Supporting Information for

Spectroscopic and DFT Studies of Second Sphere Variants of the Type 1 Copper Site in Azurin: Covalent and Non-Local Electrostatic Contributions to Reduction Potentials

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Figure S1. **L-** (left) and **S-** (right) type structural models. Atom coloring: Cu (brown); S (yellow); O (red); N (blue); C (green); F (magenta). Hydrogen atoms are omitted, and the S(Met) orientation is out of the page.

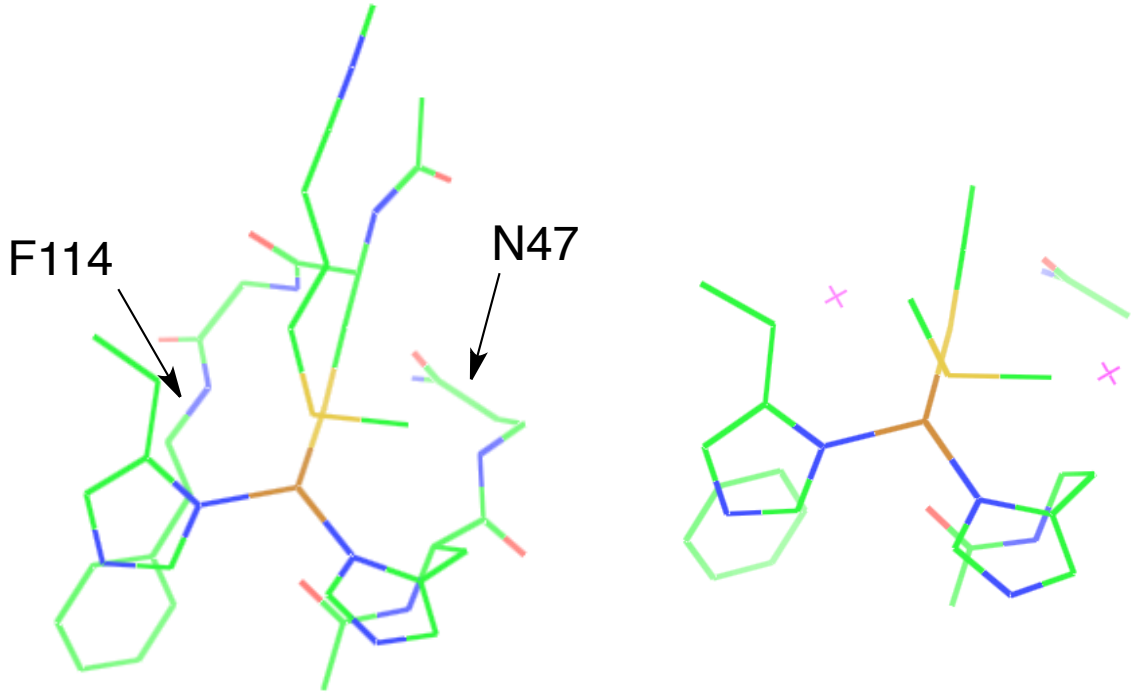


Figure S2. Orientation dependence of N114. Atom coloring as in Figure S1. Dotted lines represent potential H-bonding interactions. The N114 R-group prefers the pictured orientation due to a preference for H-bonding to the carbonyl of the S(Cys)-N(His) loop.

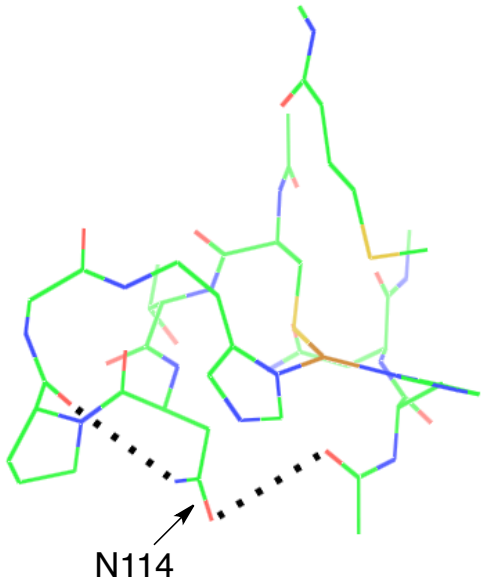
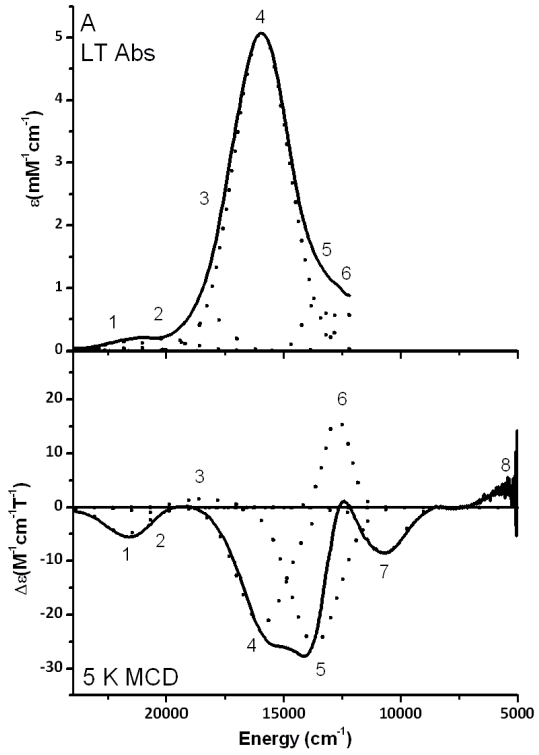
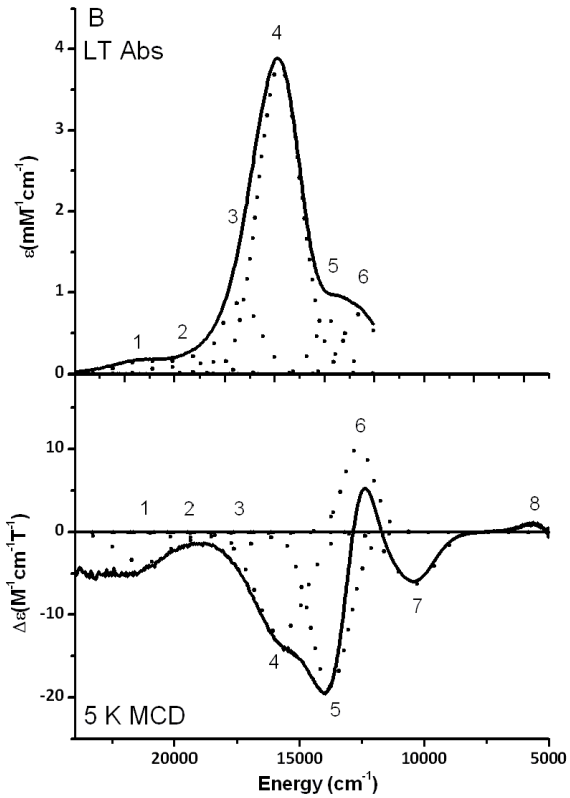
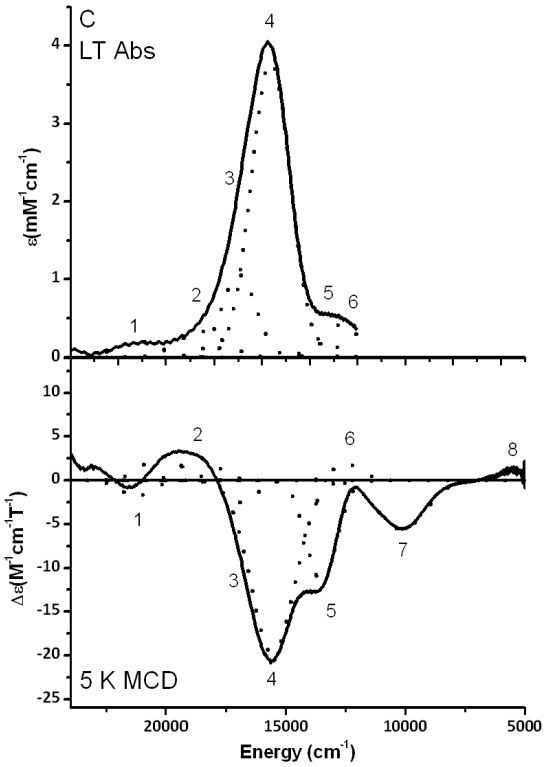


Figure S3. Low-temperature electronic absorption (top) and MCD (bottom) spectra of (A) WT Az, (B) F114N Az, (C) N47S Az, and (D) F114P Az. Simultaneous Gaussian fits are shown as dotted lines.






C
LT Abs
ε(mM⁻¹cm⁻¹)
Δε(M⁻¹cm⁻¹T⁻¹)
5 K MCD
Energy (cm⁻¹)

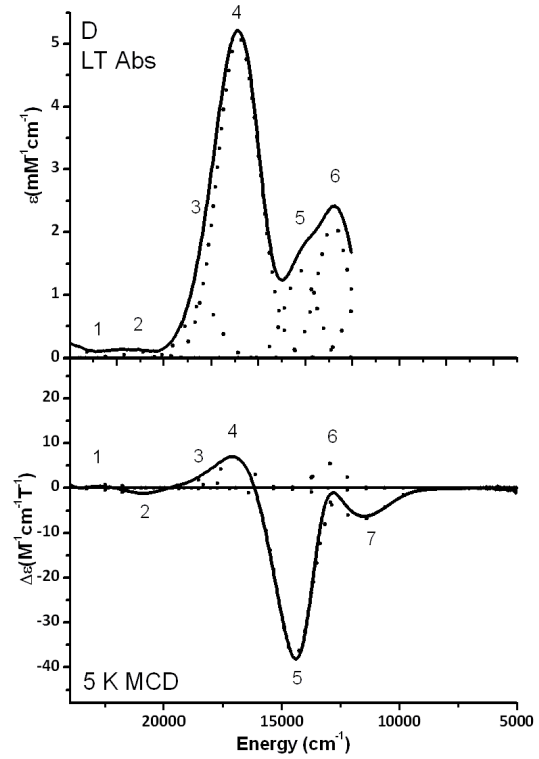

D
LT Abs
ε(mM⁻¹cm⁻¹)
Δε(M⁻¹cm⁻¹T⁻¹)
5 K MCD
Energy (cm⁻¹)

Figure S4. Geometric parameters for different dipole orientations considered in Section 3.2.3. Bonds are given in Å and angles in degrees. Note that orientation 1 and 2 are the same as 5 and 4, respectively, except on the opposite side of the Cu-S bond.

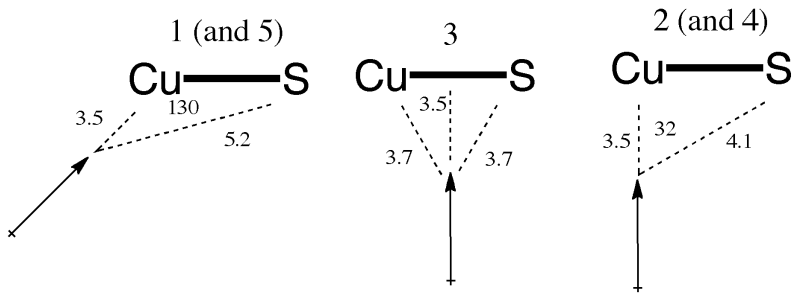


Figure S5. TDDFT calculated electronic absorption spectra of T1 sites taken from 1JZF and 2GHZ crystal structures.

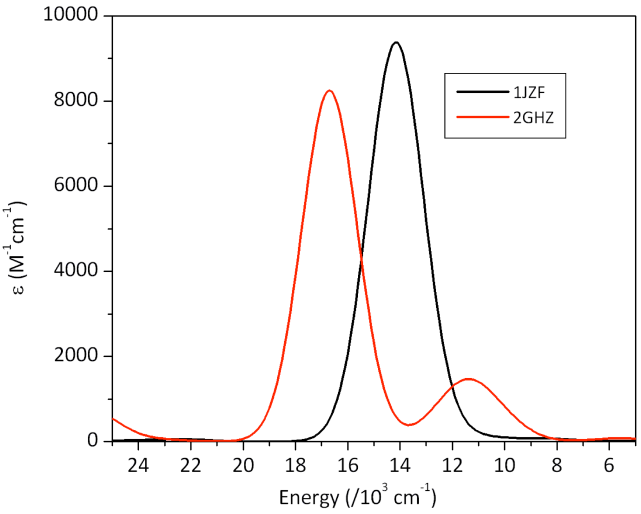


Figure S5 was obtained as follows: the T1 active sites were extracted from the X-ray crystal structures of 1JZF (WT Az) and 2GHZ (F114P) and hydrogen atoms were added at the clipping points. No second sphere interactions are included. Partial geometry optimization involved optimization of all hydrogen atoms while constraining all heavy atoms. The three structural changes to the thiolate orientation in F114P relative to WT Az are: 1) the N_l-Cu-S(Cys) angle opens up from ~123° to ~139° (note the notation of N_l (or N_r) refers to the His ligand on the left

(or right) side as viewed along the Cu-S(Cys) bond (see Figure 1 of main text); 2) the N_r-Cu-S-C_β dihedral angle rotates from ~-83° to ~128°; and 3) the Cu-S-C_β-C_α dihedral rotates from ~-174° to ~-146°. These were each applied separately and additively to the WT Az model (1JZF) and the TDDFT calculation was repeated (Figure S6). Models that contain perturbation 2 (i.e. rotation of the N_r-Cu-S-C_β dihedral angle from ~-83° to ~128°) show an increased intensity of the ligand field $d_{xz/yz}$ transitions.

Figure S6. TDDFT calculated electronic absorption spectra for perturbed WT Az models.

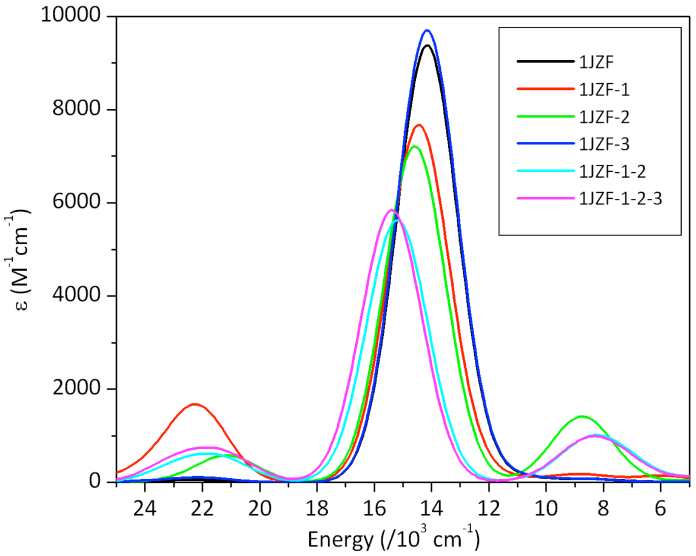


Table S1. DFT calculated H-Bond IE distance dependence (values relative to H-bond at 10 Å).

H-Bond Distance (Å)	ΔIE (eV)	
	Active	Passive
3.25	0.301	0.181
3.50	0.250	0.160
3.75	0.203	0.131
4.00	0.165	0.116
4.25	0.129	0.083
4.50	0.103	0.069
4.75	0.081	0.056

Table S2. DFT calculated H-Bond S_p-character distance dependence (values relative to H-bond at 10 Å).

H-Bond Distance (Å)	ΔS_p (%)	
	Active	Passive
3.25	-12.3	-3.6
3.50	-10.0	-2.4
3.75	-7.7	-1.7
4.00	-5.6	-1.3
4.25	-4.0	-1.0
4.50	-2.9	-0.4
4.75	-1.9	-0.2

Table S3. DFT calculated covalent and non-local electrostatic contributions to E^0.

H-Bond Distance (Å)	$\Delta\Delta S_p$ (%)	$\Delta\Delta$IE (eV)	Slope (eV/%S_p)	Active Covalent[a] (eV)	Passive Covalent[b] (eV)	Active Non-Local Electrostatic[c] (eV)	Passive Non-Local Electrostatic[d] (eV)
3.25	-8.7	0.120	-0.014	0.123	0.036	0.178	0.145
3.50	-7.6	0.090	-0.012	0.100	0.024	0.150	0.136
3.75	-6.0	0.072	-0.012	0.077	0.017	0.126	0.114
4.00	-4.3	0.050	-0.012	0.056	0.013	0.109	0.103
4.25	-3.0	0.046	-0.015	0.040	0.010	0.089	0.073
4.50	-2.5	0.034	-0.013	0.029	0.004	0.074	0.065
4.75	-1.7	0.025	-0.015	0.019	0.002	0.062	0.054

[a] Determined from: -10 mV/ % S_p x ΔS_p (from Active Table S2).

[b] Determined from: Slope x ΔS_p (from Passive Table S2).

[c] Determined from ΔIE(Active) – Active Covalent.

[d] Determined from ΔIE(Passive) – Passive Covalent

Table S4. DFT calculated dipole 1 ΔIE and ΔS_p distance dependence.

Distance (Å)	ΔIE(negative orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.	ΔIE(positive orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.
3.0	-0.188	-3.4	0.034	-0.222	0.184	3.9	-0.039	0.224
3.5	-0.153	-2.6	0.026	-0.179	0.152	2.9	-0.029	0.181
4.0	-0.125	-2.0	0.020	-0.145	0.125	2.2	-0.022	0.147
4.5	-0.104	-1.5	0.015	-0.119	0.104	1.7	-0.017	0.121
5.0	-0.089	-1.2	0.012	-0.101	0.088	1.3	-0.013	0.101

Table S5. DFT calculated dipole 2 ΔIE and ΔS_p distance dependence.

Distance (Å)	ΔIE(negative orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.	ΔIE(positive orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.
3.0	-0.220	-2.5	0.025	-0.245	0.225	2.8	-0.028	0.253
3.5	-0.176	-1.5	0.015	-0.191	0.179	1.7	-0.017	0.196
4.0	-0.145	-1.0	0.010	-0.155	0.146	1.1	-0.011	0.157
4.5	-0.121	-0.6	0.006	-0.127	0.121	0.7	-0.007	0.128
5.0	-0.102	-0.4	0.004	-0.106	0.103	0.5	-0.005	0.108

Table S6. DFT calculated dipole 3 ΔIE and ΔS_p distance dependence.

Distance (Å)	ΔIE(negative orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.	ΔIE(positive orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.
3.0	-0.229	0.1	-0.001	-0.228	0.236	0	0	0.236
3.5	-0.186	0.1	-0.001	-0.185	0.190	-0.1	0.001	0.189
4.0	-0.153	0.2	-0.002	-0.151	0.155	-0.1	0.001	0.154
4.5	-0.128	0.2	-0.002	-0.126	0.129	-0.1	0.001	0.128
5.0	-0.108	0.2	-0.002	-0.106	0.108	-0.1	0.001	0.107

Table S7. DFT calculated dipole 4 ΔIE and ΔS_p distance dependence

Distance (Å)	ΔIE(negative orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.	ΔIE(positive orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.
3.0	-0.211	2.7	-0.027	-0.184	0.213	-2.6	0.026	0.187
3.5	-0.176	1.9	-0.019	-0.157	0.178	-1.8	0.018	0.160
4.0	-0.147	1.4	-0.014	-0.133	0.148	-1.3	0.013	0.135
4.5	-0.124	1.0	-0.010	-0.114	0.124	-0.9	0.009	0.115
5.0	-0.105	0.8	-0.008	-0.097	0.105	-0.7	0.007	0.098

Table S8. DFT calculated dipole 5 ΔIE and ΔS_p distance dependence

Distance (Å)	ΔIE(negative orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.	ΔIE(positive orientation)	ΔS_p	ΔS_p Corr.	ΔIE Corr.
3.0	-0.212	3.4	-0.034	-0.178	0.218	-3.2	0.032	0.186
3.5	-0.172	2.6	-0.026	-0.146	0.174	-2.5	0.025	0.149
4.0	-0.140	2.1	-0.021	-0.119	0.141	-1.9	0.019	0.122
4.5	-0.116	1.6	-0.016	-0.100	0.116	-1.5	0.015	0.101
5.0	-0.097	1.3	-0.013	-0.084	0.097	-1.2	0.012	0.085

Table S9. S_p-characters for vacuum and PCM solvated small BC site models.

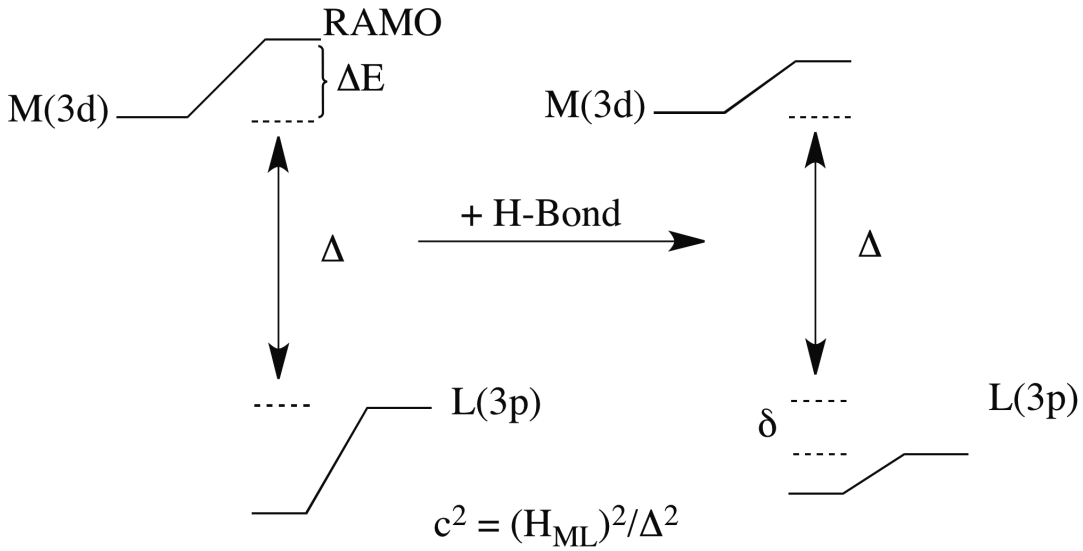
H-bond orientation/distance	ΔS_p-character (%)
Active (10 Å)	9.2[a]
Active (3.5 Å)	7.0[a]
Δ solvation[b] (active)	2.2
Passive (10 Å)	9.4[a]
Passive (3.5 Å)	7.2[a]
Δ solvation[b] (passive)	2.2
Δ (active-passive) (vacuum)	7.6
Δ (active-passive) (ε = 4.0)	7.6

[a] Value is (vacuum – PCM).

[b] Value is (10 – 3.5 Å)

Table S9 gives the S_p-characters for both vacuum and PCM solvated small models of the BC site with active and passive H-bonds at 10 and 3.5 Å. We note that the effects of H-bonding can be sensitive to solvation through imparting partial ionic or covalent character.[1,2] Solvating the T1 site with an H-bond at 10 Å results in a much more ionic Cu^{2+}-S(Et) bond (decrease in S_p-character by 9.2 and 9.4 % in active and passive orientations, respectively). This result is similar to those found elsewhere for H-bonding in general.[1,2] Solvating the T1 site with an active H-bond (S-F distance = 3.5 Å) decreases the S_p-character by 7.0 % (Δ solvation (active) = 2.2 % S_p) while for a passive H-bond at the same distance the S_p-character decreases by 7.2 % (Δ solvation (passive) = 2.2 % S_p). Furthermore, the difference in S_p-character between active and passive H-bonding (S-F distance = 3.5 Å) in both the gas phase and a PCM is 7.6 %. Therefore, with respect to solvation in a PCM formalism, the H-bonding considered is insensitive to solvation and is relatively ionic in nature, which is in agreement with previous studies.[3-8]

Figure S7. VBCI analysis.



In the VBCI model, the amount of ligand character in the ground state wavefunction (c^2) is $(H_{ML})^2/\Delta^2$, where H_{ML} is the resonance integral reflecting ligand-metal overlap and Δ is the energy difference between the M_{3d} and L_{3p} orbitals before bonding. The difference in c^2 upon H-bonding is then

$$c^2_L - c^2_{L'} = [(H_{ML})^2/\Delta^2] - [(H_{ML})^2/(\Delta + \delta)^2] \qquad \text{eqn 1}$$

where the subscripts L and L' represent the non-H-bonded and H-bonded thiolate ligand, respectively. Simplifying this expression and substituting c^2_L for $(H_{ML})^2/\Delta^2$ gives

$$c^2_L - c^2_{L'} = c^2_L[(\delta^2 + 2\Delta\delta)/(\Delta + \delta)^2], \qquad \text{eqn 2}$$

which further simplifies to

$$c^2_L - c^2_{L'} = c^2_L[(2\delta)/(\Delta)] \qquad \text{eqn 3}$$

when $\delta < \Delta$, which should be the case for H-bonding to a ligand-metal bond. Therefore, VBCI modeling predicts that the change in covalency due to H-bonding ($c^2_L - c^2_{L'}$) is linear in δ.

The change in reduction potential can also be related to δ by considering the effect of the H-bond on both oxidized and reduced bond energies (BEs) (i.e., E(RAMO) in Figure S7):

$$\Delta E_{redox} = {}^{o}(BE_L - BE_{L'}) - {}^{r}(BE_L - BE_{L'}) \qquad \text{eqn 4}$$

where the superscripts o and r represent oxidized and reduced states, respectively. Substitution of BE_L with $(H_{ML})^2/\Delta_L$, $BE_{L'}$ with $(H_{ML})^2/\Delta_{L'}$, and $\Delta_{L'}$ as $(\Delta_L + \delta)$ and simplifying gives:

$$\Delta E_{redox} = ({}^{o}c_L{}^2)({}^{o}\Delta_L)[\delta/({}^{o}\Delta_L + \delta)] - ({}^{r}c_L{}^2)({}^{r}\Delta_L)[\delta/({}^{r}\Delta_L + \delta)] \qquad \text{eqn 5}$$

When $\delta < \Delta$ this expression simplifies to

$$\Delta E_{redox} = \delta({}^{o}c_L{}^2 - {}^{r}c_L{}^2). \qquad \text{eqn 6}$$

Thus, VBCI modeling predicts that ΔE_{redox} varies linearly with δ as well.

Complete Reference 58:

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates for the **S-** and **L-** DFT structures discussed in the manuscript:

L-WT oxidized

C	5.389355	0.038965	1.970633
C	3.88961	0.172803	1.918539
O	3.257844	-0.176802	0.911132
N	3.28101	0.6357	3.040023
C	1.839186	0.72487	3.123506
C	1.40954	2.066406	3.697102
O	1.992801	2.560039	4.654361
C	1.217631	-0.40974	3.975724
C	1.594363	-1.795131	3.542536
N	1.459943	-2.266578	2.239314
C	2.058921	-2.819443	4.327822
C	1.828393	-3.540062	2.251869
N	2.19784	-3.912739	3.496878
N	0.310038	2.602457	3.120927
C	-0.232366	3.858779	3.592559
C	0.289655	5.068298	2.80948
C	-0.067436	5.008998	1.328481
O	-0.751645	4.10801	0.83609
N	0.426917	5.996533	0.55905
C	-6.438004	2.063168	-0.098783
C	-5.00135	2.460572	0.135866
O	-4.691717	3.539268	0.619618
N	-4.074845	1.512909	-0.221558
C	-2.658133	1.830237	-0.263409
C	-2.269579	2.251313	-1.68296
O	-2.696163	1.621905	-2.643
C	-1.930727	0.512807	0.091787
S	-0.106875	0.660343	0.13671
N	-1.417918	3.295911	-1.79667
C	-0.978316	3.72616	-3.102911
C	0.393053	3.226741	-3.564907
O	0.903893	3.662324	-4.588459
N	0.987188	2.279749	-2.798606
C	2.278586	1.74651	-3.187969
C	2.809442	0.793237	-2.115322
C	4.192786	0.27069	-2.395966
C	4.383567	-0.822433	-3.23538
C	5.307773	0.886957	-1.83697
C	5.661866	-1.294358	-3.51629
C	6.591667	0.420585	-2.112322

C	6.767781	-0.668961	-2.952785
C	-0.979194	-2.733884	-3.819858
C	-0.402506	-2.185557	-2.511478
C	0.944076	-2.743751	-2.153152
N	1.605644	-2.404422	-0.974565
C	1.765911	-3.572042	-2.875619
C	2.795356	-2.989682	-1.007204
N	2.921712	-3.722115	-2.132331
C	-5.292697	-3.284932	-0.435507
C	-6.220443	-2.108901	-0.636267
O	-5.794397	-1.000893	-0.964133
C	-4.008981	-2.875625	0.265087
C	-2.98216	-3.996779	0.229093
S	-1.397849	-3.502691	0.970648
C	-1.870471	-3.447396	2.73729
N	-7.532522	-2.377664	-0.459991
C	-8.548912	-1.37302	-0.673394
Cu	0.965094	-1.216134	0.530461
H	3.575332	-2.86271	-0.272385
H	3.757796	-4.208959	-2.424066
H	1.632509	-4.055913	-3.82993
H	-1.099649	-2.37407	-1.685806
H	-0.319886	-1.09245	-2.584441
H	-1.948459	-2.270817	-4.024846
H	-1.122631	-3.819979	-3.775063
H	3.518067	-1.297906	-3.692251
H	5.79771	-2.137198	-4.190334
H	7.769123	-1.028535	-3.175276
H	7.454913	0.919116	-1.678562
H	5.171721	1.749124	-1.187853
H	2.810318	1.306723	-1.148014
H	2.114477	-0.046689	-2.018033
H	2.979162	2.575806	-3.347386
H	0.550569	1.979571	-1.937101
H	-0.957923	4.820051	-3.159536
H	-1.710321	3.37699	-3.83619
H	-1.129308	3.777052	-0.946463
H	-2.463954	2.614672	0.467016
H	-2.279821	0.143236	1.060002
H	-2.179826	-0.237219	-0.665993
H	-4.394673	0.743769	-0.802487
H	-6.87605	2.76653	-0.815995
H	-6.55411	1.045359	-0.471156

H	-6.991366	2.183496	0.838883
H	-8.302361	-0.782026	-1.558755
H	-9.513482	-1.862312	-0.828559
H	-8.633749	-0.691223	0.181273
H	-7.810101	-3.304446	-0.173949
H	-5.054014	-3.678342	-1.434788
H	-5.792146	-4.099673	0.104996
H	-4.229562	-2.587459	1.299868
H	-3.608821	-1.987867	-0.230284
H	-3.341298	-4.90465	0.727947
H	-2.746019	-4.271559	-0.805478
H	-2.603839	-2.662304	2.936541
H	-0.964439	-3.231118	3.307375
H	-2.267461	-4.414673	3.058467
H	1.818697	-4.205499	1.402607
H	2.50622	-4.835748	3.770526
H	2.289374	-2.862341	5.381208
H	0.126234	-0.291686	3.939902
H	1.514243	-0.272601	5.021403
H	1.472702	0.637137	2.106692
H	3.815909	1.026414	3.806385
H	5.857933	0.722421	2.685864
H	5.645272	-0.985771	2.266448
H	5.798398	0.210306	0.972878
H	-0.011404	2.267078	2.21994
H	0.041671	3.963434	4.643386
H	1.379336	5.141037	2.915892
H	-0.130811	5.989171	3.235648
H	0.931599	6.781051	0.946771
H	0.165211	6.044673	-0.416325
H	-1.322914	3.814912	3.517385
H	-0.32415	-2.511225	-4.66949
H	2.194481	1.23387	-4.155308

L-WT reduced

C	5.385547	0.1543	1.942845
C	3.880291	0.27614	1.885204
O	3.25203	-0.11773	0.900472
N	3.275622	0.77979	2.992681
C	1.832835	0.83477	3.091095
C	1.385498	2.187904	3.620725
O	1.97212	2.717318	4.564722
C	1.264476	-0.267189	4.022865

C	1.685183	-1.657782	3.655563
N	1.504964	-2.193191	2.38686
C	2.253722	-2.609954	4.465643
C	1.948954	-3.435103	2.438566
N	2.413062	-3.735552	3.679777
N	0.283324	2.694311	3.030945
C	-0.272404	3.957866	3.47446
C	0.234868	5.14666	2.651926
C	-0.127483	5.030577	1.174853
O	-0.806565	4.117166	0.714173
N	0.349065	6.009594	0.374296
C	-6.473166	1.980595	-0.131245
C	-5.034871	2.399136	0.076117
O	-4.740773	3.497549	0.533702
N	-4.110004	1.46424	-0.270449
C	-2.691632	1.785547	-0.306569
C	-2.312924	2.16392	-1.736678
O	-2.73769	1.504446	-2.678522
C	-1.917914	0.524465	0.125569
S	-0.101534	0.775548	0.162357
N	-1.498618	3.235204	-1.895756
C	-1.046088	3.613025	-3.210288
C	0.331297	3.107486	-3.65733
O	0.830209	3.525293	-4.702084
N	0.938905	2.199249	-2.862767
C	2.232873	1.668685	-3.25052
C	2.779303	0.754579	-2.151915
C	4.1673	0.239416	-2.423078
C	4.366912	-0.876528	-3.229772
C	5.277591	0.884995	-1.888345
C	5.649292	-1.342291	-3.502244
C	6.565525	0.425013	-2.155457
C	6.750426	-0.687553	-2.963238
C	-0.97611	-2.865447	-3.730544
C	-0.376028	-2.341022	-2.425686
C	0.987048	-2.883475	-2.11376
N	1.655948	-2.530588	-0.947732
C	1.798487	-3.709009	-2.854005
C	2.840852	-3.110946	-0.997476
N	2.967605	-3.85259	-2.126316
C	-5.268162	-3.361975	-0.310669
C	-6.206471	-2.205178	-0.5543
O	-5.7983	-1.100912	-0.906097

C	-3.970713	-2.905277	0.335515
C	-2.976048	-4.050074	0.454263
S	-1.364957	-3.492734	1.08304
C	-1.840757	-3.004988	2.778268
N	-7.522445	-2.490276	-0.385019
C	-8.547073	-1.49516	-0.591173
Cu	0.971057	-1.203657	0.52737
H	3.628438	-2.986473	-0.269289
H	3.804385	-4.328178	-2.429997
H	1.654626	-4.197067	-3.805067
H	-1.043222	-2.564586	-1.585043
H	-0.317121	-1.245266	-2.45509
H	-1.958387	-2.415174	-3.902898
H	-1.099808	-3.955892	-3.711075
H	3.50291	-1.383009	-3.654153
H	5.790876	-2.209098	-4.144733
H	7.755409	-1.044848	-3.176231
H	7.425219	0.943039	-1.736322
H	5.131673	1.760288	-1.259704
H	2.777394	1.297418	-1.202193
H	2.092822	-0.084822	-2.00913
H	2.921231	2.5023	-3.441172
H	0.487752	1.84367	-2.017647
H	-1.028528	4.704814	-3.312288
H	-1.773428	3.23159	-3.932521
H	-1.155179	3.698178	-1.057635
H	-2.518727	2.607679	0.384847
H	-2.284411	0.223537	1.112338
H	-2.158135	-0.278268	-0.580411
H	-4.415322	0.657394	-0.803195
H	-6.915973	2.627676	-0.897817
H	-6.579918	0.938846	-0.433464
H	-7.028685	2.160868	0.795666
H	-8.250725	-0.843282	-1.41538
H	-9.49029	-1.987065	-0.845719
H	-8.703714	-0.870428	0.297665
H	-7.782611	-3.397459	-0.029013
H	-5.049657	-3.817221	-1.288251
H	-5.753393	-4.143629	0.29039
H	-4.183807	-2.48063	1.323493
H	-3.541401	-2.097308	-0.261792
H	-3.362685	-4.862418	1.08318
H	-2.764451	-4.478761	-0.532808

H	-2.441284	-2.091956	2.782307
H	-0.913366	-2.812391	3.319178
H	-2.384836	-3.81266	3.278491
H	1.938192	-4.137187	1.6181
H	2.789618	-4.624123	3.976192
H	2.544672	-2.587722	5.504877
H	0.169906	-0.188559	3.987481
H	1.568511	-0.05947	5.055678
H	1.431837	0.674057	2.092113
H	3.808973	1.201852	3.741977
H	5.851505	0.873692	2.625331
H	5.64866	-0.854035	2.285263
H	5.79215	0.282831	0.937705
H	-0.04207	2.279929	2.149947
H	0.007791	4.096168	4.520318
H	1.325198	5.224391	2.750481
H	-0.187905	6.081472	3.045704
H	0.936055	6.754718	0.718423
H	0.152331	5.976497	-0.616218
H	-1.362921	3.902132	3.401904
H	-0.345375	-2.613914	-4.59165
H	2.14956	1.125794	-4.202887

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C	-6.575463	-0.81205	-0.496376
C	-5.077283	-0.58296	-0.615992
O	-4.311819	-0.680508	0.350323
N	-4.620529	-0.318314	-1.869761
C	-3.211398	-0.123478	-2.135589
C	-3.056385	1.113621	-3.064994
O	-3.954557	1.445105	-3.839033
C	-2.588739	-1.364418	-2.837449
C	-2.758044	-2.647667	-2.083688
N	-2.108398	-2.922948	-0.884232
C	-3.536467	-3.729086	-2.4086
C	-2.487599	-4.134735	-0.505159
N	-3.352691	-4.656609	-1.40235
N	-1.855914	1.731925	-2.979071
C	-1.473236	2.871563	-3.799889
C	-1.792087	4.216885	-3.143603
C	-1.068064	4.449916	-1.821287
O	-0.080667	3.784424	-1.493899
N	-1.60348	5.433015	-1.028996

C	5.832086	2.213899	-1.744461
C	4.337852	2.492278	-1.721299
O	3.811158	3.375575	-2.386853
N	3.656332	1.646731	-0.877838
C	2.229628	1.712481	-0.59335
C	2.062342	2.205321	0.843833
O	2.626251	1.590399	1.741283
C	1.685492	0.287284	-0.748366
S	-0.128644	0.213063	-0.593993
N	1.340322	3.330404	1.049497
C	1.301677	3.942778	2.364072
C	0.215161	3.531893	3.39053
O	0.36396	3.870346	4.562224
N	-0.853844	2.770018	2.995494
C	-1.753865	2.24928	4.03809
C	-2.910354	1.622152	3.253689
C	-2.978134	2.48265	1.984753
C	-1.496403	2.748541	1.671563
C	1.752513	-1.944587	4.125104
C	0.84632	-1.430853	3.008387
C	-0.600688	-1.784921	3.184293
N	-1.448482	-1.927023	2.092329
C	-1.345413	-1.960905	4.323025
C	-2.672008	-2.153079	2.555913
N	-2.644273	-2.189914	3.904712
C	5.232391	-3.011118	-0.171283
C	6.05495	-1.762182	-0.49248
O	5.603887	-0.613966	-0.43185
C	3.748085	-2.683081	-0.178634
C	2.877758	-3.887058	0.150528
S	1.11858	-3.61167	-0.261713
C	1.19275	-3.696252	-2.084908
N	7.334007	-2.016126	-0.846723
C	8.243053	-0.945163	-1.188556
Cu	-0.907761	-1.662949	0.186038
H	8.086536	-0.587617	-2.21379
H	9.272208	-1.300167	-1.094634
H	8.090985	-0.106001	-0.506789
H	7.644621	-2.972969	-0.931154
H	5.464574	-3.802397	-0.896384
H	5.542966	-3.389155	0.813256
H	3.488147	-2.284603	-1.164559
H	3.558488	-1.878426	0.536594

H	3.197078	-4.787675	-0.386837
H	2.901136	-4.124104	1.219263
H	0.165373	-3.627432	-2.447757
H	1.616755	-4.652827	-2.402215
H	1.773727	-2.873625	-2.509711
H	6.03558	1.153953	-1.901507
H	6.282564	2.492226	-0.784133
H	6.285054	2.815862	-2.534315
H	4.20059	0.982327	-0.336543
H	1.782615	2.390799	-1.321786
H	2.136934	-0.360704	0.002306
H	1.945507	-0.086745	-1.743718
H	0.88845	3.758219	0.244612
H	1.244423	5.03143	2.247501
H	2.244478	3.724076	2.870183
H	-1.079873	1.950667	1.046012
H	-1.351962	3.691526	1.139627
H	-3.494504	1.981613	1.160999
H	-3.495212	3.427353	2.193093
H	-3.844382	1.619228	3.823746
H	-2.674931	0.587841	2.982214
H	-2.091936	3.069983	4.683138
H	1.709921	-3.036692	4.209421
H	2.789401	-1.651289	3.934793
H	0.953465	-0.34084	2.921193
H	1.181512	-1.83509	2.046285
H	-1.076353	-1.940642	5.367099
H	-3.445644	-2.325594	4.505093
H	-3.568387	-2.205713	1.955213
H	-6.757028	-1.880141	-0.332672
H	-6.95406	-0.275791	0.37786
H	-7.132073	-0.497863	-1.383802
H	-5.248932	-0.025857	-2.610246
H	-2.72565	0.049961	-1.176743
H	-1.52442	-1.168528	-3.010057
H	-3.058108	-1.471285	-3.821771
H	-4.185623	-3.91338	-3.25052
H	-3.772436	-5.574868	-1.353
H	-2.151365	-4.651183	0.381313
H	-1.214387	1.458579	-2.24039
H	-2.012318	2.801434	-4.747037
H	-1.499763	5.025371	-3.829244
H	-2.875145	4.308952	-2.996427

H	-1.053393	5.78054	-0.254343
H	-2.314625	6.051684	-1.393908
H	1.475025	-1.52143	5.097342
H	-1.218371	1.539587	4.676919
H	-0.400757	2.799856	-3.998793

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C	-6.57597	-0.70039	-0.461122
C	-5.071131	-0.487606	-0.585487
O	-4.306965	-0.605003	0.376018
N	-4.62155	-0.220793	-1.837363
C	-3.206941	-0.078509	-2.116716
C	-3.0288	1.151009	-3.04739
O	-3.92923	1.49534	-3.824274
C	-2.643607	-1.33657	-2.838118
C	-2.890642	-2.621319	-2.109523
N	-2.249105	-2.942691	-0.920558
C	-3.732353	-3.651075	-2.450522
C	-2.692282	-4.1322	-0.560018
N	-3.595965	-4.60392	-1.458122
N	-1.826052	1.749105	-2.95313
C	-1.420801	2.866638	-3.786083
C	-1.715506	4.23164	-3.149922
C	-0.981109	4.452356	-1.829891
O	-0.005326	3.77642	-1.505063
N	-1.496989	5.453645	-1.04159
C	5.8778	2.100828	-1.771906
C	4.386598	2.410937	-1.728897
O	3.875064	3.295076	-2.411542
N	3.70732	1.606492	-0.866438
C	2.271743	1.668103	-0.604308
C	2.112286	2.16278	0.829607
O	2.675567	1.549429	1.729266
C	1.699683	0.255411	-0.767899
S	-0.124137	0.221757	-0.698546
N	1.426812	3.314732	1.035217
C	1.39514	3.927533	2.346659
C	0.299278	3.540054	3.375714
O	0.465165	3.881411	4.548805
N	-0.7865	2.81128	2.99385
C	-1.68297	2.29561	4.040374
C	-2.812287	1.621292	3.255454
C	-2.897024	2.459055	1.972592

C	-1.422021	2.760161	1.658533
C	1.749345	-1.958977	4.132461
C	0.825314	-1.414165	3.044885
C	-0.623793	-1.735977	3.258733
N	-1.476343	-1.915619	2.179906
C	-1.353895	-1.847913	4.417024
C	-2.690319	-2.107193	2.667745
N	-2.660893	-2.083168	4.02439
C	5.192549	-3.105763	-0.172792
C	6.032781	-1.870958	-0.495003
O	5.605141	-0.716713	-0.445648
C	3.710996	-2.769883	-0.189982
C	2.834157	-3.989309	0.050239
S	1.068471	-3.634111	-0.244243
C	1.089688	-3.420315	-2.056771
N	7.317883	-2.148349	-0.836666
C	8.234993	-1.097734	-1.21128
Cu	-0.961268	-1.686401	0.192365
H	8.124244	-0.805795	-2.264032
H	9.263209	-1.432365	-1.046249
H	8.040928	-0.218434	-0.594655
H	7.598265	-3.111192	-0.950148
H	5.424036	-3.901772	-0.894544
H	5.496374	-3.485173	0.813786
H	3.469296	-2.316513	-1.15581
H	3.501963	-2.003804	0.561181
H	3.128967	-4.833102	-0.587096
H	2.899366	-4.330478	1.089625
H	0.047574	-3.408229	-2.378122
H	1.605277	-4.258011	-2.537569
H	1.549862	-2.472171	-2.343548
H	6.050731	1.052923	-2.025995
H	6.336466	2.273796	-0.791192
H	6.349167	2.753856	-2.5093
H	4.230706	0.910428	-0.347224
H	1.838683	2.355048	-1.331028
H	2.1069	-0.369429	0.029555
H	2.053401	-0.137519	-1.727322
H	0.936893	3.716129	0.240356
H	1.360493	5.018392	2.232212
H	2.330936	3.685414	2.855167
H	-0.981051	1.975558	1.038732
H	-1.308471	3.714327	1.136728

H	-3.389445	1.923214	1.156609
H	-3.448518	3.389757	2.162175
H	-3.75124	1.594039	3.818877
H	-2.536738	0.594573	2.999031
H	-2.050503	3.121877	4.664327
H	1.682493	-3.051425	4.20806
H	2.788992	-1.690184	3.917718
H	0.957388	-0.327751	2.955662
H	1.113083	-1.81739	2.06867
H	-1.074543	-1.777365	5.456584
H	-3.459262	-2.169323	4.635668
H	-3.592895	-2.184652	2.079299
H	-6.77183	-1.773631	-0.357004
H	-6.936414	-0.206948	0.445403
H	-7.136379	-0.32913	-1.324879
H	-5.243963	0.08383	-2.576895
H	-2.690486	0.06161	-1.169432
H	-1.566398	-1.187585	-2.966261
H	-3.100632	-1.398246	-3.833225
H	-4.3948	-3.787509	-3.2916
H	-4.062032	-5.498552	-1.419652
H	-2.382729	-4.676415	0.320308
H	-1.146713	1.37632	-2.270835
H	-1.952982	2.801072	-4.738945
H	-1.407607	5.027719	-3.84362
H	-2.796524	4.341996	-2.999547
H	-0.966747	5.763927	-0.239073
H	-2.224505	6.062612	-1.385872
H	1.508071	-1.541802	5.118016
H	-1.136899	1.61285	4.699255
H	-0.34709	2.775936	-3.971603

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C	-5.864615	-0.260753	-0.984357
C	-4.381184	-0.082097	-1.168003
O	-3.592144	-0.352403	-0.249569
N	-3.962964	0.333511	-2.390335
C	-2.555099	0.464489	-2.694447
C	-2.267879	1.78364	-3.394865
O	-3.005298	2.2046	-4.276943
C	-2.023997	-0.696719	-3.571751
C	-2.277415	-2.06663	-3.016555
N	-1.934712	-2.459855	-1.725519

C	-2.81174	-3.147793	-3.670151
C	-2.250401	-3.743006	-1.617808
N	-2.783671	-4.196462	-2.773148
N	-1.114446	2.383069	-3.020766
C	-0.69757	3.627277	-3.632041
C	-1.14421	4.862039	-2.841569
C	-0.567595	4.898062	-1.430821
O	0.217633	4.047626	-1.002288
N	-0.977338	5.912762	-0.647897
C	6.053475	2.229776	-0.833728
C	4.584067	2.57008	-0.869884
O	4.164608	3.609998	-1.354937
N	3.757682	1.616628	-0.327408
C	2.352196	1.893746	-0.087804
C	2.164344	2.383205	1.350434
O	2.75303	1.821751	2.266225
C	1.630488	0.536987	-0.255203
S	-0.184927	0.628857	-0.042002
N	1.297926	3.405358	1.538053
C	1.044315	3.896424	2.871554
C	-0.21825	3.379327	3.564457
O	-0.591156	3.860637	4.625862
N	-0.873856	2.358767	2.95584
C	-2.085664	1.828374	3.549829
C	-2.692876	0.765867	2.630644
C	-4.042746	0.283528	3.122259
C	1.398031	-2.50973	3.911864
C	0.608322	-2.052871	2.68122
C	-0.768675	-2.642238	2.577185
N	-1.602017	-2.407294	1.48477
C	-1.458029	-3.417999	3.475629
C	-2.759377	-3.004021	1.736412
N	-2.704834	-3.642909	2.921937
C	5.175613	-3.122488	-0.052755
C	6.078143	-1.910654	-0.051126
O	5.663354	-0.79821	0.275613
C	3.773187	-2.776204	-0.520229
C	2.817711	-3.940865	-0.314619
S	1.125597	-3.535776	-0.840851
C	1.350195	-3.505847	-2.655847
N	7.361059	-2.151592	-0.399598
C	8.355714	-1.103765	-0.408638
Cu	-1.231982	-1.300017	-0.170921

H	-3.640097	-2.946848	1.115303
H	-3.475289	-4.124062	3.364415
H	-1.171892	-3.831382	4.429706
H	1.163796	-2.29373	1.766727
H	0.524134	-0.95748	2.694115
H	2.38048	-2.029749	3.924942
H	1.54828	-3.595651	3.915868
H	-2.862415	1.178644	1.634399
H	-2.003668	-0.077428	2.534362
H	-2.802058	2.642303	3.716474
H	-0.57856	2.042016	2.041489
H	0.98491	4.990194	2.872818
H	1.89351	3.617007	3.501245
H	0.871647	3.833302	0.717146
H	2.021608	2.627684	-0.821363
H	1.850569	0.115634	-1.239771
H	2.015156	-0.153535	0.502173
H	4.189264	0.891351	0.23755
H	6.557339	2.945524	-0.173794
H	6.25309	1.216449	-0.485362
H	6.470711	2.374297	-1.835588
H	8.186224	-0.434653	0.437663
H	9.350525	-1.547074	-0.318789
H	8.316802	-0.509751	-1.329942
H	7.623805	-3.079897	-0.695134
H	5.136672	-3.498391	0.980538
H	5.601381	-3.933066	-0.658678
H	3.800896	-2.482966	-1.576481
H	3.423479	-1.904287	0.037577
H	3.146106	-4.845376	-0.840017
H	2.740727	-4.197311	0.748234
H	2.007016	-2.691254	-2.970323
H	0.364645	-3.35057	-3.099391
H	1.750057	-4.460703	-3.008755
H	-2.089262	-4.359009	-0.746828
H	-3.094174	-5.142088	-2.950007
H	-3.192565	-3.257251	-4.673913
H	-0.945308	-0.542948	-3.709769
H	-2.480124	-0.628212	-4.565482
H	-2.036822	0.447304	-1.742361
H	-4.621294	0.664886	-3.085046
H	-6.461696	0.254118	-1.742799
H	-6.101255	-1.330398	-1.027456

H	-6.137703	0.102075	0.010749
H	-0.655004	2.111127	-2.159144
H	-1.130456	3.66382	-4.632804
H	-2.239485	4.893784	-2.784998
H	-0.829394	5.770254	-3.37291
H	-1.57493	6.651813	-0.990214
H	-0.581625	6.020658	0.27603
H	0.392759	3.621615	-3.721273
H	0.887626	-2.233185	4.841272
H	-1.856586	1.413924	4.540658
O	-5.106398	0.739279	2.766891
N	-4.059732	-0.749384	4.006993
H	-4.943531	-0.872369	4.486363
H	-3.232866	-0.967251	4.549923

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C	-5.858685	-0.147586	-0.967627
C	-4.368118	0.018762	-1.145268
O	-3.585297	-0.293976	-0.244638
N	-3.952382	0.470567	-2.357593
C	-2.544171	0.565762	-2.673035
C	-2.232086	1.89632	-3.338806
O	-2.971864	2.351221	-4.210622
C	-2.074164	-0.575005	-3.613379
C	-2.382853	-1.952797	-3.110498
N	-1.998468	-2.407906	-1.855515
C	-3.02865	-2.966846	-3.773955
C	-2.399076	-3.663059	-1.773557
N	-3.029255	-4.048467	-2.913813
N	-1.073668	2.468903	-2.950969
C	-0.638919	3.720139	-3.540586
C	-1.06574	4.939278	-2.716931
C	-0.485076	4.922436	-1.30676
O	0.292747	4.060997	-0.905116
N	-0.870397	5.935962	-0.500295
C	6.098825	2.145407	-0.805044
C	4.631213	2.510783	-0.811396
O	4.230744	3.568369	-1.284569
N	3.804006	1.570649	-0.280495
C	2.39536	1.85109	-0.052375
C	2.218449	2.303597	1.395427
O	2.803697	1.7149	2.297523
C	1.613098	0.544411	-0.291957

S	-0.196981	0.736252	-0.062652
N	1.393653	3.355919	1.61601
C	1.131219	3.801466	2.96044
C	-0.141516	3.28237	3.639255
O	-0.498101	3.749115	4.720047
N	-0.821155	2.30373	3.001447
C	-2.029456	1.768296	3.600761
C	-2.656534	0.735763	2.654247
C	-4.009491	0.261637	3.137938
C	1.384516	-2.633161	3.842244
C	0.556787	-2.164292	2.644352
C	-0.820158	-2.756269	2.577473
N	-1.656188	-2.521838	1.492195
C	-1.492194	-3.532388	3.491573
C	-2.800081	-3.12603	1.754832
N	-2.744585	-3.767279	2.94858
C	5.1369	-3.209504	-0.151656
C	6.056767	-2.013749	-0.113974
O	5.663607	-0.902173	0.231474
C	3.740771	-2.829389	-0.614885
C	2.786822	-4.011545	-0.536145
S	1.077801	-3.537777	-0.932992
C	1.284698	-3.071157	-2.687845
N	7.34344	-2.271009	-0.460225
C	8.348083	-1.234359	-0.471096
Cu	-1.239961	-1.289348	-0.172627
H	-3.684423	-3.084278	1.136442
H	-3.50596	-4.258442	3.392909
H	-1.196124	-3.943896	4.44387
H	1.076973	-2.393792	1.707258
H	0.471328	-1.069827	2.65573
H	2.367452	-2.152638	3.83333
H	1.535167	-3.720112	3.83039
H	-2.817797	1.177179	1.670034
H	-1.976386	-0.108638	2.517736
H	-2.734277	2.585763	3.797554
H	-0.496369	1.924519	2.109893
H	1.084796	4.896283	3.001302
H	1.974027	3.488869	3.58347
H	0.915783	3.761245	0.814145
H	2.093978	2.624997	-0.755378
H	1.837915	0.198022	-1.305936
H	1.989157	-0.206822	0.411491

H	4.213779	0.805052	0.24279
H	6.651038	2.942378	-0.294984
H	6.304557	1.188144	-0.325716
H	6.461103	2.121136	-1.839659
H	8.220674	-0.593599	0.404579
H	9.340825	-1.691136	-0.436679
H	8.279963	-0.6028	-1.36582
H	7.58292	-3.191032	-0.796926
H	5.086953	-3.616306	0.869492
H	5.554911	-4.008227	-0.780056
H	3.789382	-2.447888	-1.641245
H	3.370476	-2.007608	0.002849
H	3.106228	-4.835942	-1.186641
H	2.74427	-4.404623	0.486742
H	1.811367	-2.119083	-2.791147
H	0.283705	-2.962285	-3.106994
H	1.817129	-3.854937	-3.236433
H	-2.241085	-4.316046	-0.928135
H	-3.413015	-4.962918	-3.102648
H	-3.469434	-3.013897	-4.758116
H	-0.990156	-0.461347	-3.746215
H	-2.533921	-0.441586	-4.599907
H	-1.99483	0.481653	-1.737292
H	-4.607441	0.829985	-3.039782
H	-6.450972	0.413877	-1.697765
H	-6.110951	-1.210313	-1.064676
H	-6.122447	0.169403	0.045279
H	-0.60795	2.119428	-2.106464
H	-1.076646	3.786825	-4.538315
H	-2.160825	4.976764	-2.65526
H	-0.743029	5.861895	-3.219057
H	-1.562825	6.615185	-0.779004
H	-0.549884	5.951494	0.457832
H	0.451646	3.70238	-3.629743
H	0.902673	-2.371487	4.792251
H	-1.796356	1.32267	4.578391
O	-5.070392	0.747734	2.80382
N	-4.043494	-0.787634	4.002821
H	-4.925575	-0.934764	4.474375
H	-3.206632	-1.106319	4.473337

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C	5.38726	-1.20778	1.724815

C	3.887511	-1.079975	1.780546
O	3.258147	-0.597274	0.826707
N	3.275233	-1.570824	2.887433
C	1.832908	-1.567334	3.005669
C	1.401232	-1.046727	4.369621
O	1.977619	-1.396771	5.389978
C	1.213195	-2.96818	2.778137
C	1.587632	-3.612225	1.476545
N	1.449961	-2.998017	0.233553
C	2.058426	-4.885106	1.278186
C	1.8224	-3.886062	-0.678464
N	2.197431	-5.040224	-0.086234
N	0.30504	-0.255347	4.349688
C	-0.250575	0.265834	5.580805
C	-6.444124	1.670456	1.704318
C	-5.012131	1.775879	2.160945
O	-4.704232	2.179362	3.272208
N	-4.078422	1.375783	1.235811
C	-2.663196	1.632722	1.436087
C	-2.281588	2.945971	0.757176
O	-2.696866	3.202148	-0.364766
C	-1.928031	0.462653	0.747902
S	-0.109494	0.525856	0.928681
N	-1.42386	3.753335	1.433805
C	-0.985878	4.995474	0.838107
C	0.387944	4.983342	0.159976
O	0.898802	6.023838	-0.231514
N	0.976376	3.772595	-0.001266
C	2.278226	3.688048	-0.63496
C	2.810867	2.254913	-0.57559
C	4.1965	2.096507	-1.141617
C	4.392472	1.943125	-2.510558
C	5.30842	2.12291	-0.305917
C	5.67288	1.819881	-3.040689
C	6.594394	1.999522	-0.828174
C	6.775688	1.849355	-2.195319
C	-0.962509	1.030727	-4.312273
C	-0.399123	0.45453	-3.009336
C	0.953962	-0.180151	-3.15131
N	1.615285	-0.783594	-2.082528
C	1.783365	-0.230987	-4.243183
C	2.811995	-1.155947	-2.517736
N	2.942551	-0.8575	-3.825672

C	-5.279142	-1.795241	-2.377233
C	-6.211011	-0.836423	-1.673561
O	-5.788224	0.1692	-1.100599
C	-3.982519	-1.983556	-1.609811
C	-2.962235	-2.758014	-2.429158
S	-1.385678	-2.953706	-1.54451
C	-1.869648	-4.203896	-0.299432
N	-7.521798	-1.150406	-1.749949
C	-8.541825	-0.302188	-1.176971
Cu	0.964555	-1.044631	-0.188988
H	3.593324	-1.584921	-1.909545
H	3.783803	-0.978373	-4.372632
H	1.653387	0.116464	-5.25562
H	-1.098051	-0.281162	-2.592198
H	-0.331039	1.256937	-2.261966
H	-1.938516	1.488317	-4.128076
H	-1.088878	0.25493	-5.076562
H	3.529621	1.942436	-3.173655
H	5.812844	1.72194	-4.11493
H	7.778618	1.762234	-2.605112
H	7.454964	2.0348	-0.164965
H	5.168687	2.25353	0.764823
H	2.807912	1.913705	0.465361
H	2.11862	1.601329	-1.116437
H	2.970364	4.37721	-0.13509
H	0.554889	2.945021	0.397833
H	-0.968566	5.789724	1.590188
H	-1.71909	5.277788	0.078135
H	-1.21603	3.560275	2.403342
H	-2.483267	1.652628	2.514311
H	-2.291197	-0.486184	1.151823
H	-2.161689	0.48661	-0.320518
H	-4.394074	1.231758	0.280833
H	-6.862017	2.682352	1.648817
H	-6.553112	1.182051	0.735905
H	-7.016773	1.132858	2.466912
H	-8.273719	0.745635	-1.329914
H	-9.497017	-0.501639	-1.668669
H	-8.658376	-0.474094	-0.099988
H	-7.796786	-2.000763	-2.218375
H	-5.060642	-1.365107	-3.365976
H	-5.768181	-2.760516	-2.562691
H	-4.186624	-2.49751	-0.662879

H	-3.582361	-0.99991	-1.352676
H	-3.329506	-3.74858	-2.721948
H	-2.717658	-2.221475	-3.353011
H	-2.641421	-3.825562	0.37497
H	-0.977703	-4.435229	0.286412
H	-2.220569	-5.116904	-0.788482
H	1.807724	-3.73366	-1.746391
H	2.509688	-5.874937	-0.563603
H	2.293503	-5.674301	1.975666
H	0.121648	-2.864163	2.843594
H	1.514252	-3.628021	3.599114
H	1.470737	-0.897617	2.234766
H	3.806072	-1.833086	3.709803
H	5.853177	-1.235604	2.71492
H	5.645739	-2.138612	1.205203
H	5.796682	-0.376856	1.146841
H	-0.004903	0.125883	3.464361
H	-0.108102	-0.472762	6.371148
H	-1.319485	0.455871	5.450327
H	-0.308028	1.808757	-4.720472
H	2.207643	4.033263	-1.674598
H	0.241131	1.196166	5.891655

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C	5.387061	-1.249045	1.663384
C	3.88257	-1.124674	1.721583
O	3.254603	-0.614198	0.790441
N	3.276814	-1.660529	2.812347
C	1.834184	-1.688019	2.923401
C	1.396584	-1.220068	4.304816
O	1.975814	-1.620768	5.313041
C	1.256985	-3.107288	2.687959
C	1.649818	-3.717904	1.377468
N	1.463147	-3.076755	0.159336
C	2.194121	-4.9579	1.150283
C	1.88159	-3.914104	-0.772381
N	2.332871	-5.070024	-0.220024
N	0.306111	-0.428468	4.317598
C	-0.263703	0.016936	5.573821
C	-6.463457	1.547921	1.755535
C	-5.026277	1.651937	2.209278
O	-4.728306	1.999535	3.346065
N	-4.100461	1.317039	1.268653

C	-2.682145	1.547295	1.490078
C	-2.301501	2.884377	0.866315
O	-2.724952	3.193602	-0.240571
C	-1.903109	0.407844	0.815843
S	-0.096658	0.559508	1.065468
N	-1.484426	3.692603	1.591641
C	-1.027077	4.944126	1.041336
C	0.349361	4.961808	0.362485
O	0.851483	6.030834	0.019712
N	0.949064	3.767584	0.163433
C	2.246965	3.724194	-0.483811
C	2.789217	2.293438	-0.486483
C	4.176345	2.169197	-1.057359
C	4.374453	2.077056	-2.431474
C	5.287386	2.166539	-0.220078
C	5.656092	1.98567	-2.96507
C	6.574585	2.074703	-0.745807
C	6.757993	1.985598	-2.118004
C	-0.97279	1.208308	-4.277206
C	-0.383903	0.560777	-3.023459
C	0.973245	-0.044155	-3.226587
N	1.629088	-0.710793	-2.199112
C	1.791678	-0.021376	-4.330095
C	2.814128	-1.059302	-2.666402
N	2.951946	-0.679653	-3.961212
C	-5.271815	-1.72835	-2.472152
C	-6.206949	-0.803081	-1.732289
O	-5.795174	0.175012	-1.111528
C	-3.970025	-1.932376	-1.715789
C	-2.97821	-2.755897	-2.523526
S	-1.371296	-2.895932	-1.686513
C	-1.85658	-3.916609	-0.250402
N	-7.521722	-1.118521	-1.831146
C	-8.545469	-0.311049	-1.211442
Cu	0.950689	-1.020774	-0.238143
H	3.593339	-1.541369	-2.095173
H	3.791949	-0.763023	-4.514582
H	1.65849	0.391077	-5.317796
H	-1.060715	-0.212849	-2.641547
H	-0.318496	1.303576	-2.217561
H	-1.95328	1.640788	-4.055706
H	-1.097166	0.480302	-5.089016
H	3.510094	2.083684	-3.091919

H	5.796569	1.927239	-4.042601
H	7.762407	1.919032	-2.529947
H	7.434666	2.080877	-0.080096
H	5.142905	2.241834	0.855084
H	2.786492	1.907375	0.537359
H	2.101283	1.650266	-1.042955
H	2.933763	4.399843	0.042141
H	0.503584	2.891572	0.438639
H	-1.005218	5.714962	1.818959
H	-1.759893	5.25357	0.291883
H	-1.104496	3.353308	2.46363
H	-2.521007	1.547585	2.570518
H	-2.273243	-0.541512	1.215056
H	-2.125785	0.433042	-0.256053
H	-4.406118	1.199685	0.308806
H	-6.919444	2.54243	1.823473
H	-6.570686	1.167115	0.739788
H	-7.006971	0.902335	2.454579
H	-8.288892	0.745798	-1.315864
H	-9.503195	-0.496604	-1.705171
H	-8.652013	-0.530517	-0.141626
H	-7.786774	-1.958911	-2.321729
H	-5.060303	-1.26671	-3.448297
H	-5.756919	-2.690893	-2.685955
H	-4.178959	-2.419283	-0.756291
H	-3.538796	-0.956433	-1.479756
H	-3.367985	-3.756125	-2.752286
H	-2.762529	-2.267018	-3.481245
H	-2.503471	-3.364574	0.435955
H	-0.935582	-4.173992	0.274032
H	-2.354108	-4.836183	-0.57472
H	1.859649	-3.728585	-1.835836
H	2.693051	-5.868647	-0.721814
H	2.482782	-5.749435	1.824995
H	0.163377	-3.027925	2.748869
H	1.575658	-3.765766	3.504512
H	1.436881	-1.026451	2.158024
H	3.807528	-1.950442	3.624181
H	5.853353	-1.316891	2.652447
H	5.647691	-2.156894	1.105416
H	5.795718	-0.394094	1.120889
H	-0.005213	-0.026429	3.427472
H	-0.298959	-0.819113	6.277114

H	-1.277421	0.385922	5.396575
H	-0.333759	2.019013	-4.647151
H	2.170382	4.113312	-1.509062
H	0.330184	0.817679	6.033713

S-WT oxidized

C	-1.113056	-2.473021	3.554109
C	-0.269213	-1.581558	2.680974
O	-0.632123	-1.280951	1.539137
N	0.914515	-1.16177	3.18274
C	1.964543	-0.643688	2.295059
C	2.273632	0.850693	2.533776
C	1.059419	1.696979	2.748532
N	0.015658	1.755505	1.834976
C	0.748433	2.5016	3.814698
C	-0.89524	2.577604	2.337062
N	-0.490129	3.047521	3.535696
C	5.320208	-3.146734	0.197589
C	4.595907	-3.239521	-1.137483
O	4.162552	-2.240433	-1.706124
N	4.465846	-4.462268	-1.644904
C	3.13533	0.400283	-3.440222
C	2.231341	1.053017	-2.397939
S	1.434635	-0.201204	-1.295567
C	-2.767432	-2.921215	-0.642892
C	-4.00442	-2.375872	-0.972122
C	-2.715355	-3.933404	0.310114
C	-5.171072	-2.830377	-0.365475
C	-3.878716	-4.394277	0.923214
C	-5.105835	-3.843251	0.584018
C	-2.43442	2.148579	-4.105638
C	-1.641793	1.750903	-2.859049
C	-2.494539	1.367819	-1.687001
N	-1.943734	0.924849	-0.489352
C	-3.860268	1.323534	-1.566604
C	-2.947538	0.599092	0.313921
N	-4.123688	0.849352	-0.294505
C	0.319982	5.240313	-1.707398
S	0.382448	4.028591	-0.351326
C	1.800537	4.708448	0.579826
Cu	-0.017197	0.76059	0.056151
H	-2.842275	0.142692	1.285546
H	-5.032226	0.597939	0.06974

H	-4.647959	1.581407	-2.256272
H	-0.972766	2.569862	-2.56438
H	-0.988637	0.900328	-3.094897
H	-1.754217	2.406758	-4.922575
H	-3.073727	3.018958	-3.91687
H	-4.061523	-1.613888	-1.746012
H	-6.135027	-2.415956	-0.652994
H	-6.016169	-4.212811	1.049501
H	-3.826347	-5.196884	1.654559
H	-1.758467	-4.384606	0.560728
H	0.563493	-2.071041	-2.751518
H	3.890376	-0.235838	-2.973062
H	2.790459	1.740957	-1.756244
H	1.428735	1.632626	-2.86391
H	0.138491	6.246918	-1.321483
H	-0.512564	4.962717	-2.359158
H	2.719715	4.65651	-0.010396
H	1.918943	4.106037	1.483573
H	1.607067	5.745089	0.86917
H	-1.819814	2.863409	1.860681
H	-0.995407	3.70708	4.111326
H	1.284227	2.723581	4.724598
H	2.861522	1.221406	1.684236
H	2.917092	0.952499	3.414706
H	1.637839	-0.850237	1.284955
H	1.199356	-1.524982	4.082329
H	-0.780855	-2.506458	4.596445
H	-2.155186	-2.145831	3.517574
H	-1.085327	-3.48848	3.144448
H	3.459284	-0.888359	0.311535
H	4.63148	-3.330155	1.021888
H	6.113501	-3.904949	0.252464
H	4.859039	-5.280678	-1.205628
H	3.983123	-4.576507	-2.526379
H	-3.070446	1.326929	-4.4526
H	1.243634	5.231445	-2.294105
H	2.8432	-1.220098	2.525542
H	-1.868772	-2.613584	-1.170301
H	5.763333	-2.163373	0.307279
H	2.554902	-0.222055	-4.129739
H	3.636136	1.179967	-4.027045
F	0.046975	-2.697466	-3.211961
F	3.926673	-1.244821	1.036579

S-WT reduced

C	-1.012289	-2.559728	3.525427
C	-0.204949	-1.623395	2.652811
O	-0.581434	-1.327196	1.523511
N	0.972477	-1.175523	3.157228
C	2.014654	-0.656991	2.252445
C	2.373431	0.8158	2.537135
C	1.180259	1.674497	2.818358
N	0.100076	1.741781	1.952671
C	0.927366	2.464887	3.912055
C	-0.779425	2.55161	2.51072
N	-0.3249	3.014422	3.703522
C	5.38187	-3.067078	0.066479
C	4.639839	-3.150994	-1.259412
O	4.181096	-2.150597	-1.805385
N	4.523429	-4.367502	-1.784824
C	3.126982	0.626206	-3.4513
C	2.186981	1.177631	-2.379658
S	1.444986	-0.161627	-1.342814
C	-2.719872	-2.969134	-0.654191
C	-3.970738	-2.440217	-0.956703
C	-2.636468	-3.995459	0.281308
C	-5.120408	-2.924698	-0.340902
C	-3.782644	-4.48635	0.903409
C	-5.023887	-3.951423	0.590885
C	-2.52477	2.160741	-4.038069
C	-1.785234	1.778372	-2.754514
C	-2.679561	1.402833	-1.611055
N	-2.146647	1.002473	-0.393431
C	-4.04991	1.33717	-1.537691
C	-3.165411	0.688451	0.383415
N	-4.343778	0.893267	-0.258823
C	0.210793	5.261059	-1.629369
S	0.262511	4.049076	-0.273605
C	2.000519	4.273711	0.229361
Cu	-0.097169	0.76897	0.068569
H	-3.086987	0.278823	1.379313
H	-5.257166	0.643244	0.090032
H	-4.823307	1.561988	-2.255378
H	-1.133126	2.6007	-2.435627
H	-1.107647	0.935111	-2.939959

H	-1.811599	2.414799	-4.828824
H	-3.178674	3.029033	-3.886198
H	-4.046974	-1.649208	-1.698725
H	-6.094209	-2.513124	-0.599306
H	-5.920698	-4.340437	1.068477
H	-3.704689	-5.294444	1.6273
H	-1.665478	-4.420565	0.522004
H	0.564761	-2.027196	-2.796176
H	3.910656	0.010079	-3.003105
H	2.736973	1.862095	-1.723112
H	1.381133	1.759442	-2.841795
H	0.435906	6.273663	-1.278562
H	-0.805364	5.251706	-2.033987
H	2.678189	3.984797	-0.579539
H	2.172311	3.619105	1.08568
H	2.195113	5.309049	0.526739
H	-1.728332	2.836685	2.082068
H	-0.796014	3.67601	4.30272
H	1.506591	2.6749	4.798355
H	2.92688	1.192975	1.668557
H	3.054073	0.879651	3.395576
H	1.645626	-0.783903	1.24068
H	1.272198	-1.551323	4.046703
H	-0.829098	-2.418053	4.597059
H	-2.074949	-2.42463	3.314729
H	-0.755951	-3.594838	3.270166
H	3.484235	-0.843622	0.243967
H	4.702811	-3.269824	0.894358
H	6.189554	-3.813544	0.098766
H	4.785957	-5.19917	-1.277663
H	3.9231	-4.47542	-2.591966
H	-3.144085	1.3336	-4.405209
H	0.90638	4.988369	-2.429671
H	2.87622	-1.276706	2.429109
H	-1.83183	-2.620902	-1.174107
H	5.801471	-2.075506	0.189729
H	2.579745	-0.006659	-4.15946
H	3.593713	1.445716	-4.017344
F	0.052422	-2.655044	-3.25934
F	3.968232	-1.203497	0.956316

S-F114P oxidized

C	0.770949	3.042014	3.109158

C	0.017411	1.99405	2.332582
O	0.429247	1.59001	1.241709
N	-1.142208	1.548145	2.866905
C	-2.118424	0.824077	2.043531
C	-2.264212	-0.660174	2.449584
C	-0.975351	-1.332817	2.805716
N	0.104835	-1.423149	1.938218
C	-0.631459	-1.93688	3.988726
C	1.067997	-2.066854	2.581744
N	0.661495	-2.394599	3.827614
C	-5.632625	2.774059	-0.35919
C	-4.89396	2.774678	-1.689609
O	-4.367835	1.757683	-2.134847
N	-4.857502	3.937775	-2.334106
C	-3.173096	-1.226955	-3.268999
C	-2.134228	-1.633663	-2.225927
S	-1.461295	-0.169363	-1.329168
C	2.459657	3.14565	-1.096812
C	3.743934	2.673869	-1.349768
C	2.305155	4.252277	-0.26798
C	4.856871	3.29298	-0.789637
C	3.414159	4.878148	0.297794
C	4.689265	4.398758	0.035511
C	2.617495	-2.297608	-3.951693
C	1.836985	-1.776046	-2.741914
C	2.691369	-1.246231	-1.627578
N	2.134836	-0.744189	-0.454541
C	4.053914	-1.106891	-1.545666
C	3.131353	-0.296102	0.294629
N	4.31098	-0.515929	-0.32188
C	0.088003	-5.317908	-1.235709
S	0.147069	-4.009853	0.025689
C	-1.37278	-4.447146	0.941094
Cu	0.173839	-0.692486	0.029166
H	3.022339	0.216548	1.237858
H	5.212942	-0.204655	0.010678
H	4.843579	-1.372487	-2.230351
H	1.189575	-2.567299	-2.3432
H	1.159229	-0.972804	-3.060999
H	1.928281	-2.660416	-4.719804
H	3.279397	-3.127357	-3.67747
H	3.879409	1.824596	-2.015814
H	5.856646	2.928136	-1.0145

H	5.556219	4.892902	0.466993
H	3.280219	5.74936	0.933969
H	1.308199	4.637254	-0.067919
H	-3.971618	-0.624554	-2.828075
H	-2.569892	-2.296185	-1.468967
H	-1.296131	-2.17485	-2.676011
H	0.103418	-6.308438	-0.77256
H	0.978489	-5.214366	-1.861677
H	-2.257306	-4.345515	0.305066
H	-1.453068	-3.758154	1.783629
H	-1.311368	-5.470245	1.322321
H	2.03395	-2.32476	2.176247
H	1.204797	-2.904348	4.510686
H	-1.181751	-2.075268	4.906559
H	-2.767756	-1.193637	1.633534
H	-2.929003	-0.734002	3.317477
H	-1.796806	0.945613	1.018098
H	-1.474887	1.992355	3.711756
H	0.391322	3.193335	4.124471
H	1.829508	2.773078	3.157575
H	0.710048	3.991434	2.566762
H	-3.591278	0.711008	0.031965
H	-4.975888	3.101797	0.44604
H	-6.483959	3.468241	-0.39714
H	-5.339985	4.760031	-2.004919
H	-4.386182	3.984126	-3.227505
H	3.230321	-1.509383	-4.403104
H	-0.800639	-5.221038	-1.866777
H	-3.057404	1.322972	2.205436
H	1.593672	2.661268	-1.536635
H	-6.000219	1.777192	-0.144046
H	-2.716278	-0.629863	-4.064554
H	-3.609657	-2.124804	-3.723386
F	-4.100318	1.107014	0.706697

S-F114P reduced

C	0.903272	2.999089	3.126489
C	0.120385	1.974796	2.334869
O	0.518557	1.575632	1.245478
N	-1.059085	1.565068	2.86331
C	-2.07677	0.934954	2.003112
C	-2.402661	-0.513514	2.424172
C	-1.205377	-1.301136	2.858372

N	-0.076242	-1.433025	2.064513
C	-1.004016	-1.978404	4.036126
C	0.778719	-2.172506	2.744491
N	0.263286	-2.526867	3.950547
C	-5.450023	3.071648	-0.442456
C	-4.691315	3.041803	-1.761209
O	-4.210024	2.001866	-2.204172
N	-4.586224	4.20484	-2.398235
C	-3.123436	-1.062678	-3.413348
C	-2.165854	-1.493299	-2.300939
S	-1.443389	-0.034319	-1.424524
C	2.661358	3.038854	-1.052052
C	3.924124	2.504265	-1.287782
C	2.549614	4.147642	-0.21925
C	5.05779	3.063677	-0.706806
C	3.679604	4.713974	0.367347
C	4.932977	4.172296	0.122104
C	2.590387	-2.390896	-3.935989
C	1.842463	-1.911763	-2.687518
C	2.728343	-1.424978	-1.578939
N	2.191106	-0.938636	-0.393595
C	4.097825	-1.329678	-1.516192
C	3.206966	-0.54905	0.351735
N	4.387724	-0.780919	-0.277712
C	-0.130428	-5.293673	-1.277387
S	-0.102969	-4.020606	0.027526
C	-1.81427	-4.220117	0.625646
Cu	0.135825	-0.71211	0.077138
H	3.125962	-0.069412	1.315927
H	5.299548	-0.50279	0.053278
H	4.873178	-1.600879	-2.215646
H	1.206001	-2.71536	-2.297883
H	1.146125	-1.102009	-2.941258
H	1.881423	-2.721673	-4.701731
H	3.257305	-3.23298	-3.711095
H	4.021864	1.637472	-1.936983
H	6.040228	2.641961	-0.909358
H	5.816537	4.616247	0.575741
H	3.5785	5.582948	1.013504
H	1.56762	4.568531	-0.019207
H	-3.91468	-0.417988	-3.019894
H	-2.701937	-2.12718	-1.583396
H	-1.356005	-2.104039	-2.719284

H	-0.348355	-6.286609	-0.870327
H	0.863531	-5.314216	-1.733286
H	-2.52948	-3.939305	-0.152982
H	-1.939318	-3.551533	1.479265
H	-1.999459	-5.249521	0.949105
H	1.752077	-2.484913	2.396419
H	0.706943	-3.119491	4.636588
H	-1.630221	-2.113908	4.904895
H	-2.888586	-0.999279	1.569415
H	-3.129403	-0.514946	3.246535
H	-1.698492	0.967452	0.987498
H	-1.374872	2.0165	3.710991
H	0.737958	2.925321	4.208023
H	1.967276	2.886067	2.910377
H	0.605551	4.005271	2.807236
H	-3.52145	0.906426	-0.031726
H	-4.785532	3.361483	0.371164
H	-6.269046	3.805114	-0.490706
H	-4.881145	5.076069	-1.984152
H	-3.988371	4.24329	-3.212877
H	3.198417	-1.58879	-4.372072
H	-0.864253	-5.043924	-2.050288
H	-2.95561	1.545751	2.110453
H	1.77727	2.582217	-1.485429
H	-5.856472	2.08947	-0.231389
H	-2.591059	-0.487103	-4.178905
H	-3.582209	-1.938131	-3.897309
F	-4.020539	1.324145	0.637324

S-F114N oxidized

C	-0.887787	1.155776	4.445049
C	-0.871507	0.38241	3.156023
O	-0.397117	0.871489	2.123226
N	-1.389106	-0.865129	3.174293
C	-1.737754	-1.55436	1.927907
C	-0.88531	-2.816123	1.673425
C	0.571193	-2.634143	1.961103
N	1.329274	-1.625905	1.38055
C	1.37821	-3.349629	2.807742
C	2.559124	-1.736707	1.861888
N	2.628647	-2.766911	2.731287
C	-5.901385	-1.362369	-0.205734
C	-5.482899	-0.297189	-1.208681

O	-4.472662	-0.421494	-1.896645
N	-6.276816	0.766856	-1.29238
C	-1.873535	-0.732406	-3.964688
C	-0.771907	-0.972581	-2.935372
S	-1.103893	-0.070901	-1.353735
C	-0.118154	4.190855	1.166541
C	3.236007	2.107416	-3.546547
C	2.437729	1.314303	-2.508584
C	2.754544	1.672829	-1.087219
N	2.081099	1.104859	-0.010589
C	3.647837	2.589247	-0.591864
C	2.538539	1.682147	1.092794
N	3.504675	2.568508	0.783046
C	3.570126	-2.631333	-2.972322
S	2.737762	-2.414923	-1.366369
C	2.13933	-4.123237	-1.116034
Cu	0.614929	-0.279829	0.02666
H	2.148228	1.521543	2.085763
H	3.946298	3.19984	1.436615
H	4.361477	3.23054	-1.084221
H	2.599026	0.239108	-2.656679
H	1.363633	1.478157	-2.667199
H	2.948583	1.80635	-4.558083
H	4.313733	1.937633	-3.441994
H	-1.859364	2.270117	-1.922653
H	-2.856141	-0.997108	-3.567347
H	-0.675319	-2.034843	-2.691199
H	0.20323	-0.639117	-3.303733
H	4.372051	-3.371325	-2.896473
H	4.011492	-1.669724	-3.246627
H	1.427771	-4.407818	-1.896211
H	1.639435	-4.15235	-0.145226
H	2.9761	-4.826878	-1.10576
H	3.400617	-1.117846	1.5937
H	3.459734	-3.069953	3.220347
H	1.175384	-4.197596	3.44337
H	-1.043676	-3.13476	0.634871
H	-1.253787	-3.635807	2.300135
H	-1.652402	-0.821533	1.137678
H	-1.858626	-1.16323	4.018553
H	-1.627413	0.788063	5.162214
H	0.100319	1.111801	4.918991
H	-1.090905	2.203752	4.205293

H	-2.983439	-1.609502	-0.23397
H	-5.547256	-1.108147	0.793193
H	-6.997047	-1.431624	-0.16175
H	-7.121675	0.861949	-0.749573
H	-6.030742	1.512101	-1.930253
H	3.050343	3.183414	-3.456917
H	2.863266	-2.932302	-3.7505
H	-2.764119	-1.852624	2.044899
H	-5.497435	-2.324349	-0.498885
H	-1.906791	0.320168	-4.265683
H	-1.6745	-1.334815	-4.859294
F	-1.955638	3.192647	-2.026937
F	-3.554128	-1.97823	0.405999
O	-0.779079	4.397748	2.181287
N	1.075047	4.767663	1.05219
H	1.248846	5.51062	1.719083
H	1.493976	4.889291	0.138511
C	-0.654144	3.29208	0.061756
H	-0.686311	2.278498	0.458923
H	-1.666139	3.625237	-0.125479
H	-0.065832	3.330085	-0.854276

S-F114N reduced

C	-0.792918	1.277466	4.43268
C	-0.830744	0.486819	3.147659
O	-0.329628	0.92595	2.11444
N	-1.434289	-0.725445	3.191679
C	-1.856272	-1.389842	1.951142
C	-1.15829	-2.747588	1.729197
C	0.307944	-2.721858	2.027687
N	1.161628	-1.794386	1.451354
C	1.025757	-3.516417	2.886655
C	2.361473	-2.025622	1.949776
N	2.330111	-3.059895	2.828501
C	-5.995446	-0.899926	-0.182475
C	-5.496466	0.116309	-1.199297
O	-4.50013	-0.095473	-1.886165
N	-6.204821	1.238064	-1.296257
C	-1.904166	-0.739178	-3.985971
C	-0.832742	-0.992196	-2.925281
S	-1.131307	-0.013305	-1.385229
C	0.206711	4.200784	1.114908
C	3.380193	1.801072	-3.572811

C	2.583408	1.117797	-2.459116
C	2.994097	1.508628	-1.070477
N	2.339106	0.990916	0.038617
C	3.963573	2.384604	-0.643866
C	2.887769	1.549815	1.100019
N	3.892373	2.388411	0.740048
C	3.343397	-2.94155	-2.937759
S	2.52388	-2.661584	-1.337339
C	1.311062	-4.021784	-1.404354
Cu	0.644149	-0.302619	0.043769
H	2.556378	1.411008	2.118431
H	4.413	2.987449	1.363219
H	4.690872	2.974303	-1.180035
H	2.661146	0.027748	-2.553388
H	1.512611	1.333929	-2.56556
H	3.022688	1.474246	-4.554473
H	4.449824	1.563741	-3.510806
H	-1.68428	2.382813	-1.948309
H	-2.902092	-0.9431	-3.589042
H	-0.814582	-2.05627	-2.662851
H	0.159305	-0.745138	-3.321061
H	3.800312	-3.935196	-2.99152
H	4.133108	-2.190752	-3.032772
H	0.605797	-3.872133	-2.227114
H	0.762959	-4.007169	-0.460449
H	1.810495	-4.989849	-1.511898
H	3.261869	-1.489696	1.69023
H	3.12345	-3.450281	3.315203
H	0.732961	-4.339186	3.520943
H	-1.338916	-3.043995	0.688518
H	-1.623601	-3.516306	2.359158
H	-1.653461	-0.703721	1.136224
H	-1.930951	-0.965747	4.038342
H	-1.565001	0.980329	5.150437
H	0.185256	1.160998	4.915608
H	-0.909987	2.33435	4.175879
H	-3.105832	-1.375	-0.20915
H	-5.607434	-0.665641	0.808539
H	-7.094238	-0.878224	-0.130946
H	-6.931746	1.470217	-0.636059
H	-5.819268	1.988718	-1.854366
H	3.275332	2.891972	-3.530134
H	2.64184	-2.816598	-3.768974

H	-2.912836	-1.551641	2.063752
H	-5.666892	-1.89322	-0.465159
H	-1.88961	0.308071	-4.309899
H	-1.732584	-1.371105	-4.869647
F	-1.708237	3.308637	-2.064418
F	-3.702621	-1.689712	0.435835
O	-0.434411	4.47174	2.127272
N	1.441207	4.680931	0.99247
H	1.721227	5.377771	1.669296
H	1.941917	4.640637	0.115698
C	-0.399689	3.332642	0.022095
H	-0.436906	2.306415	0.386846
H	-1.411389	3.690155	-0.119245
H	0.149722	3.371182	-0.916153

S-N47S oxidized

C	2.526546	-3.686396	-0.517283
C	1.299622	-2.96294	-0.030065
O	1.303284	-1.736446	0.125962
N	0.210323	-3.710652	0.252073
C	-0.880066	-3.169904	1.07379
C	-2.202473	-3.035597	0.291805
C	-2.027233	-2.460375	-1.077463
N	-1.417943	-1.23235	-1.303183
C	-2.384845	-2.994386	-2.288134
C	-1.412923	-1.035315	-2.615349
N	-1.98686	-2.081321	-3.244858
C	-2.48053	1.775785	4.129585
C	-2.362131	1.422574	2.648196
S	-0.921644	0.30974	2.330127
C	3.933423	0.42806	0.765141
C	4.333728	1.361424	-0.18592
C	4.666293	-0.746916	0.898529
C	5.445533	1.131721	-0.99016
C	5.780762	-0.985533	0.096827
C	6.170257	-0.045443	-0.846055
C	-0.121915	4.953296	-0.173359
C	-0.22873	3.446449	0.072899
C	0.557044	2.616977	-0.897764
N	0.522976	1.227149	-0.885582
C	1.454743	3.006588	-1.859348
C	1.393597	0.796361	-1.789944
N	1.95897	1.845917	-2.416127

C	-4.252047	2.840252	-1.345607
S	-3.216858	1.356733	-1.426237
C	-4.504762	0.11947	-1.035728
Cu	-0.646106	-0.020575	0.154829
H	1.651967	-0.236876	-1.958952
H	2.731103	1.787285	-3.06589
H	1.767214	3.98491	-2.187408
H	-1.282525	3.142533	0.047289
H	0.131647	3.215137	1.084763
H	-0.722844	5.501496	0.557791
H	-0.481598	5.222493	-1.172893
H	3.795652	2.303054	-0.268501
H	5.765211	1.882368	-1.709605
H	7.048921	-0.222674	-1.461004
H	6.355433	-1.899421	0.223377
H	4.379803	-1.473695	1.654611
H	1.094799	1.263618	3.505254
H	-2.622446	0.881723	4.744912
H	-3.261942	0.917486	2.285018
H	-2.22322	2.321185	2.041183
H	-5.077731	2.775334	-2.059561
H	-3.629481	3.698011	-1.612986
H	-4.841086	0.213866	0.000658
H	-4.063366	-0.865356	-1.1894
H	-5.357806	0.235372	-1.709583
H	-1.037955	-0.159665	-3.120869
H	-2.133339	-2.160112	-4.242082
H	-2.865406	-3.926877	-2.540385
H	-2.897975	-2.428886	0.885273
H	-2.666764	-4.022185	0.191172
H	-0.525787	-2.229608	1.473568
H	0.311348	-4.716344	0.221781
H	2.38268	-4.764682	-0.632905
H	2.845761	-3.266548	-1.475753
H	3.340121	-3.508668	0.191986
H	-1.686326	-2.101861	3.180377
H	0.911543	5.303244	-0.076967
H	-4.651626	2.996777	-0.339031
H	-1.014954	-3.881065	1.87
H	3.1066	0.640489	1.436651
H	-1.586325	2.296555	4.485992
H	-3.343282	2.433457	4.284958
F	1.904417	1.653903	3.757049

F	-1.721619	-3.023385	3.324435

S-N47S reduced

C	2.483273	-3.728564	-0.533006
C	1.250771	-2.982715	-0.072037
O	1.281286	-1.77093	0.126793
N	0.136355	-3.719637	0.154646
C	-0.949238	-3.18406	0.99168
C	-2.278692	-3.039831	0.225972
C	-2.100837	-2.464474	-1.142685
N	-1.435772	-1.266506	-1.352862
C	-2.479425	-2.986131	-2.354495
C	-1.414182	-1.07357	-2.65816
N	-2.034509	-2.089934	-3.309865
C	-2.713262	1.763996	4.079268
C	-2.462435	1.418404	2.61192
S	-1.008857	0.29897	2.399753
C	3.935038	0.328847	0.874988
C	4.374229	1.275676	-0.045098
C	4.643035	-0.862395	0.998033
C	5.499963	1.043265	-0.828923
C	5.771211	-1.103823	0.2166
C	6.19953	-0.150252	-0.695401
C	-0.014142	4.94945	-0.051467
C	-0.146439	3.42895	0.039905
C	0.684694	2.675142	-0.954534
N	0.632774	1.290087	-1.01803
C	1.598506	3.126623	-1.875741
C	1.503919	0.916924	-1.935506
N	2.102041	1.996833	-2.498988
C	-4.15396	2.941286	-1.365351
S	-3.165329	1.415252	-1.424011
C	-4.469269	0.250941	-0.896398
Cu	-0.595183	0.02452	0.146228
H	1.749923	-0.105569	-2.179583
H	2.858451	1.971717	-3.166562
H	1.926303	4.119509	-2.141021
H	-1.19358	3.12989	-0.087642
H	0.130438	3.083737	1.044428
H	-0.642595	5.435038	0.701744
H	-0.321291	5.323592	-1.036099
H	3.839997	2.218291	-0.133619

H	5.842135	1.799869	-1.532208
H	7.086088	-0.332978	-1.298814
H	6.320928	-2.03548	0.329052
H	4.315014	-1.606173	1.719561
H	1.049509	1.155768	3.56833
H	-2.903634	0.859963	4.668281
H	-3.347949	0.93505	2.184614
H	-2.287141	2.334193	2.037416
H	-5.01744	2.884771	-2.035787
H	-3.510826	3.76257	-1.693638
H	-4.71039	0.389001	0.161684
H	-4.082206	-0.756951	-1.049328
H	-5.370895	0.382111	-1.502663
H	-0.981533	-0.220609	-3.158356
H	-2.173178	-2.15955	-4.307204
H	-3.005074	-3.891944	-2.615618
H	-2.943861	-2.411822	0.830533
H	-2.768709	-4.01682	0.130973
H	-0.607576	-2.227007	1.37053
H	0.215215	-4.724559	0.080421
H	2.266859	-4.722639	-0.939979
H	3.007988	-3.134572	-1.2848
H	3.162714	-3.843012	0.318955
H	-1.784378	-2.148698	3.103326
H	1.018859	5.273149	0.123285
H	-4.494718	3.152844	-0.346799
H	-1.06874	-3.888517	1.795422
H	3.086216	0.536748	1.520076
H	-1.843906	2.267516	4.515818
H	-3.582229	2.428898	4.182243
F	1.860081	1.52501	3.84733
F	-1.839827	-3.072403	3.225392

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