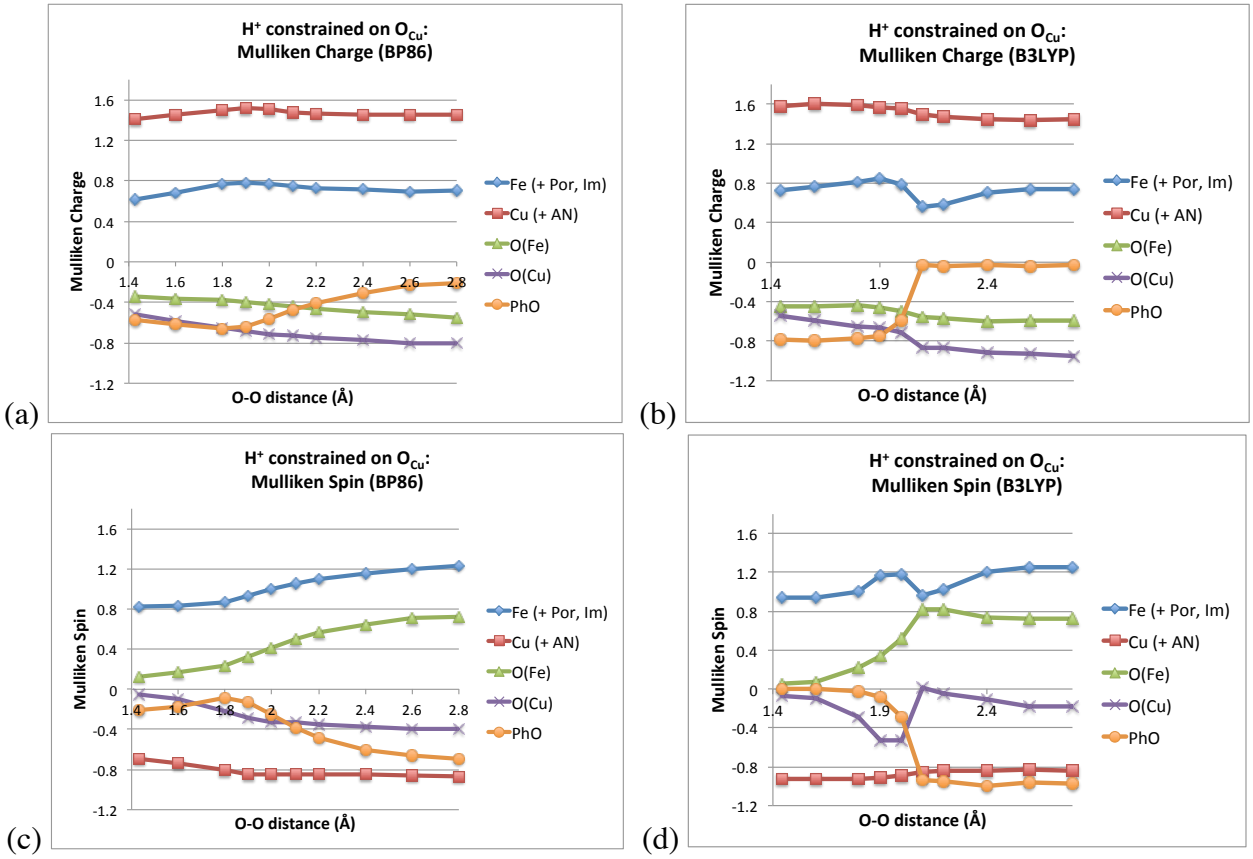


Figure S10. Mayer bond orders calculated along the PESs for (a)/(b) the H^+ remaining on phenol, and (c)/(d) the H^+ constrained on the peroxo using BP86/B3LYP, respectively. Note that an increase in Fe–O MBO and decrease in O–O MBO is observed at shorter O–O distances using BP86, but not B3LYP. This difference is attributable to the lower covalency in B3LYP, and is directly related to the larger O–O cleavage barriers calculated in B3LYP. The apparent discontinuity at O–O = 2.0-2.1 Å in (d) is due to dissociation of the phenoxy radical from the (AN)Cu^{II}–OH fragment (See Figure S9 and caption).



(a) (b)

Figure S11. Orbital occupancy of σ^*_{O-O} correlated to the energy gap between the unoccupied σ^*_{O-O} and occupied Fe d_{yz} orbitals, plotted against O–O elongation for the "H^+ constrained on O_{Cu}" PES. The orbital occupancies (dotted lines, "σ*(O–O)") and energy gaps (solid lines, "ΔE(σ*(O–O) - Fe dπ)") were obtained from a Natural Bonding Orbital analysis, and are given for both α (blue) and β (green) spin. Note that the β-spin values are only reported in the calculations until an O–O distance of 1.6 Å in BP86 and 1.8 Å in B3LYP.



(a) (b) (c) (d)

Figure S12. Mulliken charge (a)/(c) and spin (b)/(d) along the "H^+ constrained on peroxo" PES for BP86/B3LYP, respectively, summed over the individual fragments (where peroxo O-atoms

are computed separately). The initial increase in negative charge on O_{Fe} observed in BP86, but not B3LYP, demonstrates the greater transfer of charge into the σ^*_{O-O} orbital in BP86. The apparent discontinuity at O–O = 2.0-2.1 Å in (b) and (d) is due to dissociation of the phenoxy radical from the (AN)Cu^{II}–OH fragment (See Figure S9 and caption).

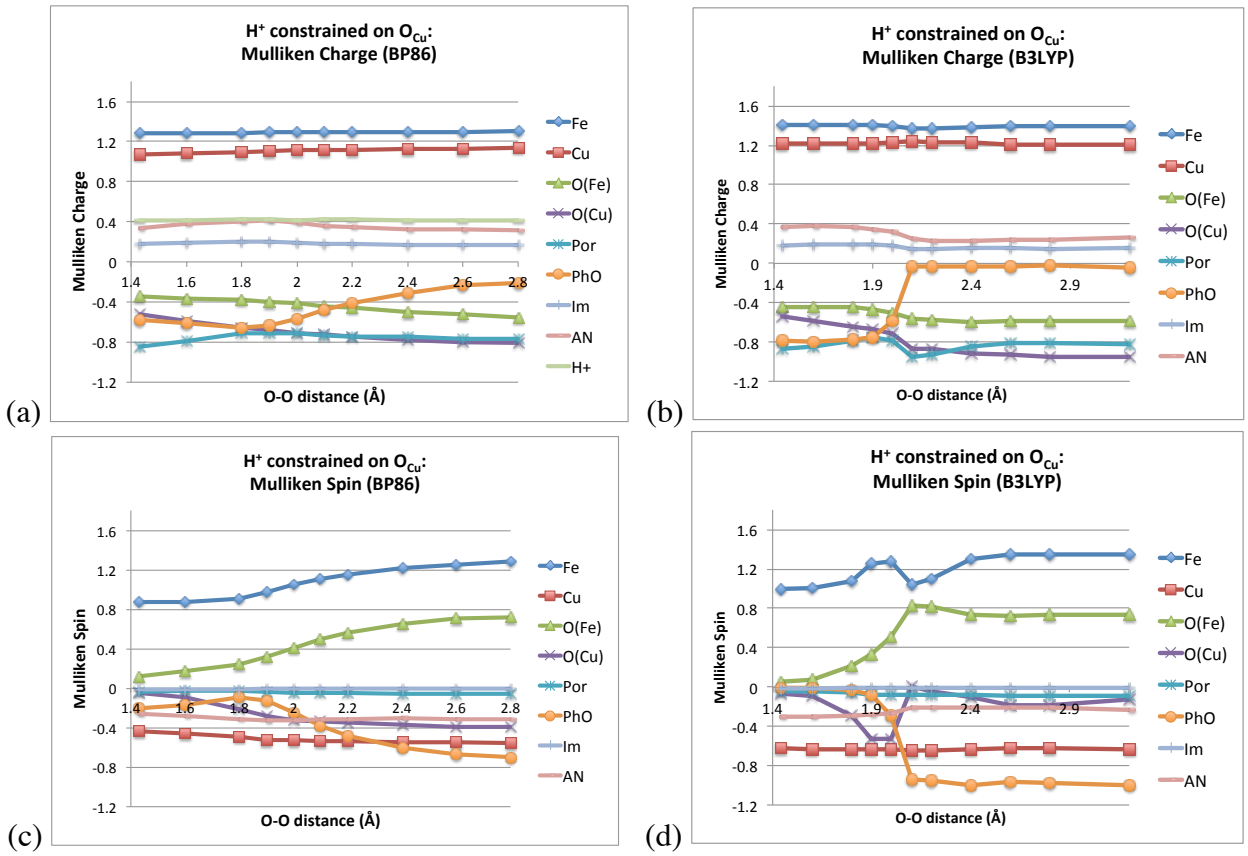


Figure S13. Mulliken charge (a)/(b) and spin (c)/(d) for all individual fragments given for the "H^+ constrained on peroxo" PES, using BP86/B3LYP, respectively. Note that the metal-bound ligands (primarily Por for Fe, and AN for Cu) exhibit a greater increase in charge in BP86 than in B3LYP, without a corresponding change in spin. This is due to greater polarization of M-L bonds in BP86 related to the higher covalency in BP86, indicating that transfer of the β electron early in O–O elongation is from Fe, rather than the porphyrin ligand.

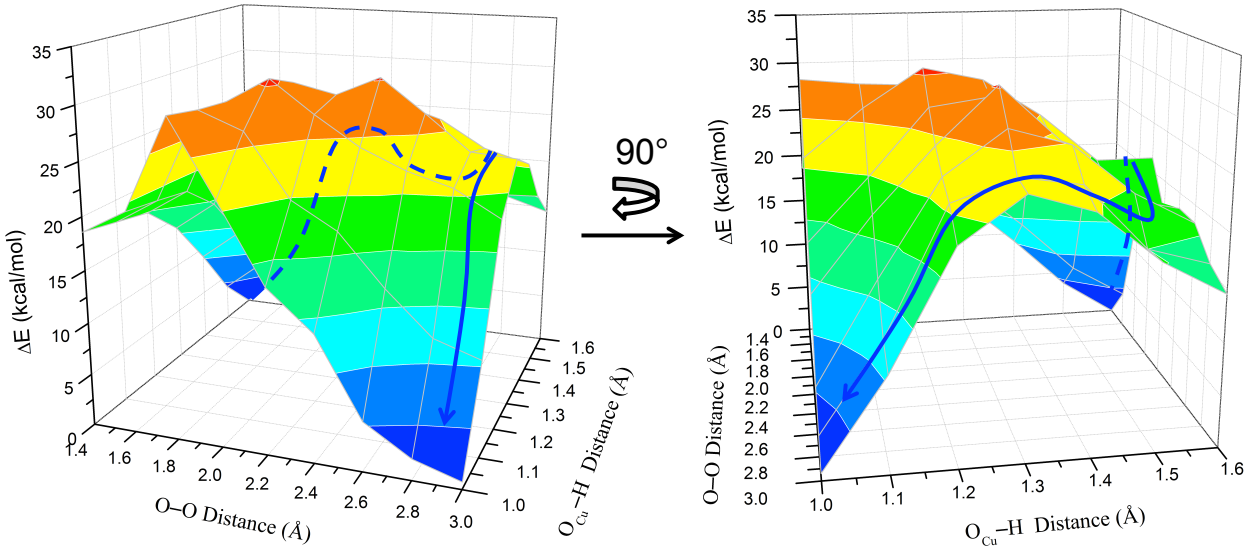


Figure S14. PESs for O_{Fe}•••O_{Cu} vs. O_{Cu}•••H(OPh) distances (two ~90° rotations to show full surface) constructed by B3LYP single-point calculations on BP86-optimized structures, where O_{Cu}•••O_{Ph} is fixed at 2.6 Å. The blue line represents an approximate reaction pathway through the H-bonded TS (**TS_{HB}**), where the dotted segment indicates that the line is behind the plot surface. Note that the second barrier (in the yellow section) along the reaction pathway is due to the O_{Cu}•••O_{Ph} constraint in the 2D PES, and allowing the phenol to optimize makes this barrier lower than the first (see main text).

6. Analysis of H^+ tunneling in the "H-bond assisted O–O homolysis" pathway for {1 + PhOH}

We evaluated the process of H^+ tunneling from the phenol to the peroxo by systematically stepping along the H-bonded O–O Homolysis coordinate, and obtaining the energy for a structure where the proton is moved to O_{Cu} and optimized, yet the rest of the structure is frozen. The minima become isoenergetic at an O_{Fe}–O_{Cu} distance of 2.22 Å (see Figure S15), earlier even than the O–O homolysis barrier (O_{Fe}–O_{Cu} = 2.3 Å). The starting structure (with the H^+ optimized on the phenol) had an O_{Cu}–H distance of 1.54, compared to a final (with the H^+ on the peroxo) distance of 1.02 Å, giving a tunneling width of 0.54 Å. A PES for the tunneling process was generated by progressively moving the H^+ from O_{Ph} to O_{Cu} (without structural relaxation), yielding a tunneling barrier of 3.7 kcal/mol (see Figure S16). Note that for the tunneling PES (used to obtain a barrier height), zero-point corrections were applied to the ΔE values. Employing a method detailed elsewhere[1], the tunneling rate can be estimated by modeling the tunneling PES as a quartic function representing a simple double-well potential and extracting the intrinsic oscillator frequency, $\hbar\omega$, which describes the motion along the O_{Ph}••H••O_{Cu} vector. Solving the vibrational Hamilitonian for a simplified 2-state double-well potential[2] yields an energy splitting of $\Delta E_{\pm}$ = 280 cm^{-1}, which relates to a tunneling rate by $k = \Delta E_{\pm} / h$, or 8.4 x10^{12} s^{-1}.

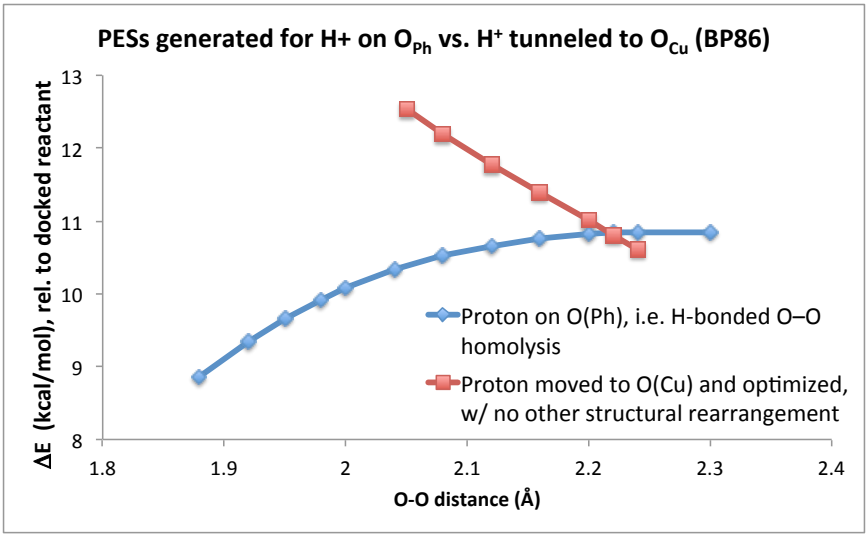


Figure S15. Potential surfaces corresponding to the H-bonded O–O homolysis (blue), and the H^+ tunneled to the peroxo (red), where the latter is a surface generated by moving the H^+ from O_{Ph} to O_{Cu}, and performing a geometry optimization where only the H^+ is unfrozen. Therefore, the surfaces cross where the two protonation states are isostructural and isoenergetic.

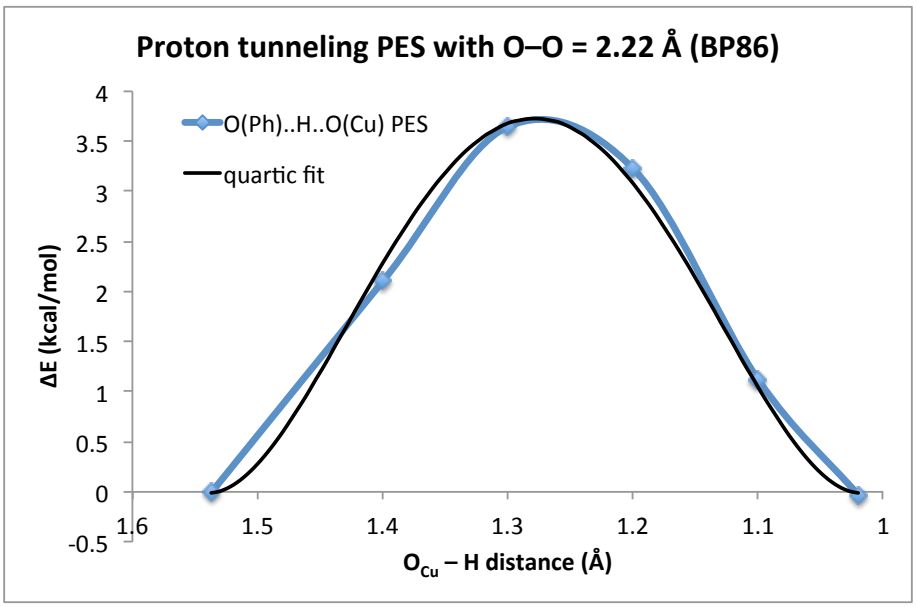
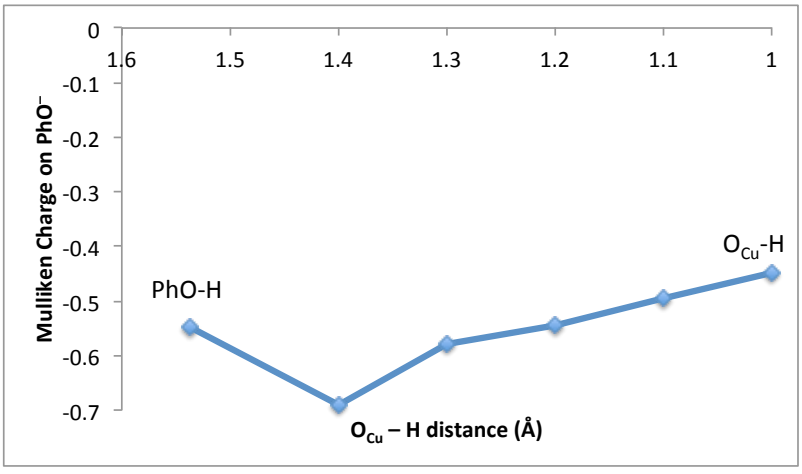


Figure S16. PES generated (using BP86) by progressively moving the H^+ from O_{Ph} to O_{Cu}, while the structure (except for the H^+) is frozen in the geometry obtained at O_{Fe}–O_{Cu} = 2.22 Å along the H-bonded O–O homolysis surface. The energies are given in zero-point-corrected ΔE obtained from a frequency calculation performed at each point.

To examine the electron flow correlated to the H^+ tunneling, the Mulliken charge and spin for the phenolate fragment were monitored along the tunneling PES given in Figure S16. As shown in Figure S17, the phenolate fragment has gained less than 10% radical character at the tunneling barrier (which occurs at an O_{Cu}–H distance ~ 1.3 Å), indicating that the electron transfer from phenolate follows the H^+ transfer.

(a)



(b)

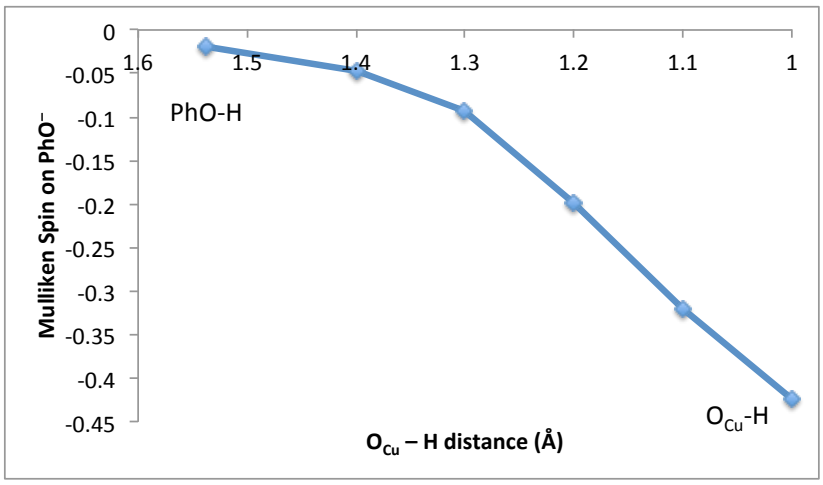
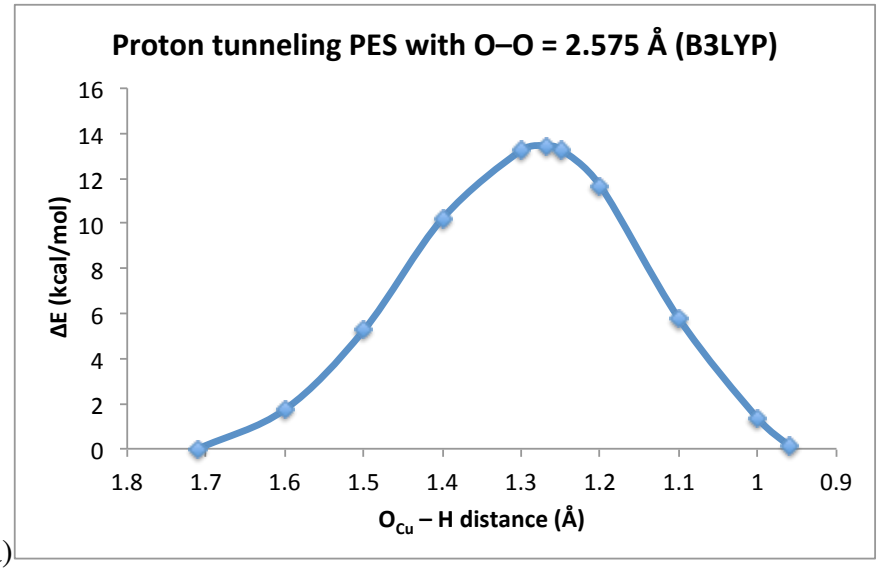


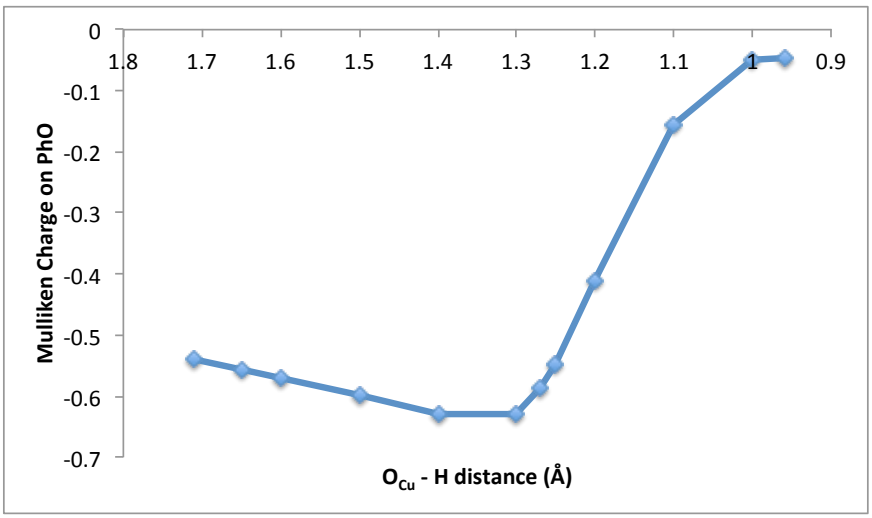
Figure S17. Mulliken charge and spin on the phenolate fragment along the PES generated for the H^+ tunneling from O_{Ph} to O_{Cu} using BP86, indicating that at the tunneling barrier (O_{Cu}–H ~ 1.3 Å) the phenolate has gained less only about 10% radical character.

A similar method was applied using B3LYP, and an isoenergetic pair of structures was found where the H^+ could tunnel from O_{Ph} to O_{Cu}. This structure had an O_{Fe}–O_{Cu} distance of 2.575 Å, and required a slight geometric modification from to the fully optimized "H^+ on O_{Ph}" structure, which involved elongation of the O_{Cu} – O_{Ph} distance from 2.67 Å to 2.70 Å. The O_{Cu} – O_{Ph} distance was then frozen and a re-optimization was performed to yield the starting structure for H^+ tunneling (this constraint only raised the energy by 0.1 kcal/mol relative to the fully optimized structure, and did not introduce any imaginary frequencies). The tunneling PES (Figure S18a) yielded a barrier in zero-point corrected ΔE of 13.4 kcal/mol, with a H^+ tunneling distance of 0.75 Å. This yields an energy splitting of $\Delta E_{\pm}$ = 6 cm^{-1}, corresponding to a tunneling rate of 1.8 x10^{11} s^{-1}. As with BP86, the electron is minimally transferred (<20% radical character, based on Mulliken spin) from the phenolate at the barrier.

(a)



(b)



(c)

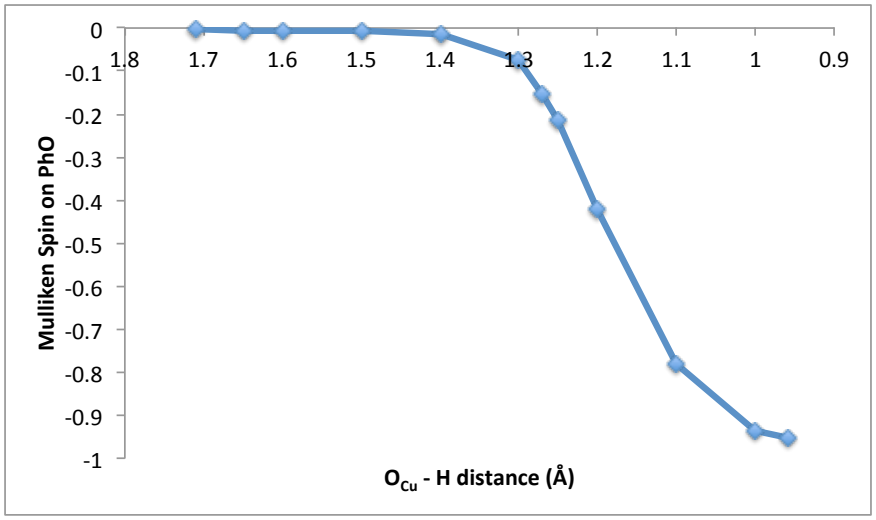


Figure S18. (a) PES for H^+ tunneling in B3LYP (analogous to Figure S16 for BP86), as well as Mulliken charge (b) and spin (c) calculated for the phenolate fragment along the tunneling PES (analogous to Figure S17(a) and (b), respectively for BP86).

It is valuable to note that if proton tunneling does not occur and the reaction coordinate therefore continues along the "H-bond assisted O–O homolysis" curve past TS_{HB}, (shown in Figure 13 in the text), the proton can transfer at a later point in O–O elongation (after the energy of this surface has come down sufficiently) over a classical barrier that remains lower in energy than TS_{HB}. Specifically, it was calculated that this can occur at an O–O distance of 2.4 Å in BP86 and 2.5 Å in B3LYP. However, since the barrier to O–O cleavage for this reaction pathway is still defined by TS_{HB}, the exact mode of H^+ transfer would not be distinguishable in the reaction of {**1** + PhOH}. Additionally, the e^- transfer from phenolate occurs after the barrier to H^+ transfer for this process.

7. Identification of phenoxyl radical products

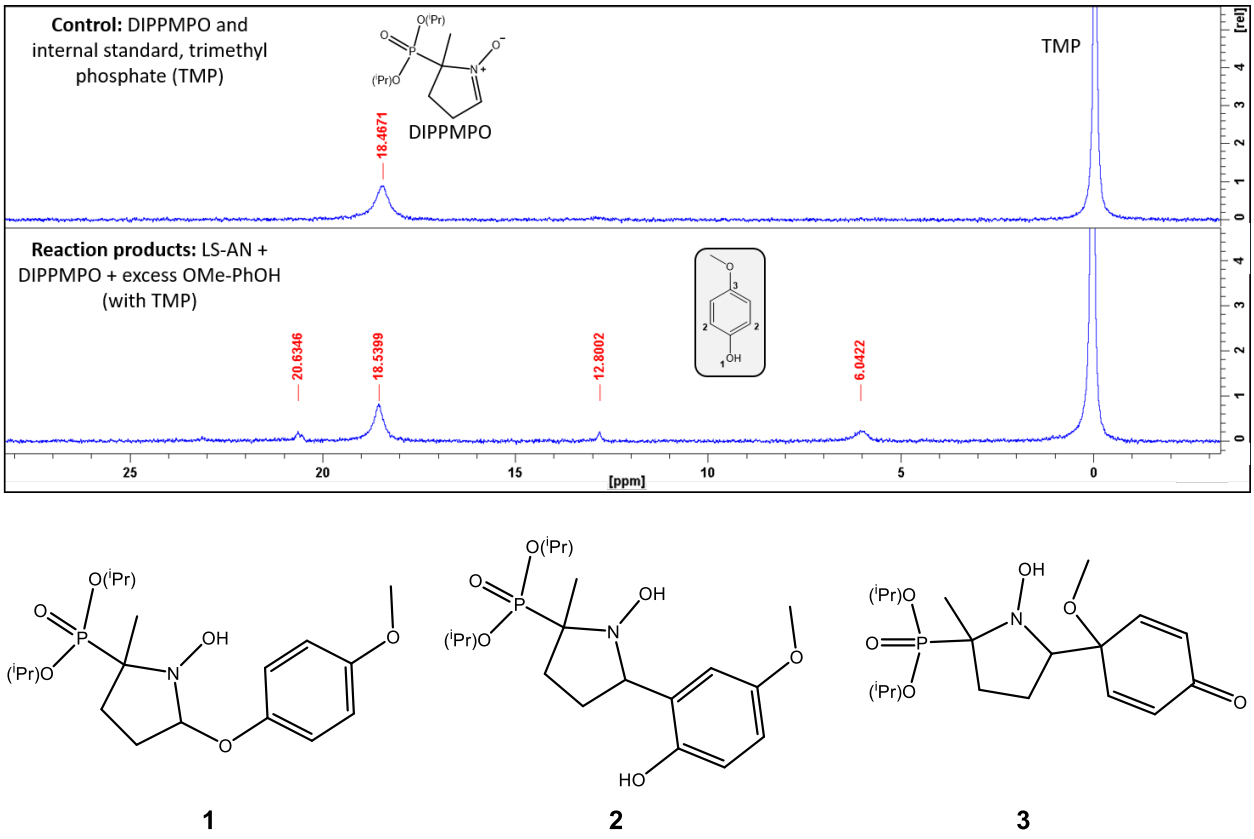


Figure S19. (top) Proton-decoupled ^{31}P-NMR spectra of (top) a control sample containing the radical trap, DIPPMPO, and internal standard, TMP, calibrated to 0 ppm, and of (bottom) the reaction products from {LS-AN + DIPPMPO + excess OMe-PhOH} which shows three new ^{31}P peaks. We attribute the multiplicity of these peaks to the three possible locations where a radical can reside on the OMe-PhOH and therefore the three distinct adducts which can be formed with the radical trap (bottom).

8. Kinetics Experiments on {**1** + 4-OMePhOH}

Table S3. Michaelis-Menten parameters calculated from the kinetic data collected at four temperatures between -70 and -77 (plotted in Figure 14B of the main text). Each data point (temperature/phenol concentration) is an average over 3 or more trials. Standard deviations are given in parentheses.

T (°C)	V_{max} (x 10^{-4} s^{-1})[a]	K_M (mM)	$\Delta G^{\ddagger}$ (kcal/mol)[b]
-70	4.93 (0.17)	1.47 (0.24)	14.79 (0.01)
-72	4.38 (0.16)	3.29 (0.43)	14.69 (0.01)
-74	3.70 (0.20)	3.97 (0.68)	14.61 (0.02)
-77	3.03 (0.33)	4.9 (1.6)	14.46 (0.04)

[a] The Eyring Analysis shown in Figure 14B was performed using a weighted least-squares fit to the values for V_{max} calculated at each temperature. The value for $\Delta G^{\ddagger}$ given in the text (14.8 kcal/mol) was then calculated at 203 K from the $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ extracted from the fit.
[b] Calculated using the Eyring equation at each temperature, using the corresponding V_{max} as the reaction rate (k). Note that the second decimal place is not significant.

Table S4. Reaction rates from individual trials for the kinetics data given in Table 2 of the main text. Reaction conditions are those given in Scheme 1.

Exp #	OMePhOH Rate	OMePhOD Rate
1	0.000417	0.000232
2	0.000440	0.000265
3	0.000400	0.000204
4	0.000429	0.000310
5	0.000389	0.000198
6	0.000431	0.000234

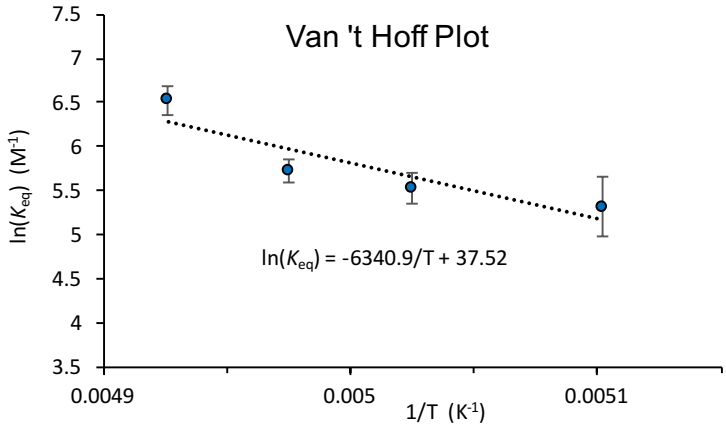


Figure S20. Van 't Hoff Plot showing the temperature dependence of the binding affinity in {**1** + p-OMe-PhOH}. The value for Keq was estimated using the assumption that $K_M \approx K_D = 1/K_{eq}$ (where the K_M is the Michaelis constant shown in Figure 14B and Table S3), which is valid when k_{cat} is small.

Table S5. Amount of phenol-bound adduct at various temperatures when 80 equivalents of 4-OMe-PhOH have been added to **1** (estimated from K_{eq} as in Figure S20); values in italics have been calculated using the fit from the Van 't Hoff Equation. These data indicate that a negligible amount of phenol would be bound in liquid N_2-frozen samples (assuming fast equilibrium), preventing direct detection of a bound adduct (by resonance Raman, for example) in samples frozen at -136 °C (f.p. of the MeTHF solvent). Qualitatively, a lower binding affinity at lower temperature corresponds to a negative slope in the Van 't Hoff plot (Figure S20).

T (°C)	**K_{eq}**	**% Phenol Bound**
-70	682	96.5
-72	304	92.4
-74	252	91.0
-77	203	89.0
-80	*106*	*80.9*
-136	*0.0002*	*0.001*

9. Evaluation of {1 + 4-OMePhOH} using different Density Functionals for comparison to kinetics data

Table S6. Calculated barriers and KIEs for {1 + 4-OMePhOH} using a range of density functionals that vary in the amount of HF exchange. All values are calculated at 203 K.

Functional	% HF exchange	$\Delta G^{\ddagger}_{PI}$ (kcal/mol)	KIE_{PI} [a] (k_H/k_D)[b]	$\Delta G^{\ddagger}_{HB}$ (kcal/mol)	KIE_{HB} [a] (k_H/k_D)[b]	KIE_{HB} (k_H/k_D)[b] (Streitweiser approx.)[c]
BP86	0	8.0	14.6	9.4	1.76	2.19
M06L	0	10.5	15.2	8.1	1.21	1.34
TPSSH	10	14.1 [d]	13.6	12.5	1.24	1.43
B3LYP	20	23.9 [d]	5.2	17.7	1.13	1.15
B3LYP-GD3	20	21.6 [e]		15.6	1.14	1.20
ωB97X-D	22	31.3 [e]		22.9	1.06	1.12
PBE0	25	28.3 [e]		20.6	1.16	1.31

[a] Calculated from the effect of H/D exchange on the barrier in $\Delta G^{\ddagger}$

[b] The deuterated 4-OMePhOD used in the kinetic experiments was also deuterated in the phenolic proton positions (4-CH_3-C_6D_4OD); calculated KIEs include this additional substitution.

[c] See Ref. 3

[d] Required a structural constraint to prevent the proton from returning to the phenolate, however the TS calculation converged to a structure with only one imaginary frequency.

[e] TS calculations yielded structures with two or more imaginary frequencies (a structural constraint was imposed to prevent the proton from returning to phenolate).

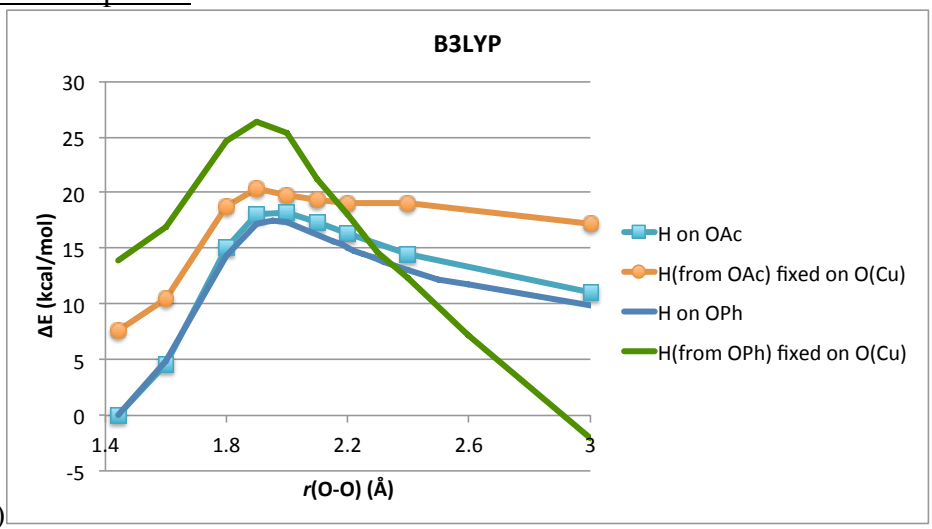
Table S7. Calculated barriers and KIEs for {1 + 4-OMePhOH} using the density functionals from Table S6 that provided the closest agreement with experiment, employing a basis set that includes both diffuse a polarization functions on all oxygen atoms and the phenolic proton, as described in the Experimental Methods. All values are calculated at 203 K. KIEs were calculated in the same manner as those in Table S6.

Functional	% HF exchange	$\Delta G^{\ddagger}_{PI}$ (kcal/mol)	KIE_{PI} (k_H/k_D)	$\Delta G^{\ddagger}_{HB}$ (kcal/mol)	KIE_{HB} (k_H/k_D)	KIE_{HB} (k_H/k_D) (Streitweiser approx.)
BP86	0	7.2	7.7	8.3	1.56	1.87
TPSSH	10	15.6[a]	9.2	12.7	1.26	1.39
B3LYP	20	20.9[a]	10.2	16.2	1.16	1.21
B3LYP-GD3	20	19.2[a]	5.9	15.7	1.25	1.27

[a] Required a structural constraint to prevent the proton from returning to the phenolate, however the TS calculation converged to a structure with only one imaginary frequency.

10. "H-bond assisted O–O Homolysis" and "H^+ fixed on O_{Cu}" PESs generated using acetic acid instead of phenol

(a)



(b)

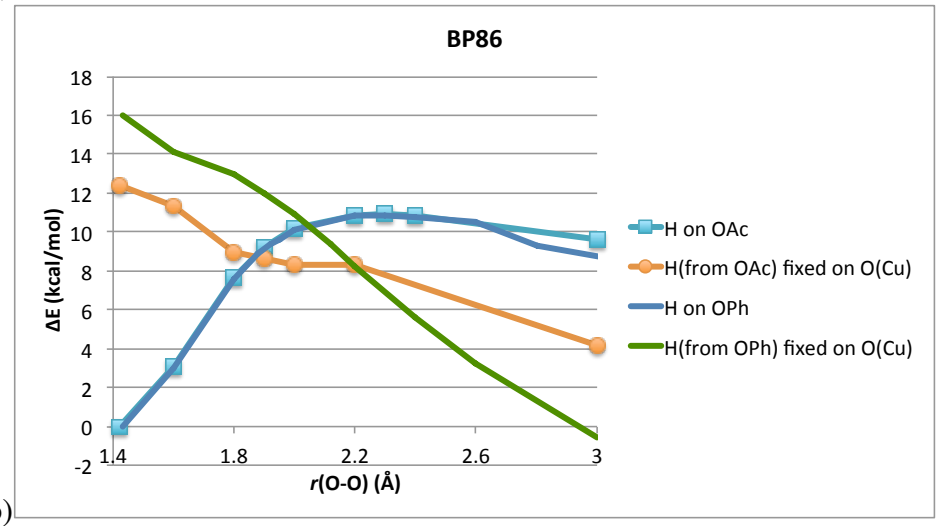


Figure S21. Comparison of PESs generated using (a) B3LYP and (b) BP86 for O–O cleavage with phenol (blue and green curves, re-plotted from Figure 13 in the text) vs. acetic acid (teal and orange curves) as the H^+ donor, where the proton is optimized on either the donor ($^-$OPh/$^-$OAc) or the peroxo O_{Cu}, respectively. Note that the electronic structure at the fully cleaved O–O distance of 3.0 Å in both acetic acid PESs (where the proton is H-bonding to the peroxo from OAc, and where it is fixed on O_{Cu}) has a hole on O_{Cu} thus the acetic acid surfaces reflect those generated using phenol without e^- transfer from phenolate.

11. Calculation of O–O bond cleavage thermodynamics in a higher dielectric (ε = 8.0)

Table S8. Overall thermodynamics of O-O bond rupture in CcO for different combinations of possible e^- source with the lowest energy H^+ donor available (Arg^+) and Tyr, calculated in ε = 4.0 and 8.0 at 298 K

Reaction {[(heme *a*)(His)Fe-O_2-Cu$(His)_3]^+$} + {HA} + {E^-} → {[(heme *a*)FeO(DMIm)]$^+$ + [$(His)_3$Cu(OH)]$^+$} + {A^-} + {E}			
H^+ Donor ({HA})	**e^- Donor ({E^-})**	**ΔG° (kcal/mol)** ε = 4.0	**ΔG° (kcal/mol)** ε = 8.0
Arg^+	Trp	+12.7	+9.0
	TyrH	+17.2	+14.5
	Tyr^-	-35.9	-27.7
Tyr	Trp	+44.0	+28.5
	Tyr^-	-4.6	-8.2

12. Cartesian Coordinates for reactants, transition states, and products

Docked reactant (**D**), BP86

Fe	0.164637	0.551695	0.707791
N	-0.110859	-1.244595	1.528702
N	-1.800772	0.884728	0.780871
N	0.469600	2.403991	-0.030613
C	-3.917601	1.826742	0.455468
C	-4.101311	0.656462	1.147558
C	-2.784373	0.074006	1.343987
C	-2.485963	1.976727	0.248040
C	-1.898189	3.112407	-0.340362
C	-2.559597	-1.154365	1.991821
C	-1.296342	-1.766553	2.054779
C	-1.056960	-3.059420	2.676759
C	0.277455	-3.334794	2.520347
C	0.863735	-2.200277	1.822084
C	2.242075	-2.075782	1.573066
C	2.839416	-0.905418	1.069364
C	4.276651	-0.721745	0.943291
C	4.476503	0.572272	0.527513
C	3.162069	1.175648	0.379967
C	2.957063	2.498980	-0.050930
C	1.681699	3.050144	-0.261769
C	1.457936	4.378794	-0.815949
C	0.101135	4.533768	-0.934541
C	-0.509255	3.306376	-0.440778
N	2.161420	0.259117	0.709208
H	0.824175	-4.210238	2.865019
H	-1.810077	-3.666866	3.173286
H	-5.039068	0.211114	1.471212
H	-4.677292	2.524041	0.110001
H	-0.443212	5.398492	-1.307690
H	2.239415	5.085589	-1.086434
H	5.422776	1.076554	0.343714
H	5.028416	-1.477847	1.160851
O	0.078893	0.050762	-1.041436
O	-0.747060	-0.999936	-1.543394
Cu	0.611041	-1.889013	-2.615729
N	-0.272782	-3.745363	-2.324279
N	2.467059	-2.717978	-2.723380
N	1.029465	-0.335881	-3.958243
H	2.492059	-3.214947	-1.817456
C	3.613725	-1.742242	-2.641201
H	3.560250	-1.269791	-1.644591
H	4.569566	-2.301317	-2.696384

C	2.692724	-3.785784	-3.764248
H	3.460277	-4.492085	-3.389615
H	3.098773	-3.311079	-4.673285
C	1.382030	-4.532458	-4.086676
H	0.757427	-3.934106	-4.775961
H	1.638140	-5.458199	-4.632525
C	0.572399	-4.899461	-2.827194
C	-0.625540	-3.990708	-0.888461
H	0.297868	-4.033922	-0.291561
H	-1.244849	-3.158732	-0.525296
H	-1.174937	-4.947306	-0.783592
C	-1.544144	-3.690308	-3.122227
H	-2.142431	-2.825369	-2.800441
H	-1.317699	-3.590556	-4.195481
H	-2.137932	-4.613488	-2.966953
C	1.025490	-0.914939	-5.341702
H	1.710865	-1.771773	-5.411504
H	0.004991	-1.253857	-5.584108
H	1.332194	-0.152850	-6.087030
C	0.011210	0.769477	-3.937417
H	-0.984561	0.362959	-4.167038
H	-0.013344	1.210048	-2.930949
H	0.280033	1.540727	-4.687985
C	3.580037	-0.654729	-3.725123
H	3.687564	-1.091631	-4.735532
H	4.474540	-0.023478	-3.572652
C	2.367378	0.289140	-3.649386
H	-0.098622	-5.759061	-3.024638
H	1.252056	-5.199025	-2.009029
H	2.523898	1.130881	-4.357184
H	2.284617	0.717559	-2.635341
C	3.142011	-3.202512	1.986964
C	3.398316	-4.322678	1.176207
C	3.796231	-3.206323	3.237318
C	4.232695	-5.382395	1.545664
C	4.644006	-4.237130	3.660622
C	4.863092	-5.334616	2.805105
H	4.383150	-6.220825	0.862863
H	5.117585	-4.177215	4.642568
H	5.520637	-6.150614	3.118027
C	4.157375	3.359078	-0.318876
C	4.924396	3.253463	-1.496723
C	4.592767	4.337448	0.600009
C	6.045481	4.048519	-1.763858
C	5.705476	5.159275	0.380018
C	6.437811	5.011399	-0.813644

H	6.591512	3.914615	-2.699949
H	5.987772	5.895941	1.135037
H	7.309717	5.644173	-1.003374
C	-2.799062	4.215832	-0.808672
C	-3.057712	4.457756	-2.173238
C	-3.432934	5.092988	0.095516
C	-3.893922	5.486763	-2.625402
C	-4.278351	6.134630	-0.305208
C	-4.510310	6.330243	-1.680927
H	-4.056731	5.615703	-3.697423
H	-4.737378	6.777715	0.448510
H	-5.167781	7.138099	-2.015355
C	-3.723961	-1.840724	2.640293
C	-4.311502	-3.012109	2.120850
C	-4.303683	-1.355452	3.832894
C	-5.394084	-3.668012	2.718578
C	-5.387387	-1.972708	4.469948
C	-5.935781	-3.141244	3.907239
H	-5.801130	-4.569403	2.255832
H	-5.784441	-1.542708	5.391794
H	-6.782325	-3.637571	4.390471
F	-2.444527	3.628545	-3.119712
F	4.539856	2.302432	-2.456130
F	2.766488	-4.385258	-0.092569
F	-3.792030	-3.541593	0.925456
F	-3.761409	-0.200492	4.407226
F	3.577326	-2.119604	4.094850
F	3.874027	4.489009	1.790956
F	-3.195633	4.909360	1.465548
N	0.324016	1.332758	2.584979
C	1.077311	0.854519	3.590166
C	-0.320929	2.469589	3.079642
H	1.719182	-0.021230	3.558924
C	0.044743	2.680729	4.402078
H	-1.004519	3.055362	2.471922
N	0.938109	1.640816	4.710995
C	-0.353271	3.738049	5.384966
H	-0.849849	3.310524	6.277743
H	0.516022	4.325327	5.739851
H	-1.060201	4.438182	4.911663
C	1.608315	1.424031	6.002682
H	2.247852	2.286476	6.254011
H	0.863432	1.279664	6.802835
H	2.235435	0.522710	5.932157
H	-2.211234	-0.363521	-2.254844
O	-2.910564	-0.042606	-2.898566

C	-4.102520	-0.725913	-2.773069
C	-5.111089	-0.459828	-3.731081
C	-4.351232	-1.671019	-1.749165
C	-6.343448	-1.133905	-3.668686
H	-4.909001	0.277037	-4.515172
C	-5.584911	-2.349033	-1.698006
H	-3.588649	-1.861683	-0.987900
C	-6.586242	-2.086697	-2.654874
H	-7.115262	-0.916987	-4.416685
H	-5.753954	-3.082650	-0.902087
H	-7.545189	-2.614588	-2.611285

$\underline{TS_{PI}, BP86}$

Fe	0.328765	0.476359	0.719822
N	-0.068480	-1.273542	1.593840
N	-1.561525	1.031241	0.934938
N	0.788152	2.317611	0.002877
C	-3.587377	2.177009	0.720846
C	-3.842569	1.041618	1.444901
C	-2.582999	0.326930	1.569984
C	-2.163791	2.181675	0.423555
C	-1.504871	3.255141	-0.200174
C	-2.452849	-0.915703	2.213590
C	-1.264357	-1.667103	2.190365
C	-1.133630	-3.000626	2.752161
C	0.137928	-3.431850	2.465994
C	0.803675	-2.349768	1.758340
C	2.160993	-2.383720	1.390211
C	2.857845	-1.268983	0.888151
C	4.292812	-1.242906	0.645116
C	4.608850	0.040155	0.269867
C	3.365179	0.795945	0.258741
C	3.272918	2.143677	-0.133916
C	2.053667	2.829878	-0.273130
C	1.944571	4.182296	-0.799897
C	0.606021	4.477761	-0.865239
C	-0.107754	3.314823	-0.359941
N	2.303043	-0.017701	0.643263
H	0.596463	-4.382120	2.731032
H	-1.912711	-3.533645	3.291888
H	-4.797810	0.697237	1.833267
H	-4.292968	2.942975	0.408838
H	0.140431	5.399486	-1.206481
H	2.783765	4.812398	-1.086289
H	5.588071	0.441309	0.017188
H	4.965462	-2.089859	0.762486

O	0.199127	-0.077158	-0.859877
O	-1.289335	-0.975725	-1.581019
Cu	0.023168	-1.773840	-2.701162
N	-0.932106	-3.646432	-2.446232
N	1.781300	-2.724004	-3.003470
N	0.491841	-0.137612	-3.921987
H	1.823019	-3.293449	-2.141822
C	3.008214	-1.849939	-2.925123
H	3.036082	-1.431203	-1.904159
H	3.908190	-2.483409	-3.056013
C	1.868682	-3.720063	-4.134274
H	2.646073	-4.467962	-3.880608
H	2.204227	-3.191567	-5.042020
C	0.513207	-4.412654	-4.383066
H	-0.146076	-3.769071	-4.994117
H	0.697498	-5.319577	-4.986591
C	-0.205323	-4.812469	-3.079822
C	-1.173044	-3.941015	-0.997085
H	-0.205368	-4.073472	-0.488337
H	-1.703070	-3.087677	-0.551173
H	-1.774007	-4.865525	-0.884623
C	-2.261315	-3.465274	-3.121446
H	-2.775271	-2.601206	-2.675110
H	-2.119970	-3.280112	-4.198704
H	-2.886167	-4.372035	-2.991447
C	0.274618	-0.586330	-5.336611
H	0.882078	-1.474893	-5.563848
H	-0.790429	-0.836013	-5.471652
H	0.544333	0.220368	-6.048168
C	-0.399759	1.047903	-3.679340
H	-1.453460	0.766834	-3.824891
H	-0.271755	1.376504	-2.638504
H	-0.124651	1.867805	-4.373462
C	3.011319	-0.707743	-3.949719
H	2.999680	-1.094859	-4.985649
H	3.972741	-0.173639	-3.837066
C	1.908772	0.338307	-3.724500
H	-0.938422	-5.622596	-3.267001
H	0.522812	-5.199014	-2.343010
H	2.076526	1.196228	-4.409467
H	1.963282	0.719857	-2.690294
C	2.935292	-3.642972	1.643384
C	2.970738	-4.715165	0.733290
C	3.687171	-3.828056	2.822663
C	3.686296	-5.897117	0.948653
C	4.423350	-4.988485	3.090751

C	4.421297	-6.031213	2.143630
H	3.666928	-6.689562	0.198061
H	4.982760	-5.069017	4.024871
H	4.989171	-6.946008	2.335454
C	4.542191	2.872126	-0.470825
C	5.079950	2.894504	-1.773177
C	5.275626	3.580264	0.503411
C	6.260929	3.567826	-2.107864
C	6.461344	4.269867	0.220186
C	6.956064	4.262129	-1.098328
H	6.621872	3.546498	-3.138168
H	6.980426	4.800294	1.021112
H	7.880005	4.796000	-1.338978
C	-2.316514	4.437759	-0.634934
C	-2.623141	4.691351	-1.987266
C	-2.811044	5.379990	0.290581
C	-3.377430	5.794071	-2.407886
C	-3.569459	6.496921	-0.079124
C	-3.855112	6.702283	-1.443354
H	-3.586103	5.928715	-3.471140
H	-3.922231	7.188382	0.688752
H	-4.447527	7.568034	-1.753452
C	-3.642287	-1.472432	2.936131
C	-4.394126	-2.561985	2.451031
C	-4.081622	-0.933987	4.164999
C	-5.504805	-3.092240	3.118084
C	-5.185754	-1.427362	4.870633
C	-5.902410	-2.517809	4.341003
H	-6.044415	-3.934550	2.680495
H	-5.469613	-0.963604	5.817563
H	-6.768271	-2.916822	4.877212
F	-2.147831	3.796954	-2.952884
F	4.392511	2.206186	-2.785773
F	2.232665	-4.591369	-0.469861
F	-4.014962	-3.138134	1.227476
F	-3.371084	0.145260	4.702380
F	3.687052	-2.793421	3.766677
F	4.788366	3.590641	1.814866
F	-2.519263	5.181885	1.647848
N	0.734223	1.251412	2.609512
C	1.511462	0.693919	3.553996
C	0.230894	2.434201	3.157741
H	2.063373	-0.237809	3.469933
C	0.708986	2.594260	4.450670
H	-0.437476	3.088211	2.604916
N	1.524290	1.472336	4.686125

C	0.483415	3.670917	5.466456
H	0.023478	3.278254	6.393910
H	1.426076	4.176378	5.753307
H	-0.194589	4.434816	5.053577
C	2.260191	1.178159	5.926606
H	2.980003	1.983954	6.145142
H	1.560364	1.076471	6.772474
H	2.809166	0.233028	5.801222
H	-2.120636	-0.332485	-1.956112
O	-3.161430	0.208229	-2.621593
C	-4.400829	-0.283667	-2.480531
C	-5.432783	0.119689	-3.388553
C	-4.763648	-1.211075	-1.452622
C	-6.743202	-0.373262	-3.270211
H	-5.169719	0.832857	-4.178520
C	-6.075229	-1.706790	-1.348331
H	-3.996529	-1.528599	-0.739271
C	-7.078941	-1.294941	-2.252452
H	-7.510748	-0.040021	-3.981253
H	-6.311760	-2.422477	-0.550402
H	-8.100480	-1.682839	-2.167190

TS_{HB}, BP86

Fe	0.466015	0.381531	0.695822
N	0.016148	-1.394827	1.513507
N	-1.395551	1.014747	1.014189
N	0.984039	2.232529	0.062336
C	-3.375368	2.251072	0.911303
C	-3.664769	1.081131	1.565133
C	-2.432029	0.311743	1.623065
C	-1.958321	2.216716	0.587665
C	-1.264158	3.297847	0.016976
C	-2.340663	-0.969491	2.194037
C	-1.185455	-1.767062	2.109323
C	-1.105686	-3.136639	2.591071
C	0.136934	-3.609069	2.249271
C	0.837138	-2.517837	1.589841
C	2.179969	-2.590760	1.178523
C	2.912395	-1.480101	0.721542
C	4.336714	-1.507377	0.428393
C	4.700459	-0.223443	0.103055
C	3.495590	0.588991	0.173445
C	3.453607	1.955287	-0.161492
C	2.263569	2.701880	-0.226348
C	2.203502	4.090910	-0.656683
C	0.880632	4.454737	-0.648615

C	0.127011	3.296376	-0.194281
N	2.410234	-0.192208	0.559688
H	0.555936	-4.593426	2.446472
H	-1.897786	-3.663317	3.117898
H	-4.626307	0.751314	1.950585
H	-4.052752	3.065150	0.665220
H	0.450627	5.419663	-0.907100
H	3.062521	4.700868	-0.926771
H	5.687131	0.142561	-0.172518
H	4.971261	-2.389585	0.478818
O	0.197146	-0.121327	-0.865183
O	-1.754221	-0.854472	-1.839727
Cu	-0.323826	-1.521683	-2.782847
N	-1.204915	-3.481040	-2.635353
N	1.459982	-2.407375	-3.149788
N	0.124755	0.206783	-3.929477
H	1.527100	-3.032420	-2.329904
C	2.667040	-1.512135	-3.028151
H	2.672394	-1.133660	-1.992388
H	3.582391	-2.118724	-3.178614
C	1.564436	-3.323727	-4.345768
H	2.361736	-4.067990	-4.148398
H	1.879745	-2.726740	-5.217602
C	0.226966	-4.032327	-4.638351
H	-0.462640	-3.350592	-5.170857
H	0.426511	-4.870853	-5.329772
C	-0.452215	-4.569818	-3.363355
C	-1.359660	-3.843987	-1.192497
H	-0.363146	-3.959342	-0.736852
H	-1.898207	-3.029097	-0.687424
H	-1.919261	-4.795219	-1.084434
C	-2.567921	-3.333458	-3.241646
H	-3.086929	-2.503623	-2.737399
H	-2.480318	-3.104886	-4.316489
H	-3.151793	-4.268829	-3.118934
C	-0.106903	-0.139037	-5.368214
H	0.526031	-0.986416	-5.672435
H	-1.164956	-0.418400	-5.502967
H	0.120539	0.726815	-6.023865
C	-0.776775	1.353208	-3.581493
H	-1.819304	1.090029	-3.804911
H	-0.690546	1.557771	-2.506192
H	-0.487634	2.250965	-4.165038
C	2.649996	-0.327888	-4.003517
H	2.635892	-0.668809	-5.055825
H	3.605139	0.213630	-3.873781

C	1.536438	0.692503	-3.722368
H	-1.156071	-5.392332	-3.603613
H	0.304967	-4.984131	-2.672253
H	1.687592	1.585578	-4.366256
H	1.594220	1.018546	-2.669514
C	2.890391	-3.905315	1.302536
C	2.843837	-4.886805	0.295355
C	3.652829	-4.241448	2.440262
C	3.491874	-6.122822	0.382955
C	4.323595	-5.462625	2.581136
C	4.240613	-6.410006	1.541969
H	3.411450	-6.838921	-0.437138
H	4.896127	-5.662543	3.489074
H	4.756749	-7.369852	1.634016
C	4.744775	2.635187	-0.509912
C	5.127288	2.900772	-1.840538
C	5.662739	3.045262	0.479725
C	6.328833	3.530339	-2.186401
C	6.877074	3.677989	0.186030
C	7.210524	3.922601	-1.160183
H	6.563620	3.704577	-3.238419
H	7.540952	3.973523	1.000982
H	8.154101	4.416756	-1.409194
C	-2.025047	4.555074	-0.281698
C	-2.417298	4.923227	-1.584202
C	-2.383511	5.457074	0.741760
C	-3.123602	6.099066	-1.868168
C	-3.088497	6.643800	0.510082
C	-3.461821	6.964556	-0.810013
H	-3.403084	6.322627	-2.899715
H	-3.333990	7.298847	1.348421
H	-4.014534	7.886463	-1.013015
C	-3.538808	-1.516249	2.910730
C	-4.353001	-2.537449	2.380275
C	-3.921388	-1.037369	4.182629
C	-5.469894	-3.058376	3.044295
C	-5.029369	-1.523819	4.886970
C	-5.809228	-2.545210	4.311184
H	-6.058814	-3.846863	2.571426
H	-5.267139	-1.108464	5.868418
H	-6.678842	-2.938124	4.845791
F	-2.084522	4.070896	-2.644042
F	4.257452	2.508469	-2.870878
F	2.093016	-4.605064	-0.871230
F	-4.034346	-3.050988	1.111600
F	-3.147834	-0.027701	4.765729

F	3.732902	-3.301199	3.474603
F	5.336319	2.806628	1.819293
F	-2.005196	5.142805	2.055190
N	0.941802	1.053499	2.642036
C	1.716068	0.419844	3.539216
C	0.506825	2.230032	3.257924
H	2.223337	-0.529990	3.395870
C	1.023941	2.309111	4.543298
H	-0.146001	2.938473	2.755277
N	1.794249	1.142891	4.705339
C	0.872326	3.344967	5.613735
H	0.417724	2.928872	6.533620
H	1.843662	3.793811	5.899039
H	0.219835	4.157116	5.255305
C	2.549775	0.763958	5.910475
H	3.310117	1.528097	6.141720
H	1.869409	0.656750	6.771450
H	3.053205	-0.197606	5.730900
H	-2.909608	0.119952	-2.150102
O	-3.705759	0.673664	-2.522223
C	-4.919978	0.122828	-2.208479
C	-6.079734	0.665337	-2.821015
C	-5.069351	-0.954950	-1.296945
C	-7.351854	0.138000	-2.536135
H	-5.959060	1.500253	-3.519614
C	-6.345188	-1.482779	-1.022019
H	-4.182386	-1.362643	-0.802851
C	-7.493745	-0.942791	-1.638078
H	-8.235928	0.570280	-3.020650
H	-6.434420	-2.319460	-0.319018
H	-8.485465	-1.355534	-1.421649

Product (**P**), BP86

Fe	1.592695	-0.157838	0.368759
N	1.718995	-2.098896	-0.143742
N	0.794383	-0.668280	2.140636
N	1.618472	1.766679	0.940956
C	-0.350797	-0.571218	4.172382
C	-0.106174	-1.895680	3.909733
C	0.581807	-1.954099	2.628572
C	0.226382	0.191993	3.076235
C	0.264403	1.598019	3.026549
C	0.894653	-3.152131	1.960298
C	1.384673	-3.196917	0.641436
C	1.507160	-4.423122	-0.133324
C	1.878891	-4.057840	-1.403303

C	2.022459	-2.610149	-1.402746
C	2.466758	-1.859521	-2.507041
C	2.739578	-0.479929	-2.442243
C	3.374027	0.272833	-3.513163
C	3.567232	1.549127	-3.044317
C	3.026868	1.590785	-1.694302
C	2.945944	2.762764	-0.918844
C	2.245516	2.832184	0.299366
C	2.001095	4.067937	1.026454
C	1.190857	3.753163	2.089545
C	0.965248	2.316753	2.039002
N	2.534181	0.339348	-1.335973
H	2.048578	-4.704592	-2.261105
H	1.307607	-5.423985	0.242945
H	-0.377369	-2.757303	4.515364
H	-0.862175	-0.145994	5.032690
H	0.806016	4.421423	2.856749
H	2.396078	5.044072	0.754159
H	4.017365	2.391399	-3.565108
H	3.652519	-0.132117	-4.483539
O	0.087566	-0.019480	-0.333021
O	-5.126533	-0.249904	-0.566339
Cu	-3.616439	0.655513	-1.218906
N	-2.957124	-1.241353	-1.979855
N	-1.840147	1.427002	-1.739321
N	-4.519745	2.514451	-0.648987
H	-1.163782	0.756816	-1.296632
C	-1.398191	2.749345	-1.167881
H	-1.183659	2.581870	-0.097375
H	-0.445425	3.042356	-1.648103
C	-1.524556	1.380120	-3.216843
H	-0.424398	1.453366	-3.327154
H	-1.971664	2.265513	-3.701541
C	-2.024018	0.084061	-3.886604
H	-3.090117	0.174669	-4.169311
H	-1.458023	-0.056712	-4.824390
C	-1.827554	-1.144235	-2.976935
C	-2.532514	-2.006119	-0.764147
H	-1.677119	-1.491928	-0.293151
H	-3.386847	-2.041051	-0.070132
H	-2.226387	-3.037625	-1.029512
C	-4.105077	-1.959078	-2.623874
H	-4.942517	-1.960402	-1.912310
H	-4.413200	-1.429082	-3.540411
H	-3.804621	-2.993622	-2.888257
C	-5.381502	2.835324	-1.835853

H	-4.758345	2.947374	-2.737064
H	-6.101809	2.016339	-1.993202
H	-5.939742	3.779048	-1.667366
C	-5.410644	2.339784	0.549165
H	-6.083603	1.493360	0.364601
H	-4.788608	2.103691	1.427146
H	-5.979666	3.273392	0.737763
C	-2.440597	3.864881	-1.316786
H	-2.783173	3.961326	-2.364414
H	-1.947196	4.821887	-1.065267
C	-3.615594	3.682496	-0.347665
H	-1.791013	-2.081873	-3.566214
H	-0.877413	-1.062694	-2.418416
H	-4.241297	4.600518	-0.316273
H	-3.213439	3.518453	0.669366
C	2.712731	-2.567448	-3.805128
C	1.816591	-2.470388	-4.889018
C	3.855400	-3.363012	-4.028774
C	2.019889	-3.114488	-6.115440
C	4.104219	-4.028871	-5.235064
C	3.175538	-3.901518	-6.286730
H	1.283819	-3.000213	-6.913774
H	5.010298	-4.628496	-5.343401
H	3.352426	-4.413101	-7.237276
C	3.571611	4.013881	-1.460488
C	2.821491	5.028061	-2.090283
C	4.960537	4.247417	-1.379926
C	3.388025	6.199830	-2.605561
C	5.575888	5.401773	-1.880275
C	4.780192	6.386124	-2.497628
H	2.747649	6.943962	-3.083520
H	6.656804	5.521131	-1.781758
H	5.242825	7.294636	-2.893964
C	-0.435530	2.376464	4.098211
C	-1.649762	3.050029	3.852708
C	0.073980	2.499086	5.407381
C	-2.331198	3.789853	4.825675
C	-0.569125	3.226311	6.416553
C	-1.783340	3.876283	6.120828
H	-3.271713	4.282495	4.571057
H	-0.119695	3.282660	7.410073
H	-2.300498	4.449022	6.896023
C	0.612975	-4.453229	2.652760
C	-0.684998	-4.996507	2.747032
C	1.638658	-5.219900	3.243716
C	-0.965643	-6.211492	3.384120

C	1.409562	-6.440704	3.890770
C	0.094061	-6.938585	3.960763
H	-1.994365	-6.575748	3.420715
H	2.249041	-6.982805	4.330873
H	-0.104845	-7.890021	4.462561
F	-2.196377	2.966043	2.560082
F	1.434625	4.846952	-2.210657
F	0.663321	-1.687785	-4.724869
F	-1.745064	-4.281308	2.173593
F	2.948022	-4.729575	3.178855
F	4.783922	-3.484837	-2.986700
F	5.757122	3.274220	-0.766264
F	1.285540	1.861759	5.703185
N	3.483485	-0.355241	1.262390
C	4.555669	-0.965711	0.730496
C	3.876582	0.105329	2.521513
H	4.604320	-1.445348	-0.242709
C	5.202304	-0.231655	2.755211
H	3.193083	0.638168	3.176552
N	5.620067	-0.914580	1.597705
C	6.100899	0.015569	3.927101
H	6.468739	-0.927834	4.375276
H	6.988188	0.617849	3.650855
H	5.551941	0.565863	4.707974
C	6.959335	-1.476863	1.358693
H	7.720490	-0.679810	1.388883
H	7.197553	-2.236128	2.121803
H	6.976931	-1.950651	0.366009
H	-5.934171	-0.130053	-1.122846
O	-7.570572	0.228616	-1.865714
C	-8.554405	-0.342965	-1.243594
C	-9.926447	-0.162463	-1.691545
C	-8.331494	-1.189682	-0.080696
C	-10.982194	-0.782648	-1.025082
H	-10.093357	0.473529	-2.566880
C	-9.400128	-1.800517	0.570641
H	-7.294271	-1.317532	0.249356
C	-10.730433	-1.603777	0.107160
H	-12.011711	-0.640155	-1.371874
H	-9.221414	-2.436339	1.445042
H	-11.565255	-2.086759	0.626107

Docked reactant (**D**), B3LYP

Fe	0.229686	0.489761	0.764605
N	-0.130164	-1.331774	1.523373
N	-1.724518	0.907720	0.850911

N	0.623384	2.363813	0.109307
C	-3.778267	1.941381	0.556823
C	-4.010829	0.772510	1.212850
C	-2.726014	0.124353	1.387551
C	-2.345176	2.034571	0.350990
C	-1.702583	3.150061	-0.200338
C	-2.553883	-1.132336	1.978289
C	-1.328972	-1.809299	2.015497
C	-1.148073	-3.140669	2.557090
C	0.160181	-3.471507	2.369037
C	0.796047	-2.333378	1.734676
C	2.168122	-2.258222	1.464979
C	2.825170	-1.100346	1.031231
C	4.265255	-0.982289	0.902054
C	4.526821	0.312938	0.567516
C	3.248948	0.989358	0.466875
C	3.096943	2.330340	0.095818
C	1.856397	2.949440	-0.090380
C	1.690301	4.298680	-0.596165
C	0.351515	4.512206	-0.718765
C	-0.311808	3.300366	-0.273531
N	2.223351	0.110079	0.753940
H	0.658058	-4.385585	2.652292
H	-1.918212	-3.735535	3.021239
H	-4.959831	0.366835	1.524455
H	-4.502280	2.672718	0.236279
H	-0.146646	5.404783	-1.061946
H	2.493593	4.977800	-0.834100
H	5.489212	0.772196	0.406236
H	4.973844	-1.779427	1.063522
O	0.175360	-0.018440	-0.981210
O	-0.859759	-0.852053	-1.537229
Cu	0.442504	-1.695954	-2.656174
N	-0.502389	-3.577310	-2.541753
N	2.263472	-2.571214	-2.898282
N	0.862617	-0.061098	-3.954038
H	2.304704	-3.118133	-2.034334
C	3.424761	-1.623897	-2.797793
H	3.402794	-1.199908	-1.789677
H	4.358992	-2.193933	-2.895156
C	2.434905	-3.571103	-4.006350
H	3.187681	-4.307684	-3.696273
H	2.832399	-3.054278	-4.883376
C	1.115092	-4.271505	-4.359977
H	0.502881	-3.626553	-5.001476
H	1.350296	-5.156002	-4.962668

C	0.306963	-4.703703	-3.128286
C	-0.857921	-3.913250	-1.131298
H	0.055758	-4.041102	-0.550094
H	-1.436098	-3.096300	-0.703746
H	-1.440889	-4.843561	-1.095201
C	-1.766674	-3.416326	-3.323212
H	-2.332033	-2.571343	-2.931288
H	-1.545702	-3.238526	-4.378032
H	-2.382959	-4.321982	-3.243611
C	0.765709	-0.532264	-5.366341
H	1.412268	-1.392521	-5.540753
H	-0.267293	-0.818774	-5.578861
H	1.053865	0.267220	-6.063533
C	-0.112456	1.060094	-3.782879
H	-1.123834	0.706933	-3.981164
H	-0.065198	1.416594	-2.755875
H	0.132063	1.876427	-4.477260
C	3.394295	-0.494201	-3.828845
H	3.443505	-0.891301	-4.849408
H	4.313180	0.087123	-3.692198
C	2.229814	0.490466	-3.672323
H	-0.375679	-5.526704	-3.380610
H	0.979657	-5.073360	-2.347286
H	2.397998	1.347930	-4.342589
H	2.205729	0.873610	-2.648709
C	3.003637	-3.464046	1.752489
C	3.178563	-4.507219	0.840718
C	3.676537	-3.629727	2.968812
C	3.946349	-5.638967	1.079071
C	4.462814	-4.734185	3.274937
C	4.594375	-5.745496	2.315936
H	4.032439	-6.407366	0.321880
H	4.953938	-4.796716	4.237316
H	5.200865	-6.616672	2.531679
C	4.329281	3.135475	-0.166535
C	5.070434	3.021210	-1.347711
C	4.823881	4.069081	0.751808
C	6.215734	3.758339	-1.622572
C	5.961723	4.838609	0.537242
C	6.660680	4.676441	-0.664148
H	6.736183	3.617064	-2.560972
H	6.286065	5.541117	1.294033
H	7.550143	5.265055	-0.854078
C	-2.546785	4.283839	-0.682382
C	-2.707209	4.577811	-2.041582
C	-3.224361	5.140142	0.193304

C	-3.485070	5.626773	-2.518398
C	-4.018255	6.203111	-0.220235
C	-4.147047	6.442138	-1.593419
H	-3.567193	5.793088	-3.584731
H	-4.513444	6.823896	0.515187
H	-4.760178	7.264604	-1.941853
C	-3.748663	-1.798109	2.579777
C	-4.374026	-2.911522	2.007213
C	-4.326813	-1.351485	3.775381
C	-5.482683	-3.548805	2.550563
C	-5.434915	-1.943370	4.370180
C	-6.013920	-3.054533	3.747314
H	-5.913588	-4.404016	2.046144
H	-5.825398	-1.542138	5.296436
H	-6.878279	-3.533005	4.191786
F	-2.038917	3.779332	-2.968703
F	4.627525	2.108738	-2.310447
F	2.526375	-4.406052	-0.406088
F	-3.859262	-3.406885	0.802854
F	-3.753109	-0.248646	4.403958
F	3.543062	-2.621526	3.923255
F	4.132166	4.232866	1.949736
F	-3.088166	4.909317	1.563048
N	0.426578	1.191485	2.698578
C	1.199286	0.674856	3.649970
C	-0.213271	2.288866	3.259509
H	1.835944	-0.189036	3.560999
C	0.179796	2.436554	4.570981
H	-0.906947	2.895545	2.702805
N	1.082410	1.395445	4.804908
C	-0.200493	3.438488	5.608664
H	-0.668818	2.968084	6.482452
H	0.665835	4.008685	5.967052
H	-0.917067	4.149645	5.190373
C	1.783291	1.121372	6.060996
H	2.423869	1.963986	6.333613
H	1.067002	0.939976	6.866242
H	2.402800	0.233144	5.932737
H	-2.313764	-0.061889	-2.080448
O	-3.043276	0.355428	-2.616030
C	-4.231702	-0.323130	-2.552853
C	-5.267373	0.104833	-3.402605
C	-4.448809	-1.408355	-1.686815
C	-6.500417	-0.552489	-3.388655
H	-5.086994	0.947047	-4.062058
C	-5.685924	-2.063366	-1.686221

H	-3.664831	-1.725034	-1.010083
C	-6.718306	-1.643684	-2.534187
H	-7.293099	-0.213345	-4.048926
H	-5.834016	-2.902224	-1.013603
H	-7.676106	-2.153589	-2.528868

TS_{PI}, B3LYP

Fe	0.359719	0.436835	0.770927
N	-0.026878	-1.349732	1.592861
N	-1.545285	0.965256	1.005289
N	0.803384	2.298747	0.113982
C	-3.565135	2.085438	0.817105
C	-3.812536	0.925408	1.481873
C	-2.551652	0.221328	1.591049
C	-2.144202	2.120580	0.537033
C	-1.489422	3.211357	-0.040652
C	-2.410070	-1.039899	2.175492
C	-1.218495	-1.771787	2.147021
C	-1.077822	-3.122571	2.647200
C	0.190851	-3.525504	2.356505
C	0.850272	-2.412316	1.705990
C	2.195595	-2.417996	1.325892
C	2.884634	-1.290235	0.867046
C	4.309781	-1.250710	0.610365
C	4.616740	0.035335	0.276445
C	3.378968	0.786760	0.302844
C	3.271213	2.135388	-0.051847
C	2.056210	2.817989	-0.155264
C	1.930771	4.180696	-0.629454
C	0.600019	4.468343	-0.667413
C	-0.100697	3.290141	-0.199016
N	2.336186	-0.039751	0.671891
H	0.650266	-4.475695	2.578486
H	-1.849289	-3.683367	3.149460
H	-4.760636	0.557312	1.838204
H	-4.271807	2.847913	0.533171
H	0.131108	5.391894	-0.966705
H	2.754768	4.822222	-0.898108
H	5.584234	0.440952	0.026341
H	4.980415	-2.091565	0.691041
O	0.220947	-0.096621	-0.812487
O	-1.327082	-0.935319	-1.539611
Cu	0.010529	-1.617757	-2.732511
N	-0.890933	-3.530674	-2.593504
N	1.803334	-2.482967	-3.107591
N	0.392323	0.095495	-3.884824

H	1.882872	-3.078481	-2.278915
C	2.982736	-1.557269	-3.014413
H	3.007896	-1.179256	-1.988921
H	3.900355	-2.137918	-3.177897
C	1.908227	-3.420809	-4.277761
H	2.696172	-4.153321	-4.060319
H	2.228393	-2.851268	-5.153328
C	0.578138	-4.130906	-4.562709
H	-0.089730	-3.472233	-5.130573
H	0.781238	-4.986541	-5.216195
C	-0.124522	-4.624167	-3.290443
C	-1.116768	-3.923004	-1.169521
H	-0.155005	-4.026770	-0.665050
H	-1.700417	-3.149582	-0.674225
H	-1.652747	-4.880469	-1.120834
C	-2.224537	-3.362926	-3.253213
H	-2.764541	-2.543678	-2.778412
H	-2.099800	-3.139307	-4.315366
H	-2.811743	-4.285736	-3.157378
C	0.144197	-0.289573	-5.306575
H	0.769588	-1.133231	-5.600478
H	-0.906177	-0.567158	-5.423804
H	0.358958	0.553581	-5.976987
C	-0.530429	1.228223	-3.553249
H	-1.570417	0.919763	-3.659761
H	-0.367053	1.525487	-2.519657
H	-0.321368	2.077763	-4.217099
C	2.919374	-0.385116	-3.992892
H	2.891635	-0.736805	-5.030648
H	3.857327	0.173360	-3.892511
C	1.792248	0.610851	-3.709574
H	-0.820638	-5.441064	-3.522669
H	0.610646	-5.023176	-2.583078
H	1.913256	1.486753	-4.364163
H	1.865029	0.961150	-2.676983
C	2.965730	-3.688795	1.482411
C	3.010629	-4.672287	0.491832
C	3.703769	-3.979215	2.635413
C	3.714794	-5.863332	0.601174
C	4.432139	-5.149804	2.811859
C	4.432832	-6.096678	1.780831
H	3.700396	-6.580628	-0.209020
H	4.979883	-5.310681	3.731298
H	4.991994	-7.017231	1.895719
C	4.526556	2.868693	-0.403139
C	4.967686	3.019096	-1.722149

C	5.350079	3.449519	0.567763
C	6.129704	3.691406	-2.080091
C	6.523976	4.134535	0.275624
C	6.911217	4.253876	-1.063885
H	6.409052	3.769028	-3.122835
H	7.111792	4.561025	1.078043
H	7.821510	4.784326	-1.316134
C	-2.305902	4.395251	-0.442437
C	-2.586988	4.704693	-1.777834
C	-2.836322	5.284451	0.499382
C	-3.343425	5.802625	-2.171529
C	-3.599948	6.397322	0.170020
C	-3.853450	6.651906	-1.183059
H	-3.526722	5.979119	-3.223474
H	-3.978813	7.042265	0.952194
H	-4.447234	7.512531	-1.466696
C	-3.606685	-1.654933	2.823906
C	-4.309199	-2.728207	2.264230
C	-4.112314	-1.192043	4.045292
C	-5.427893	-3.312585	2.845251
C	-5.225409	-1.732774	4.677747
C	-5.885511	-2.804643	4.066562
H	-5.922872	-4.137646	2.349656
H	-5.558559	-1.322529	5.622227
H	-6.756352	-3.241987	4.539781
F	-2.072661	3.869215	-2.767780
F	4.191550	2.453838	-2.738815
F	2.285722	-4.440434	-0.695369
F	-3.863240	-3.236458	1.040320
F	-3.457195	-0.126271	4.658396
F	3.699779	-3.033142	3.658734
F	4.966488	3.329826	1.901310
F	-2.575321	5.032122	1.847204
N	0.748073	1.154471	2.696882
C	1.566959	0.607325	3.592443
C	0.194865	2.278450	3.297437
H	2.158408	-0.282548	3.460230
C	0.688342	2.410878	4.575471
H	-0.512425	2.913195	2.791567
N	1.563276	1.333507	4.747428
C	0.423944	3.426843	5.634939
H	-0.002542	2.975023	6.539289
H	1.336676	3.958461	5.931465
H	-0.288873	4.168318	5.266041
C	2.344752	1.038044	5.950925
H	3.041677	1.852849	6.162613

H	1.682969	0.899218	6.809206
H	2.911179	0.120633	5.788691
H	-2.092772	-0.278469	-1.809876
O	-3.238313	0.305944	-2.455225
C	-4.480538	-0.149973	-2.365377
C	-5.501860	0.387818	-3.201501
C	-4.867546	-1.176314	-1.457215
C	-6.818432	-0.070313	-3.127415
H	-5.224914	1.173190	-3.899142
C	-6.187894	-1.629601	-1.396910
H	-4.115835	-1.602814	-0.802477
C	-7.179645	-1.085583	-2.226806
H	-7.572045	0.366168	-3.779249
H	-6.443488	-2.416608	-0.690688
H	-8.204044	-1.441443	-2.174789

TS_{HB}, B3LYP

Fe	0.358611	0.388992	0.748611
N	-0.061041	-1.419979	1.516893
N	-1.546314	0.936925	0.980834
N	0.833518	2.265675	0.161086
C	-3.548004	2.093027	0.817945
C	-3.817956	0.914027	1.439048
C	-2.566238	0.188709	1.533257
C	-2.122958	2.116145	0.551251
C	-1.444764	3.216943	0.018089
C	-2.447340	-1.094673	2.075071
C	-1.266252	-1.844313	2.036991
C	-1.152227	-3.214555	2.491802
C	0.116338	-3.623680	2.209120
C	0.800444	-2.495861	1.609589
C	2.154411	-2.500943	1.258828
C	2.864230	-1.365570	0.852237
C	4.298192	-1.330045	0.644234
C	4.624038	-0.038154	0.355481
C	3.389601	0.721010	0.362053
C	3.302044	2.081008	0.044825
C	2.095926	2.779130	-0.067557
C	1.995137	4.160040	-0.494877
C	0.668983	4.465832	-0.542230
C	-0.053181	3.279901	-0.126601
N	2.329779	-0.107216	0.671491
H	0.559598	-4.587338	2.404792
H	-1.939419	-3.782589	2.960594
H	-4.773626	0.548999	1.778475
H	-4.241169	2.876215	0.557705

H	0.216851	5.406477	-0.812910
H	2.830576	4.801609	-0.725473
H	5.601675	0.366874	0.147394
H	4.960104	-2.177717	0.726153
O	0.218367	-0.104179	-0.853775
O	-1.377008	-0.796289	-1.742077
Cu	0.034877	-1.469344	-2.779752
N	-0.840065	-3.417565	-2.751920
N	1.857295	-2.305657	-3.131752
N	0.434111	0.271381	-3.933080
H	1.923304	-2.920277	-2.316372
C	3.015365	-1.362335	-2.982083
H	2.995123	-1.000382	-1.951197
H	3.951034	-1.920820	-3.121500
C	2.016622	-3.212261	-4.319231
H	2.801324	-3.945975	-4.092074
H	2.366442	-2.617431	-5.166433
C	0.706684	-3.925805	-4.680124
H	0.049011	-3.252245	-5.242533
H	0.944299	-4.751775	-5.360042
C	-0.035635	-4.476226	-3.454605
C	-1.104756	-3.845541	-1.347904
H	-0.155707	-3.985242	-0.827905
H	-1.676673	-3.067862	-0.844872
H	-1.663280	-4.791905	-1.332155
C	-2.148027	-3.241325	-3.451084
H	-2.720279	-2.462063	-2.947586
H	-1.987739	-2.948930	-4.491559
H	-2.722643	-4.177759	-3.433741
C	0.254739	-0.082949	-5.370269
H	0.910186	-0.906459	-5.655573
H	-0.782765	-0.383973	-5.538208
H	0.476365	0.778902	-6.015659
C	-0.520827	1.373126	-3.608133
H	-1.539559	1.061154	-3.831688
H	-0.455116	1.600734	-2.546937
H	-0.275775	2.267110	-4.198465
C	2.967718	-0.172214	-3.940802
H	2.985219	-0.504143	-4.985535
H	3.892321	0.398181	-3.794454
C	1.814837	0.802785	-3.684259
H	-0.708315	-5.296014	-3.742403
H	0.680035	-4.888066	-2.734963
H	1.955875	1.696729	-4.311473
H	1.836930	1.127095	-2.640649
C	2.911068	-3.782606	1.393638

C	3.003866	-4.717391	0.359995
C	3.588541	-4.132341	2.567109
C	3.698465	-5.916090	0.447631
C	4.304078	-5.313684	2.723638
C	4.354881	-6.209806	1.649388
H	3.723573	-6.593292	-0.396142
H	4.804392	-5.521080	3.660636
H	4.905286	-7.137542	1.747896
C	4.573436	2.814797	-0.240924
C	5.025928	3.066048	-1.540602
C	5.404038	3.295313	0.778097
C	6.204368	3.740241	-1.836355
C	6.594209	3.976273	0.549280
C	6.992127	4.198546	-0.773858
H	6.491367	3.898126	-2.867912
H	7.185754	4.321825	1.387164
H	7.915172	4.728000	-0.977163
C	-2.237915	4.430320	-0.340330
C	-2.478096	4.816301	-1.663722
C	-2.784957	5.275117	0.632750
C	-3.211976	5.942298	-2.018823
C	-3.528485	6.412523	0.343046
C	-3.742029	6.742639	-1.000489
H	-3.362107	6.177981	-3.064438
H	-3.921567	7.019171	1.148513
H	-4.318825	7.624197	-1.253275
C	-3.658138	-1.714167	2.693656
C	-4.379106	-2.750445	2.089729
C	-4.155702	-1.296973	3.934842
C	-5.505888	-3.342382	2.647073
C	-5.276697	-1.846818	4.545341
C	-5.954096	-2.881136	3.890119
H	-6.014038	-4.138117	2.117899
H	-5.602018	-1.472661	5.507390
H	-6.830736	-3.325505	4.345780
F	-1.940934	4.031797	-2.683577
F	4.244683	2.605454	-2.605071
F	2.341814	-4.425756	-0.849711
F	-3.945252	-3.211921	0.841892
F	-3.483302	-0.269917	4.593363
F	3.535560	-3.236781	3.633940
F	5.011074	3.073765	2.095939
F	-2.562567	4.951360	1.972143
N	0.720206	1.042071	2.719033
C	1.492491	0.440040	3.619444
C	0.192635	2.167443	3.338920

H	2.054304	-0.467481	3.476733
C	0.655173	2.245895	4.633240
H	-0.478014	2.841617	2.833793
N	1.484643	1.132000	4.796604
C	0.403631	3.243645	5.713126
H	-0.047381	2.783578	6.601190
H	1.326400	3.743227	6.034219
H	-0.283264	4.013192	5.352343
C	2.213603	0.766979	6.013364
H	2.911709	1.560049	6.292481
H	1.517512	0.594889	6.838248
H	2.775219	-0.149054	5.827767
H	-2.686192	0.189290	-2.061547
O	-3.464443	0.690609	-2.451826
C	-4.653728	0.032577	-2.302205
C	-5.782087	0.565512	-2.952248
C	-4.787368	-1.135297	-1.529669
C	-7.022459	-0.067590	-2.835123
H	-5.666429	1.469017	-3.541594
C	-6.033898	-1.762715	-1.423459
H	-3.925864	-1.534585	-1.008798
C	-7.158257	-1.237817	-2.073257
H	-7.885897	0.353026	-3.342268
H	-6.117881	-2.663641	-0.823467
H	-8.122730	-1.727655	-1.986954

Product (**D**), B3LYP

Fe	0.753110	0.325773	0.734646
N	0.649182	-1.551532	1.469264
N	-1.058355	0.731111	1.526304
N	0.941191	2.261722	0.186489
C	-3.054103	1.781466	2.060175
C	-3.114560	0.522771	2.573976
C	-1.868016	-0.134230	2.236060
C	-1.762840	1.914042	1.416570
C	-1.295689	3.099072	0.839896
C	-1.557834	-1.451257	2.587488
C	-0.378700	-2.101133	2.207566
C	-0.098905	-3.496789	2.478968
C	1.085543	-3.790926	1.873692
C	1.550673	-2.571857	1.243578
C	2.756251	-2.461410	0.544018
C	3.264572	-1.259641	0.042129
C	4.559155	-1.125301	-0.593146
C	4.714235	0.192517	-0.902526
C	3.508433	0.873083	-0.476357

C	3.257287	2.231906	-0.693971
C	2.047072	2.860222	-0.384642
C	1.770897	4.258677	-0.646960
C	0.493295	4.494957	-0.241469
C	-0.021969	3.245597	0.281224
N	2.642746	-0.028758	0.110092
H	1.605248	-4.735794	1.858937
H	-0.735978	-4.159897	3.041913
H	-3.920689	0.075926	3.132873
H	-3.804028	2.554298	2.111527
H	-0.051884	5.424538	-0.276955
H	2.468342	4.959440	-1.076881
H	5.554956	0.663499	-1.386231
H	5.253002	-1.932428	-0.766835
O	0.130567	-0.124456	-0.715236
O	-2.596959	-0.875101	-1.688350
Cu	-1.038325	-1.297342	-2.639747
N	-1.595952	-3.379311	-2.396182
N	0.774366	-1.932052	-3.321752
N	-0.973436	0.580748	-3.658178
H	1.066772	-2.493643	-2.518501
C	1.839195	-0.880512	-3.437790
H	1.993749	-0.481167	-2.433561
H	2.772432	-1.359345	-3.763655
C	0.825741	-2.875719	-4.491452
H	1.757576	-3.452226	-4.418099
H	0.878334	-2.284177	-5.408809
C	-0.380741	-3.822126	-4.543633
H	-1.242359	-3.316699	-4.995645
H	-0.132336	-4.654955	-5.211548
C	-0.769833	-4.368225	-3.163848
C	-1.530796	-3.679042	-0.940109
H	-0.497844	-3.598330	-0.594294
H	-2.149546	-2.952921	-0.413576
H	-1.892051	-4.697455	-0.734180
C	-3.019724	-3.478641	-2.834615
H	-3.589454	-2.717210	-2.305142
H	-3.098001	-3.302644	-3.910267
H	-3.415776	-4.480296	-2.613158
C	-1.591013	0.286079	-4.983778
H	-1.013489	-0.469369	-5.520655
H	-2.605764	-0.086184	-4.825055
H	-1.641274	1.193217	-5.602847
C	-1.818175	1.604458	-2.973206
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H	-1.410601	1.795485	-1.981121

H	-1.816558	2.540630	-3.548818
C	1.467736	0.258899	-4.386609
H	1.201658	-0.119602	-5.381028
H	2.363724	0.874361	-4.528914
C	0.386291	1.186900	-3.830093
H	-1.334089	-5.306802	-3.259660
H	0.128684	-4.595709	-2.580187
H	0.288785	2.069472	-4.481939
H	0.697186	1.537810	-2.842465
C	3.557875	-3.703410	0.329539
C	3.366447	-4.529451	-0.781217
C	4.552876	-4.124177	1.217800
C	4.086413	-5.691730	-1.021830
C	5.310785	-5.275479	1.037466
C	5.069513	-6.061669	-0.095348
H	3.883889	-6.283957	-1.904660
H	6.065628	-5.543792	1.765106
H	5.647448	-6.963442	-0.257251
C	4.328235	3.046360	-1.344627
C	4.271627	3.423055	-2.691341
C	5.464749	3.483898	-0.654551
C	5.249739	4.176587	-3.328322
C	6.477878	4.239126	-1.233744
C	6.362541	4.586552	-2.584467
H	5.139024	4.430316	-4.374588
H	7.327648	4.545620	-0.637659
H	7.138934	5.175721	-3.057434
C	-2.177007	4.304554	0.903623
C	-2.933301	4.760043	-0.180750
C	-2.293416	5.066212	2.072104
C	-3.753742	5.881431	-0.133040
C	-3.094910	6.195348	2.184597
C	-3.831056	6.600930	1.064803
H	-4.314341	6.175301	-1.010944
H	-3.135872	6.737139	3.120578
H	-4.464277	7.477841	1.125855
C	-2.563547	-2.226554	3.375867
C	-3.743054	-2.725196	2.811271
C	-2.392828	-2.512258	4.735731
C	-4.696926	-3.448822	3.515823
C	-3.307436	-3.231963	5.495823
C	-4.469676	-3.701659	4.873805
H	-5.585710	-3.805082	3.011219
H	-3.110437	-3.412652	6.544594
H	-5.197522	-4.264118	5.446043
F	-2.857246	4.047509	-1.376786

F	3.163856	3.011702	-3.438385
F	2.380326	-4.155024	-1.711613
F	-3.971230	-2.476403	1.453463
F	-1.236637	-2.046709	5.357788
F	4.788368	-3.337077	2.343526
F	5.582279	3.138462	0.689760
F	-1.555080	4.661108	3.186050
N	1.589921	0.897220	2.619088
C	2.592244	0.281603	3.240029
C	1.211900	1.955504	3.435733
H	3.126477	-0.585245	2.889740
C	1.998670	1.977814	4.565485
H	0.411784	2.628240	3.176885
N	2.877066	0.898931	4.424082
C	2.007670	2.891761	5.744390
H	1.809061	2.356209	6.681299
H	2.969285	3.407799	5.858212
H	1.233096	3.653562	5.626137
C	3.919793	0.500121	5.372012
H	4.651932	1.302273	5.494962
H	3.480889	0.262501	6.344221
H	4.426735	-0.385279	4.987033
H	-2.362602	-0.224825	-1.011922
O	-5.759692	0.735543	-3.789331
C	-6.387301	0.296201	-2.769165
C	-7.823366	0.470232	-2.647386
C	-5.691507	-0.390353	-1.696759
C	-8.497962	-0.006773	-1.539446
H	-8.337632	0.984236	-3.452420
C	-6.394801	-0.857597	-0.597856
H	-4.610945	-0.528713	-1.783410
C	-7.791938	-0.672229	-0.508622
H	-9.571417	0.125882	-1.452837
H	-5.864789	-1.369565	0.198972
H	-8.331916	-1.042414	0.356846

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