Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Quantifying flattening distortion on the thermodynamics and kinetics of electron transfers of Cu(I) photoredox catalysts

Christian Sandoval–Pauker[†], Gabriela Molina–Aguirre[†], Dino Villagrán[†,] and Balazs Pinter[†,‡,*]*

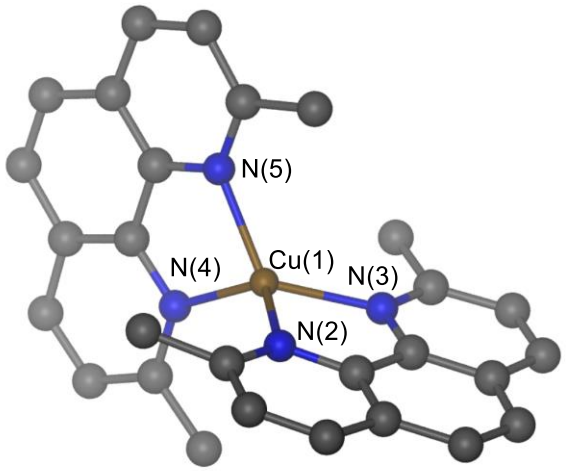
†Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, TX, 79968, USA, dino@utep.edu, bpinter@utep.edu

‡Current affiliation: European Research Council Executive Agency. Disclaimer: The views expressed are purely those of the authors and may not in any circumstances be regarded as stating an official position of the ERCEA and the European Commission.

Table of Contents

1. Calculated and experimental X-ray structural metrics

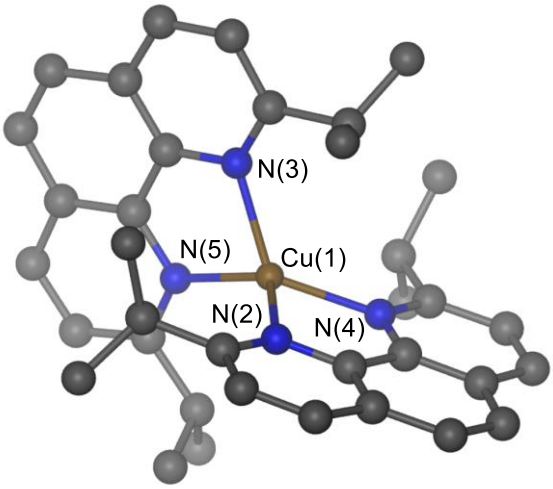
Table S1. Experimental and calculated distances for the Cu(I) cation **2** (S_0). Hydrogen atoms attached to carbons are omitted for clarity (TPSSh-D3/def2-TZVP(-f)/defgrid2)



Bond	Length (exp.) (Å)	Length (calc.) (Å)	Δ (Å)
Cu(1)–N(2)	2.028	2.029	0.001
Cu(1)–N(3)	2.070	2.025	0.045
Cu(1)–N(4)	2.042	2.025	0.017
Cu(1)–N(5)	2.053	2.026	0.027
Angle	**Angle (exp.) (°)**	**Angle (calc.) (°)**	**Δ (°)**
N(2)–Cu(1)–N(3)	82	83	1
N(2)–Cu(1)–N(4)	128	123	5
N(2)–Cu(1)–N(5)	132	125	7
N(3)–Cu(1)–N(4)	127	126	1
N(3)–Cu(1)–N(5)	111	123	12
N(4)–Cu(1)–N(5)	82	83	1
Θ	80	88	8
β	133	138	5
γ	144	139	5

*Experimental XRD structural metrics from ref. 1

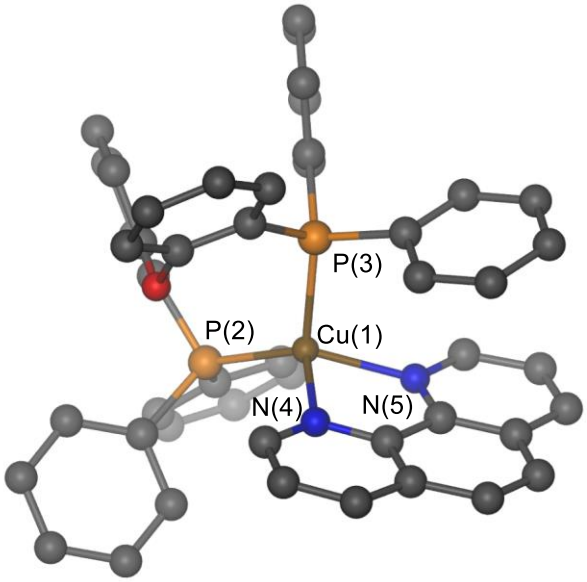
Table S2. Experimental and calculated distances for the Cu(I) cation **3** (S_0). Hydrogen atoms attached to carbons are omitted for clarity (TPSSh-D3/def2-TZVP(-f)/defgrid2)



Bond	Length (exp.) (Å)	Length (calc.) (Å)	Δ (Å)
Cu(1)–N(2)	2.067	2.046	0.021
Cu(1)–N(3)	2.053	2.043	0.010
Cu(1)–N(4)	2.006	2.016	0.010
Cu(1)–N(5)	2.020	2.019	0.001
Angle	**Angle (exp.) (°)**	**Angle (calc.) (°)**	**Δ (°)**
N(2)–Cu(1)–N(3)	118	114	3
N(2)–Cu(1)–N(4)	83	83	0
N(2)–Cu(1)–N(5)	123	123	0
N(3)–Cu(1)–N(4)	123	126	3
N(3)–Cu(1)–N(5)	83	82	1
N(4)–Cu(1)–N(5)	133	133	0
Θ	88	89	1
β	132	129	3
γ	145	147	2

*Experimental XRD structural metrics from ref. 2

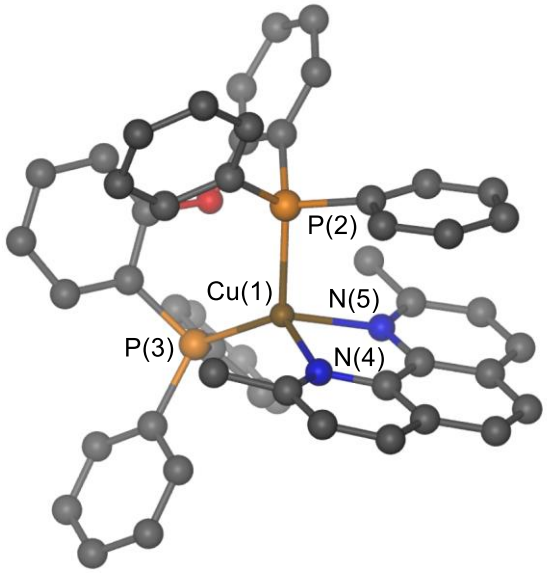
Table S3. Experimental and calculated distances for the Cu(I) cation **4** (S_0). Hydrogen atoms attached to carbons are omitted for clarity (TPSSh-D3/def2-TZVP(-f)/defgrid2)



Bond	Length (exp.) (Å)	Length (calc.) (Å)	|Δ| (Å)
Cu(1)–P(2)	2.195	2.217	0.022
Cu(1)–P(3)	2.270	2.278	0.008
Cu(1)–N(5)	2.079	2.059	0.020
Cu(1)–N(4)	2.054	2.062	0.008
Angle	**Angle (exp.) (°)**	**Angle (calc.) (°)**	**|Δ| (°)**
P(2)–Cu(1)–P(3)	118	115	3
P(2)–Cu(1)–N(5)	123	133	10
P(2)–Cu(1)–N(4)	124	116	8
N(3)–Cu(1)–N(5)	101	102	1
N(3)–Cu(1)–N(4)	103	101	2
N(5)–Cu(1)–N(4)	82	82	0
Θ	89	85	4
B	106	105	1
γ	137	138	1

*Experimental XRD structural metrics from ref. 3

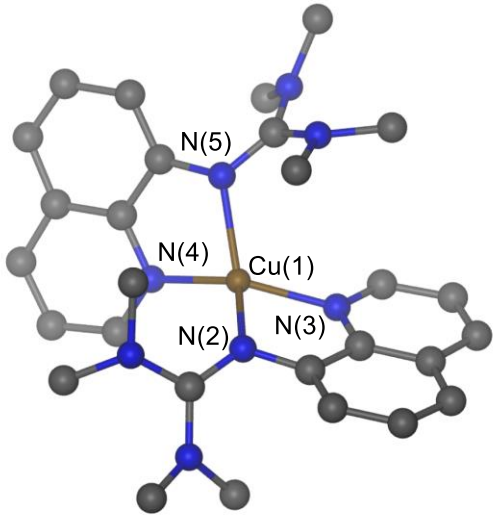
Table S4. Experimental and calculated distances for the Cu(I) cation **5** (**S_0**). Hydrogen atoms attached to carbons are omitted for clarity (TPSSh-D3/def2-TZVP(-f)/defgrid2)



Bond	**Length (exp.) (Å)**	**Length (calc.) (Å)**	**|Δ| (Å)**
Cu(1)–P(2)	2.315	2.288	0.027
Cu(1)–P(3)	2.228	2.227	0.001
Cu(1)–N(4)	2.093	2.072	0.021
Cu(1)–N(5)	2.087	2.075	0.012
Angle	**Angle (exp.) (°)**	**Angle (calc.) (°)**	**|Δ| (°)**
P(2)–Cu(1)–P(3)	118	118	0
P(2)–Cu(1)–N(4)	104	103	1
P(2)–Cu(1)–N(5)	100	101	1
N(3)–Cu(1)–N(4)	123	125	2
N(3)–Cu(1)–N(5)	123	121	2
N(4)–Cu(1)–N(5)	81	81	0
Θ	88	89	1
B	106	106	0
γ	136	136	0

*Experimental XRD structural metrics from ref. 4

Table S5. Experimental and calculated distances for the Cu(I) cation **7** (**S_0**). Hydrogen atoms attached to carbons are omitted for clarity (TPSSh-D3/def2-TZVP(-f)/defgrid2)



Bond	**Length (exp.) (Å)**	**Length (calc.) (Å)**	**Δ (Å)**
Cu(1)–N(2)	2.095	2.070	0.025
Cu(1)–N(3)	1.966	2.002	0.036
Cu(1)–N(4)	1.999	1.999	0.000
Cu(1)–N(5)	2.068	2.072	0.004
Angle	**Angle (exp.) (°)**	**Angle (calc.) (°)**	**Δ (°)**
N(2)–Cu(1)–N(4)	108	117	9
N(2)–Cu(1)–N(5)	129	128	1
N(2)–Cu(1)–N(3)	83	82	1
N(4)–Cu(1)–N(3)	149	140	9
N(4)–Cu(1)–N(5)	82	82	0
N(3)–Cu(1)–N(5)	114	114	0
Θ	64	72	8
β	134	133	1
γ	140	144	4

*Experimental XRD structural metrics from ref. 5

2. Calculated and experimental ground- and excited-state reduction potentials in MeCN

Table S6. Calculated reduction potentials of the investigated Cu(I) complexes in MeCN (V vs. SCE). The experimental ground- and excited-state reduction potentials are reported in parentheses.

Complex	E^0_{ox} ($D^{ox} \rightarrow S_0$)	E^0_{red} ($S_0 \rightarrow D^{red}$)	$^*E^0_{ox}$ ($D^{ox} \rightarrow T_1$)	$^*E^0_{red}$ ($T_1 \rightarrow D^{red}$)
2	0.66 (0.65[a])	–1.8 (–1.80[a])	–1.1 (–1.05[e])	–0.04 (–0.10[e])
3	0.78 (0.87[a])	–1.87 (–1.83[a])	–0.96 (–0.96[f])	–0.12 (0.00[f])
7	–0.14 (–0.06[b])	–2.04	–1.46	–0.72
8	–0.03 (0.16[b])	–2.17	–1.61	–0.60

Experimental reduction potentials were taken from a) ref.[6] and b) ref.[7] Experimental $^*E^0_{ox}$ and $^*E^0_{red}$ values were obtained from the corresponding E^0_{ox} and E^0_{red} values using the following equations $^*E^0_{ox} = E^0_{ox} - E_{0,0}$ and $^*E^0_{red} = E^0_{red} + E_{0,0}$ where $E_{0,0}$ was estimated from the maximum emission of the photocatalyst (λ^{em}) taken from e) ref.[8] and f) ref[9].

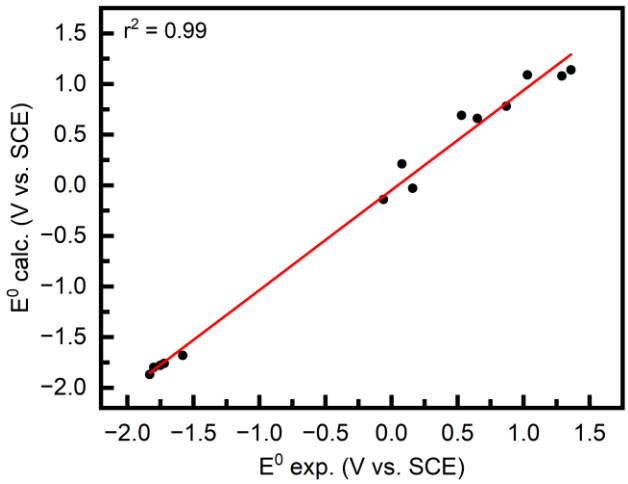


Figure S1. Correlation between calculated and experimental ground-state redox potentials E^0_{red} and E^0_{ox}

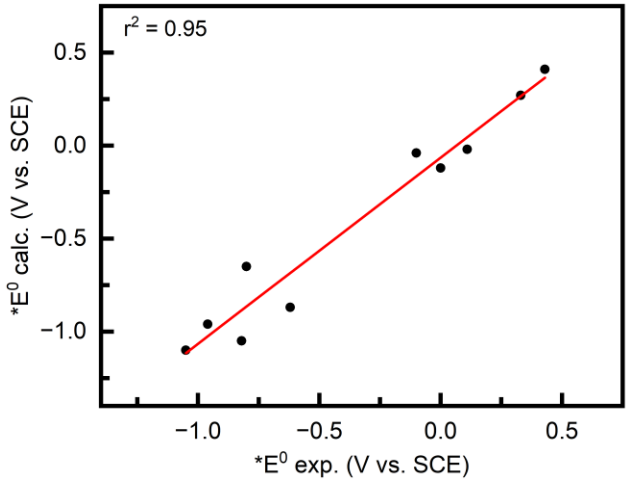
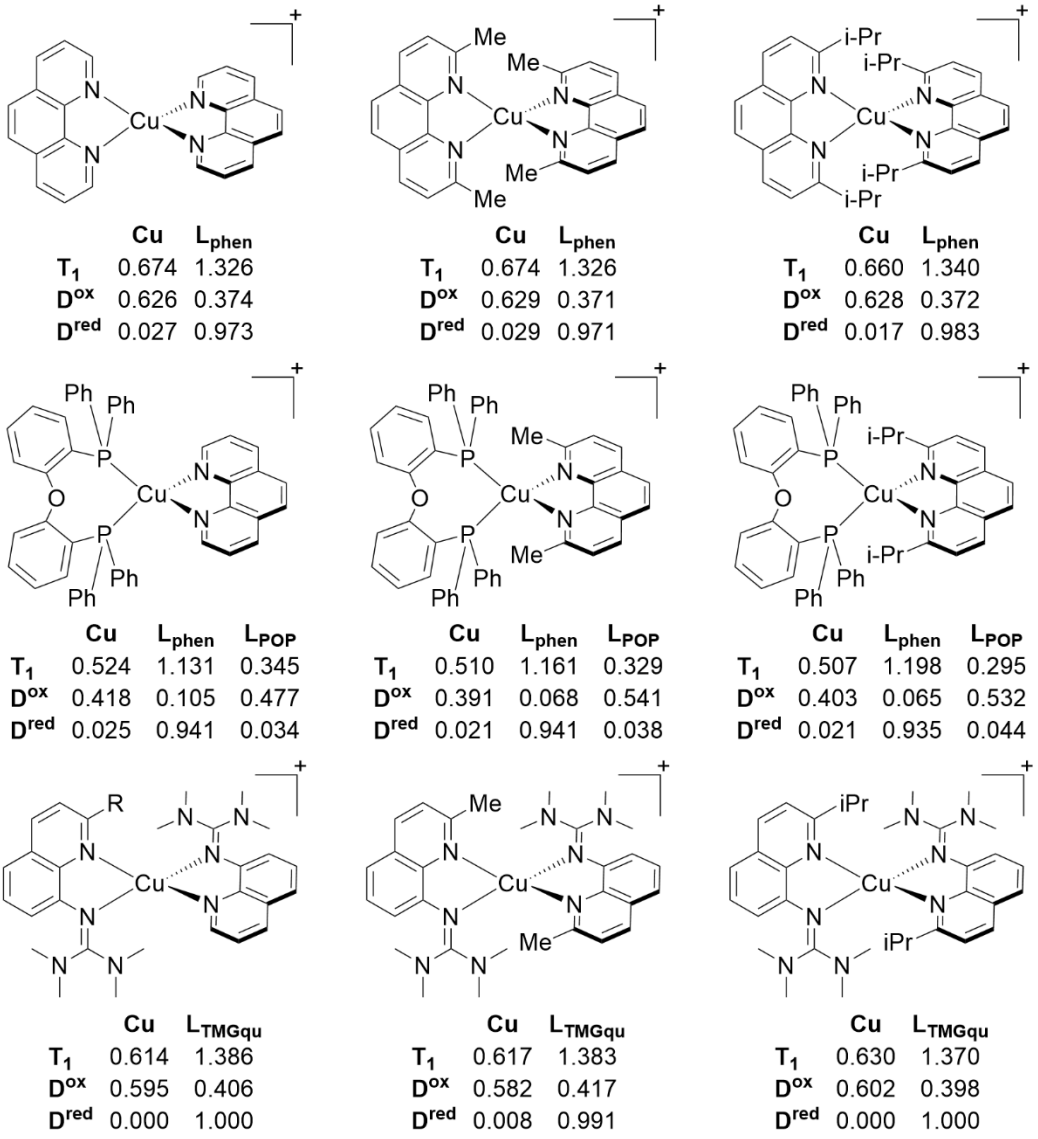


Figure S2. Correlation between calculated and experimental excited state reduction potentials $^*E^0_{red}$ and $^*E^0_{ox}$

3. Condensed spin density populations for T_1, D^{ox} and D^{red} states of complexes 1-9



	Cu	L_{phen}
T_1	0.674	1.326
D^{ox}	0.626	0.374
D^{red}	0.027	0.973

	Cu	L_{phen}
T_1	0.674	1.326
D^{ox}	0.629	0.371
D^{red}	0.029	0.971

	Cu	L_{phen}
T_1	0.660	1.340
D^{ox}	0.628	0.372
D^{red}	0.017	0.983

	Cu	L_{phen}	L_{POP}
T_1	0.524	1.131	0.345
D^{ox}	0.418	0.105	0.477
D^{red}	0.025	0.941	0.034

	Cu	L_{phen}	L_{POP}
T_1	0.510	1.161	0.329
D^{ox}	0.391	0.068	0.541
D^{red}	0.021	0.941	0.038

	Cu	L_{phen}	L_{POP}
T_1	0.507	1.198	0.295
D^{ox}	0.403	0.065	0.532
D^{red}	0.021	0.935	0.044

	Cu	L_{TMGqu}
T_1	0.614	1.386
D^{ox}	0.595	0.406
D^{red}	0.000	1.000

	Cu	L_{TMGqu}
T_1	0.617	1.383
D^{ox}	0.582	0.417
D^{red}	0.008	0.991

	Cu	L_{TMGqu}
T_1	0.630	1.370
D^{ox}	0.602	0.398
D^{red}	0.000	1.000

Figure S3. Condensed spin density populations at the metal and the ligand(s) in the open-shell T_1, D^{ox}, and D^{red} states of complexes **1-9**

4. Computational protocol for the calculation of reduction potentials

All calculations were carried out using density functional theory (DFT) implemented in Orca software package v.5.0.3.[10,11] Geometry optimizations on the non-truncated models of the complexes were performed using the meta-GGA hybrid functional TPSSh[12] combined with the triple-ζ valence basis set def2-TZVP(-f)[13] and the auxiliary basis set def2/J[13]. A tight convergence of the wavefunction (energy change, TolE = 1×10^{-8}; RMS density change, TolRMSP = 5×10^{-9}; maximum density change, TolMaxP = 1×10^{-7}; DIIS error convergence, TolErr = 5×10^{-7}) and a defgrid2 DFT integration grid were requested. The RI-J approximation for the Coulomb integrals and COSX numerical chain-of-sphere integration for the HF exchange integrals (RIJCOSX)[14] was employed to accelerate the DFT calculations. Dispersion effects were considered in all calculations via Grimme's D3 protocol in combination with the Becke-Johnson (D3BJ) damping scheme.[15]

Analytical frequency calculations at the same theoretical level as optimizations (TPSSh-D3/def2-TZVP(-f)) were conducted to confirm that the optimized equilibrium structures represent local minima of the potential energy surface identified by the absence of imaginary vibrational modes, and to obtain the thermodynamic corrections to the electronic energy within the ideal gas–rigid rotor–harmonic oscillator approximation at T = 273.15 K. The electronic energies and wavefunctions of all species computed were refined by subsequent single-point calculations at the TPSSh-D3/def2-TZVP level.

We employed the general procedure described by Baik and Friesner[16] and Roy et al.[17] to calculate standard reduction potentials (E^0). Equation 1 shows the defining equation of the half-cell potential $E^0_{1/2}$ (A/A^-) for a one-electron reduction process ($A + e^- \rightarrow A^-$). $\Delta G^{0,sol}$ corresponds to the solution state reaction Gibbs free energy of the reduction process, n is the number of electrons transferred (n = 1), and F is the Faraday constant (F = 96500 C mol^{-1}).

$$E^0_{1/2}(A/A^-) = \frac{-\Delta G^{0,sol}(A/A^-)}{nF} \quad (1)$$

The Born-Haber thermodynamic cycle was used to evaluate $\Delta G^{0,sol}$ (A/A^-) of the different reduction processes studied. As shown in equation 2, $\Delta G^{0,sol}$ (A/A^-) values are calculated from the Gibbs free energy change of the electron attachment process in the gas phase ($\Delta G^{0,gas}(A/A^-)$) and the standard solvation free energies of oxidized ($\Delta G^0_{solv}(A)$) and reduced ($\Delta G^0_{solv}(A^-)$) species.[16,17]

$$\Delta G^{0,sol}(A/A^-) = -\Delta G^0_{solv}(A) + \Delta G^{0,gas}(A/A^-) + \Delta G^0_{solv}(A^-) \quad (2)$$

We employed equations 3 and 4 to calculate the value of $\Delta G^{0,gas}(A/A^-)$, where E^{gas} is the refined electronic energy from the single point calculations, ZPE is the zero-point energy correction, and $\Delta G_{0\rightarrow 298K}$ is the thermal correction. The latter two values are obtained at 298.15 K from the analytical frequency calculations.

$$G^{0,gas} = E^{gas} + ZPE + \Delta G_{0\rightarrow 298\ K} \quad (3)$$

$$\Delta G^{0,gas}(A/A^-) = G^{0,gas}(A^-) - G^{0,gas}(A) \quad (4)$$

The individual standard solvation-free energies of the oxidized (A) and reduced (A^-) species (ΔG^0_{solv}) were obtained by subtracting the solution-state electronic energies (E^{sol}) and the refined electronic energies in the gas phase (E^{gas}), as shown in equation 5. The universal solvation model based on solute electron density (SMD)[18] implemented in Orca 5.0.3 at the same level of theory as the single-point calculations (TPSSh-D3/def2-TZVP) was employed to compute the solution state energies (E^{sol}) of the species. The GEPOL algorithm[19–21] generated the solvent cavity as a solvent-excluded surface, and the atomic radii of the default method were adjusted to H (1.250 Å), C (2.000 Å), N (1.600 Å), O (1.600), P (2.074 Å) and Cu (1.748). The radii of the solvents were set at 2.19 Å and 2.33 for acetonitrile and dichloromethane, respectively.

$$\Delta G^0_{solv}(A) = E^{sol}(A) - E^{gas}(A) \quad (5)$$

The resulting $\Delta G^{0,gas}(A/A^-)$, $\Delta G^0_{solv}(A)$ and $\Delta G^0_{solv}(A^-)$ values were inserted into equation 2, and the $E^0_{1/2}$ (A/A^-) obtained from equation 1. The standard reduction potentials (E^0) were then determined from equation 6, where $E^0(REF)$ is the reference electrode, which is the standard calomel electrode (SCE) in our manuscript. The absolute half-cell potential of the SCE electrode is 4.429 V.[22]

$$E^0 = E^0(A/A^-) - E^0(REF) \quad (6)$$

The above protocol was initially developed to calculate ground-state reduction potentials (i.e., E^0_{ox} and E^0_{red}).[16,17] Our recent reports show that the same robust framework can be employed to calculate excited-state reduction potentials (i.e., $^*E^0_{ox}$ and $^*E^0_{red}$) of Ru, Ir, and Cu complexes typically within 0.15 V to experimental data when a ^{3}MLCT state defines the excited state redox properties.[23–26] Therefore, we employed the same method described above (i.e., equations 1-6) to directly compute the solution state reaction Gibbs free energies of excited-state electron transfers ($\Delta G^{0,sol}(T_1/D^{red})$ and $\Delta G^{0,sol}(D^{ox}/T_1)$).[22,27,28] For this, we directly access the gas phase and solution state energetics of the ^{3}MLCT state and use those values to compute $\Delta G^{0,sol}$ of the redox process of interest and excited state reduction potentials (equations 1-6). This approach fundamentally differs from other reported protocols for calculating excited state reduction potentials, which are based on computing $E_{0,0}$ values using TD-DFT methodologies.[22,27,28]

Here, we provide a step-by-step tutorial for the protocol we used for the calculation of reduction potentials using the ground state $\mathbf{D^{ox}} \rightarrow \mathbf{S_0}$ redox step (E^0_{ox}) of $[Cu(dmp)_2]^+$ (**2**) in DCM as an example. The same protocol can be used for the other redox events by changing the XYZ coordinates, charge, and multiplicity appropriately.

The optimized structures for the $\mathbf{D^{ox}}$ and $\mathbf{S_0}$ species were obtained through *geometry optimizations* using the following input files in Orca 5.0.3 (In all examples provided herein, the lines for controlling the RAM allocation (%maxcore) and processors (%pal) are omitted for simplicity). The initial geometries were either taken from experimental X-ray structures or built *in silico*.

Input file for the $\mathbf{S_0}$ state:

```
!TPSSh def2-TZVP(-f) Opt d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 1 1
Cu       3.775315      8.721786      1.035774
N        3.902955      6.703423      1.142789
N        5.763053      8.606687      1.414008
```

```
N        2.936746      9.717854     -0.513148
N        2.510285      9.872399      2.123970
C        2.943197      5.787994      0.994628
C        3.230632      4.413738      1.095037
H        2.429145      3.697455      0.966424
.
.
.
H        3.328423      8.059850      3.769686
H        2.740440      8.844015      5.262242
H        4.177491      9.456630      4.430406
*
```

Input file for the **D^{ox}** state:

```
!TPSSh def2-TZVP(-f) Opt d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 2 2
Cu       3.633165      8.552478      0.905332
N        3.975450      6.556050      1.012719
N        5.634046      8.623082      1.431591
N        2.728021      9.605868     -0.591076
N        2.527604      9.824432      2.077359
C        3.148232      5.547657      0.753119
C        3.553039      4.207349      0.903336
H        2.951693      3.503445      0.689189
.
.
.
H        2.616440      7.953999      4.016880
H        2.991785      9.011461      5.158753
H        4.016815      8.727543      3.963297
*
```

As a result of the previous calculations, a file with the extension .xyz containing the XYZ coordinates for the optimized equilibrium structures is generated. Those XYZ coordinates are used to perform the next set of calculations. Besides, the gas phase dispersion corrected electronic energy at the TPSSh-D3/def2-TZVP(-f) level (E^{gas})was obtained from the .out files. *Frequency calculations* were performed at the same level of theory as optimizations using the subsequent input files (The lines for controlling the RAM allocation (%maxcore) and processors (%pal) are omitted for simplicity). $G^{0,gas}$ values are obtained from the .out file of these calculations.

Input file for the **S_0** state:

```
!TPSSh def2-TZVP(-f) freq d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 1 1
Cu   3.78618454890123      8.73585660105153      1.04731521051368
N    3.90208830350401      6.71293562409774      1.14666985784901
N    5.77051366583172      8.60757917889728      1.42773688549201
N    2.93747318909698      9.71983662178366     -0.50551149761289
N    2.51820235163825      9.88479643309250      2.13183007265793
C    2.93897002448102      5.80234039852265      0.99266436014885
C    3.22163291603248      4.42617167281352      1.08106976936983
H    2.41753091721533      3.71387792414380      0.94693449633693
.
```

```
.
.
H    3.31486723296830      8.06978047771496      3.81341544613296
H    2.80887077200594      8.92504045306826      5.29405513411201
H    4.21854137172579      9.47235397735990      4.37493688551659
*
```

Input file for the **D^{ox}** state:

```
!TPSSh def2-TZVP(-f) freq d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 2 2
Cu    3.81080208108758      8.75271149460812      1.02539382047211
N     3.94009921789056      6.75620521048136      0.88367367431585
N     5.68679183273613      8.61262607642444      1.70013139646962
N     2.77362342342012      9.49762691641693     -0.51167644551542
N     2.76085499924761     10.08280511105058      2.10043302301560
C     3.00597114509435      5.87113254008780      0.52522630254695
C     3.29183008917623      4.49036411089094      0.55316206040174
.
.
.
H     4.02519646125763      8.59920785297405      3.79768892839755
H     3.18960114949372      9.24054981033882      5.22458972696069
H     4.56237356601734     10.10983624215874      4.55228276923024
*
```

Single-point calculations were computed at the TPSSh-D3/def2-TZVP level of theory to refine the gas phase electronic energy (E^{gas}) and to obtain solution state energies (E^{sol}).

The refinement of E^{gas} values was carried out using the following input files.

Input file for the **S$_0$** state:

```
!TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 1 1
Cu    3.78618454890123      8.73585660105153      1.04731521051368
N     3.90208830350401      6.71293562409774      1.14666985784901
N     5.77051366583172      8.60757917889728      1.42773688549201
N     2.93747318909698      9.71983662178366     -0.50551149761289
N     2.51820235163825      9.88479643309250      2.13183007265793
C     2.93897002448102      5.80234039852265      0.99266436014885
C     3.22163291603248      4.42617167281352      1.08106976936983
H     2.41753091721533      3.71387792414380      0.94693449633693
.
.
.
H     3.31486723296830      8.06978047771496      3.81341544613296
H     2.80887077200594      8.92504045306826      5.29405513411201
H     4.21854137172579      9.47235397735990      4.37493688551659
*
```

Input file for the **D^{ox}** state:

```
!TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

* xyz 2 2
Cu     3.81080208108758      8.75271149460812      1.02539382047211
N      3.94009921789056      6.75620521048136      0.88367367431585
N      5.68679183273613      8.61262607642444      1.70013139646962
N      2.77362342342012      9.49762691641693     -0.51167644551542
N      2.76085499924761     10.08280511105058      2.10043302301560
C      3.00597114509435      5.87113254008780      0.52522630254695
C      3.29183008917623      4.49036411089094      0.55316206040174
.
.
.
H      4.02519646125763      8.59920785297405      3.79768892839755
H      3.18960114949372      9.24054981033882      5.22458972696069
H      4.56237356601734     10.10983624215874      4.55228276923024
*
```

The following input files were employed to obtain solution state energies (E^{sol})

Input file for the $\mathbf{S_0}$ state:

```
!TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

 !CPCM
%cpcm smd true
SMDsolvent "DICHLOROMETHANE"
surfacetype gepol_ses
rsolv 2.33
radius[1] 1.250
radius[6] 2.000
radius[7] 1.600
radius[29] 1.748
end

* xyz 1 1
Cu     3.78618454890123      8.73585660105153      1.04731521051368
N      3.90208830350401      6.71293562409774      1.14666985784901
N      5.77051366583172      8.60757917889728      1.42773688549201
N      2.93747318909698      9.71983662178366     -0.50551149761289
N      2.51820235163825      9.88479643309250      2.13183007265793
C      2.93897002448102      5.80234039852265      0.99266436014885
C      3.22163291603248      4.42617167281352      1.08106976936983
H      2.41753091721533      3.71387792414380      0.94693449633693
.
.
.
H      3.31486723296830      8.06978047771496      3.81341544613296
H      2.80887077200594      8.92504045306826      5.29405513411201
H      4.21854137172579      9.47235397735990      4.37493688551659
*
```

Input file for the $\mathbf{D^{ox}}$ state:

```
!TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2
```

```
!CPCM
%cpcm smd true
SMDsolvent "DICHLOROMETHANE"
surfacetype gepol_ses
rsolv 2.33
radius[1] 1.250
radius[6] 2.000
radius[7] 1.600
radius[29] 1.748
end

* xyz 2 2
Cu     3.81080208108758      8.75271149460812      1.02539382047211
N      3.94009921789056      6.75620521048136      0.88367367431585
N      5.68679183273613      8.61262607642444      1.70013139646962
N      2.77362342342012      9.49762691641693     -0.51167644551542
N      2.76085499924761     10.08280511105058      2.10043302301560
C      3.00597114509435      5.87113254008780      0.52522630254695
C      3.29183008917623      4.49036411089094      0.55316206040174
.
.
.
H      4.02519646125763      8.59920785297405      3.79768892839755
H      3.18960114949372      9.24054981033882      5.22458972696069
H      4.56237356601734     10.10983624215874      4.55228276923024
*
```

Table S7 collects all the data that was extracted from the corresponding output files of the previous calculations for **S_0**, **T_1**, **D^{ox}**, and **D^{red}** states of complexes **1**-**9**

Table S7. DFT calculated energies of the **S_0**, **T_1**, **D^{ox}**, and **D^{red}** states of complexes **1**-**9**. Values are reported in kcal/mol

Complex	State	E^{gas}	$G^{0,gas}$	E^{gas}	E^{sol} - DCM
		TPSSh-D3/ def2-TZVP(-f)	TPSSh-D3/ def2-TZVP(-f)	TPSSh-D3/ def2-TZVP	TPSSh-D3/ def2-TZVP
1	**S_0**	–1747124.69	–1746939.01	–1747144.01	–1747189.47
	T_1	–1747092.46	–1746907.12	–1747112.35	–1747158.72
	D^{ox}	–1746919.55	–1746731.98	–1746939.34	–1747073.26
	D^{red}	–1747212.23	–1747030.71	–1747231.71	–1747250.57
2	**S_0**	–1845879.60	–1845630.58	–1845900.56	–1845946.38
	T_1	–1845838.47	–1845589.44	–1845859.92	–1845905.45
	D^{ox}	–1845672.98	–1845422.10	–1845694.29	–1845822.55
	D^{red}	–1845965.16	–1845719.78	–1845986.30	–1846005.67
3	**S_0**	–2883912.94	–2883413.17	–2883950.70	–2884000.70
	T_1	–2883857.30	–2883359.80	–2883895.52	–2883945.57
	D^{ox}	–2883713.37	–2883213.50	–2883751.26	–2883869.35
	D^{red}	–2883990.80	–2883494.68	–2884028.89	–2884057.72
4	**S_0**	–2735806.50	–2735409.32	–2735842.14	–2735893.19
	T_1	–2735759.48	–2735363.93	–2735795.53	–2735846.65

	D^{ox}	–2735610.19	–2735212.23	–2735645.98	–2735766.98
	D^{red}	–2735888.42	–2735494.61	–2735924.35	–2735953.29
5	**S_0**	–2785182.58	–2784752.16	–2785219.03	–2785269.96
	T_1	–2785129.66	–2784701.12	–2785166.44	–2785217.51
	D^{ox}	–2784985.75	–2784554.86	–2785022.34	–2785142.04
	D^{red}	–2785261.82	–2784834.93	–2785298.57	–2785327.55
6	**S_0**	–2043344.39	–2042958.87	–2043368.00	–2043413.27
	T_1	–2043300.21	–2042916.72	–2043325.87	–2043371.05
	D^{ox}	–2043141.53	–2042754.02	–2043165.47	–2043287.88
	D^{red}	–2043428.04	–2043045.30	–2043451.84	–2043471.98
7	**S_0**	–1987862.74	–1987520.20	–1987888.12	–1987933.72
	T_1	–1987828.59	–1987486.26	–1987854.64	–1987902.67
	D^{ox}	–1987678.92	–1987333.38	–1987704.72	–1987829.82
	D^{red}	–1987940.52	–1987602.16	–1987965.99	–1987986.74
8	**S_0**	–2037239.93	–2036865.27	–2037266.12	–2037310.57
	T_1	–2037200.31	–2036825.96	–2037227.06	–2037273.58
	D^{ox}	–2037054.62	–2036677.10	–2037081.13	–2037204.41
	D^{red}	–2037315.44	–2036944.35	–2037341.69	–2037361.24
9	**S_0**	–2135961.72	–2135517.43	–2135989.21	–2136033.88
	T_1	–2135920.04	–2135476.84	–2135948.08	–2135993.94
	D^{ox}	–2135776.79	–2135330.24	–2135804.57	–2135925.49
	D^{red}	–2136035.29	–2135595.27	–2136062.90	–2136083.86

The solutions state reaction Gibbs free energies and reduction potentials of the different electron transfer events of the photoredox cycle $\mathbf{D^{ox}} \rightarrow \mathbf{S_0}$ (E^0_{ox}), $\mathbf{S_0} \rightarrow \mathbf{D^{red}}$ (E^0_{red}), $\mathbf{D^{ox}} \rightarrow \mathbf{T_1}$ ($^*E^0_{ox}$), and $\mathbf{T_1} \rightarrow \mathbf{D^{red}}$ ($^*E^0_{red}$) can be calculated from the values reported in Table S7 using equations 1-6. For consistency, the calculations are always performed in the direction of reduction (i.e., $\mathbf{D^{ox}} \rightarrow \mathbf{T_1}$), even though ligand-centered redox processes of the cycle take place in the direction of oxidation. The results of the calculations are provided in Table S8.

Since generally single point calculations are performed with more sophisticated levels of theory than optimizations and frequency calculations (in our case, we only refined the basis set), a correction to $G^{0,gas}$ needs to be computed for each species to account for the differences in the levels of theory of $G^{0,gas}$ and E^{gas}, E^{sol} values obtained from single point calculations. The corrected $G^{0,gas}$ can be calculated using equations 7 and 8. $G^{0,gas}_{LT1}$ and E^{gas}_{LT1} correspond to the gas phase electronic energy and Gibbs free energy at the TPSSh-D3/def2-TZVP(-f) level, respectively. $G^{0,gas}_{LT2}$ is the corrected gas phase Gibbs free energy at the TPSSh-D3/def2-TZVP level of theory, and G_{corr} is the correction factor.

$$G^{0,gas}_{LT2} = G^{0,gas}_{LT1} + G_{corr} \quad (7)$$

$$G_{corr} = G^{0,gas}_{LT1} - E^{gas}_{LT1} \quad (8)$$

Table S8. Calculated values for the application of the Born Haber cycle for computing reduction potentials of the redox events of the photoredox cycle of complexes **1-9**. E^0 values are computed in DCM and referenced to the standard calomel electrode (SCE)

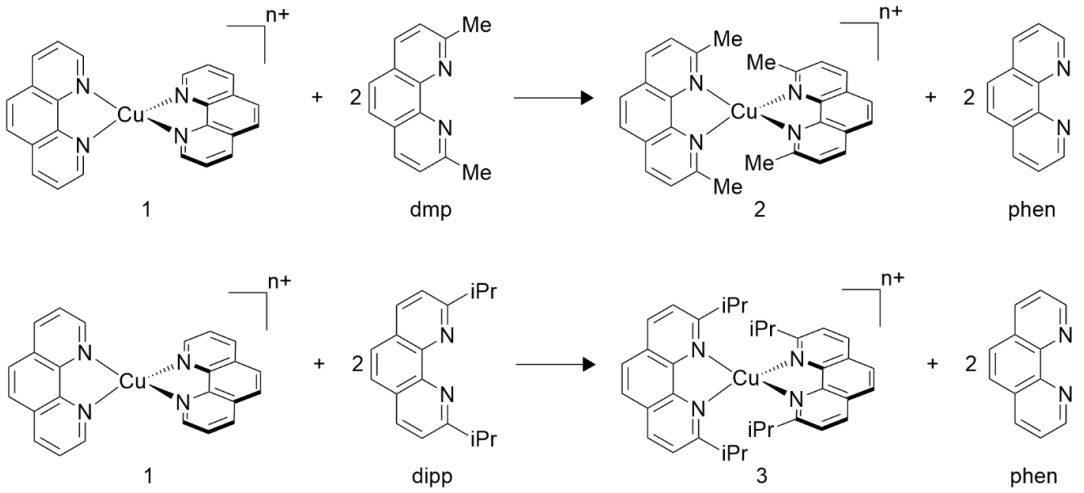
Complex	Redox event	$\Delta G^{0,gas}(A/A^-)$ (kcal/mol)	$\Delta G^0_{solv}(A)$ (kcal/mol)	$\Delta G^0_{solv}(A^-)$ (kcal/mol)	$\Delta G^{0,sol}$ (A/A^-) (kcal/mol)	$E^0_{1/2}$ (A/A^-) (V)	E^0 (V)
1	$D^{ox} \rightarrow S_0$ $(\mathbf{E^0_{ox}})$	–206.56	–133.92	–45.46	–118.10	5.12	0.69
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–91.86	–45.46	–18.86	–65.26	2.83	–1.60
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–175.24	–133.92	–46.37	–87.69	3.80	–0.63
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–123.18	–46.37	–18.86	–95.67	4.15	–0.28
2	$D^{ox} \rightarrow S_0$ (E^0_{ox})	–208.13	–128.26	–45.82	–125.69	5.45	1.02
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–89.38	–45.82	–19.37	–62.93	2.73	–1.70
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–167.48	–128.26	–45.53	–84.75	3.68	–0.75
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–130.03	–45.53	–19.37	–103.87	4.50	0.08
3	$D^{ox} \rightarrow S_0$ $(\mathbf{E^0_{ox}})$	–204.52	–122.41	–45.27	–127.38	5.52	1.09
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–86.62	–45.27	–20.14	–61.49	2.67	–1.76
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–164.42	–122.41	–45.18	–87.19	3.78	–0.65
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–126.72	–45.18	–20.14	–101.68	4.41	–0.02
4	$D^{ox} \rightarrow S_0$ $(\mathbf{E^0_{ox}})$	–196.94	–121.00	–51.05	–126.99	5.51	1.08
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–85.58	–51.05	–28.94	–63.47	2.75	–1.68
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–151.96	–121.00	–51.12	–82.08	3.56	–0.87
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–130.56	–51.12	–28.94	–108.38	4.70	0.27
5	$D^{ox} \rightarrow S_0$ $(\mathbf{E^0_{ox}})$	–197.16	–119.70	–50.93	–128.39	5.57	1.14
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–83.07	–50.93	–28.98	–61.12	2.65	–1.78
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–146.45	–119.70	–51.07	–77.82	3.37	–1.05
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–133.78	–51.07	–28.98	–111.69	4.84	0.41
6	$D^{ox} \rightarrow S_0$ $(\mathbf{E^0_{ox}})$	–199.54	–118.09	–50.00	–131.45	5.70	1.27
	$S_0 \rightarrow D^{red}$ $(\mathbf{E^0_{red}})$	–81.84	–50.00	–28.83	–60.67	2.63	–1.80
	$D^{ox} \rightarrow T_1$ $(^*\mathbf{E^0_{ox}})$	–146.63	–118.09	–50.05	–78.59	3.41	–1.02
	$T_1 \rightarrow D^{red}$ $(^*\mathbf{E^0_{red}})$	–134.75	–50.05	–28.83	–113.53	4.92	0.49

7	$D^{ox} \rightarrow S_0$ ($\mathbf{E^0_{ox}}$)	–186.40	–125.10	–45.60	–106.90	4.64	0.21
	$S_0 \rightarrow D^{red}$ ($\mathbf{E^0_{red}}$)	–82.05	–45.60	–20.75	–57.20	2.48	–1.95
	$D^{ox} \rightarrow T_1$ ($\mathbf{^*E^0_{ox}}$)	–153.13	–125.10	–48.03	–76.06	3.30	–1.13
	$T_1 \rightarrow D^{red}$ ($\mathbf{^*E^0_{red}}$)	–115.32	–48.03	–20.75	–88.04	3.82	–0.61
8	$D^{ox} \rightarrow S_0$ ($\mathbf{E^0_{ox}}$)	–187.85	–123.28	–44.45	–109.02	4.73	0.30
	$S_0 \rightarrow D^{red}$ (E^0_{red})	–79.14	–44.45	–19.55	–54.24	2.35	–2.08
	$D^{ox} \rightarrow T_1$ ($^*E^0_{ox}$)	–149.10	–123.28	–46.52	–72.34	3.14	–1.29
	$T_1 \rightarrow D^{red}$ ($^*E^0_{red}$)	–117.89	–46.52	–19.55	–90.92	3.94	–0.49
9	$D^{ox} \rightarrow S_0$ (E^0_{ox})	–186.90	–120.92	–44.67	–110.65	4.80	0.37
	$S_0 \rightarrow D^{red}$ (E^0_{red})	–77.96	–44.67	–20.96	–54.25	2.35	–2.08
	$D^{ox} \rightarrow T_1$ ($^*E^0_{ox}$)	–146.86	–120.92	–45.86	–71.80	3.11	–1.32
	$T_1 \rightarrow D^{red}$ ($^*E^0_{red}$)	–118.00	–45.86	–20.96	–93.10	4.04	–0.39

The same procedure was followed to calculate the reduction potentials of complexes **2**, **3**, **7**, and **8** in MeCN for validation purposes (see Table S6).

5. Homodesmotic reactions

Homodesmotic reactions in DCM were employed, using complex **1** as a reference, to quantify the stabilization/destabilization effect of the substitution of H for −CH_3 or −i-Pr in the 2,9 positions of the phenanthroline redox-active ligand in both $\mathbf{S_0}$ and $\mathbf{D^{ox}}$ states of complexes **1**-**3**. As shown in Scheme S1, to calculate the homodesmotic stabilization energies (HSE) of complex **2** and **3** vs. **1**, the solution state energies of $\mathbf{S_0}$ and $\mathbf{D^{ox}}$ states (see Table S7), as well as the energies of the free ligands, are required. Optimization, frequencies, and single-point calculations to obtain the solution state electronic energy of the free ligands were carried out at the TPSSh-D3/def2-TZVP level of theory.



Scheme S1. Homodesmotic reactions to evaluate the homodesmotic stabilization energies (HSE) for the substitution of H for −CH_3 or −i-Pr in the 2,9 positions of the phenanthroline redox-active ligand in both $\mathbf{S_0}$ (n=1) and $\mathbf{D^{ox}}$ (n=2) states of complexes **1**-**3**.

Table S9 compiles the solution state electronic energy of the complexes and the free ligands used for the calculation of homodesmotic reactions.

Table S9. DFT calculated solution state electronic energies in DCM of the $\mathbf{S_0}$ and $\mathbf{D^{ox}}$ states of complexes **1-3** together with the E^{sol} values of the free ligands. Values are reported in kcal/mol

Complex	State	E^{sol}
$\mathbf{[Cu(phen)_2]^+}$ **(1)**	$\mathbf{S_0}$	–1747189.47
	$\mathbf{D^{ox}}$	–1747073.26
$\mathbf{[Cu(dmp)_2]^+}$ **(2)**	$\mathbf{S_0}$	–1845946.38
	$\mathbf{D^{ox}}$	–1845822.55
$\mathbf{[Cu(dipp)_2]^+}$ **(3)**	$\mathbf{S_0}$	–2043413.27
	$\mathbf{D^{ox}}$	–2043287.88
phen	–	–358876.80
dmp	–	–408250.70
dipp	–	–506982.02

The resulting HSE values are provided in Table S10.

Table S10. Calculated homodesmotic stabilization energies (HSE) in DCM

$[Cu(phen)_2]^{n+}$ + 2 dmp → $[Cu(dmp)_2]^{n+}$ + 2 phen:		
State	**HSE (kcal/mol)**	**HSE (eV)**
D^{ox} (n = 2)	–1.50	–0.07
S_0 (n = 1)	–9.13	–0.40
$[Cu(phen)_2]^{n+}$ + 2 dipp → $[Cu(dipp)_2]^{n+}$ + 2 phen:		
State	**HSE (kcal/mol)**	**HSE (eV)**
D^{ox} (n = 2)	–4.19	–0.18
S_0 (n = 1)	–13.37	–0.58

Figure S4 provides a depiction of the relative stability of the S_0 and D^{ox} states of complexes **1**-**3** in DCM based on the HSE values, showcasing the overall effect of substituting H for $-CH_3$ or –i-Pr on the thermodynamic driving force of the reduction processes.

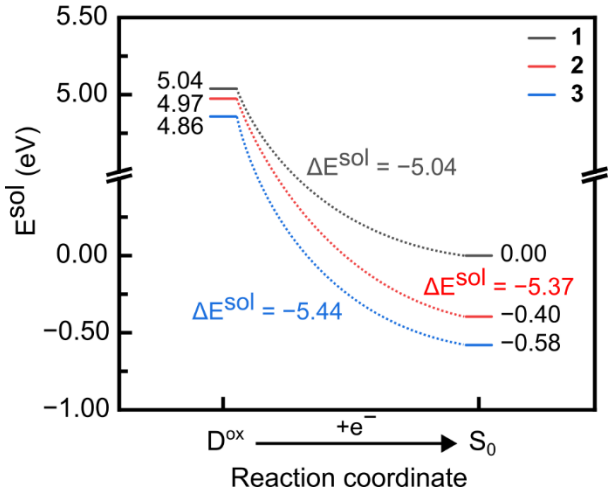


Figure S4. Effect of substituting H for $-CH_3$ and –i-Pr on the thermodynamic driving force of the ground state metal centered $D^{ox} \rightarrow S_0$ redox process of complexes **1**-**3**

6. Calculated structural metrics

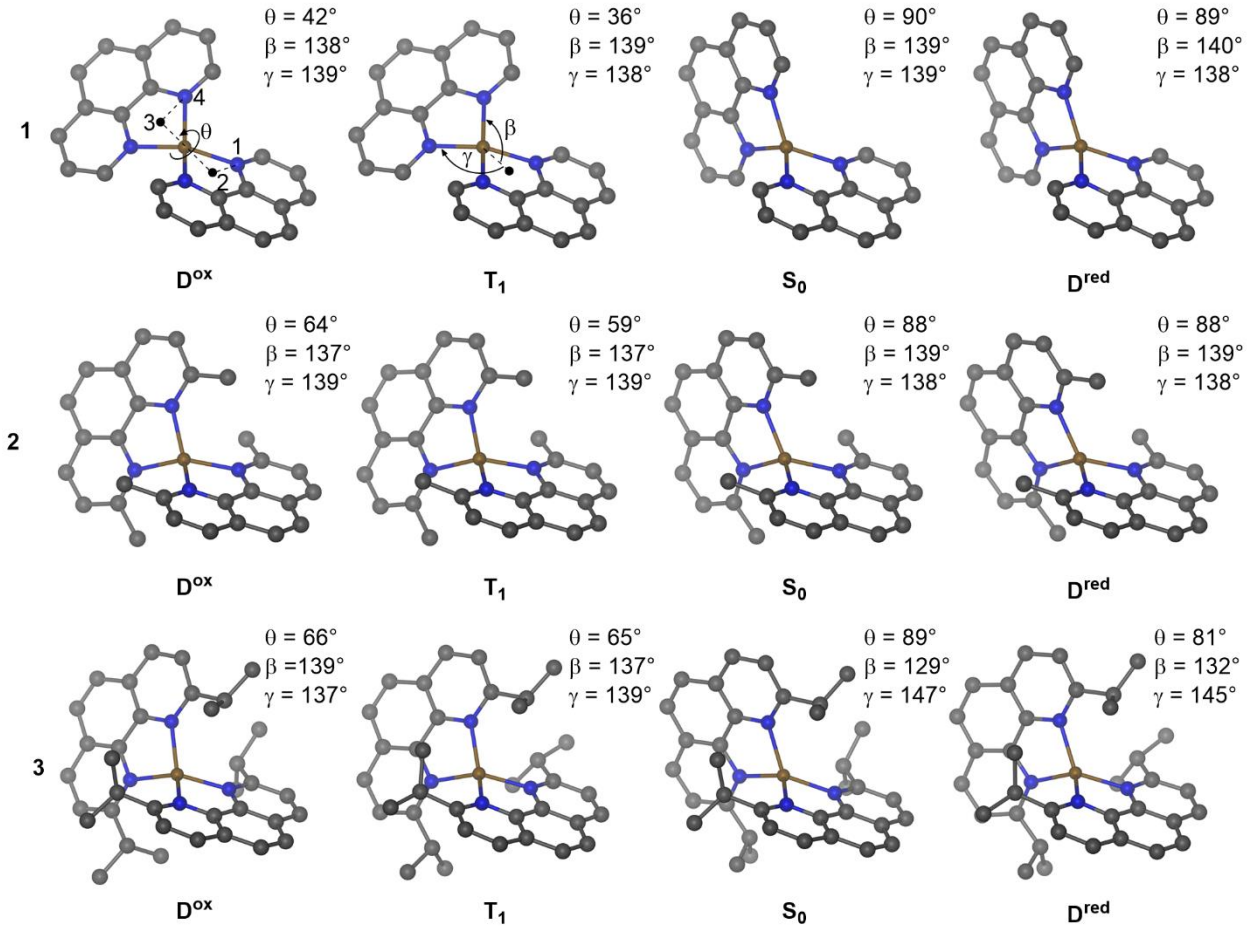


Figure S5. Computed equilibrium structures at the $\mathbf{S_0}$, $\mathbf{T_1}$, $\mathbf{D^{ox}}$, and $\mathbf{D^{red}}$ states of complexes **1**, **2,** and **3**. The angles Θ, β, and γ (°) that characterize the first coordination sphere of the metal complexes are provided.

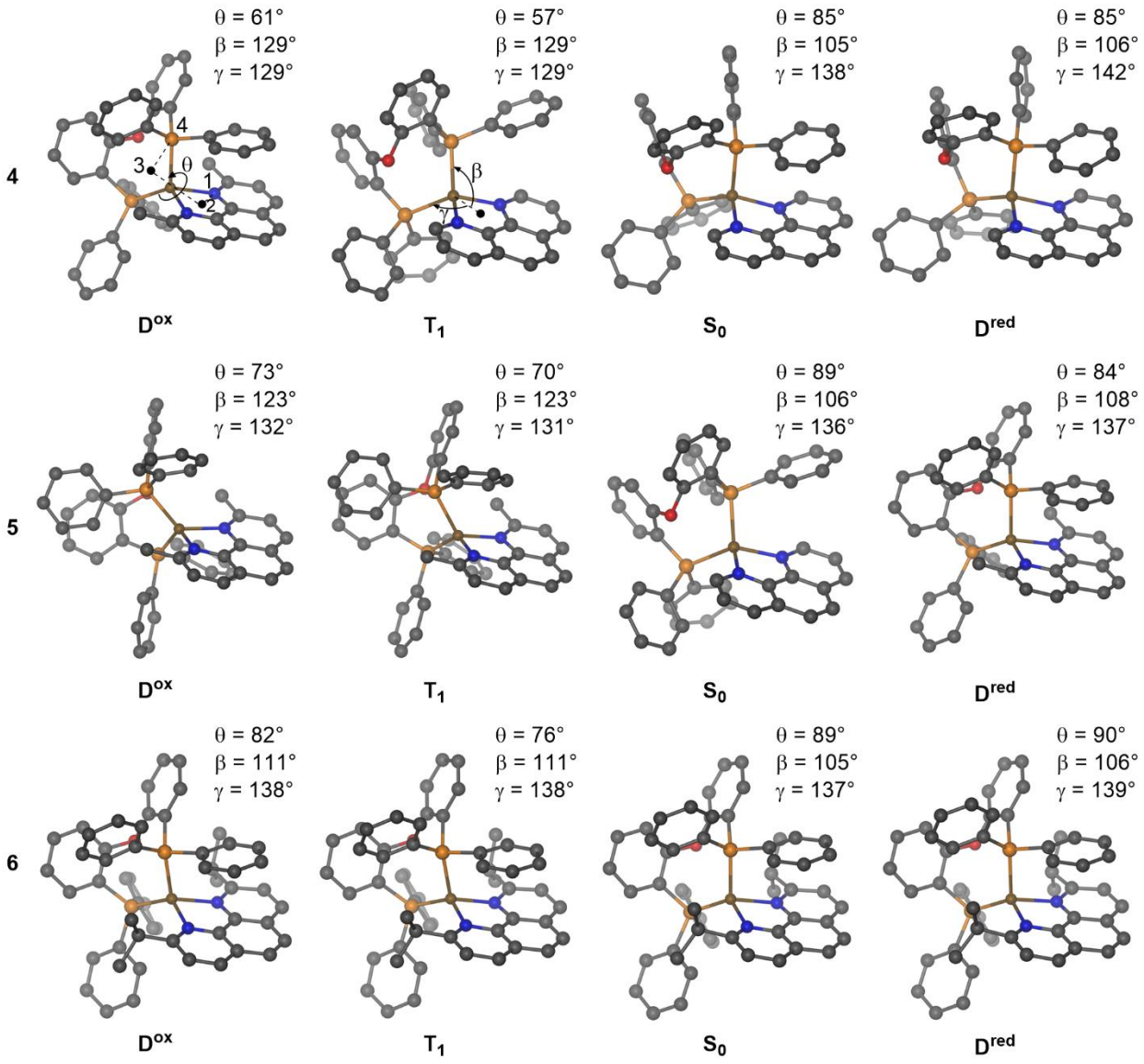


Figure S6. Computed equilibrium structures at the S_0, T_1, D^{ox}, and D^{red} states of complexes **4**, **5,** and **6**. The angles Θ, β, and γ (°) that characterize the first coordination sphere of the metal complexes are provided

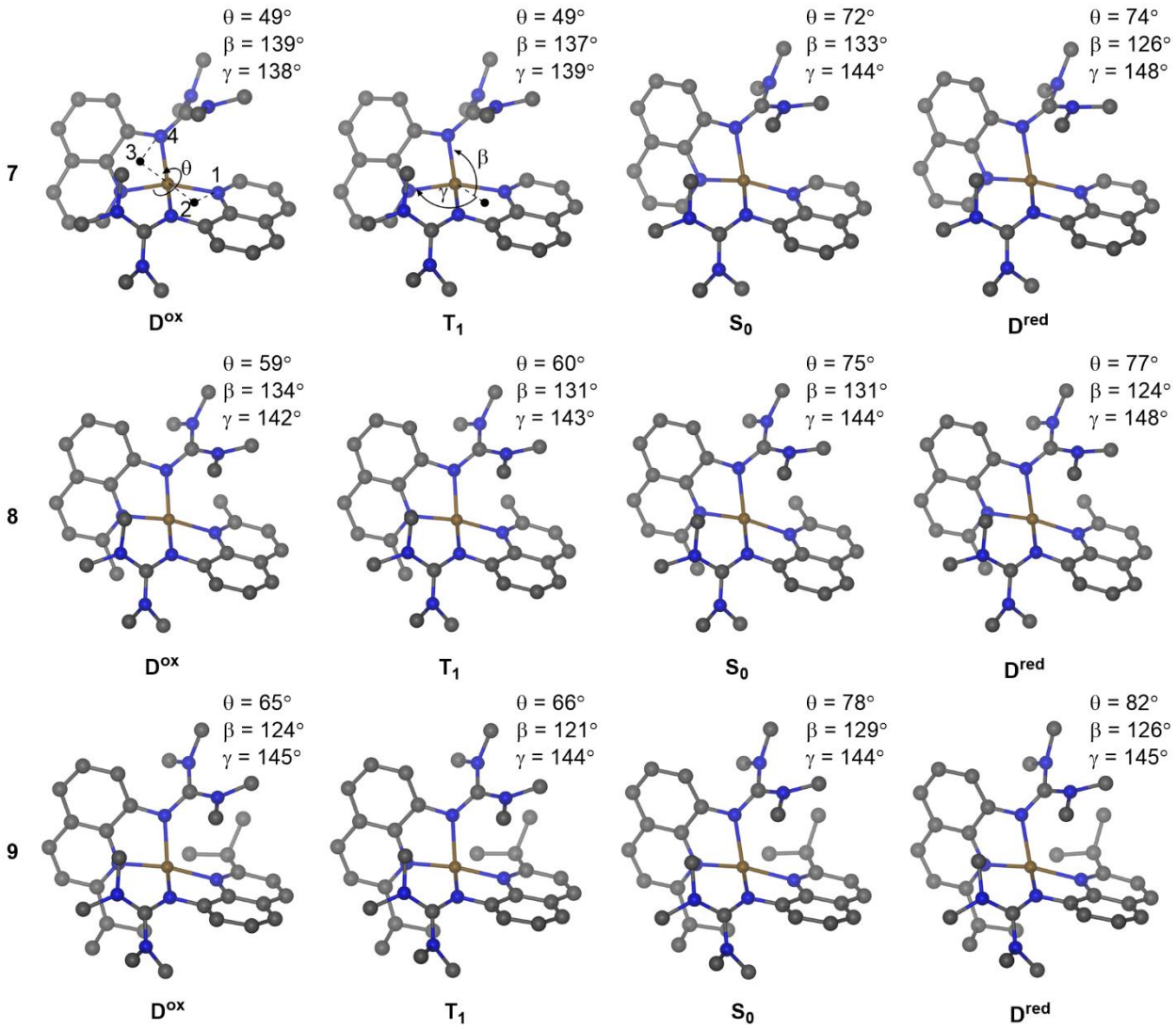


Figure S7. Computed equilibrium structures at the $\mathbf{S_0}$, $\mathbf{T_1}$, $\mathbf{D^{ox}}$, and $\mathbf{D^{red}}$ states of complexes **7**, **8,** and **9**. The angles Θ, β, and γ (°) that characterize the first coordination sphere of the metal complexes are provided.

Table S11. Compilation of structural metrics for the equilibrium geometries of the S_0, T_1, D^{ox}, and D^{red} states for complexes **1-9**. d_{Cu-N} and d_{Cu-P} correspond to the average Cu–N and Cu–P distances in Å. Angles Θ, β, and γ are provided in degrees

Complex	**1**				**2**				**3**			
State	d_{Cu-N}	**Θ**	**β**	**γ**	d_{Cu-N}	**Θ**	**β**	**γ**	d_{Cu-N}	**Θ**	**β**	**γ**
S_0	2.028	90	139	139	2.026	88	138	139	2.031	89	129	147
T_1	1.982	36	139	138	1.985	59	137	139	1.998	65	137	139
D^{ox}	1.997	42	139	138	2.003	64	137	139	2.007	66	139	137
D^{red}	2.022	89	140	137	2.019	88	139	138	2.023	81	132	145
Complex	**4**				**5**				**6**			
State	d_{Cu-N} / d_{Cu-P}	**Θ**	**β**	**γ**	d_{Cu-N} / d_{Cu-P}	**Θ**	**β**	**γ**	d_{Cu-N} / d_{Cu-P}	**Θ**	**β**	**γ**
S_0	2.061 / 2.248	85	105	138	2.074 / 2.258	89	106	136	2.085 / 2.269	89	105	137
T_1	1.975 / 2.315	57	129	129	1.995 / 2.330	70	123	131	1.995 / 2.346	76	111	138
D^{ox}	2.043 / 2.297	61	129	129	2.073 / 2.308	73	123	132	2.073 / 2.317	82	111	138
D^{red}	2.029 / 2.244	85	106	142	2.032 / 2.249	84	108	137	2.042 / 2.263	90	106	139
Complex	**7**				**8**				**9**			
State	d_{Cu-N}	**Θ**	**β**	**γ**	d_{Cu-N}	**Θ**	**β**	**γ**	d_{Cu-N}	**Θ**	**β**	**γ**
S_0	2.036	72	133	144	2.044	75	131	144	2.072	78	129	144
T_1	1.969	49	137	139	1.985	60	131	143	2.003	66	121	144
D^{ox}	1.981	49	139	138	1.993	59	134	142	2.011	65	124	145
D^{red}	2.041	74	126	148	2.053	77	124	148	2.069	82	126	145

Table S12. Dihedral angles change (ΔΘ) upon each one of the redox events of the photoredox cycle for complexes **1-9**

PC	$\lvert\Delta\Theta\rvert$ ($D^{ox} \rightarrow S_0$)	$\lvert\Delta\Theta\rvert$ ($S_0 \rightarrow D^{red}$)	$\lvert\Delta\Theta\rvert$ ($D^{ox} \rightarrow T_1$)	$\lvert\Delta\Theta\rvert$ ($T_1 \rightarrow D^{red}$)
1	48.41	0.95	5.62	53.08
2	24.33	0.17	4.37	28.87
3	22.52	7.99	1.39	15.93
4	23.66	0.19	3.92	27.77
5	16.17	5.54	2.78	13.41
6	7.67	0.45	5.44	13.56
7	23.70	1.85	0.02	25.53
8	15.69	2.44	1.21	16.92
9	13.19	3.11	0.29	16.01

7. Theoretical square schemes

For an A/A^- redox couple, the contributions of vertical electron transfer (ET) and structural relaxation (SR) were estimated following equations 9 and 10, respectively. Where $E^{sol}(A_{(A)})$ represents the solution state energy of species A, $E^{sol}(A^-_{(A)})$ is the solution state energy of compound A^- and $E^{sol}(A^-_{(A)})$ is the solution state energy of a nonequilibrium structure with the charge and multiplicity of A^- and the geometry of A. E^{sol} values were calculated through single-point calculations on the respective geometry at the TPSSh-D3/def2-TZVP level of theory.

$$EA = E^{sol}(A^-_{(A)}) - E^{sol}(A_{(A)}) \quad (9)$$

$$SR = E^{sol}(A^-_{(A)}) - E^{sol}(A^-_{(A)}) \quad (10)$$

Let us use the $\mathbf{D^{ox} \rightarrow S_0}$ redox event of complex **2** as a tutorial example. In this case, $E^{sol}(A_{(A)})$ and $E^{sol}(A^-_{(A)})$ correspond to the solution state energies of the $\mathbf{D^{ox}}$ and $\mathbf{S_0}$ states, respectively. These values are obtained as indicated in section S1.1 (see input files specified before). A single-point calculation is required to compute $E^{sol}(A^-_{(A)})$. For the $\mathbf{D^{ox} \rightarrow S_0}$ redox event, this corresponds to computing the solution state energy on the geometry of $\mathbf{D^{ox}}$ and the charge and multiplicity of the $\mathbf{S_0}$ state using the following input file (The lines for controlling the RAM allocation (%maxcore) and processors (%pal) are omitted for simplicity).

```
! TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

!CPCM
%cpcm smd true
SMDsolvent "DICHLOROMETHANE"
surfacetype gepol_ses
rsolv 2.33
radius[1] 1.250
radius[6] 2.000
radius[7] 1.600
radius[29] 1.748
end

* xyz 1 1
Cu   3.81080208108758      8.75271149460812      1.02539382047211
N     3.94009921789056      6.75620521048136      0.88367367431585
N     5.68679183273613      8.61262607642444      1.70013139646962
N     2.77362342342012      9.49762691641693     -0.51167644551542
N     2.76085499924761     10.08280511105058     2.10043302301560
C     3.00597114509435      5.87113254008780      0.52522630254695
C     3.29183008917623      4.49036411089094      0.55316206040174
.
.
.
H     4.02519646125763      8.59920785297405      3.79768892839755
H     3.18960114949372      9.24054981033882      5.22458972696069
H     4.56237356601734     10.10983624215874     4.55228276923024
*
```

Table S13 compiles the resulting energies and the calculated vertical electron transfer (ET) and structural relaxation (SR) contributions to the driving force of the reduction process.

Table S13. Solution state energies and energy decomposition for the redox events of the photoredox cycle of complexes **1**-**9** into vertical electron attachment (EA) and structural relaxation (SR) steps. Energies are calculated in DCM and provided in kcal/mol

Complex	Redox event	$E^{sol}(A_{(A)})$	$E^{sol}(A^{-}_{(A-)})$	$E^{sol}(A^{-}_{(A)})$	EA	SR
1	$D^{ox} \rightarrow S_0$	–1747073.26	–1747189.47	–1747180.08	–106.82	–9.39
	$S_0 \rightarrow D^{red}$	–1747189.47	–1747250.57	–1747248.88	–59.41	–1.69
	$D^{ox} \rightarrow T_1$	–1747073.26	–1747158.72	–1747157.00	–83.74	–1.72
	$T_1 \rightarrow D^{red}$	–1747158.72	–1747250.57	–1747240.81	–82.09	–9.76
2	$D^{ox} \rightarrow S_0$	–1845822.55	–1845946.38	–1845939.981	–117.43	–6.40
	$S_0 \rightarrow D^{red}$	–1845946.38	–1846005.67	–1846003.748	–57.37	–1.92
	$D^{ox} \rightarrow T_1$	–1845822.55	–1845905.45	–1845903.076	–80.53	–2.37
	$T_1 \rightarrow D^{red}$	–1845905.45	–1846005.67	–1845996.841	–91.39	–8.83
3	$D^{ox} \rightarrow S_0$	–2043287.88	–2043413.27	–2043407.878	–120.00	–5.39
	$S_0 \rightarrow D^{red}$	–2043413.27	–2043471.98	–2043470.16	–56.89	–1.82
	$D^{ox} \rightarrow T_1$	–2043287.88	–2043371.05	–2043369.433	–81.55	–1.62
	$T_1 \rightarrow D^{red}$	–2043371.05	–2043471.98	–2043467.059	–96.01	–4.92
4	$D^{ox} \rightarrow S_0$	–2735766.98	–2735893.19	–2735883.744	–116.76	–9.45
	$S_0 \rightarrow D^{red}$	–2735893.19	–2735953.29	–2735949.911	–56.72	–3.38
	$D^{ox} \rightarrow T_1$	–2735766.98	–2735846.65	–2735842.715	–75.73	–3.94
	$T_1 \rightarrow D^{red}$	–2735846.65	–2735953.29	–2735941.594	–94.94	–11.70
5	$D^{ox} \rightarrow S_0$	–2785142.04	–2785269.96	–2785263.333	–121.29	–6.63
	$S_0 \rightarrow D^{red}$	–2785269.96	–2785327.55	–2785324.152	–54.19	–3.40
	$D^{ox} \rightarrow T_1$	–2785142.04	–2785217.51	–2785213.462	–71.42	–4.05
	$T_1 \rightarrow D^{red}$	–2785217.51	–2785327.55	–2785321.194	–103.68	–6.36
6	$D^{ox} \rightarrow S_0$	–2883869.35	–2884000.70	–2883995.525	–126.18	–5.17
	$S_0 \rightarrow D^{red}$	–2884000.70	–2884057.72	–2884054.361	–53.66	–3.36
	$D^{ox} \rightarrow T_1$	–2883869.35	–2883945.57	–2883940.534	–71.18	–5.04
	$T_1 \rightarrow D^{red}$	–2883945.57	–2884057.72	–2884051.026	–105.46	–6.69
7	$D^{ox} \rightarrow S_0$	–1987829.82	–1987933.72	–1987926.478	–96.66	–7.24
	$S_0 \rightarrow D^{red}$	–1987933.72	–1987986.74	–1987985.924	–52.20	–0.82
	$D^{ox} \rightarrow T_1$	–1987829.82	–1987902.67	–1987901.07	–71.25	–1.60
	$T_1 \rightarrow D^{red}$	–1987902.67	–1987986.74	–1987979.953	–77.28	–6.79
8	$D^{ox} \rightarrow S_0$	–2037204.41	–2037310.57	–2037305.528	–101.12	–5.04
	$S_0 \rightarrow D^{red}$	–2037310.57	–2037361.24	–2037359.767	–49.20	–1.47
	$D^{ox} \rightarrow T_1$	–2037204.41	–2037273.58	–2037271.86	–67.45	–1.72
	$T_1 \rightarrow D^{red}$	–2037273.58	–2037361.24	–2037355.86	–82.28	–5.38
9	$D^{ox} \rightarrow S_0$	–2135925.49	–2136033.88	–2136028.83	–103.34	–5.05
	$S_0 \rightarrow D^{red}$	–2136033.88	–2136083.86	–2136082.49	–48.61	–1.37

$\mathbf{D^{ox} \rightarrow T_1}$	–2135925.49	–2135993.94	–2135992.40	–66.91	–1.54
$\mathbf{T_1 \rightarrow D^{red}}$	–2135993.94	–2136083.86	–2136077.32	–83.38	–6.54

Figure S8 shows the theoretical square scheme for the $\mathbf{T_1 \rightarrow D^{red}}$ process. A similar protocol to the one shown before can be employed to build the theoretical square schemes for this reduction process as well as the ligand-centered reductions $\mathbf{D^{ox} \rightarrow T_1}$ and $\mathbf{S_0 \rightarrow D^{red}}$. Note that for all calculations reported herein, the analyses are always carried out in the reduction direction.

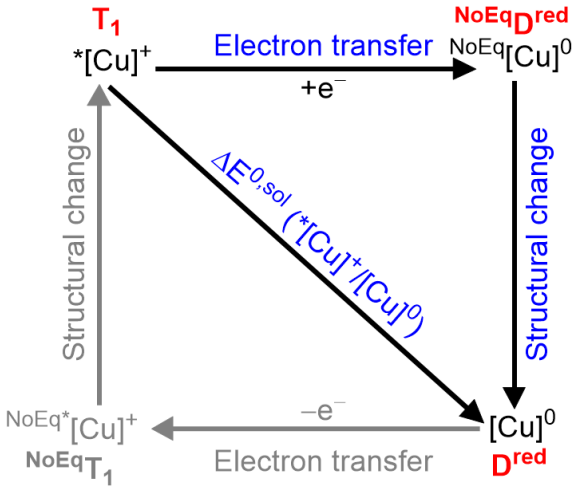


Figure S8. Theoretical square scheme that was implemented to separate the redox events of the photoredox cycle into vertical electron transfer (ET) and structural relaxation (SR) steps. The picture exemplifies the separation for the excited state metal-centered *[Cu(II)]$^{+}$ ($\mathbf{T_1}$) → [Cu(I)]^{0} ($\mathbf{D^{red}}$) reduction. ^{NoEq}[Cu]^{0} denotes a non-equilibrium structure with the geometry of *[Cu(II)]$^{+}$

8. Internal reorganization energies for the electron self-exchange reaction

Internal reorganization energies (λ_T) for the electron self-exchange reaction were calculated in DCM using Nelsen's four-point method (Figure S9) at the =TPSSh-D3/def2-TZVP level of theory. The total internal reorganization energy is the sum of the individual reorganization energies (λ_i) of the oxidized (A) and reduced (A^-) species (equations 11-13).

$$\lambda_T = \lambda_A + \lambda_{A^-} \quad (11)$$

$$\lambda_A = E^{sol}(A_{(A^-)}) - E^{sol}(A_{(A)}) \quad (12)$$

$$\lambda_{A^-} = E^{sol}(A^-_{(A)}) - E^{sol}(A^-_{(A^-)}) \quad (13)$$

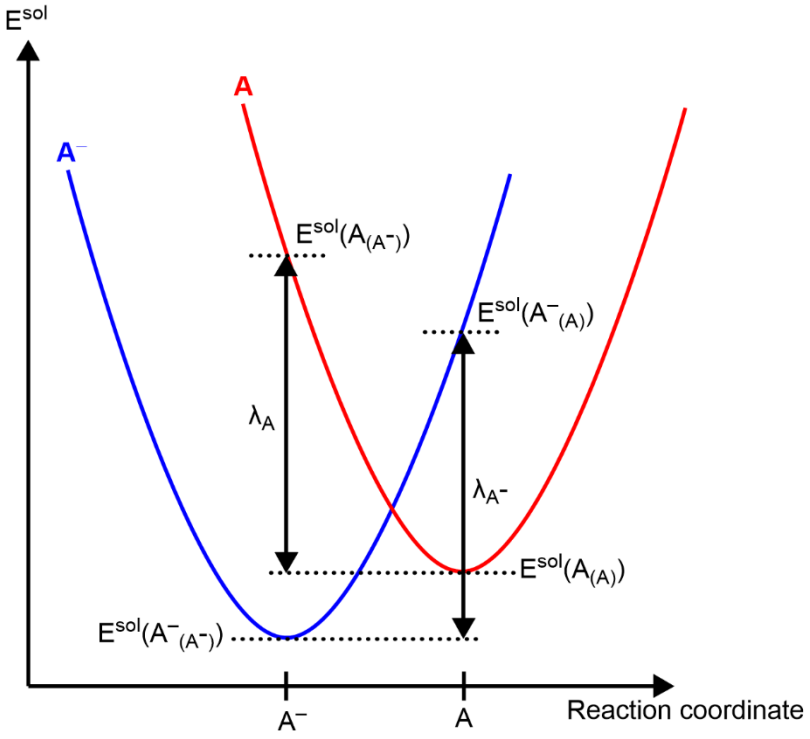


Figure S9. Representation of Nelsen's four-point method for the calculation of the internal reorganization energies (λ_i) of the oxidized (A) and reduced (A^-) species in the context of an electron self-exchange reaction

Again, for the $\mathbf{D^{ox}} \rightarrow \mathbf{S_0}$ redox event of complex **2**, $E^{sol}(A_{(A)})$ and $E^{sol}(A^-_{(A^-)})$ are the solution state energies of the $\mathbf{D^{ox}}$ and $\mathbf{S_0}$ states, respectively (*vide supra*). $E^{sol}(A^-_{(A)})$ and $E^{sol}(A_{(A^-)})$ are calculated with single-point calculations using the provided inputs (The lines for controlling the RAM allocation (%maxcore) and processors (%pal) are omitted for simplicity). As mentioned above, $E^{sol}(A_{(A^-)})$ is the solution state energy of a non-equilibrium species with the geometry of $\mathbf{D^{ox}}$ and the charge and multiplicity of $\mathbf{S_0}$. Conversely, $E^{sol}(A^-_{(A)})$ corresponds to the non-equilibrium species with $\mathbf{S_0}$ geometry and the charge and multiplicity of $\mathbf{D^{ox}}$.

Input file to calculate $E^{sol}(A_{(A^-)})$

```
! TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

!CPCM
%cpcm smd true
SMDsolvent "DICHLOROMETHANE"
surfacetype gepol_ses
rsolv 2.33
radius[1] 1.250
radius[6] 2.000
radius[7] 1.600
radius[29] 1.748
end

* xyz 1 1
Cu    3.81080208108758      8.75271149460812      1.02539382047211
N     3.94009921789056      6.75620521048136      0.88367367431585
N     5.68679183273613      8.61262607642444      1.70013139646962
N     2.77362342342012      9.49762691641693     -0.51167644551542
N     2.76085499924761     10.08280511105058      2.10043302301560
C     3.00597114509435      5.87113254008780      0.52522630254695
C     3.29183008917623      4.49036411089094      0.55316206040174
.
.
.
H     4.02519646125763      8.59920785297405      3.79768892839755
H     3.18960114949372      9.24054981033882      5.22458972696069
H     4.56237356601734     10.10983624215874      4.55228276923024
*
```

Input file to calculate $E^{sol}(A^{-}_{(A)})$

```
! TPSSh def2-TZVP d3 TightSCF SlowConv RIJCOSX defgrid2

!CPCM
%cpcm smd true
SMDsolvent "DICHLOROMETHANE"
surfacetype gepol_ses
rsolv 2.33
radius[1] 1.250
radius[6] 2.000
radius[7] 1.600
radius[29] 1.748
end

* xyz 2 2
Cu    3.78618454890123      8.73585660105153      1.04731521051368
N     3.90208830350401      6.71293562409774      1.14666985784901
N     5.77051366583172      8.60757917889728      1.42773688549201
N     2.93747318909698      9.71983662178366     -0.50551149761289
N     2.51820235163825      9.88479643309250      2.13183007265793
C     2.93897002448102      5.80234039852265      0.99266436014885
C     3.22163291603248      4.42617167281352      1.08106976936983
H     2.41753091721533      3.71387792414380      0.94693449633693
.
```

```
.
.
H     3.31486723296830      8.06978047771496      3.81341544613296
H     2.80887077200594      8.92504045306826      5.29405513411201
H     4.21854137172579      9.47235397735990      4.37493688551659
*
```

Table S14 compiles the resulting energies and the calculated internal reorganization energies for the electron self-exchange reaction.

Table S14. Calculated internal reorganization energies (kcal/mol) for the electron self-exchange reaction of the redox events of the photoredox cycle of complexes **1**-**9**

Complex	Redox event	$E^{sol}(A_{(A)})$	$E^{sol}(A_{(A^-)})$	$E^{sol}(A^-_{(A^-)})$	$E^{sol}(A^-_{(A)})$	λ_A	λ_{A^-}	λ_T
1	$D^{ox} \rightarrow S_0$	–1747073.26	–1747056.30	–1747189.47	–1747180.08	16.96	9.39	26.35
	$S_0 \rightarrow D^{red}$	–1747189.47	–1747187.76	–1747250.57	–1747248.88	1.71	1.69	3.40
	$D^{ox} \rightarrow T_1$	–1747073.26	–1747071.66	–1747158.72	–1747157.00	1.60	1.72	3.32
	$T_1 \rightarrow D^{red}$	–1747158.72	–1747138.90	–1747250.57	–1747240.81	19.82	9.76	29.58
2	$D^{ox} \rightarrow S_0$	–1845822.55	–1845815.17	–1845946.38	–1845939.98	7.38	6.40	13.78
	$S_0 \rightarrow D^{red}$	–1845946.38	–1845944.55	–1846005.67	–1846003.75	1.83	1.92	3.75
	$D^{ox} \rightarrow T_1$	–1845822.55	–1845820.30	–1845905.45	–1845903.08	2.25	2.37	4.63
	$T_1 \rightarrow D^{red}$	–1845905.45	–1845895.93	–1846005.67	–1845996.84	9.52	8.83	18.34
3	$D^{ox} \rightarrow S_0$	–2043287.88	–2043280.86	–2043413.27	–2043407.88	7.02	5.39	12.41
	$S_0 \rightarrow D^{red}$	–2043413.27	–2043410.64	–2043471.98	–2043470.16	2.63	1.82	4.45
	$D^{ox} \rightarrow T_1$	–2043287.88	–2043286.15	–2043371.05	–2043369.43	1.73	1.62	3.35
	$T_1 \rightarrow D^{red}$	–2043371.05	–2043364.45	–2043471.98	–2043467.06	6.60	4.92	11.53
4	$D^{ox} \rightarrow S_0$	–2735766.98	–2735758.68	–2735893.19	–2735883.74	8.30	9.45	17.74
	$S_0 \rightarrow D^{red}$	–2735893.19	–2735889.54	–2735953.29	–2735949.91	3.65	3.38	7.03
	$D^{ox} \rightarrow T_1$	–2735766.98	–2735762.58	–2735846.65	–2735842.71	4.40	3.94	8.33
	$T_1 \rightarrow D^{red}$	–2735846.65	–2735835.81	–2735953.29	–2735941.59	10.84	11.70	22.54
5	$D^{ox} \rightarrow S_0$	–2785142.04	–2785134.18	–2785269.96	–2785263.33	7.86	6.63	14.49
	$S_0 \rightarrow D^{red}$	–2785269.96	–2785266.13	–2785327.55	–2785324.15	3.83	3.40	7.22
	$D^{ox} \rightarrow T_1$	–2785142.04	–2785135.67	–2785217.51	–2785213.46	6.37	4.05	10.42
	$T_1 \rightarrow D^{red}$	–2785217.51	–2785209.38	–2785327.55	–2785321.19	8.13	6.36	14.49
6	$D^{ox} \rightarrow S_0$	–2883869.35	–2883864.93	–2884000.70	–2883995.53	4.42	5.17	9.60
	$S_0 \rightarrow D^{red}$	–2884000.70	–2883997.12	–2884057.72	–2884054.36	3.58	3.36	6.94
	$D^{ox} \rightarrow T_1$	–2883869.35	–2883865.04	–2883945.57	–2883940.53	4.31	5.04	9.34
	$T_1 \rightarrow D^{red}$	–2883945.57	–2883939.99	–2884057.72	–2884051.03	5.58	6.69	12.28
7	$D^{ox} \rightarrow S_0$	–1987829.82	–1987820.24	–1987933.72	–1987926.48	9.58	7.24	16.82
	$S_0 \rightarrow D^{red}$	–1987933.72	–1987930.03	–1987986.74	–1987985.92	3.69	0.82	4.51
	$D^{ox} \rightarrow T_1$	–1987829.82	–1987827.66	–1987902.67	–1987901.07	2.16	1.60	3.76

	$T_1 \rightarrow D^{red}$	–1987902.67	–1987889.78	–1987986.74	–1987979.95	12.89	6.79	19.67
8	$D^{ox} \rightarrow S_0$	–2037204.41	–2037196.71	–2037310.57	–2037305.53	7.70	5.04	12.74
	$S_0 \rightarrow D^{red}$	–2037310.57	–2037306.38	–2037361.24	–2037359.77	4.19	1.47	5.66
	$D^{ox} \rightarrow T_1$	–2037204.41	–2037200.72	–2037273.58	–2037271.86	3.69	1.72	5.41
	$T_1 \rightarrow D^{red}$	–2037273.58	–2037263.76	–2037361.24	–2037355.86	9.82	5.38	15.20
9	$D^{ox} \rightarrow S_0$	–2135925.49	–2135918.93	–2136033.88	–2136028.83	6.56	5.05	11.60
	$S_0 \rightarrow D^{red}$	–2136033.88	–2136030.89	–2136083.86	–2136082.49	2.99	1.37	4.36
	$D^{ox} \rightarrow T_1$	–2135925.49	–2135922.74	–2135993.94	–2135992.40	2.75	1.54	4.29
	$T_1 \rightarrow D^{red}$	–2135993.94	–2135986.38	–2136083.86	–2136077.32	7.56	6.54	14.10

9. S_0 – T_1 energy gaps

Table S15. Compilation of the available experimental ^{3}MLCT lifetimes for the species studied. Values are reported in DCM at 298 K.

Complex	τ (ns)	Ref.
1	No emission	-
2	90	[29]
3	365	[9]
4	190	[30]
5	320	[31]

Table S16. Calculated $\mathbf{S_0}$ – $\mathbf{T_1}$ energy gaps (ΔG^{sol}_{S0-T1}) in DCM for complexes **1**-**9**. Experimental $E_{0,0}$ energies estimated from the maximum emission spectra of the complexes at 298K are provided in parentheses

Complex	G^{sol} **(S_0) (kcal/mol)**	G^{sol} **(T_1) (kcal/mol)**	ΔG^{sol}_{S0-T1} **(eV)**
1	-1747003.79	-1746973.38	1.32
2	-1845697.36	-1845656.42	1.78 (1.70)
3	-2043027.75	-2042987.56	1.74 (1.83)
4	-2735496.01	-2735451.10	1.95 (1.91)
5	-2784839.54	-2784788.97	2.19 (2.18)
6	-2883500.93	-2883448.07	2.29
7	-1987591.18	-1987560.34	1.34
8	-2036935.91	-2036899.23	1.59
9	-2135589.59	-2135550.74	1.68

10. Cartesian coordinates of optimized structures

Cartesian coordinates of the gas-phase optimized equilibrium structures (in Å) at TPSSh-D3/def2-TZVP(-f)/defgrid2 level of theory. S is the total spin angular momentum (M=2S+1).

$[1]^{2+}$ - D^{ox} (S = 1)

Eh = -2783.893877975775

Cu	3.80094923904876	8.75352839061488	1.06445487192206
N	4.06602922316402	6.81506945660716	0.66816228408882
N	5.58215255016417	8.57905282163593	1.95231755064803
N	2.62715275082806	9.36415567442165	-0.43133850996107
N	2.94250509736615	10.26498321505448	2.04817059773646
C	3.24716197710438	5.95084258534986	0.07280101667686
C	3.57396665155672	4.59743269590527	-0.07137465812840
H	2.87283928543073	3.93422867164584	-0.56013878289474
C	4.78229763668209	4.13443676951673	0.40577031646835
H	5.05691205252504	3.09228049272090	0.29202598992032
C	5.66320503401758	5.02526603262375	1.05294782606411
C	6.93542649550250	4.65048871809012	1.59287903908882
H	7.25461715325594	3.61987708000497	1.49757329540711
C	7.73318203467514	5.56474033168937	2.20957453732204
H	8.69729753132654	5.27187989177562	2.60687481099300
C	7.32003699719832	6.92828194383580	2.35308083449234
C	8.09272433381815	7.93011583378817	2.97555959573998
H	9.06637307808187	7.68448744191185	3.38314434779381
C	7.60377196497092	9.21723589095124	3.05385463503390
H	8.17985031664310	10.00876852163524	3.51423179626086
C	6.33710719201229	9.50831756289431	2.53386804375289
C	5.24617649064007	6.36409218948677	1.17034962460531
C	6.06667564672177	7.31328651647836	1.84203665469793
C	2.54678454790502	8.91963352055771	-1.68341045325219
C	1.70295012873984	9.51330665153787	-2.62943803319171
H	1.67634891289958	9.11649956709826	-3.63552242782033
C	0.91884125922052	10.58703789390996	-2.26300918349931
H	0.25087769979933	11.05171976562003	-2.97877733038181
C	0.99443044613730	11.08756025367949	-0.94697260221345
C	0.23408183801452	12.20058540158900	-0.46384759014725
H	-0.45121955774344	12.69303534521164	-1.14280792240361
C	0.36121984678151	12.63312852055993	0.82044537288332
H	-0.22508800679265	13.47082239784637	1.17766610181581
C	1.27110266670828	11.99969191612569	1.72661588879772
C	1.45341295857185	12.38895668646422	3.06966208618049
H	0.88455949502426	13.21877127190121	3.47242955077430
C	2.35099040420802	11.70380286846621	3.86143761888339
H	2.50191913236992	11.97155473202274	4.89867994848340
C	3.08603646083544	10.64472272060313	3.31588283877445
C	1.88284420198183	10.44205921057782	-0.06723311320240
C	2.03827984727694	10.91327074904788	1.26661832946907
H	3.17115710415084	8.07475757956212	-1.94520880204709
H	3.79760095910330	10.09205298424432	3.91631918017247
H	2.30598907928364	6.34004719364082	-0.29448020972958
H	5.93046122678981	10.51046022509521	2.58401792892549

$[1]^{0}$ - D^{red} (S = 1)

Eh = -2784.360286925258

Cu	3.77297982980538	8.73235596023766	1.09399859098975
N	3.88927657974401	6.71651800690688	1.20570447036160

N	5.76475736692893	8.61699190471867	1.42643336923442
N	2.96785054246021	9.72701240144733	-0.47171062511453
N	2.47952259708923	9.86325081258254	2.15978925825177
C	2.94347542893831	5.77690977930520	1.13951881315261
C	3.19889682459704	4.41442236308669	1.27519454037049
H	2.38259019561292	3.70799335279804	1.19677431530060
C	4.50673511562901	3.98652733574452	1.49028174919106
H	4.74125876565667	2.93275380370923	1.58908931596156
C	5.52860215138276	4.93748952625425	1.57446198256695
C	6.90683765027158	4.60288059741866	1.77649861803117
H	7.17218475613777	3.55604172409568	1.87789178947293
C	7.86611341991487	5.56382165814754	1.83093558372753
H	8.90644752504091	5.29314233428404	1.97585052266239
C	7.53688320825417	6.95280233173947	1.70834493373958
C	8.48349717591081	7.98005589648589	1.77379393922985
H	9.53086499439167	7.74020553354615	1.91741603270113
C	8.05835037178601	9.30137937174387	1.65593660299898
H	8.76006971819959	10.12379563782406	1.70877768132206
C	6.70183172378254	9.56631529481533	1.48642974800927
C	5.18014875969535	6.30623485545656	1.43690250784415
C	6.17608949858288	7.30935126514500	1.52197876443174
C	3.25237818319820	9.68985015481200	-1.77539285393381
C	2.62880193445748	10.49669402232563	-2.72396870723285
H	2.90144753983063	10.40248089767404	-3.76720460265261
C	1.64982005059220	11.39737600863638	-2.31116048328751
H	1.13699080335557	12.03185129044326	-3.02508469497953
C	1.32594430862495	11.47557681209276	-0.95303103369648
C	0.32496681887189	12.35537303225782	-0.42730459507473
H	-0.20598327496476	13.00147839673097	-1.11810146365933
C	0.03363084598069	12.38029841604122	0.89977960835080
H	-0.73323577992873	13.04585529465252	1.28119542021615
C	0.72986028215022	11.54340421811371	1.83114092888381
C	0.47999012950771	11.54427690566630	3.20703807344154
H	-0.28225078504660	12.19727924230396	3.61661896225542
C	1.22371978315714	10.70253294358421	4.03091904770412
H	1.06404563557271	10.68007880892393	5.10122605059655
C	2.20365058498478	9.89024654954865	3.46599567223546
C	2.01839512617452	10.62663416911124	-0.05125556160513
C	1.73678320470125	10.67460972147618	1.33567554699612
H	2.80539217611371	9.23698060472764	4.08793865430918
H	4.00780128638944	8.97080468229723	-2.07212783489470
H	1.93604760698593	6.13458227304026	0.95821962282030
H	6.34414334847838	10.58672732304664	1.40580265577017

$[1]^+$ - S_0 (S = 0)

Eh = -2784.220779973

Cu	3.78097711899206	8.73184049448938	1.05890097652368
N	3.89760327143545	6.71106021088169	1.17689763917553
N	5.77287933714030	8.61143151603986	1.41973453210364
N	2.95292704503478	9.73240613881555	-0.49649621930002
N	2.49616610732579	9.86894536747737	2.14225584429677
C	2.95480438687188	5.78155668077197	1.05076486069720
C	3.21924466140400	4.41056050524264	1.15461841861379
H	2.40873822266838	3.70243724550858	1.04184137833411
C	4.50775936196451	3.98814619290629	1.39866013648381
H	4.74171613786408	2.93344232326905	1.48402399995039
C	5.53129722463845	4.94426932276143	1.53806097914892

C	6.89782049879219	4.60367036832145	1.79247879187651
H	7.16122250686549	3.55645213199804	1.88279047256393
C	7.84791822360803	5.56714072276757	1.91915832532317
H	8.88007615482159	5.29958047837952	2.11216608927521
C	7.51294739436922	6.95354975421055	1.80108246887890
C	8.45580482087330	7.99143681583902	1.92388531303306
H	9.49505082223753	7.75380274963683	2.11860575028758
C	8.04015480161851	9.29859357344620	1.79430791777546
H	8.73834548747095	10.12055872691539	1.88363606014687
C	6.68946090371152	9.56731888770636	1.54166211306830
C	5.17175025394355	6.30315575467125	1.41701846383975
C	6.17393535262618	7.31901377654490	1.54831106852883
C	3.19253574415656	9.65074744536483	-1.80211761719121
C	2.51472515767127	10.42699305152247	-2.74983615504680
H	2.75461086803420	10.31495500140275	-3.79911128290555
C	1.55420302389556	11.32019140232068	-2.32811300973903
H	1.01375928888141	11.93416352471134	-3.03904087022475
C	1.27430088006297	11.43301120226667	-0.95327472319631
C	0.29498754335240	12.33026446803530	-0.42020827984168
H	-0.26083576716137	12.95661505837013	-1.10792434198369
C	0.06262453289892	12.39923051392918	0.91701753733336
H	-0.68121622582040	13.08121457958575	1.31167528005200
C	0.79003593674839	11.57730199230717	1.83541696298450
C	0.58963140370964	11.60779674557779	3.22831453319981
H	-0.14802244744475	12.27975740357101	3.65115345610981
C	1.33796864576613	10.77884540850586	4.03525193839325
H	1.20930641472583	10.77677226957309	5.10974604714243
C	2.28159279296475	9.92340286885487	3.45360924866614
C	2.00672959596958	10.61073398095215	-0.07150869738848
C	1.76232318430670	10.68347452609565	1.33870648300402
H	3.95214231209280	8.94105858605126	-2.10683106528362
H	2.88230934262570	9.26181256850739	4.06599686605860
H	1.95055761405817	6.13977804760099	0.85916746072870
H	6.33726566022767	10.58613553329256	1.43443807950307

$[1]^+$ - T_1 (S = 2)

Eh = -2784.169430621353

Cu	3.79899751006794	8.75196358672548	1.06594846052722
N	4.09059674348253	6.84448798440381	0.61825303780424
N	5.53536841254584	8.56407395908435	2.00298335660066
N	2.58914243374126	9.31774921161079	-0.39774328420605
N	2.99504916454937	10.29125895686555	2.02045411339909
C	3.28694572316828	5.97409205897925	-0.00881810991259
C	3.61845817840753	4.63502638429235	-0.17181719726566
H	2.93141237373940	3.98163591596248	-0.69229896731634
C	4.82745033903992	4.15656191875208	0.32612141658256
H	5.10872685133177	3.11898295149764	0.19355756873936
C	5.67878967240405	5.03153562266177	1.01164181074377
C	6.94277076993923	4.65771401199358	1.57583446566480
H	7.27123426955921	3.63102998822112	1.46623819542919
C	7.72189629259912	5.56259005744364	2.22654994227127
H	8.67952221610763	5.26548593381424	2.63723433839945
C	7.30163331121540	6.92288234566548	2.39601521807384
C	8.04861440314565	7.90630554062233	3.05549635697267
H	9.01466452843772	7.66031201502489	3.47917840503321
C	7.53809384307778	9.19811492003762	3.15041732780568
H	8.09660431714656	9.98434614942680	3.64009989850420

C	6.28807775377261	9.48710200278918	2.61767891910312
C	5.26143771102523	6.37397263794835	1.15293151414232
C	6.04857299005118	7.30060559411209	1.86345053221567
C	2.47972483445668	8.85667081953060	-1.65151975990799
C	1.63090235279226	9.43269480113177	-2.58832562539617
H	1.58193912626104	9.01210413577116	-3.58362216993622
C	0.85324689243772	10.53147583210257	-2.23298099631864
H	0.17449615978913	10.98321974331273	-2.94606762061881
C	0.96335886630540	11.05729637600613	-0.94011075452392
C	0.22442586062946	12.18783813845905	-0.45910114329758
H	-0.47206279971614	12.67184020238268	-1.13336925428376
C	0.37963087068807	12.64482916914985	0.81231731470196
H	-0.19482359508316	13.49399677690888	1.16285144272395
C	1.30589300990365	12.03006241216526	1.71765030337726
C	1.52107207644770	12.44845801550628	3.03639834375591
H	0.96822604494531	13.29008614322948	3.43545262087283
C	2.44419511371853	11.76566220559379	3.82392619762470
H	2.62288997089243	12.05388955370335	4.85099559233399
C	3.15714695323629	10.70153955882400	3.28618271337267
C	1.86394954543950	10.42799844633290	-0.05186087343051
C	2.05611102885845	10.92744924682310	1.25079011180950
H	3.09390955885436	8.00241288807843	-1.90613535217375
H	3.87908120466135	10.15630419960291	3.88069754486165
H	2.35237938940757	6.36803473393712	-0.38730812655174
H	5.87223911051915	10.48463304051296	2.67962506769299

[2]$^{2+}$ - D^{ox} (S = 1)

Eh = -2941.267509927296

Cu	3.81080208108758	8.75271149460812	1.02539382047211
N	3.94009921789056	6.75620521048136	0.88367367431585
N	5.68679183273613	8.61262607642444	1.70013139646962
N	2.77362342342012	9.49762691641693	-0.51167644551542
N	2.76085499924761	10.08280511105058	2.10043302301560
C	3.00597114509435	5.87113254008780	0.52522630254695
C	3.29183008917623	4.49036411089094	0.55316206040174
H	2.51602127099857	3.79458490766967	0.26055363617982
C	4.52924264289076	4.03830570176988	0.94087890752085
H	4.74934115433133	2.97716638091413	0.95052277054526
C	5.51660236003964	4.96239888857582	1.34473172463381
C	6.82218692867651	4.59272124816152	1.78994351525076
H	7.08430742774695	3.54212494945798	1.81445235039148
C	7.72252114797146	5.53978403891412	2.17415439460464
H	8.71499474895244	5.25520175543927	2.50139759999693
C	7.37917368282587	6.92579873445779	2.15542704298771
C	8.26196529627375	7.96261555321577	2.52869818353611
H	9.26415635197013	7.72156125107483	2.86351231085601
C	7.84766921243047	9.26889157333545	2.45223581378019
H	8.51742103245643	10.07770164423207	2.71529528440463
C	6.53906331550803	9.58616696775606	2.03073716444942
C	5.16250237545384	6.32289640241003	1.30779446523291
C	6.09439020686428	7.31010244019385	1.73343683795863
C	1.65955941872157	6.35869076847836	0.09162511138040
H	1.46380209324453	7.36574559610862	0.45647394653433
H	0.88154782171652	5.69024805608003	0.46167836005117
H	1.58930281616274	6.36472274231741	-0.99997226823204
C	6.10740627793626	11.01393523238402	1.92332254114960
H	5.05801951159774	11.09755010253849	1.64747816400500

H	6.70827144510071	11.52035299515167	1.16297987486399
H	6.27422889711423	11.54121621442970	2.86506050998667
C	2.87266161544764	9.21158571137424	-1.81221577736579
C	2.05810428894027	9.88280693576080	-2.74881241918103
H	2.15797094919114	9.63067281652848	-3.79684435556790
C	1.15627291111370	10.83268501402021	-2.33877754231065
H	0.52303624315395	11.33796468179432	-3.05871961656091
C	1.06207724362329	11.16340474563217	-0.96933886167856
C	0.17705504921055	12.15489828233630	-0.44681108818740
H	-0.47299507452869	12.68436848888977	-1.13250169469962
C	0.14832973925006	12.43117496976422	0.88664987651004
H	-0.53036348294006	13.17825273385080	1.27947387382760
C	1.01205574596365	11.74652917289778	1.79461128362522
C	1.03305035958287	11.97409077778368	3.18740233666041
H	0.37124800583800	12.71419789733688	3.62196801156945
C	1.88254229462582	11.24515918163581	3.98281792460906
H	1.89746253508026	11.39200313526677	5.05512666471846
C	2.75602435078545	10.29144632509320	3.42003213565947
C	1.90987964539997	10.46723045637963	-0.09028522271203
C	1.89772329291751	10.77254613475412	1.29928915297952
C	3.87035321950282	8.19683410995991	-2.27215818666861
H	4.38353583401256	7.72828949780836	-1.43467950576169
H	4.61493729326184	8.67976032798206	-2.91073809826355
H	3.38699042103058	7.42437071786624	-2.87438639983657
C	3.68656911713023	9.50851337478461	4.29163101027172
H	4.02519646125763	8.59920785297405	3.79768892839755
H	3.18960114949372	9.24054981033882	5.22458972696069
H	4.56237356601734	10.10983624215874	4.55228276923024

[2]^{0} - D^{red} (S = 1)

Eh = -2941.733122685201

Cu	3.78800402388567	8.73574423727180	1.04516300225897
N	3.89313620135679	6.72461079646885	1.18473349787216
N	5.77388559823442	8.61080753647105	1.37874298450253
N	2.97571920346925	9.75216630096721	-0.49597039963168
N	2.48727061806780	9.83713601060910	2.12978744308121
C	2.91661639384662	5.80942051173170	1.12680255024754
C	3.17405106094442	4.44665696279114	1.30497676654213
H	2.35557066403900	3.74079472725333	1.23808017074791
C	4.47378347024902	4.00822529249687	1.54383300570081
H	4.68854255051342	2.95310482466813	1.67156013016058
C	5.51095877705443	4.94348781799501	1.61477097992393
C	6.88435086984744	4.60301458167825	1.83920367957994
H	7.14092680727761	3.55721881242360	1.97050208046887
C	7.85083005181124	5.55880597813795	1.87874590297836
H	8.88765594962249	5.28446202988858	2.04146096035542
C	7.53151900538250	6.94619814583820	1.71812844632069
C	8.47448486517547	7.97763148793577	1.76871314492731
H	9.52123429115024	7.74490075891297	1.92948240143450
C	8.05334775800997	9.29579716969439	1.61563186860825
H	8.76383352633563	10.11192262891108	1.65802169480735
C	6.69756692095584	9.58000808176304	1.42527264341147
C	5.17501788674301	6.30879144007923	1.43792911726008
C	6.17713302035718	7.30648767459583	1.50873176888338
C	1.53910565135549	6.33115085112521	0.84814363158541
H	1.52161547675623	6.85447601677847	-0.11179432334175
H	1.25505966366518	7.06446952207368	1.60820277076599

H	0.80349799129566	5.52652274003221	0.83049987477071
C	6.18949272758135	10.98273267973780	1.27844283721246
H	5.61477097929707	11.07795147403440	0.35311228113995
H	7.00625249043078	11.70507465595688	1.27346131487115
H	5.50520472655359	11.22242465695881	2.09718785775733
C	3.28091355888988	9.71793785043658	-1.80001654638624
C	2.64507573769486	10.54991409662870	-2.72648598842522
H	2.91597862902935	10.48040788731639	-3.77262813949465
C	1.66043973057948	11.43874839075189	-2.30380649922834
H	1.15042176543795	12.08036617711731	-3.01370057819444
C	1.32554785616864	11.49721132149226	-0.94735906822474
C	0.31705516169031	12.35964671095465	-0.40718950388232
H	-0.21708017483324	13.01578863828730	-1.08610955068117
C	0.02216108128489	12.35519038031895	0.92026705682409
H	-0.75078142472248	13.00686462529577	1.31345808862743
C	0.72419833970178	11.50483594027783	1.83485194569165
C	0.48216376155579	11.46680088278011	3.21167019861959
H	-0.28453160092508	12.10076851201011	3.64293107648205
C	1.23577573982305	10.61430716196285	4.01400354072979
H	1.07128971083896	10.57214181925601	5.08347858023854
C	2.23283504063424	9.81616908258902	3.44474782266688
C	2.02152152658294	10.63662719986705	-0.06264783925547
C	1.73808196088841	10.65618788252486	1.32454442591768
C	4.32759084761536	8.72513536707702	-2.20692622083104
H	5.23986457291693	8.88171590915069	-1.62485242008163
H	4.55812744006991	8.80086656771314	-3.26994466065158
H	3.98719725756773	7.70937139410489	-1.98679102702908
C	3.09026958713820	8.90326555563494	4.26867547200013
H	3.04601191890832	7.88598182115535	3.87010067087155
H	2.77824067677930	8.89742908224849	5.31346852668797
H	4.13655507741938	9.21645833776655	4.21075755180559

$[2]^+$ - S_0 (S = 0)

Eh = -2941.596778167522

Cu	3.78618454890123	8.73585660105153	1.04731521051368
N	3.90208830350401	6.71293562409774	1.14666985784901
N	5.77051366583172	8.60757917889728	1.42773688549201
N	2.93747318909698	9.71983662178366	-0.50551149761289
N	2.51820235163825	9.88479643309250	2.13183007265793
C	2.93897002448102	5.80234039852265	0.99266436014885
C	3.22163291603248	4.42617167281352	1.08106976936983
H	2.41753091721533	3.71387792414380	0.94693449633693
C	4.50371620891892	3.99648761256305	1.33593946656115
H	4.72920821590576	2.93867811183040	1.40622107813399
C	5.53217345212608	4.94307229466558	1.50539820872106
C	6.89322818655512	4.59863387087893	1.77690167490185
H	7.15591026759622	3.55045418760451	1.85753455909744
C	7.84020775072834	5.56230839483152	1.93492765394145
H	8.86902633523459	5.29405348315720	2.14407069085880
C	7.50339469802812	6.94810679234998	1.82957399235715
C	8.43382233462425	7.99409533484321	1.98220890448810
H	9.47170195866288	7.76408341012422	2.19348668683608
C	8.01411482936983	9.29850817168598	1.85841839058556
H	8.71406546832835	10.11661126127968	1.97143419710610
C	6.66504624075284	9.58620513960763	1.57731066036037
C	5.17232354246481	6.30137613485387	1.39699114861763
C	6.17098448008398	7.31546519533337	1.55496811549100

C	1.55269921992770	6.31129153254078	0.74382195201032
H	1.58199854666270	7.15393364825448	0.05041075929922
H	1.11323238509955	6.67393499856875	1.67819433147591
H	0.90699883837139	5.53006632581853	0.34375387830118
C	6.16458195448441	10.99230998791791	1.45285719591114
H	5.41201923519863	11.05269485997092	0.66467857965545
H	6.97574101969568	11.68847831220434	1.24162985454834
H	5.68465310773669	11.30175595700331	2.38682338814794
C	3.17522710911352	9.59735382686603	-1.81301809097239
C	2.46689416369544	10.36927566331380	-2.75315500436479
H	2.68701017568424	10.24872709815800	-3.80624788281499
C	1.51103880037069	11.26619723855547	-2.33473974129309
H	0.96395179781530	11.86648855954178	-3.05245695957991
C	1.24526976187601	11.40684847525125	-0.95906840366312
C	0.27644741666032	12.31277067452105	-0.42448365757866
H	-0.29136293494127	12.92869213599229	-1.11181270808087
C	0.06919618265059	12.40325932026658	0.91685733577659
H	-0.66678490320350	13.09178505806667	1.31485264956896
C	0.81366738147587	11.59501527730916	1.83204368221623
C	0.64647266193869	11.63694697246826	3.22946954628195
H	-0.08149400373469	12.31191663888509	3.66449742476287
C	1.40887057678475	10.81602769944385	4.02851261588559
H	1.29347337510009	10.83258668941676	5.10480659649270
C	2.34905964122456	9.93978343575043	3.45406825630356
C	1.99366637588453	10.59959467638471	-0.07961783889828
C	1.77412329207595	10.69257322178665	1.33249347422450
C	4.20752686467099	8.59511128912120	-2.22793255636020
H	5.04029643521741	8.60160763552799	-1.52216130799645
H	4.57643458122570	8.79605193372133	-3.23341662574851
H	3.77771831972472	7.58853912860645	-2.21713532141879
C	3.21364785873200	9.04693847061062	4.28976702933290
H	3.31486723296830	8.06978047771496	3.81341544613296
H	2.80887077200594	8.92504045306826	5.29405513411201
H	4.21854137172579	9.47235397735990	4.37493688551659

[2]$^{+}$ - T_1 (S = 2)

Eh = -2941.531222730112

Cu	3.72837184780810	8.68285311692400	1.03848244713727
N	3.95178602036164	6.71404975653980	0.83980603682475
N	5.57717197780329	8.61077775889166	1.75115056975760
N	2.70675344580674	9.43967878100309	-0.49385232282740
N	2.76832150065678	10.05330007861354	2.08861393373038
C	3.05969641407816	5.78097568329631	0.47097118070620
C	3.40576620489335	4.42362345672229	0.46445139208396
H	2.66451211104906	3.70196682433628	0.14641999255900
C	4.67006011988421	4.01267688619047	0.85184893531401
H	4.94068952672994	2.96389008597334	0.82941622797573
C	5.60050331505697	4.96599956165295	1.28827245435072
C	6.92374432125921	4.65446107219251	1.73213802057667
H	7.23693203044218	3.61731115738429	1.73325123389835
C	7.77681893844847	5.63398927122172	2.13716153902152
H	8.78170117096989	5.38863827921196	2.45943906310586
C	7.37293766680035	7.00673976414285	2.15353450905233
C	8.19802084968930	8.06860002318182	2.54997619181167
H	9.21118195008156	7.87316707890310	2.87949854958180
C	7.71134462439775	9.36700092791657	2.49139963255137
H	8.34280052848083	10.20323519301061	2.76142793787135

C	6.39894985345342	9.62474026372616	2.08736616012454
C	5.19186512043562	6.31720265746056	1.28200841875746
C	6.06243257080283	7.32789263648225	1.73945945300316
C	1.66998554014212	6.21128076317161	0.11085732931377
H	1.61654900836625	7.28425997640028	-0.05906180938841
H	0.98921302601007	5.96173946326682	0.93051245854655
H	1.31524904883472	5.68551190016665	-0.77697499119820
C	5.87936810537353	11.02743431844318	1.99680366159288
H	5.28690139720815	11.15665017526135	1.08860578817503
H	6.70675762054445	11.73550429892510	1.98454978053882
H	5.23447788686925	11.27668026836046	2.84293669737888
C	2.79715725579361	9.16119310180169	-1.80852698438265
C	2.09011030950379	9.91750557936525	-2.74666059258128
H	2.18477798932187	9.66238829456155	-3.79393427781369
C	1.27128786800872	10.96469877791032	-2.34626899090342
H	0.70886478337926	11.53491513454162	-3.07562007006586
C	1.18898991015988	11.29173311530049	-0.98682738859937
C	0.39696524726136	12.36118801377479	-0.45944480435840
H	-0.18837296549125	12.95754397807200	-1.14911623405625
C	0.36765093262338	12.62368374564517	0.87511492651572
H	-0.24694767730899	13.42703752197436	1.26336214463528
C	1.15006730180723	11.85765231664643	1.79697345214412
C	1.17554455079073	12.06809200251076	3.18179488466573
H	0.57766144879920	12.85754104230309	3.62078675218019
C	1.95712602685069	11.24534532485942	3.98278675787447
H	1.96724357169313	11.37371444816929	5.05718925652225
C	2.75012952996478	10.24131111594792	3.42183084899138
C	1.94653746527150	10.51087148128748	-0.08715250938446
C	1.95371810636341	10.81432351769180	1.28843183215330
C	3.66467583886638	8.01710321979556	-2.23370524401225
H	4.58247981660525	7.98641055769756	-1.64353407328420
H	3.92100282563246	8.10623126114775	-3.28844100619021
H	3.15131981755502	7.06247790296020	-2.09200992139227
C	3.58984902820098	9.34399002779466	4.27966810172196
H	3.53816380832462	8.31294533549559	3.92303179760474
H	3.24702373562361	9.37967797470945	5.31283767584094
H	4.64147273166096	9.64092872906172	4.26302019424653

[3]$^{2+}$ - D^{ox} (S = 1)

Eh = -3255.953713460561

Cu	11.04978771268972	10.50752280136921	-4.45181175351290
N	11.01473717704224	9.19344266196451	-5.98302854596127
N	11.85044876572113	10.53286678493032	-2.60359253513027
N	12.17448006397843	11.58872806787998	-5.69472329114938
N	9.31480093251088	10.65012247524471	-3.46481492240837
C	10.47225305298078	7.97356988977875	-6.04164827814798
C	10.69248439422510	7.15787023786114	-7.17246803655998
C	11.44754622770624	7.60600156079482	-8.22710351489270
C	12.03767501943875	8.88725010759732	-8.16966581964557
C	12.85213861609518	9.43983562303575	-9.20477540647028
C	13.39915051199552	10.68115076900807	-9.07776832869498
C	13.18754879297221	11.45472904335608	-7.89660038953198
C	13.71331655531714	12.74898286144811	-7.69087752753693
C	13.12930562534802	10.39144397214628	-2.23272354462280
C	13.46371976843893	10.39641086902767	-0.86472815535023
C	12.49372089073904	10.55093960051994	0.09737119442282
C	11.14304489763971	10.67585360290428	-0.28311818517756

C	10.06153288651772	10.82402857566832	0.63965549701939
C	8.77892174083420	10.93616847100479	0.19899440707981
C	8.47809327032969	10.88906993572317	-1.19767952199231
C	7.17816216162726	11.00093511125317	-1.73019135642398
C	13.43147142713494	13.42395334074572	-6.52878901610677
C	12.64888140596529	12.82509708158153	-5.51939235470680
C	12.40259549367485	10.92036056727409	-6.86009746849224
C	11.80162495442828	9.63932662366566	-7.00570937800050
C	9.65911775025482	7.48025141514304	-4.87410937830396
C	8.30823110260911	6.89873620016498	-5.31161385484686
C	10.46887883299412	6.44689682542244	-4.06951278571429
C	12.29826933022653	13.56315487075069	-4.25461576536851
C	11.37987471918469	14.75503940098585	-4.57871689096915
C	13.54446866094244	14.02102363747636	-3.48599001477703
C	6.98895057881698	10.95829091334923	-3.09191853191826
C	8.07891780749036	10.77665886620552	-3.96408013671937
C	9.52594748269866	10.72777627014001	-2.12250915398245
C	10.87227805439843	10.64413806506714	-1.66351698855205
C	14.15939195978580	10.17697424657342	-3.31519426059572
C	14.02462084314647	8.74569015517819	-3.86845687713362
C	15.59525528169663	10.45579176585139	-2.87048882304552
C	7.92951796623998	10.76282972938263	-5.46518742220767
C	6.50804067253954	10.47010703208636	-5.94373901708025
C	8.44113827819734	12.09868516267636	-6.03739118762540
H	10.24549503349104	6.17336106476148	-7.19774145021584
H	11.59950727901365	6.98243494323770	-9.10045565315711
H	13.02466100360636	8.85209825366770	-10.09809868889917
H	14.00567548979370	11.09894624591369	-9.87194395807093
H	14.32779667779459	13.20670342427700	-8.45743190234785
H	14.50014337046213	10.28762367522354	-0.57912657174422
H	12.76125477785199	10.57106983789421	1.14754068147056
H	10.28413368154466	10.84897204873772	1.69933875966421
H	7.96366884135050	11.05952986907300	0.90131387606902
H	6.33307538579732	11.12532964545105	-1.06297164324500
H	13.81176742513519	14.42410112113358	-6.36953306951797
H	9.47765317267602	8.34370045260385	-4.22994906631719
H	11.74005375952503	12.86276603725524	-3.62614377786690
H	8.43664669060019	5.96618567548084	-5.86394071817391
H	7.70660355992080	6.67517197103069	-4.42935557251939
H	7.75135835030418	7.59365723226736	-5.94218272294083
H	11.40611886650467	6.86798676649774	-3.70102049566199
H	9.88154148883278	6.11188713140356	-3.21292213847612
H	10.70357191576858	5.57250350839662	-4.67981857829867
H	10.48046546414926	14.43720034518312	-5.10848758656142
H	11.08031277627078	15.24506058708184	-3.65087843130139
H	11.89739835525495	15.49250796759656	-5.19507094423041
H	14.11561751291745	14.75590840527555	-4.05670420129200
H	13.24178405161996	14.49363242031688	-2.55031101159550
H	14.20521179784243	13.18550381724688	-3.25135508961787
H	5.99602629070507	11.05412811767516	-3.50728857240503
H	13.90659050095689	10.86734393992252	-4.12302435036875
H	8.59333835887866	9.97482166832689	-5.83224335076592
H	14.26831121252832	8.00844715592548	-3.10084458152604
H	14.71049061781051	8.60720531064346	-4.70571033073852
H	13.00873777556857	8.55064878181915	-4.21946785091256
H	15.70329001271184	11.44949658256307	-2.43115459867482
H	16.25826712274715	10.39601117340137	-3.73447815081584

H	15.94255813884339	9.71681370662421	-2.14521447031292
H	6.11209201766599	9.55008383384573	-5.50943446040798
H	6.50773068995193	10.35944174129996	-7.02880553978065
H	5.82720425154797	11.28921463560529	-5.70238351635708
H	7.83121451186692	12.93222359611297	-5.68360363857899
H	9.47715589591303	12.28260936448345	-5.74114633010747
H	8.39478925370097	12.07640661550534	-7.12717442556508

[3]^{0} - D^{red} (S = 1)

Eh = -3256.410297100027

Cu	11.12267716738514	10.59140608292402	-4.43362807007211
N	11.07772944971944	9.14153417303451	-5.87121694125594
N	11.82195483687301	10.33682385431059	-2.55135405462996
N	12.13627305774216	11.60826344812728	-5.83572286432567
N	9.37549402732476	10.92397916176942	-3.48015361440793
C	10.45549669840250	7.95309776332861	-5.88764433373321
C	10.48044021008481	7.13209061135700	-7.01912660243760
C	11.16605909268819	7.53605970338965	-8.16069616177016
C	11.80006908525784	8.78140730222023	-8.17765311959118
C	12.52825909404786	9.29296985868344	-9.29977715771442
C	13.13314272633088	10.50953592562708	-9.25200590301482
C	13.04279593669946	11.33823428172987	-8.08698731130235
C	13.62709375199230	12.60393890863183	-7.98124771537136
C	13.07590202621957	10.16567177729523	-2.10562951685318
C	13.34253620715681	9.93717159381254	-0.75287004933795
C	12.29765318274508	9.88196834308659	0.16592385832320
C	10.98674926761683	10.09990528446135	-0.26825994570270
C	9.84189333420086	10.07651767696065	0.59226015218698
C	8.58953069183450	10.29239495177206	0.10760413095160
C	8.36995753828208	10.57764490020817	-1.27801781712851
C	7.11191413389325	10.83113558082758	-1.83479562485694
C	13.47014693555272	13.33635751259543	-6.80737157012713
C	12.71409207909281	12.81661353981164	-5.75399974562454
C	12.31063231495373	10.85969275556173	-6.97159800593445
C	11.71722142193871	9.57332400688975	-7.00460947991151
C	9.75998744474548	7.55800124446705	-4.60407718027390
C	8.62431724946831	6.55461676106082	-4.80318939522140
C	10.77653495596828	7.03995327423865	-3.57559166535608
C	12.44615553822686	13.57137036740781	-4.47292448679965
C	11.03812314923742	14.18522382929777	-4.51571664947057
C	13.50591920883823	14.61938100574004	-4.13741303408350
C	7.01021422217454	11.11903449501607	-3.19142257838037
C	8.16028520807545	11.16425390474023	-3.98828619284638
C	9.49049036451745	10.61913361361306	-2.14455024194498
C	10.78912853624647	10.35003446596321	-1.64925941637031
C	14.15646020753024	10.21797951070972	-3.16251415374659
C	14.23234863226893	8.89303751640301	-3.93626732552508
C	15.52659911559586	10.61905635146253	-2.61661419242569
C	8.09918751289157	11.48177723576516	-5.46427316034158
C	7.49102411816479	10.31519464649296	-6.25499900845047
C	7.34678451027088	12.78744382306502	-5.74495896448836
H	9.97867697246301	6.17430227967635	-6.99485940132790
H	11.20702548135147	6.89801731468978	-9.03650703903529
H	12.59381594287935	8.68145161035048	-10.19330341576632
H	13.69023862064296	10.88003383549610	-10.10577513672302
H	14.19707634043278	13.00555473954375	-8.81161138722368
H	14.36296984652831	9.78843366531710	-0.42673686354828

H	12.49286549425944	9.68290619751273	1.21377922748710
H	9.99459707717706	9.87411394198291	1.64694790153915
H	7.73132778260419	10.26180502184865	0.77029587464593
H	6.22931539845643	10.80742976495563	-1.20533307538094
H	13.91843631912540	14.31589977458919	-6.71120716488538
H	9.34167690999499	8.48666784993033	-4.20435116477939
H	12.43655972889667	12.81190463272614	-3.68196133616112
H	9.00210293818599	5.57366365994031	-5.10508185670974
H	8.08417596110702	6.42225716228377	-3.86308889052557
H	7.91273228760359	6.89423380833360	-5.55949118849990
H	11.54225782265982	7.79043831661065	-3.38261233148937
H	10.27427506126310	6.81710406073159	-2.63079519082048
H	11.25944262946048	6.12738832934832	-3.93564658468980
H	10.29818968700772	13.40615545273920	-4.70212098158866
H	10.80138776902179	14.65971964873723	-3.56012066469995
H	10.96760904923040	14.93803103731631	-5.30563839207726
H	13.49318825804640	15.44932555511490	-4.84942109006133
H	13.31202510852944	15.03583964830037	-3.14641111916364
H	14.50926287914286	14.18644913319940	-4.13469314401492
H	6.04669664214398	11.32934630418803	-3.63807032538963
H	13.82588046679609	10.98092856390274	-3.87491201171400
H	9.14089934886805	11.59748853457478	-5.78223722836553
H	14.49180604586610	8.06705133098342	-3.26837270725830
H	14.99405048800192	8.95883049613091	-4.71739093018515
H	13.27645635250880	8.67378247449717	-4.41365530136289
H	15.47395921442800	11.54760488079512	-2.04309120724060
H	16.22194130438305	10.76822122504001	-3.44575935777777
H	15.94785924446814	9.84197953651223	-1.97269601754365
H	8.06028620103746	9.39911359642098	-6.09690341595215
H	7.50035951829407	10.54036444555917	-7.32446226511466
H	6.45568178327459	10.13593490334950	-5.95200734918460
H	6.29125250692478	12.70409925881409	-5.47263494826583
H	7.77691420656639	13.62050537861974	-5.18523303836700
H	7.39801406810949	13.02632258547558	-6.81016337141072

$[3]^+$ - S_0 (S = 0)

Eh = -3256.276981225595

Cu	10.99894055510957	10.66679969901128	-4.47238699569218
N	11.15354762985591	9.13724778697425	-5.82268766019227
N	11.76800462096623	10.23891855462427	-2.62853859408212
N	11.94121802221263	11.69587666006423	-5.92797506195134
N	9.32527829134949	11.01890652980959	-3.39971818629962
C	10.74082456459764	7.87358045463989	-5.72213422186023
C	11.06717066601166	6.92815695816555	-6.71484320822662
C	11.80499344858110	7.30054052626665	-7.81352481750577
C	12.23384042126370	8.63678610652045	-7.94344836630298
C	12.99197701955989	9.12654489993159	-9.05162769042927
C	13.37383684763396	10.43137012280715	-9.11571286412630
C	13.03318245684901	11.34868520683413	-8.07362476263226
C	13.40086660630412	12.70959405620627	-8.07462093077064
C	13.00248857644088	9.86497778572815	-2.29360704209066
C	13.28968365098488	9.41653800033350	-0.98853202158149
C	12.30114969724412	9.37646380266842	-0.03405372001137
C	10.99591387912488	9.79145221086944	-0.36603953508480
C	9.90381992305340	9.80474495638220	0.55625663279229
C	8.66680559411095	10.21955108298678	0.16905762348465
C	8.42142192329078	10.64843743517157	-1.17256573536694

C	7.16611582172437	11.08408780601811	-1.64140610649930
C	13.03251642264556	13.51252599742845	-7.02155185005676
C	12.29703992715266	12.98097293239793	-5.94367221472463
C	12.29183034100656	10.89059695245631	-6.96739909204168
C	11.88058515952798	9.52050352976435	-6.90456307901616
C	9.92923457162354	7.50683085935677	-4.50397669404242
C	8.64872864475112	6.74485879960548	-4.86502562677851
C	10.77808709977361	6.71003958905208	-3.50169077481538
C	11.89043902436810	13.82111211926969	-4.76008185931044
C	11.01776306213272	15.00971616891046	-5.18277441976395
C	13.11958194052499	14.28111080259027	-3.96424861957137
C	7.02884542742023	11.47703027191098	-2.95227358752457
C	8.13257711884395	11.43770524902650	-3.82626039925165
C	9.47881458421231	10.63951668671188	-2.10301931363392
C	10.78287032736476	10.21248809671765	-1.69327568166735
C	14.06102695067414	9.93800480179795	-3.36613506910777
C	14.40069496215254	8.53946722361075	-3.90294066432481
C	15.32204385118493	10.66248872708860	-2.88017902073738
C	8.03473153118556	11.82001166684201	-5.28161482154144
C	7.56883525401344	10.61241934792821	-6.11164105410215
C	7.14784543521427	13.04335802746990	-5.52519619744179
H	10.72552209627533	5.90696922943570	-6.60590729119467
H	12.05582014698472	6.57859306349533	-8.58218886217749
H	13.25702551364712	8.43645219735766	-9.84395506520139
H	13.94682389580771	10.79587780704299	-9.96011134018602
H	13.97083520661320	13.11148822099121	-8.90436098549755
H	14.29866555013209	9.11008508307906	-0.74476943829239
H	12.51694154079784	9.03508391128486	0.97186305870226
H	10.08067383833261	9.47798557895599	1.57418039204592
H	7.84412885422446	10.22858176074868	0.87433308719354
H	6.31908358513341	11.10865752419464	-0.96547547468014
H	13.30688083822233	14.55961382772152	-7.00929979691443
H	9.65340441693392	8.45758621200652	-4.03789621385650
H	11.29610461511844	13.15736451192774	-4.12153176297651
H	8.87246346525355	5.75706459447327	-5.27464979799482
H	8.04400102134489	6.59911376089253	-3.96772133762329
H	8.04940564024980	7.28932898444482	-5.59705969749987
H	11.65907716131725	7.27422468949938	-3.19411923779054
H	10.18733015327734	6.48436459179433	-2.61132213123333
H	11.11041212756755	5.76408103679044	-3.93652624033762
H	10.13927268148088	14.67781116012241	-5.73969922617756
H	10.67947605712212	15.55436689760713	-4.29897168521728
H	11.57475078855241	15.70887733769070	-5.81120586421449
H	13.74874124648287	14.94950468542027	-4.55735717017753
H	12.80298600352513	14.82321869340946	-3.07092138975777
H	13.72623666996601	13.42903089071011	-3.65241847798913
H	6.07223330976843	11.82054304928332	-3.32287481269843
H	13.61394896020822	10.51704389029682	-4.17984893687082
H	9.05973950297768	12.05480885534686	-5.58904245696336
H	14.80210908663337	7.90321307148075	-3.11012674710922
H	15.15488580536306	8.61581764576669	-4.68916803906142
H	13.51923888973003	8.05219191721168	-4.32139726660608
H	15.08401609154577	11.64290916378402	-2.46282969983990
H	16.01160980942076	10.80251493940353	-3.71491777607867
H	15.84583409838898	10.08575516661119	-2.11403529460474
H	8.25466432848500	9.77314137380815	-5.98786069566830
H	7.53800649408178	10.87681954454079	-7.17074425776512

H	6.56830341455480	10.29285159087936	-5.80981986044787
H	6.09711144298896	12.82824651569697	-5.31653704449086
H	7.45392585218906	13.88911150416169	-4.90586475360556
H	7.21570094725795	13.34361802868075	-6.57255610525733

$[3]^{+}$ - T_1 (S = 2)

Eh = -3256.206586074729

Cu	11.10204654360671	10.49447158303024	-4.45374619067327
N	10.94592736277472	9.20556355593125	-5.97702319774991
N	11.85556392668231	10.48926111773603	-2.59534762465304
N	12.24651218160514	11.52689061224716	-5.70791497631883
N	9.34971586556512	10.68108374329010	-3.51403979046722
C	10.30930549947287	8.01999101788721	-6.04579581253045
C	10.38053943391096	7.24832155500465	-7.20691212857583
C	11.10838902954391	7.68557758566056	-8.30838049006341
C	11.78977223958552	8.90474234648079	-8.24749909873996
C	12.58230063312539	9.44016023206426	-9.31337475309906
C	13.22738745435433	10.62967868871761	-9.18202823064363
C	13.14090056786332	11.38892255917516	-7.97096074094979
C	13.75606120043325	12.62884723441717	-7.77117695653751
C	13.13200560056370	10.35112461919877	-2.18453899470742
C	13.43015737062999	10.28086586820177	-0.82251870845751
C	12.42099553900545	10.35230888072007	0.13028758261145
C	11.08901031098654	10.48180371500457	-0.27969174515110
C	9.97334378538221	10.55071187450734	0.61502503567414
C	8.70141276302484	10.67204471796336	0.14835779089107
C	8.43325017983184	10.72830351979643	-1.25578954814667
C	7.15603828349718	10.88341399350979	-1.81084370379312
C	13.57893206290882	13.30103434917579	-6.56553589212200
C	12.81735183752676	12.73650630331142	-5.54253651315424
C	12.37265975744470	10.86791584420807	-6.90431553991231
C	11.68983555907712	9.64272051538787	-7.04562304155668
C	9.56526759363545	7.56631449430120	-4.81199047145983
C	8.57240031360571	6.43343305665137	-5.06964402969083
C	10.55741814361969	7.17675937190188	-3.70323969759944
C	12.54806763712106	13.43611345206488	-4.23317765304153
C	11.10827273089410	13.97895103040809	-4.22349866803034
C	13.55690168000980	14.53300457168287	-3.89717103367373
C	7.00996042396703	10.96427645860340	-3.18770714899465
C	8.12409360900991	10.86211553303929	-4.02910178462379
C	9.52169831740256	10.64345553200677	-2.15287969561757
C	10.84361360949037	10.53901336053712	-1.67037257199095
C	14.18788862797545	10.24494853959607	-3.25787092705431
C	14.15620398107530	8.84568678498399	-3.89584773926663
C	15.59362982423014	10.60232030169483	-2.77705367469792
C	7.99851057364161	10.99343451836464	-5.52674909946259
C	6.97093560578745	10.01953098530202	-6.11517341124697
C	7.65372146930908	12.44315588022891	-5.90706528592436
H	9.86205082761482	6.30135568869305	-7.24054346282575
H	11.15451043504789	7.08570487416977	-9.20949936429423
H	12.65729916014683	8.87315383761629	-10.23381084724739
H	13.81873752226682	11.02696764298584	-9.99853729936370
H	14.35770156326561	13.06574903137711	-8.55929588199366
H	14.46035029267855	10.17248323276554	-0.51519211630706
H	12.65858976875152	10.30543239886751	1.18638695106876
H	10.16492620789510	10.50661057707165	1.68065421586266
H	7.86686768452618	10.73254184089166	0.83686290914646

H	6.29186410713513	10.95394803212925	-1.16083999535747
H	14.03322351388764	14.26912340981832	-6.41129703659106
H	9.01049275050279	8.43742387492335	-4.45506261727207
H	12.60160933383862	12.66738785297104	-3.45655504877240
H	9.08302728889105	5.50126651245257	-5.32294235282687
H	7.98918795753384	6.25095689949353	-4.16551109973493
H	7.87864156885649	6.67587570551606	-5.87717402709396
H	11.21027272200188	8.01180860609890	-3.44165137681891
H	10.01355483587277	6.88005766841962	-2.80431825867795
H	11.18494971058982	6.34065887581792	-4.02003104183477
H	10.38998829000059	13.17693452546371	-4.40726553633207
H	10.88107772601894	14.42210204435767	-3.25197753859205
H	10.97513470501000	14.74259038912090	-4.99319698075067
H	13.47274130818416	15.38102722549835	-4.58089647964201
H	13.36579196750477	14.90674722115624	-2.88984163970069
H	14.58290729767651	14.16067054170847	-3.93250149425975
H	6.03313816759515	11.11077867666309	-3.62853822174399
H	13.89994541966736	10.95514216817068	-4.03606191196952
H	8.98025749000914	10.75496954842994	-5.94483627265884
H	14.39417735850007	8.07553081585799	-3.15863075831567
H	14.88795445718005	8.78920171800342	-4.70413522433027
H	13.17185406615664	8.62638111881910	-4.31443974018309
H	15.61609523178361	11.58017693765876	-2.29142784753821
H	16.27190227513870	10.63184079442765	-3.63155594265475
H	15.98321129090251	9.85934592995225	-2.07706806729431
H	7.19551120490820	8.98686845756757	-5.84644319320465
H	6.97210301663410	10.09814191590309	-7.20401256926302
H	5.96194922010281	10.24975259579251	-5.76596468714020
H	6.66901485734193	12.72086969649676	-5.52494716398615
H	8.38480292976897	13.14738623127074	-5.50727051390842
H	7.63714833943357	12.54418598160591	-6.99413330439505

[4]$^{2+}$ - D^{ox} (S = 1)

Eh = -4359.472910490747

Cu	1.37199772057258	14.75276771727535	7.89631015453648
P	2.10558222688648	13.98881097010600	9.93264695712370
P	1.86733551910234	16.99437920359457	8.02303360949383
O	4.29560753557729	15.31288083530455	8.64124052006841
N	-0.36909981899019	14.70496104669832	6.80758890042867
C	-1.46109371154916	15.45465116236057	6.90717567338724
H	-1.43089851296341	16.26437014871643	7.62555342434602
C	-2.59549925068140	15.23963319092477	6.11650868703481
H	-3.45887737124492	15.87921016119322	6.24160144743297
C	-2.58638062730837	14.22373796247037	5.18553189266782
H	-3.44930802827741	14.04221998325430	4.55554688069276
C	-1.43899266543749	13.41735506207147	5.04761224034265
C	-0.34798921187817	13.69979507276724	5.89480460927979
N	1.86680542453388	13.23416250698800	6.63935417187951
C	1.71302070290081	17.85110577650831	9.60103847612004
C	0.66022069872011	17.49692673962198	10.44985674653974
H	0.01404821705057	16.66591861483250	10.19548661168750
C	0.44514826154201	18.20350073057857	11.62453114592808
H	-0.37251739448157	17.92802814898996	12.27910407063103
C	1.28778444147768	19.26031878852541	11.96037850720934
H	1.12321498240685	19.81236702495885	12.87755140575721
C	2.34459924577408	19.60712939282093	11.12298711151517
H	3.00028248795296	20.42760148441496	11.38716244933579

C	2.56148549351064	18.90701264078931	9.94230186745210
H	3.38178966450621	19.17987088877409	9.28984420485812
C	0.79162654673174	17.86621220049754	6.85864438045628
C	-0.08197298568369	18.87099357218130	7.28295857525448
H	-0.07516011734000	19.19668282609025	8.31540298196412
C	-0.95039585820142	19.46200608684165	6.36988073511043
H	-1.61846819303580	20.24880802023669	6.69783514275151
C	-0.94924369188241	19.05639407683763	5.03915413694554
H	-1.62142100768058	19.52464641046021	4.33060821311897
C	-0.07525606976096	18.05598481449239	4.61210452623750
H	-0.06706850952777	17.74801394853916	3.57374706866128
C	0.78564258683858	17.45598388454483	5.51744722882401
H	1.46072192285999	16.67491767680121	5.18477464011784
C	3.54521976279474	17.21610074152920	7.36428770802488
C	3.83658025049295	18.21824547418396	6.43006318136093
H	3.06462251783967	18.91931185606146	6.14059223023216
C	5.10317023625434	18.30986119853549	5.86674689597896
H	5.31682968636864	19.09485617532539	5.15261213843854
C	6.08872185488610	17.38913320951691	6.20993537529139
H	7.07111914634688	17.45044571426716	5.75856409503512
C	5.82148195434958	16.38959303380433	7.14265296000225
H	6.57751907039443	15.67098175893306	7.43307204685631
C	4.56478546689790	16.32212948767885	7.71767207494189
C	4.23594371554773	15.71482867532222	9.97547163787921
C	5.12632156019406	16.63291819007928	10.50944709991236
H	5.89403853286080	17.07381929086384	9.88692756549984
C	5.00532962984891	16.97973930676450	11.85045965926399
H	5.69700411841484	17.69506538819300	12.27772350879238
C	4.00517319918668	16.41997869333063	12.64134050452047
H	3.91155845105551	16.70382444954214	13.68148847374513
C	3.12437960970789	15.49653799197402	12.09640136079711
H	2.33599078905952	15.07295242542396	12.70463196632857
C	3.23706968143316	15.12579713587468	10.75336097143045
C	2.95632257533612	12.39993363906329	9.79289693445703
C	4.34080734366216	12.28449207908212	9.94282210959104
H	4.93486922433678	13.14911643643890	10.20938687138229
C	4.95310219201969	11.04777726637708	9.77042658529610
H	6.02404667757426	10.95586117913470	9.90335477490298
C	4.19127509382914	9.92854607924789	9.44616834815622
H	4.67125170774927	8.96563731374389	9.32147378016155
C	2.80928494728906	10.04121206449013	9.29792540418754
H	2.21486131125825	9.16749036560848	9.06059341608243
C	2.19187371861326	11.27193009788098	9.46438449164836
H	1.11629522948000	11.35732456721709	9.35679860801632
C	0.70059028124219	13.66313376056895	11.02154713460488
C	0.87254736710616	12.93602960233172	12.20647228088980
H	1.85158831257011	12.55891037181360	12.47729992997897
C	-0.21925274028932	12.68818372090264	13.02767369596678
H	-0.08456421206767	12.13161839738808	13.94689967802576
C	-1.48582015274358	13.14400065269050	12.66604415070100
H	-2.33476604431547	12.94139136107091	13.30729433304068
C	-1.66586413240606	13.84339568798549	11.47661980499064
H	-2.65418752238762	14.17869920511010	11.18708586593414
C	-0.57460770663590	14.10070954663408	10.65556031588274
H	-0.71363616462726	14.62422648429619	9.71557342771693
C	-1.32914067225664	12.34696970361144	4.10415698650330
H	-2.17504673339648	12.13423398483255	3.46180092801209

C	-0.18831825734073	11.61250990035425	4.00794375632923
H	-0.11265720585808	10.80873727430172	3.28563183075503
C	0.84715560275683	12.92115968259005	5.79912547237751
C	0.93666541974194	11.88405142406590	4.84985361354031
C	2.15362066238779	11.17499742013086	4.78488200557811
H	2.26688704062998	10.36822048506552	4.07018829058014
C	3.18707055822616	11.51883217161352	5.62804975973473
H	4.13439463857529	10.99777501690928	5.59710745320187
C	3.00501210760513	12.55469508141007	6.55246453931110
H	3.78955264538041	12.83460800676689	7.24319657293763

[4]^{0} - D^{red} (S = 1)

Eh = -4359.916294904858

Cu	1.18969538114738	14.50987851968899	8.28448474770948
P	1.97895577555263	13.68737291546813	10.16597530617585
P	2.03509694930928	16.59316241537421	7.86186867761569
O	4.30542397702547	15.10318373256749	9.16085249723765
N	-0.70935925883964	14.73626341642332	7.59088567225576
C	-1.77140625697126	15.39472269674470	8.07435218306418
H	-1.68023694558975	15.75325309159079	9.09489337348655
C	-2.93123366969101	15.63743039682065	7.35905327877467
H	-3.74703607080070	16.17452329521734	7.82507185202519
C	-3.01719010669405	15.17847864360295	6.03365962636824
H	-3.90576937060458	15.35442020386991	5.43795636645552
C	-1.93487399403216	14.50587996274161	5.47784733084178
C	-0.77364842550989	14.28986430967594	6.27768175300246
N	1.48200637022663	13.53366321632467	6.53612086001999
C	1.77410415378537	17.92563108826645	9.08432746963190
C	0.87540279753146	17.68807853620068	10.12471194581769
H	0.38475329797942	16.72287841905824	10.18517770138990
C	0.63409482656826	18.66701796431607	11.08258730375943
H	-0.06043460830170	18.47092762402530	11.89108173577160
C	1.29830517469143	19.88658385195147	11.01160820637875
H	1.11783369254329	20.64731582818828	11.76231766120617
C	2.20268526680348	20.12784661360947	9.97907304765233
H	2.72354156299233	21.07701573619016	9.92431456389978
C	2.43785503379963	19.15352948378577	9.01800572202260
H	3.14493233902823	19.34053064842787	8.21838037018245
C	1.19531422898845	17.20440342749158	6.36518836615308
C	0.17702832463126	18.15634475598871	6.44424119330807
H	-0.02464119609896	18.65329007929273	7.38501695820178
C	-0.59095787359917	18.45514291305145	5.32370442327717
H	-1.38626941651595	19.18746639284430	5.39987527317621
C	-0.35021489810508	17.80813192940499	4.11699530841265
H	-0.95858771894928	18.03215380180763	3.24863708551463
C	0.66526047690637	16.85948068605570	4.03072754737441
H	0.84582789887004	16.33479847949418	3.10040333267085
C	1.42897204807702	16.55199044673922	5.14759623332847
H	2.19501509647525	15.78885931262881	5.08144020809861
C	3.81274698389438	16.73531232207551	7.44658760525162
C	4.29511362367715	17.51941880836156	6.39431417937762
H	3.59602769955338	18.12140859377055	5.82661848606475
C	5.64216703979342	17.51170408533641	6.05076949914530
H	5.99179211783144	18.12617954521846	5.22978725487439
C	6.53386995300422	16.70456717768055	6.75024515433463
H	7.58235523787456	16.68429767636296	6.47782567078501
C	6.07975175505533	15.91839153977147	7.80406982773349

H	6.74887604495719	15.27698935363074	8.36404715955545
C	4.73594977988482	15.94818011830791	8.14666387771653
C	3.90399674377397	15.66900335007226	10.35724332769855
C	4.48076545048757	16.82821453959607	10.85695761444890
H	5.23286281739781	17.34759521151438	10.27661469443399
C	4.06303747871676	17.31542369738470	12.09047879879954
H	4.49899256029048	18.22888350631751	12.47635673983413
C	3.09520951834148	16.63656183012231	12.82190081340658
H	2.77213182536870	17.01653442622645	13.78336253009712
C	2.51853017410577	15.48188548243532	12.30425478199644
H	1.73755288763894	14.97356545466120	12.85572810499308
C	2.90166057953638	14.98497401966650	11.05777042426470
C	3.15545353146189	12.29954653105462	10.02457997145766
C	4.34024086978757	12.22694293265738	10.75777756305288
H	4.59605541817700	13.02416417720162	11.44627189817271
C	5.19588153138427	11.14197157883795	10.59795286615262
H	6.11687233053851	11.09329201587633	11.16779775925656
C	4.87255488874380	10.12300143427873	9.70668123188595
H	5.54129158116885	9.27924177565684	9.58145767021088
C	3.69339447031494	10.19322535887191	8.96898916073320
H	3.44307922280462	9.40839034062272	8.26475785602301
C	2.84143045537897	11.28029182864650	9.12087787250695
H	1.93602044572486	11.35458236190412	8.52855834365498
C	0.79070987552998	13.08611333832551	11.41642223748215
C	1.16840603613102	12.32914209130335	12.52908568911770
H	2.20941572560845	12.06191158881172	12.66971291150168
C	0.21210064632562	11.91207901056214	13.44652142273975
H	0.50978169286324	11.32308536740472	14.30645162627900
C	-1.12852808153122	12.24403007115774	13.25836017295978
H	-1.87289363722668	11.91350515088447	13.97360729505234
C	-1.51261109515042	12.98581955304257	12.14605027544110
H	-2.55642804298792	13.23042080356847	11.98720963126930
C	-0.55572400752937	13.40084237694865	11.22510748848826
H	-0.84393615829145	13.95245167985067	10.33688452835952
C	-1.91523879784706	14.03397731412368	4.12395212358001
H	-2.79997896395713	14.19118654197606	3.51552002721156
C	-0.82467318363885	13.41713182055881	3.60138168526393
H	-0.82785307311966	13.07616099843855	2.57106377097074
C	0.35640696538819	13.65895051445561	5.73452603187076
C	0.36273688033573	13.21376225571635	4.37863642562140
C	1.52344404941255	12.64271148940303	3.86848267615120
H	1.54818369634182	12.30375298884501	2.83871670935748
C	2.65580903581669	12.52626878528597	4.69539780932920
H	3.57792552309255	12.09243011264533	4.33129613471150
C	2.57993546701375	12.98442743994127	6.00105604269442
H	3.43844256812139	12.91647179769602	6.66060736436486

[4]$^{+}$ - S_0 (S = 0)

Eh = -4359.78575513344

Cu	1.14705950946459	14.58379729212471	8.34162563765487
P	1.90802487597823	13.71660473499917	10.23455010612396
P	1.91357624877456	16.67820606174844	7.87755812966348
O	4.16809257645531	15.06606963479917	9.01977036978133
N	-0.70374507972226	14.60104510873049	7.43962895892325
C	-1.84491224670862	15.14688405838039	7.84556328030811
H	-1.87577391807222	15.48654255981591	8.87357860452583
C	-2.96063742741424	15.29275383030697	7.01452138753089

H	-3.86325226275985	15.74151980815414	7.40799787114749
C	-2.88618216692584	14.86320933863569	5.70796173953993
H	-3.73179246729236	14.96546053087260	5.03804246748337
C	-1.69028294565230	14.29068484400532	5.23907727389675
C	-0.61869894899086	14.17982995457059	6.15095416080323
N	1.64540915666162	13.58323191145526	6.60831501112718
C	1.71029499208896	17.96276790734467	9.14825695986633
C	0.92712586277917	17.66412776193052	10.26354801486374
H	0.48791897075792	16.67654465105987	10.35160855015764
C	0.73727293349403	18.61326462131617	11.26177957404709
H	0.13552931746158	18.37211225218365	12.12974647185750
C	1.33475350419286	19.86371828860830	11.14948153830392
H	1.19310655269898	20.60342361471427	11.92833445193130
C	2.12293923479900	20.16584353327180	10.04002187912514
H	2.59101716147710	21.13935718204563	9.95623212838065
C	2.31152299233208	19.21991994729949	9.04161779957025
H	2.93165656637368	19.45320225350362	8.18432655927042
C	1.02156911502047	17.30091878986320	6.41819071764444
C	-0.06315880832555	18.16890688268950	6.56452851388808
H	-0.27892112583553	18.60233525248114	7.53375225335134
C	-0.86121803490338	18.48412312541945	5.46922945462067
H	-1.69511207506257	19.16496872691467	5.59261051272877
C	-0.58734281784896	17.93670088329391	4.22026164748846
H	-1.20721767313272	18.18841784180088	3.36822954280820
C	0.49465196888851	17.07362712498451	4.06615283476482
H	0.71849349039681	16.64883387360772	3.09493649611183
C	1.29000421649956	16.75108350076130	5.15727758671706
H	2.13069656908237	16.07948015462111	5.02888596567124
C	3.67046552152430	16.77019211893323	7.38695128989042
C	4.13843508926331	17.60445260464274	6.36635739317453
H	3.44361580028530	18.26235065381505	5.85915067151707
C	5.47345579175589	17.58209721923772	5.98052468030401
H	5.81528795674666	18.23763136018897	5.18914836500929
C	6.36454543259504	16.71334568903869	6.60317369555573
H	7.40344574418121	16.68635468393365	6.29809602823101
C	5.92477883611635	15.88186570851088	7.62818433155458
H	6.59834190322537	15.20392208757524	8.13734250087754
C	4.59449329992418	15.92832753890855	8.01689639058935
C	3.92688800946476	15.61005877136996	10.27327240969696
C	4.60878748356544	16.72233009680531	10.74406201301997
H	5.33071205602513	17.22312442168046	10.11209187732122
C	4.34052865860901	17.18410821646857	12.02849148908633
H	4.86421617516208	18.05699637527510	12.39829676585075
C	3.41510195526560	16.52979946706471	12.83355609579645
H	3.21420974582510	16.88801549471254	13.83531499108858
C	2.73220968254322	15.42216901964368	12.34441475953256
H	1.98809836202049	14.93014381371139	12.95786339370961
C	2.96658968268351	14.95285351019596	11.05083378812605
C	2.95831304424160	12.25004332259862	9.99058943508645
C	4.23159876205049	12.13002477894677	10.54873537706817
H	4.62659184141782	12.92742250947171	11.16701929449834
C	4.99272281138853	10.99000058053297	10.30984994959615
H	5.98082764441582	10.90247688834272	10.74585957012066
C	4.48586391761327	9.96387029567328	9.51873236726546
H	5.07962230677793	9.07599357708071	9.33719317931162
C	3.21459763972436	10.07851034099949	8.96038082525178
H	2.81725546436727	9.28034608761595	8.34461958425456

C	2.45712945312589	11.21993276592201	9.18809093306184
H	1.47340417232797	11.31869258381558	8.74170508964625
C	0.74352142819448	13.22423534124519	11.54242128038193
C	1.07830719059367	12.30055555273997	12.53594967892363
H	2.05281381174064	11.82694575295714	12.52572585810494
C	0.15992616409393	11.98491766373073	13.53032219331882
H	0.42253082441074	11.26528220977195	14.29644221252880
C	-1.09474400603849	12.58954643285652	13.54211030888203
H	-1.80817178655469	12.34002335352038	14.31825033871418
C	-1.43623312188894	13.50635637108492	12.55211327335564
H	-2.41566844993944	13.96981468358389	12.55472261380244
C	-0.52147669931033	13.81561170602863	11.55248681970190
H	-0.78347701959640	14.51513657795163	10.76603717118765
C	-1.51431820229883	13.83727756359186	3.89373720908872
H	-2.34655572508456	13.92951069464939	3.20584616132380
C	-0.33333879944309	13.30727965878450	3.47976904149121
H	-0.21002994005983	12.96954357494767	2.45740296650424
C	0.63032941637315	13.62825514108485	5.71087601157926
C	0.77525535181498	13.19127420696855	4.37638909507474
C	2.03115930883884	12.68217951138510	3.99652538192055
H	2.18474938247192	12.33633636298751	2.98085494912831
C	3.05239927779711	12.63556683568487	4.92146909956586
H	4.02884803941170	12.24959279903674	4.65934764346864
C	2.82073328368392	13.09909749236330	6.22211688160333
H	3.60018120952635	13.08057909201641	6.97359482357659

[4]$^{+}$ - T_1 (S = 2)

Eh = -4359.710820951739

Cu	1.38231032574932	14.70805210918575	7.84959532386350
P	2.15485250775926	13.91513478767049	9.87963074673723
P	1.90903703569402	16.96114398732342	7.98977055135090
O	4.36254396482923	15.29721454882136	8.70376561567198
N	-0.32905175176881	14.79004866779127	6.85690725829630
C	-1.40192738380938	15.59673811488794	6.99812408522917
H	-1.29566695550353	16.41502184767169	7.70028093677906
C	-2.56506314430914	15.43139411429724	6.27705358176677
H	-3.38505812934941	16.11932153890804	6.43300645951384
C	-2.65831552726235	14.39298237797970	5.33159114954293
H	-3.55674978059778	14.26081447138761	4.74128831797061
C	-1.57340380889408	13.53633932517422	5.15560610951807
C	-0.41639851927870	13.74729114805818	5.94993853655769
N	1.75476561657769	13.15851469399471	6.69244218444848
C	1.72545547781896	17.86807124094622	9.54548898182107
C	0.68184984129307	17.49634035247407	10.39651584532724
H	0.06936998919774	16.63572815135112	10.15533246905379
C	0.43214225106546	18.22131165175043	11.55415349551676
H	-0.37938957552132	17.92899394379606	12.20942305021590
C	1.23180511988544	19.31520574660297	11.87207021219210
H	1.04090090852393	19.88108466651324	12.77588426682610
C	2.28205239865559	19.67992607551884	11.03396191536977
H	2.90782045598630	20.52789414225869	11.28480144713602
C	2.53137050952547	18.96061322800754	9.87137806269002
H	3.34754799902747	19.24541643076873	9.21833524369832
C	0.91607869709692	17.88331589480629	6.78592724709552
C	0.16295928369915	19.00205523564630	7.14497655083432
H	0.20720243159630	19.38514087315033	8.15664503773624
C	-0.64878376908377	19.62226040419827	6.19945623329625

H	-1.23292997963581	20.48993332031415	6.48107660624517
C	-0.70975202218602	19.13037016587030	4.90045662424526
H	-1.34643595578093	19.61210626950282	4.16835035801144
C	0.04779976723662	18.01760081619404	4.53775006841493
H	-0.00093320405296	17.63126927346330	3.52713270365438
C	0.85382204244766	17.39171999886554	5.47561222281267
H	1.42379847341555	16.51250313710479	5.19762643654294
C	3.62041679186617	17.18616008594263	7.39405168942847
C	3.93379172864463	18.17310283663626	6.45238704225416
H	3.16270766431106	18.86081489279358	6.13021638981601
C	5.21103419639476	18.26114226842791	5.91182610897917
H	5.43382686185820	19.03294173520860	5.18589252166606
C	6.19159552446033	17.34912226377665	6.28770702565468
H	7.18223159720687	17.40317511463474	5.85345946932358
C	5.90476005023306	16.36429578658883	7.22849191944779
H	6.65124525849940	15.64589856571170	7.54294866666946
C	4.63589708730794	16.30170235296580	7.77922014583360
C	4.22333137001119	15.70820213896609	10.02479163094403
C	5.04178682151591	16.67897050678675	10.58363009145054
H	5.80447009362967	17.15603513338700	9.98179797471751
C	4.85069315918262	17.03160860726581	11.91405653327218
H	5.48204319029432	17.79104309086833	12.35861688687747
C	3.85376839031644	16.42235852020607	12.67110526797877
H	3.70105560188233	16.71122174529740	13.70306528719908
C	3.04588742427706	15.44878352602907	12.10008022429436
H	2.25329918003108	14.99450284607998	12.68014046100965
C	3.22564602160430	15.07262258948150	10.76712971641536
C	3.03183276380305	12.33249602317626	9.83541169278092
C	4.40655161056701	12.23801334382649	10.05686292333866
H	4.97496521410910	13.11715553430207	10.33315585941385
C	5.04459623313211	11.00855031865751	9.92999428097782
H	6.11058320357270	10.93617451704861	10.10886930993322
C	4.31630903895606	9.87536692139039	9.58177877277678
H	4.81649435701846	8.91946288984855	9.48442687705891
C	2.94322156832326	9.96761503698432	9.36350740029945
H	2.37444918830891	9.08660806547580	9.09267224291168
C	2.30112660369243	11.19086930394558	9.48492033417989
H	1.23521335575892	11.26407679175805	9.30290195856284
C	0.71770903899349	13.58850305818219	10.93805875809164
C	0.84487854524742	12.88203638652795	12.13990654580503
H	1.81460002796547	12.51006680507287	12.44934831492021
C	-0.27541429488922	12.64207981572035	12.92434252373830
H	-0.17367836315100	12.09751003685199	13.85523149460664
C	-1.52896666487585	13.08849272437367	12.50941591439802
H	-2.40121583331087	12.89131183071651	13.12086925928105
C	-1.66498405253100	13.76741307559515	11.30314340751445
H	-2.64173411585555	14.09245449428510	10.96606921083317
C	-0.54420637764584	14.01498239812397	10.51827441720579
H	-0.65339505126580	14.51251793160319	9.56004008388430
C	-1.53856017695462	12.44895381579441	4.21866166957460
H	-2.41583621065243	12.27316364899739	3.60647380987162
C	-0.43953878608196	11.65969938102378	4.08174884332313
H	-0.43169813216995	10.85650821391815	3.35370686535709
C	0.69294622414970	12.90997892676210	5.84014851741738
C	0.73157603556172	11.85962708466730	4.88574644904314
C	1.89861171091036	11.10573834300011	4.78657011401877
H	1.96129410279266	10.29679389064920	4.06866459803793

C	2.98808679889508	11.41132446568708	5.61836646219881
H	3.91178563223722	10.85211581398211	5.55853818027222
C	2.87293284940565	12.42437457221146	6.55172503066202
H	3.68569335240834	12.65727618052556	7.22794088849366

[5]$^{2+}$ - D^{ox} (S = 1)

Eh = -4438.157879345236

Cu	3.40656684750851	11.83124907228011	13.74735259874155
P	3.69136306122369	9.55596224724671	13.85906570480121
P	4.83694743571418	12.67762083101370	15.36605461127075
N	1.38891839834423	12.36450732266671	13.50384327267448
N	3.62395273518454	13.10198457458339	12.16041423896504
O	6.43604505175239	10.58998877179736	14.29895741253448
C	0.28522931710117	11.94644200729208	14.12530145450869
C	-0.95684022808636	12.58336986864695	13.92322510108603
H	-1.82505928393094	12.21301604168127	14.45337837862144
C	-1.05729000310705	13.64811783591109	13.06745543403925
H	-2.00672115430043	14.14572832933932	12.90773634139934
C	0.08904066725729	14.09051337595946	12.37605571082440
C	1.29694436770660	13.40798620055126	12.62816168118635
C	0.05982674430342	15.16942376679009	11.44281569389653
H	-0.87803763927784	15.68547870216927	11.27686364543704
C	1.18097599045091	15.53185816483685	10.76372065235777
H	1.15490879479597	16.34035240739189	10.04331933583079
C	2.47632066923428	13.79589636011219	11.91716082194356
C	2.41134843957390	14.84160059834218	10.97457748861373
C	3.59215028105970	15.13831164648486	10.26107031612440
H	3.58827414511260	15.93760597280794	9.52900703646967
C	4.72540690630127	14.40168129341158	10.48907637847781
H	5.63657506475811	14.59780203617270	9.93886718810459
C	4.72312549605579	13.37371680487785	11.45374415888272
C	0.35762835677635	10.77045323520349	15.04309512252501
H	1.38220637890716	10.42917293120187	15.16344369785650
H	-0.23072381227654	9.94378032221758	14.63840270018392
H	-0.05653664821853	11.01680729909535	16.02366942859991
C	5.94224902253771	12.54505468689428	11.67810829984911
H	5.85244723074617	11.97303420100386	12.59739653749557
H	6.83298894984930	13.17205429611745	11.73374813000536
H	6.07454494629255	11.84980059147637	10.84321241014583
C	5.20252170266799	8.96840678232643	13.04211126000483
C	6.43545702185850	9.49859050025037	13.43647190738301
C	7.62752068545470	9.05369448244007	12.89361110687414
H	8.56058542015901	9.50193456141705	13.21089876754514
C	7.59527716290443	8.04482346326356	11.93330555928396
H	8.52226631639877	7.68734335356710	11.50279033313658
C	6.38008916477183	7.50685688794230	11.51890366587881
H	6.35968550469413	6.72749186031026	10.76776408363554
C	5.18780051368826	7.96771165785319	12.06531237916605
H	4.24290401522459	7.55314423384429	11.73770229022138
C	3.64776630064401	8.65267882420811	15.42650146804971
C	4.01977295898845	7.30226801947857	15.45051971246067
H	4.36155142815332	6.81470446884349	14.54549955237496
C	3.95237849397490	6.58769080445202	16.63828776061558
H	4.23253942881849	5.54162757720624	16.65223551305836
C	3.52827935371507	7.21464308111236	17.80831368931444
H	3.48128359185099	6.65474411553971	18.73424997117948
C	3.17534946402441	8.56011486033004	17.79127920797517

H	2.86260345218303	9.05307233076785	18.70333012732080
C	3.23653838890018	9.27820791443392	16.60403077685778
H	2.98845135902483	10.33149687490388	16.60026880360985
C	2.33757477731155	8.93554262353622	12.83059064530274
C	1.46922200465211	7.92807205218815	13.25779179594358
H	1.61286097635046	7.45861093603394	14.22277781363068
C	0.42191996681086	7.52679105534023	12.43546758898505
H	-0.24388572308870	6.73700932258784	12.76115876947754
C	0.23259381863335	8.13146397753211	11.19569894740686
H	-0.58361923522560	7.81374707281409	10.55860642551603
C	1.09388437993061	9.14145735971141	10.76909585521063
H	0.94834581999052	9.60837272172824	9.80278387812309
C	2.14018693637638	9.54713266482585	11.58400126982509
H	2.81051889494257	10.33423205755724	11.25370290389609
C	5.70851648878318	11.44493044808056	16.34789757036446
C	6.36753300237542	10.41574635967962	15.66871040376676
C	6.93089396559715	9.34322021192656	16.33910944592837
H	7.41635706258266	8.54742281840355	15.78921094016765
C	6.85322615642997	9.31717069853094	17.72802382231708
H	7.28993810275985	8.48479001500942	18.26562845208671
C	6.23548958018680	10.35050080476786	18.43075724958769
H	6.19892127391097	10.32453761496996	19.51210334689575
C	5.65466791350029	11.40738654755178	17.74480780119401
H	5.14790613663035	12.19802576917030	18.28327630806930
C	6.03821546515409	13.84898038717276	14.70685345569858
C	5.56063984796297	15.01005668742793	14.08364996740270
H	4.49525282074781	15.20409231104145	14.03631937223001
C	6.45412503776629	15.92351912315376	13.54434446961444
H	6.08409996213366	16.82667849961495	13.07495230345663
C	7.82556322021904	15.68145503825725	13.61426834573468
H	8.52246090413346	16.39638199766651	13.19436236624446
C	8.30221516394539	14.53038627254566	14.23646079296305
H	9.36821504385469	14.35269847935977	14.30612146197196
C	7.41335512651346	13.61213608539490	14.78222926020815
H	7.78665824080811	12.72385982949572	15.27484424366448
C	3.81026124984996	13.62553183347866	16.51371226346245
C	2.50676392403388	13.19146414487734	16.77528868384858
H	2.11687517934167	12.32579349027604	16.25424423044486
C	1.71278057152984	13.87168106496778	17.68802646784193
H	0.70363088069813	13.53321871032492	17.88898320637449
C	2.21536839860501	14.99519810510709	18.33998507675668
H	1.59681528931385	15.52938590216494	19.05060985222169
C	3.51049388688911	15.43671347369018	18.07796129454297
H	3.89986718316146	16.30923573115787	18.58782271351633
C	4.30955551463267	14.76014450380713	17.16496817648733
H	5.31563753181376	15.10515774700065	16.96315384221569

[5]^{0} - D^{red} (S = 1)

Eh = -4438.597821723871

Cu	3.44911993185535	12.02225517103192	14.14155024626345
P	3.81148865062055	9.79610988707633	13.74792599752983
P	4.82273552548343	12.95243787140797	15.59738860614371
N	1.43156054435164	12.20844715767028	14.16344416188987
N	3.28042517974756	12.74593897251999	12.24446140738421
O	6.53835161549228	10.90202008269826	14.53475846473776
C	0.51491012552571	11.88679593158531	15.09945628690376
C	-0.84745524655642	12.05156444307672	14.89520686833658

H	-1.53760892955216	11.78457542136395	15.68583830535844
C	-1.31538683839387	12.54258672094397	13.66330261786489
H	-2.37694588127179	12.66843931682460	13.48205528492421
C	-0.39992599921381	12.85728120166638	12.66484127413658
C	0.98836758029556	12.68237927857818	12.93586704167626
C	-0.78188448058859	13.33121539313085	11.36660356043884
H	-1.83910629905827	13.46962019308525	11.16417146153443
C	0.14177062212233	13.59184426246107	10.40537689089601
H	-0.16699852581021	13.93934689950366	9.42472512955555
C	1.94263485690878	12.95730788777147	11.94340022069953
C	1.53844915280152	13.40544703193696	10.65040996089576
C	2.52153505043936	13.61770399655015	9.68988062599291
H	2.23896422976833	13.95740580994384	8.69912064941563
C	3.86131922257186	13.37133601714232	10.00632950600695
H	4.64428975938060	13.50947823145978	9.27106099797763
C	4.19712213903116	12.92670598360607	11.28713119971485
C	1.03555350673347	11.28704736524828	16.37226844330569
H	2.01690775062226	11.69897612411943	16.61536576030128
H	1.15754048911690	10.20579810777836	16.26032935745516
H	0.35165037477105	11.46619554222058	17.20358173328452
C	5.61779987077684	12.57947313887886	11.62557351825233
H	5.72160628105817	12.42593048815250	12.69827193193386
H	6.30816353022370	13.36363487885563	11.30854554989419
H	5.91212809660743	11.65451004516870	11.11878489560600
C	5.46154615118150	9.20948557322985	13.18466482406618
C	6.62370206666866	9.82929482475709	13.65589166928700
C	7.88496053642126	9.45980783923375	13.20839182515402
H	8.74978710065074	9.99081566494947	13.58612928065119
C	8.00897592792226	8.42659268193126	12.28768711233177
H	8.99097031513644	8.13439874440562	11.93526235790657
C	6.87147127629066	7.77132930674086	11.82415455995640
H	6.96140374781526	6.96169160779232	11.10984987727646
C	5.61549886359148	8.16406247122062	12.26817741577745
H	4.73207322999183	7.67040601410180	11.88217795766137
C	3.34180734656219	8.46560975738328	14.91581804137881
C	2.93593988244571	7.19697966477384	14.49086704139590
H	2.84066070353410	6.98904166986390	13.43180885358717
C	2.63482471824042	6.21043295779609	15.42110968011406
H	2.31606960469802	5.23076012888796	15.08383372113129
C	2.74153928585886	6.47924308829711	16.78455653451302
H	2.50564244474020	5.70769487787163	17.50850756765649
C	3.14359152161909	7.73920755483508	17.21349122055557
H	3.22457971158750	7.95808418519674	18.27173352924506
C	3.43589594847311	8.73023799780180	16.28226025790064
H	3.73953506707300	9.71509777432936	16.61409544863068
C	2.72778924903584	9.52293302315279	12.30958768247510
C	1.36156945164194	9.32503619591662	12.53963671166989
H	1.00351161141161	9.14790062597342	13.54650150768631
C	0.45368383747766	9.39716359756919	11.49151554133428
H	-0.60293480463354	9.26509046849285	11.69112094499087
C	0.89450622600274	9.67391582266889	10.20139393876478
H	0.18245913120605	9.75511699854148	9.38893264957246
C	2.25072009126530	9.87024139327500	9.96354427776245
H	2.60117162961412	10.10839106329316	8.96654076360947
C	3.16155626015244	9.79903178283750	11.00949002618544
H	4.20937550636300	9.99083210792808	10.81804407041598
C	5.63203219023868	11.64644115592614	16.57844532548907

C	6.31408703694224	10.64369464237876	15.87191718746359
C	6.75631952300997	9.48368847084098	16.49177417516516
H	7.25811409022297	8.72087767235094	15.91040987297034
C	6.52341660471036	9.31195600997347	17.85268026177531
H	6.85793365333619	8.40342254140775	18.33865938709214
C	5.85821962891744	10.29296047028960	18.58007145885347
H	5.67331915998602	10.15675524290432	19.63873488679883
C	5.41390940114663	11.44844095759243	17.94390298343172
H	4.86825465967559	12.19713217771923	18.50429074565395
C	6.18254672556295	13.97742210473530	14.93765110507279
C	5.82890007202840	14.96241400411507	14.01008237052709
H	4.79249484922116	15.06057547514501	13.70460782431185
C	6.79999726380600	15.79050178320128	13.46379802507061
H	6.51663167945083	16.55055035300023	12.74494373872618
C	8.13585592105572	15.63151303677183	13.82560582399184
H	8.89561780044994	16.27186498880929	13.39266509235240
C	8.49367764682031	14.64524196642065	14.73940696680950
H	9.53285288440573	14.51597558050518	15.02016579041884
C	7.52029045129313	13.82194807196653	15.29741782277015
H	7.80191249934443	13.05320654065966	16.00772898171241
C	4.11192174541743	14.09168752830627	16.83707325735762
C	2.75077512247499	14.38579410616798	16.74630990691904
H	2.16082618987411	13.91954423206064	15.96451187643100
C	2.16679289319469	15.28199778813778	17.63766326541188
H	1.10946576427928	15.50614117999020	17.55838759836217
C	2.94057301105725	15.88926240230994	18.61990797028950
H	2.48697116743344	16.58755879337122	19.31392665243060
C	4.30481735839740	15.61218718116215	18.70479391960799
H	4.91141952671690	16.09737939588217	19.46090027247609
C	4.88991955109943	14.72330609773829	17.81328492647847
H	5.95446940252969	14.52437272965238	17.86652768082204

$[5]^+$ - S_0 (S = 0)

Eh = -4438.471551175498

Cu	3.47640153525550	12.00418134023041	14.15877006469101
P	3.78455608318137	9.77992317141245	13.72187797430361
P	4.83772176823704	12.97657398156522	15.62901764633417
N	1.41458400003671	12.20789741191113	14.12429700217054
N	3.27146973990182	12.76740130876173	12.24022555284214
O	6.48774995697675	10.90572715396495	14.50569512052472
C	0.52310424630948	11.86420415973480	15.05333153503809
C	-0.86101178312571	11.96917239774984	14.81066153803188
H	-1.55443523141035	11.68667410246562	15.59290476085941
C	-1.31568726432362	12.42476677314760	13.59803017528964
H	-2.37793803342380	12.51108789927715	13.39998614759541
C	-0.38971779304248	12.77566827928037	12.59694917170419
C	0.97906259598407	12.64412455761634	12.91185322429883
C	-0.77784460139936	13.22989658931104	11.30040374048489
H	-1.83436654855209	13.33200431761834	11.08210028581237
C	0.15652905390583	13.51877643810114	10.35618574951190
H	-0.14052794235360	13.85518007592018	9.36978921966550
C	1.96411044756456	12.94617537888414	11.91476231453509
C	1.54843843264419	13.37270629502988	10.63683388529525
C	2.55645198073846	13.61838588331228	9.68395778966420
H	2.28385011595524	13.95316663142562	8.68959584234963
C	3.87018308959681	13.41542796152192	10.02252982990182
H	4.66124919408964	13.58364647529434	9.30231648882356

C	4.20957996839667	12.97331978245158	11.31811148712455
C	1.03208398930631	11.33437243505274	16.35683107630655
H	2.08932791783211	11.57107916247851	16.47133880633139
H	0.92341202706520	10.24654833354042	16.38798344088423
H	0.47268219229251	11.75005058924486	17.19684746208552
C	5.63302734991143	12.68797923055166	11.67811351781738
H	5.70679786885414	12.39134198680195	12.72228095298024
H	6.26268519213189	13.56509213706543	11.51534238052150
H	6.02370670756911	11.88102338613716	11.05140711564594
C	5.43161320362024	9.19812122524983	13.16880358674165
C	6.58987090625924	9.82649051701663	13.63551828488925
C	7.85278516533442	9.45054554208099	13.20034605005396
H	8.71804431984048	9.98290705228357	13.57481627516422
C	7.97866742331285	8.40009439087521	12.29917240232205
H	8.96167065432464	8.09966477235949	11.95789458645715
C	6.84356334526571	7.73408549622805	11.84395244861307
H	6.93832574040530	6.90875906134852	11.14923988716796
C	5.58525463393368	8.13300067256212	12.27433192104298
H	4.70521325947421	7.62542683463313	11.89897758535279
C	3.28411609852565	8.49811190227194	14.91972941896283
C	2.86069845816311	7.22680328328666	14.51884922569569
H	2.77384651401641	6.99141162049794	13.46489490619533
C	2.53631279162940	6.26824498035014	15.46973483828056
H	2.20417322331511	5.28674640273108	15.15310581538104
C	2.64110366896426	6.56621366481022	16.82721716576458
H	2.38952594125600	5.81506832612557	17.56638042661899
C	3.06852980005820	7.82631851040151	17.23126436701816
H	3.15695503812037	8.06243866422195	18.28487823062701
C	3.38411485926123	8.79091678276697	16.28067577222248
H	3.72033483736316	9.77104328106335	16.59462027577619
C	2.70900535372860	9.51178723719357	12.27536853452896
C	1.34282850161807	9.28706232368539	12.48009996520603
H	0.97304408917195	9.09139972275022	13.47962409346189
C	0.45474884880067	9.32045685085663	11.41207053880116
H	-0.59944515042691	9.14118472321202	11.58684363870510
C	0.91527042807193	9.58551812172010	10.12593652494462
H	0.22179745998561	9.61408291157881	9.29438798576194
C	2.27191851004418	9.81054560921221	9.91345082234388
H	2.63986543407274	10.01496002420325	8.91505710067690
C	3.16286447414264	9.77647369734303	10.97899644068393
H	4.21504545348667	9.96170341855996	10.80324944343005
C	5.64856441763722	11.64873187213053	16.57699103178356
C	6.30924507855006	10.64716619147970	15.85207266906594
C	6.76821459309846	9.48770346408853	16.45990465283176
H	7.25883504847258	8.72466280956803	15.86985690695741
C	6.57344128160079	9.31994105643087	17.82714758723647
H	6.92596317328828	8.41459780493308	18.30564172388236
C	5.93077284409426	10.30175194448284	18.57296502317785
H	5.78188253704001	10.16905484247456	19.63724838546831
C	5.46910192227712	11.45648880393059	17.94874881454554
H	4.94571369909012	12.20887903292595	18.52472988575850
C	6.17883983124580	14.00622628013252	14.94450116096348
C	5.79992430151642	15.07912205214806	14.13132786714652
H	4.74811179506927	15.25884498364740	13.93403655520550
C	6.76247719121167	15.91264291501391	13.57867725131059
H	6.46112536153043	16.74710458143302	12.95648126562475
C	8.11345252234554	15.67338488039627	13.82275386131448

H	8.86595009500861	16.32071709181607	13.38877628118044
C	8.49411745177320	14.60611417260042	14.62935067083781
H	9.54364868369364	14.42196439356168	14.82618925033118
C	7.53035462095112	13.77511867703351	15.19324476180143
H	7.83117764760987	12.94940951493471	15.82651677372350
C	4.13922540451748	14.09558627852596	16.88597072606189
C	2.77425148646100	14.38131466383474	16.85021058380937
H	2.15822379969173	13.92344239155696	16.08542809816765
C	2.21643360616044	15.26395797991546	17.77061420004472
H	1.15630803256368	15.48527776586918	17.73419861835065
C	3.02291331202443	15.86674172461517	18.72909970727333
H	2.59107585293719	16.55456196658165	19.44616973542208
C	4.39110281529685	15.59951596191799	18.75930172887707
H	5.02184625599679	16.08201133631056	19.49626781025650
C	4.94948281750448	14.72425068010677	17.83814901281528
H	6.01662397849538	14.53409963526109	17.84965954045494

[5]$^{+}$ - T_1 (S = 2)

Eh = -4438.387213389165

Cu	3.37102446610548	11.96932691307158	13.86719299072590
P	3.61881160963965	9.65263702506924	13.91419074616021
P	4.88623217324836	12.78560733935232	15.43614569751758
N	1.41785964463859	12.24661157776715	13.59045321024186
N	3.57108709805492	13.10017559510842	12.23213456760196
O	6.42886838399564	10.69119816768285	14.34638444067247
C	0.33110092632503	11.80314833980381	14.28334022977083
C	-0.94889117295575	12.22156128628572	13.97300184631241
H	-1.77511238859925	11.83986092405599	14.55827547743823
C	-1.17648166265484	13.10629070057488	12.90807829970617
H	-2.18130564440115	13.41730625525922	12.64983793824979
C	-0.08925771467191	13.57754724051323	12.17801872418347
C	1.21107370410179	13.13287165333291	12.54008492754797
C	-0.21096503920413	14.48251026108185	11.07488619730616
H	-1.20226713283419	14.82790471855418	10.80425768016993
C	0.87741828552829	14.89436977990483	10.37248559692105
H	0.76447531778980	15.55770759079152	9.52336673592405
C	2.32997943605295	13.57711784631375	11.83322258969145
C	2.19134806172158	14.45132435225677	10.71958848452608
C	3.33921410479128	14.79954276452143	10.01278409254340
H	3.26940965828072	15.47477498481460	9.16820489749159
C	4.56675185950549	14.24147173216103	10.38103124920137
H	5.46547152844479	14.45592934700276	9.81760203283545
C	4.65335176999514	13.38940003201218	11.47652716109896
C	0.56134672000629	10.85497388904519	15.41402704600555
H	1.19570205479511	11.30848888859371	16.18060674954825
H	1.05128834506737	9.94235270809959	15.07156652731094
H	-0.38477250377765	10.57752627088785	15.87688514306282
C	5.94075598619671	12.69973937638784	11.79889029320526
H	5.94035812613572	12.31976990568888	12.81567311169307
H	6.79294571471003	13.36698057114366	11.66906812917603
H	6.06916826365070	11.84829450751481	11.12222239525188
C	5.14331968182963	9.10676561831633	13.06965118344658
C	6.38180735692690	9.63901949456358	13.43990079904417
C	7.56050665446775	9.23432717857310	12.83582230482680
H	8.49361295175828	9.69136017779215	13.13994357637303
C	7.51478704679897	8.26588556624870	11.83760646727465
H	8.43195589474561	7.94539395453024	11.35934589992430

C	6.29452879960674	7.72320659865443	11.44743012943952
H	6.25580122454172	6.97702674856557	10.66379858578566
C	5.11752172794490	8.14438500956018	12.05539127495490
H	4.16657002167890	7.73618744799489	11.73715127837680
C	3.56645481666952	8.59934790430031	15.39437756683929
C	3.89968050483199	7.24312651787527	15.30265543540590
H	4.19898638581383	6.82073721663998	14.35094396797127
C	3.85403538435596	6.43880038859475	16.43303017439669
H	4.10752317327936	5.38832587939254	16.35681682250731
C	3.48408700515997	6.98189593471102	17.66157498682372
H	3.45197970385321	6.35286957764348	18.54298742736127
C	3.16688486239775	8.33243234254384	17.75881099062002
H	2.89588554572831	8.76148089663546	18.71548407522311
C	3.21062693661150	9.14060484520157	16.62938079735324
H	2.98443749053674	10.19469797369658	16.70951229710085
C	2.29481324521126	9.08745454907242	12.80897906432023
C	1.39004943374681	8.08405440648903	13.15430462248099
H	1.50646749207203	7.54388205986162	14.08592342201987
C	0.32771256808724	7.78792080603279	12.30456106827692
H	-0.37649465289646	7.01144448486144	12.57744606371736
C	0.16780312623687	8.48982417572901	11.11428933649268
H	-0.66599630919763	8.26799173084049	10.45980190609728
C	1.07543407875787	9.48753150404496	10.76385461635873
H	0.94963638120595	10.04147988916342	9.84169040215705
C	2.13105140683404	9.79069577436435	11.60861356689779
H	2.81974611387261	10.58763040310237	11.35082409357744
C	5.67613526110362	11.47999846144838	16.41495588582609
C	6.30281664367593	10.45344116528141	15.70118561740622
C	6.79483383426136	9.31763894504565	16.32472078494517
H	7.25311963895926	8.53078234116188	15.73961445526482
C	6.67675227328222	9.21620203964773	17.70653326255236
H	7.05254004714627	8.33294462147419	18.20767912036220
C	6.08273543317453	10.23604950847261	18.44551447974028
H	6.00063067990943	10.14905889343111	19.52149015653431
C	5.57542733328197	11.35857167436898	17.80288386948045
H	5.08221152870789	12.13573447341362	18.37261340891402
C	6.19651519237814	13.88799622040275	14.84477401986222
C	5.80320253117475	15.04541626617551	14.16304458807577
H	4.75049239429806	15.26402312182621	14.02572350201929
C	6.76273590081503	15.90972299564168	13.65664640908753
H	6.45507419173696	16.80385228246631	13.12843874900235
C	8.11661658607265	15.62393607754350	13.82375441197842
H	8.86491012202513	16.29857501031577	13.42572795932909
C	8.50836460245539	14.47551523717018	14.50490943406873
H	9.56055936271994	14.25841900407650	14.64402796710616
C	7.55121648106138	13.60472396677419	15.01484941912582
H	7.85760575575877	12.71225979794213	15.54590796839303
C	3.97398859063642	13.82163727410306	16.61537054835303
C	2.58041381780299	13.86589920004891	16.55808862263028
H	2.05586498297764	13.30481626085325	15.79362581070610
C	1.86893776247160	14.65899117305189	17.45257735363952
H	0.78775137841665	14.69466072564139	17.39769847991384
C	2.54951856104294	15.41101632479916	18.40363721606492
H	1.99735922037738	16.03060055901041	19.10000239237311
C	3.94267428899318	15.38489914808003	18.45250627570447
H	4.47167491991048	15.98474675464576	19.18317000364110
C	4.65698211572690	14.59996735988013	17.55778842110226

H	5.74043353449366	14.59734451555351	17.58065199425623

[6]$^{2+}$ - D^{ox} (S = 1)

Eh = -4595.49037254323

Cu	3.47415494985438	11.95887612890035	14.04691396853444
P	3.79171249266927	9.66994480714310	13.80121242212776
P	4.99211647200609	12.84870510032281	15.54304270062479
N	1.39801339440569	12.08092585104696	14.02877610908290
N	3.27111198964417	12.84898415005295	12.19304995025235
O	6.51860434358100	10.76378226606939	14.46865395156110
C	0.50409249247815	11.71406496175790	14.95238927784582
C	-0.87823168271855	11.84728465431664	14.70725997709138
H	-1.57836065391466	11.55463417847439	15.47811286824813
C	-1.32750799049163	12.32898045375904	13.50615641689024
H	-2.38909951971586	12.42076347932182	13.30730161352677
C	-0.39885281709550	12.70707082431862	12.51542035195538
C	0.96923883303609	12.57806604206210	12.83183005602951
C	-0.79554128640232	13.19512693493683	11.23628317824701
H	-1.85312170469009	13.28828027595140	11.02093161938610
C	0.13680809423816	13.53012853675336	10.30481000001004
H	-0.16082193549404	13.88984074477611	9.32724597273656
C	1.95174763384383	12.96218699534448	11.86189420643760
C	1.52742567770048	13.41626776266890	10.59635351877449
C	2.52915223126383	13.72365427400432	9.65285437320451
H	2.24603260368635	14.07275405766148	8.66645225186200
C	3.84715535389919	13.57015987063073	9.99122300709514
H	4.62774912238827	13.79547136634967	9.27693095309510
C	4.20709573042855	13.13365472381875	11.28371551696316
C	0.97786468585481	11.14913055015675	16.26647374747458
H	2.07024404523877	11.08928357526886	16.20836817589767
C	5.65914096253253	12.98651088803099	11.64851107285838
H	5.69691991691547	12.72905352675089	12.70983129094980
C	5.39208092357594	9.11551336242990	13.13859332238380
C	6.58186130418297	9.69076037273294	13.58814347826388
C	7.81635287865528	9.27817828196488	13.11439043426311
H	8.71424990896344	9.76313953235549	13.47591223707874
C	7.87325243713700	8.25145891898904	12.17783390159339
H	8.83348875273806	7.92200981014671	11.80125755080899
C	6.70151723292852	7.64780619891010	11.72785076858267
H	6.74719263670336	6.84372089865354	11.00442885285035
C	5.46941551328348	8.07565842899083	12.20345580355857
H	4.56178033377824	7.60925303858316	11.84209465709869
C	3.35126400864529	8.45431567501871	15.06780150569436
C	2.90522544029269	7.18191346042444	14.68597508852137
H	2.75990967702773	6.94257162006908	13.63985991101644
C	2.64314661548517	6.22390360644730	15.65519954512753
H	2.29449381642489	5.24233995277909	15.35877740388481
C	2.83449055648829	6.52172746116061	17.00338266814119
H	2.63049903976882	5.76971380428219	17.75563633553162
C	3.28819919322048	7.78044977939523	17.38170320788830
H	3.44155880738455	8.01359644929620	18.42812167299226
C	3.54411984644919	8.74794107557697	16.41788784718068
H	3.89541606223965	9.72578225698255	16.71757053178782
C	2.61405463228682	9.47326972090405	12.44033621715061
C	1.27554089167459	9.15398801963962	12.70888383064442
H	0.97109067542611	8.90326709788021	13.71558966463260

C	0.33858921772502	9.14942700627202	11.68696292492148
H	-0.68979019458679	8.88829686393601	11.90382115421039
C	0.71976739228028	9.47290957638474	10.38591027851303
H	-0.01354837953770	9.46658245633920	9.58897654613543
C	2.04628517599220	9.79617345632223	10.11043113392904
H	2.34892094613634	10.04050985088009	9.09977174540267
C	2.98709712203280	9.80419935986851	11.12952901697607
H	4.01338925816723	10.06218298096063	10.90753952738005
C	5.70489310123892	11.51498642876151	16.53103725574445
C	6.37112850058313	10.50972123922486	15.82131710885561
C	6.85153539169762	9.37019410918930	16.44561154992908
H	7.34978069204578	8.60016164707044	15.87119797888137
C	6.67142134160676	9.23876609611098	17.81941380626950
H	7.04698951816156	8.35486454466940	18.31953851739187
C	6.01324955558393	10.22521178899676	18.54938654324495
H	5.87804807075740	10.11227490829699	19.61741258865701
C	5.52315104690893	11.35675164902447	17.90770260562486
H	4.98456033819371	12.10793081254716	18.46994182055726
C	6.35551554397055	13.92656093587632	15.00667010654263
C	6.03440084174945	15.25004539611732	14.67122608037378
H	5.00217073172115	15.57898796090302	14.68095822541106
C	7.03997870755818	16.15484991956601	14.36544480472939
H	6.78594106912983	17.17975819848228	14.12477300281884
C	8.37180916961013	15.74758607544280	14.37785391334492
H	9.15735692296298	16.45591641523192	14.14535711272405
C	8.69409721040211	14.43119911181451	14.69934410379192
H	9.73035539893901	14.11715171407973	14.72475000114567
C	7.69311692820212	13.51982581021734	15.01178824651680
H	7.95835080831081	12.50936473235959	15.28689933251668
C	4.08541035871575	13.98825495068691	16.62455441616413
C	2.82993807578265	14.44448851131644	16.22041119372948
H	2.35816460588078	14.01991690187366	15.34164362396722
C	2.18860595699082	15.45532912696063	16.92994871276919
H	1.21957486715916	15.81346413557490	16.60417170331469
C	2.79412307077342	16.00306233394289	18.05433228974361
H	2.29596999831242	16.78760775779077	18.61041091723180
C	4.05157558434271	15.55602086567568	18.45939902348398
H	4.53059521098740	15.99518251451345	19.32577636662738
C	4.70698940454357	14.56771570697707	17.73938955329726
H	5.70793757922927	14.26867073376899	18.02616738489493
C	0.58903594993860	12.06233423457049	17.44059414139091
H	-0.49675165656801	12.11925211428011	17.54419981077300
H	0.98846959720150	11.64669962732644	18.36759064909970
H	0.97870471626569	13.07130262671691	17.32211222656309
C	0.40027116335853	9.74615872286514	16.50847466940388
H	0.69845990955141	9.03424600050213	15.73962828825183
H	0.75380105582244	9.36595052774909	17.46698900462128
H	-0.69032109685026	9.77856486301328	16.54709686007409
C	6.41264771588897	14.30516485062477	11.42346236109822
H	7.41073741091868	14.23279999779718	11.85665875390514
H	6.52372769609379	14.51420719431909	10.35724786226476
H	5.89960773987694	15.14620559495891	11.88775394732813
C	6.33089934009268	11.86209250817842	10.84496950638686
H	7.38482907358696	11.80164580906190	11.12103000283972
H	5.88022691988674	10.88905784663098	11.04027922759042
H	6.27729484677035	12.06061141311313	9.77235170720397

[6]^{0} - D^{red} (S = 1)

Eh = -4595.932493053311

Cu	3.47448213288617	12.02106822380316	14.08262781303719
P	3.78449303926435	9.76601439161998	13.72122116260418
P	4.86592263741428	12.94947150531715	15.54367467154002
N	1.43440137234116	12.16774661343344	14.14058835472047
N	3.26086738401260	12.69028553809614	12.17076732719044
O	6.51558188108213	10.84600076072936	14.49714274988357
C	0.52742496502117	11.86749390125130	15.09315579799456
C	-0.83808790420015	12.03253407827752	14.89863080518668
H	-1.52247054845035	11.78597698607469	15.70046517945707
C	-1.32136990346099	12.48131878747378	13.66060433275299
H	-2.38533207332148	12.59874799116967	13.48729732864506
C	-0.42050798308781	12.74484392169854	12.63575080582653
C	0.97369277794793	12.59074991132035	12.89644475403933
C	-0.83056711091056	13.13773893439620	11.32071392754423
H	-1.89248870010758	13.25597823672754	11.13065657388333
C	0.07396045356195	13.34108912966658	10.32958868321393
H	-0.25222334862670	13.62235338345631	9.33347022619530
C	1.91103640352683	12.82845321523784	11.87666938414090
C	1.47611082376031	13.18690499352111	10.56479619395324
C	2.43529962800302	13.35214861647257	9.57262510338623
H	2.12658004636116	13.61065420732562	8.56540475860860
C	3.78743164755736	13.18234872653348	9.88625508886112
H	4.55138884649759	13.31546873169660	9.13096978021099
C	4.16076725082114	12.86886313914285	11.19273585530225
C	1.03996951712055	11.26650859512286	16.38510602561450
H	2.13163266532876	11.22856557572932	16.29152979527736
C	5.62202091970495	12.77543638835898	11.57113868716113
H	5.64661624161889	12.48624401767706	12.62610273892549
C	5.42547460703844	9.16112254933799	13.15106354723117
C	6.59332038876112	9.76395239297299	13.62796130875209
C	7.85201858323862	9.37030606628930	13.19497012628899
H	8.72304774005821	9.88815590449639	13.57678032398307
C	7.96622670240100	8.33306802751088	12.27786878860907
H	8.94579532343220	8.02430693417097	11.93317113257554
C	6.82162757537058	7.69513218826852	11.80759981175357
H	6.90419065111358	6.88216609728901	11.09627478357065
C	5.56878948175908	8.10704599873873	12.24268937765554
H	4.68034478329365	7.62243910304490	11.85706590238656
C	3.34424229972687	8.41909397084712	14.88666984620355
C	2.88781417899468	7.17102049933386	14.45070788820124
H	2.71959750559714	6.99848291742533	13.39454985902821
C	2.62994083852515	6.15950594615614	15.36683794761960
H	2.26927895960716	5.19796357897630	15.01977185255671
C	2.83718626767887	6.37862217784407	16.72736453159488
H	2.63681799746269	5.58744802141986	17.44066562893988
C	3.29306394486589	7.61607015516649	17.16645642360120
H	3.45033672193458	7.79856829991888	18.22302654074148
C	3.53645403575591	8.63407105707859	16.25109896651883
H	3.87270556301379	9.60206084726370	16.59914391190652
C	2.67810984359093	9.48027419710108	12.29981601043584
C	1.31414609151823	9.29725329194656	12.55390136862494
H	0.96806344927957	9.15856196988542	13.56993623915532

C	0.39120405501894	9.33163445236330	11.51748984560678
H	-0.66255977580376	9.21150508639143	11.73831324812840
C	0.81443933686832	9.55442266898213	10.21138779871056
H	0.09163817591768	9.60515219166009	9.40601693585317
C	2.16772011306700	9.73589432422874	9.94855828955764
H	2.50649957711543	9.93298164635584	8.93873038304158
C	3.09265009150219	9.70430198090285	10.98420422060647
H	4.13595297167689	9.88602198737447	10.76710468118630
C	5.60996190954906	11.61094893755133	16.53562950775580
C	6.29259203155588	10.60223885827340	15.83864963520653
C	6.74028241940312	9.45043740156289	16.47032064882837
H	7.24754671263420	8.68529273406232	15.89695537722518
C	6.49948149472442	9.28706044804146	17.83035945182839
H	6.83712350663376	8.38459774211054	18.32527548710123
C	5.81461186052830	10.26480999910793	18.54409491660487
H	5.61544403564919	10.13122890524870	19.60047432957984
C	5.37172941034999	11.41514774018736	17.89767929635810
H	4.81133801060252	12.16009031652712	18.44815566004817
C	6.28918325356909	14.01018785061214	15.06873011781093
C	5.99200582287192	15.29736524852738	14.60699376415935
H	4.95793251207220	15.61426935392443	14.52927570274087
C	7.00843006931691	16.17649813572805	14.26124271674918
H	6.76096998582698	17.17153481626161	13.91009327937928
C	8.33917425587113	15.77775032183924	14.35481396273680
H	9.13363620591664	16.46146215297241	14.07964000355906
C	8.64221096900567	14.49839708400797	14.80746843083200
H	9.67580986038326	14.18202643316753	14.89092352435591
C	7.62450466757052	13.62010614096479	15.16891533163940
H	7.87712198316264	12.63695127039105	15.54182654399403
C	4.09464211685896	14.10344952127820	16.73366041820201
C	2.80766238688983	14.55168561962778	16.43688755345011
H	2.28214017490081	14.11856376833860	15.59185473866758
C	2.21338003198848	15.54536057037584	17.21154487200737
H	1.21583498568343	15.89180785155745	16.96784671759141
C	2.89777168318988	16.08428466622028	18.29374408045902
H	2.43579196505885	16.85515892143796	18.89972081569849
C	4.18649446362797	15.64247694849507	18.59437436846891
H	4.72640245385800	16.07243453263672	19.43020703904478
C	4.78849739247408	14.66870205810916	17.81018285265224
H	5.80758646642942	14.36237684732588	18.01705747203345
C	0.66890662391718	12.09527734074584	17.62076436836715
H	-0.41655984651454	12.13670028209322	17.74427367762884
H	1.09014839160388	11.63530890107774	18.51949140070586
H	1.04328740328656	13.11512803612812	17.55409507330945
C	0.50070812030988	9.83943182743351	16.56099727607567
H	0.76156915884428	9.19830727815367	15.71908465383343
H	0.91069547419395	9.38520512109099	17.46598105327604
H	-0.58816901523532	9.85685162182520	16.65169214380973
C	6.29635753654186	14.14597117904814	11.41985174388632
H	7.29126645561197	14.13228632627752	11.87122491587355
H	6.39915595393898	14.40849402339326	10.36328096624744
H	5.71272959891602	14.92559155335113	11.90774768117150
C	6.39009983199742	11.73180164579185	10.75299144960409
H	7.44103566089730	11.72419647267825	11.05307170388600
H	5.99696453128077	10.72588605889741	10.90170844858932
H	6.34586902320481	11.96350842346778	9.68570962318275

$[6]^+$ – S_0 (S = 0)

Eh = -4595.808419331483

Cu	3.49680396390942	11.98248111300488	14.10089584461542
P	3.76907549669182	9.73899335054351	13.69324615804376
P	4.87542442701416	12.95943462663394	15.57485622211605
N	1.40880706442856	12.16153419139120	14.10934418517278
N	3.24596934289350	12.70557214767503	12.17215847475036
O	6.47374121608603	10.85001940308962	14.47257962966393
C	0.52307312190502	11.85206376528687	15.05805232275768
C	-0.86079039139264	12.01385279874550	14.84335289421443
H	-1.54799975191163	11.77696101936245	15.64501963434260
C	-1.32690621187684	12.45008613590485	13.63050399776817
H	-2.38960256924330	12.56784202656012	13.45137536383111
C	-0.41238363227774	12.72572135638625	12.59670305056335
C	0.96035943429361	12.57729487385110	12.89108124725154
C	-0.82571339038300	13.11748333682450	11.28860812816086
H	-1.88580388593894	13.22656587748262	11.09189221024298
C	0.08929510067458	13.33281821193482	10.30787607052818
H	-0.22382565859013	13.61558967036786	9.30968280958249
C	1.92774652624007	12.83431495322930	11.86198687161789
C	1.48394511729135	13.18984800945274	10.57018457243810
C	2.46802135723965	13.38127023270991	9.58171994210847
H	2.16943252489216	13.64454541643689	8.57334622955299
C	3.79061782677927	13.23291353913981	9.90850708137437
H	4.56198309949668	13.37902215032678	9.16352416404799
C	4.16490041230350	12.90172909972424	11.22679813328061
C	1.01613570508060	11.26380136053878	16.35607701479277
H	2.10798268749162	11.22053544100309	16.27981370390600
C	5.61977901373414	12.80975325727647	11.60651517096884
H	5.64679970625099	12.52884952547497	12.66292375783949
C	5.41095057071552	9.14967071074746	13.13234197299695
C	6.57208772691773	9.76383354061319	13.61013110546937
C	7.83418517800103	9.37069407850124	13.18881332174152
H	8.70312858751019	9.89041013276037	13.57258562188518
C	7.95563244952055	8.32382508715992	12.28321063687298
H	8.93781888196564	8.01283981125326	11.94923425960485
C	6.81656375362646	7.67464249143067	11.81394969535184
H	6.90762075596910	6.85162305240346	11.11603722968638
C	5.55939678676279	8.08390508931851	12.23813431709637
H	4.67654650133430	7.58334796698523	11.86001318111182
C	3.31783739065746	8.43723494962599	14.89338594045183
C	2.84843981404112	7.18442476368626	14.48484852780200
H	2.68169891933677	6.98484667171192	13.43329901810067
C	2.58147073127197	6.19802430986960	15.42511151414841
H	2.21081844127979	5.23269903392539	15.10156572851431
C	2.79755479921583	6.44584805288096	16.77928463279270
H	2.59318928424656	5.67270025817286	17.51025308594698
C	3.27334938841104	7.68591580181133	17.18937889421611
H	3.44421005137597	7.88586484147143	18.24035381765513
C	3.52391380675905	8.68136200819200	16.25181077568389
H	3.88238771428581	9.64889179872549	16.57870540780482
C	2.66495201780067	9.45275457009856	12.26931699804783
C	1.30064182667284	9.25078054985531	12.50947380506787
H	0.94940899036639	9.09543771647952	13.52181965461803

C	0.38846720312541	9.25532726778689	11.46210484683945
H	-0.66305222601339	9.09480147167852	11.66814033847516
C	0.82207332546841	9.46871884175778	10.15717394540728
H	0.11035872660613	9.47503921935993	9.34069627081815
C	2.17546597009028	9.67095699070883	9.90809836823352
H	2.52434488960453	9.83670817122477	8.89582499623169
C	3.08974800099854	9.66650266737498	10.95450124180051
H	4.13673707164675	9.83726185843985	10.74444688842749
C	5.62886334022674	11.60691372990502	16.53845392975744
C	6.29743388374222	10.60385356665429	15.82280516600431
C	6.76448367614084	9.45256169012688	16.44018911900224
H	7.26437029815031	8.69053564426639	15.85671379382793
C	6.55868564185710	9.28788624118357	17.80572740310798
H	6.91700645315919	8.38886393892520	18.29170854616502
C	5.88869390320766	10.26119980132921	18.53868207802947
H	5.72202141873795	10.12724453676092	19.60023031885052
C	5.42550095517113	11.41083272765648	17.90619466422555
H	4.88138729219770	12.15456915156809	18.47377872545376
C	6.27964729811247	14.02205786809539	15.05642255779999
C	5.97146793985980	15.32198267922798	14.64051697352697
H	4.93792804002898	15.64930491138172	14.61467392900018
C	6.98080333857506	16.20650233288774	14.28664311040211
H	6.72884253167439	17.21397993840691	13.97756252394662
C	8.31176124488121	15.79976037864049	14.33020707122308
H	9.10058893457297	16.48923629562255	14.05473953653605
C	8.62419615084650	14.50814399976327	14.73892101049853
H	9.65869376525030	14.18905898839786	14.78744021616832
C	7.61470114453985	13.62262170531229	15.10670807581877
H	7.87494943329531	12.63086732247960	15.44955268647960
C	4.11800343024599	14.09924064156548	16.77937575880718
C	2.83412211073126	14.57137946030401	16.50815823049100
H	2.29555722922894	14.17047945208961	15.65674292352486
C	2.26117761667612	15.55673255223571	17.30841838392459
H	1.26706532399004	15.92523848773457	17.08415468490896
C	2.96669047880643	16.06544993955533	18.39183288369541
H	2.52278448078373	16.83015247078177	19.01784218245362
C	4.25446260720658	15.60415804915849	18.66466252015476
H	4.81130103064176	16.01320507699997	19.49917444109057
C	4.83463464430190	14.63851403764078	17.85477636368874
H	5.85336177854218	14.31977283174815	18.04194287506163
C	0.62265615487184	12.11006115586793	17.57405461723329
H	-0.46390455059114	12.15037357169092	17.68607673381409
H	1.03101209495234	11.65573611229611	18.47937259619520
H	1.00143680818412	13.12787465555717	17.50503807869613
C	0.46105905739735	9.84035528720015	16.52596979840185
H	0.74357918132854	9.18826603809050	15.69991761381978
H	0.84768358244598	9.39978565334306	17.44557407014511
H	-0.62935296401240	9.86022108533706	16.59483880971460
C	6.29074783545489	14.18126964984667	11.43821544798525
H	7.28763447303141	14.15985812823014	11.88103632885009
H	6.39040767466381	14.43746512556242	10.38012382280806
H	5.71985058512435	14.96682077428585	11.93112505647784
C	6.37770411854939	11.75709775865071	10.78814488414295
H	7.42747685663505	11.75275740781665	11.08645522178472
H	5.98447584873024	10.75329983350057	10.94669250331284
H	6.33566198719730	11.98293096794679	9.71963703055586

$[6]^+$ - T_1 (S = 2)

Eh = -4595.719742787328

Cu	3.42767881040591	12.00539085492498	14.02113063856509
P	3.70321332447700	9.66554278261454	13.84775542776740
P	5.00236251207191	12.94311658925859	15.45783001280449
N	1.44259266138595	12.02834094757814	14.01577259228344
N	3.27078467929252	12.91824687355282	12.24445902398369
O	6.46809314653673	10.78118095157154	14.45852502757024
C	0.54021347087500	11.58532749375286	14.93146034189916
C	-0.82015521652372	11.64838982163653	14.68382762454689
H	-1.50795872294576	11.30420863921893	15.44432823015218
C	-1.30642962143571	12.13053151581884	13.45940600719047
H	-2.37007314501663	12.14737340801722	13.25465133057379
C	-0.40479669616299	12.57837661121797	12.49905990792516
C	0.98237462254573	12.53153046236158	12.80479290762300
C	-0.79670755111715	13.07256616547637	11.21565722167385
H	-1.85495346383457	13.11773702378606	10.98439673043601
C	0.12765412258168	13.46914295831269	10.29997098256067
H	-0.18158328030412	13.81675148027698	9.32068234692094
C	1.92951941459654	12.97945005583212	11.88274851172395
C	1.52443366632676	13.43189100935656	10.59510044577878
C	2.51322275325028	13.76830376320991	9.67591906172976
H	2.23736010485948	14.11585988749564	8.68728876176632
C	3.85567310645227	13.63748094296638	10.03879694039199
H	4.63929983092919	13.88349316482313	9.33491524618562
C	4.20765864258466	13.22739958431481	11.32078861593266
C	1.05730594523391	11.04710971855775	16.24584064585824
H	2.14444702968011	10.95074473204547	16.14100386670128
C	5.66244749441414	13.10563736098795	11.70053980986652
H	5.69748438075553	12.88788135547227	12.76965521528542
C	5.30908398754742	9.11248280828929	13.16719864110657
C	6.50461704932440	9.69291546669398	13.59431644750253
C	7.73465119532711	9.28067863214189	13.10576862988694
H	8.63320563309415	9.77542637516954	13.45200625587961
C	7.78446278911316	8.25387890171028	12.17052063053673
H	8.74086364953330	7.92880100014703	11.78027936635200
C	6.60784723888620	7.65047777213546	11.73472479065447
H	6.64371746826207	6.85141777559143	11.00489726506960
C	5.38249836705987	8.07627326972836	12.22950192890257
H	4.46898305256191	7.61716501244088	11.87341788175069
C	3.31639820565099	8.37094517150344	15.06541495830458
C	2.88621252714793	7.10380145288657	14.65563565935379
H	2.71158665771419	6.90129913142401	13.60625310912537
C	2.66999269007428	6.10681037316494	15.59690562533333
H	2.33073455496123	5.12938124437959	15.27596333751546
C	2.89236966411051	6.36153257655251	16.94888275585285
H	2.72281712443419	5.58088471882159	17.68060086392896
C	3.32871947013618	7.61637768148542	17.35730549133517
H	3.50171683573450	7.81980388774438	18.40709212549933
C	3.53623104849507	8.62091008917514	16.41957040371991
H	3.86604082450834	9.59948964862303	16.74286300242374
C	2.53357058432855	9.44788466647313	12.47545041321849
C	1.20419437669303	9.09544987290003	12.73388501058698
H	0.90417767436856	8.79987668305429	13.73001667411771
C	0.25818409072889	9.14445369724067	11.72018951964032
H	-0.76894519672917	8.87759068932835	11.93545942919814
C	0.62305283686554	9.55457855877715	10.44075842742745

H	-0.12029101099698	9.60612357389752	9.65494068609771
C	1.94260965714465	9.90485872451312	10.17571777142318
H	2.23273117487399	10.23470475448498	9.18600138569664
C	2.89293350061896	9.85873323163428	11.18683129701876
H	3.91040125510283	10.15893325203477	10.97520518350434
C	5.63831934164920	11.59465163509608	16.49243969816724
C	6.28536979695646	10.55739551373167	15.80982459114833
C	6.73092154816425	9.41747013019707	16.46102047507143
H	7.21522693578496	8.62665654791660	15.90300504383027
C	6.52615839923443	9.31091078144427	17.83292414753529
H	6.87024458878433	8.42512631901038	18.35222335595312
C	5.87399635470094	10.32147885776775	18.53366606311531
H	5.70906404281787	10.22576210509137	19.59941726801078
C	5.42565892074078	11.45623661954365	17.86498705809806
H	4.89382300007784	12.22872175996114	18.40495420260460
C	6.45034292375421	13.96743573840252	15.02344348898839
C	6.21611287633850	15.30305084132505	14.67632975979254
H	5.20304037620316	15.68611712882071	14.64554993755051
C	7.27963332196780	16.14898854623874	14.39371685934161
H	7.08732312593412	17.18308049109488	14.13480623980271
C	8.58536364769295	15.66992390318745	14.44275164924467
H	9.41503644990695	16.33095803943109	14.22384157678010
C	8.82216952906584	14.34122711280868	14.78054965170159
H	9.83724317034268	13.96588032510511	14.83091338011049
C	7.76157423281436	13.49085763868650	15.07275081457272
H	7.96229038337986	12.46759950289826	15.35623967395894
C	4.09960737225619	14.10749075135295	16.52241026633975
C	2.83998113389798	14.54450383436665	16.10970376351096
H	2.37796488801689	14.10684840298407	15.23109590085418
C	2.17838399996186	15.54405649481619	16.81765077477600
H	1.20393657583494	15.88199190310432	16.48661696492885
C	2.76854696626660	16.10149389278372	17.94497423031902
H	2.25403148566525	16.87759077808215	18.49859839784200
C	4.03028064207283	15.67398271244791	18.35815123238623
H	4.49682924355598	16.12040016083939	19.22795758280670
C	4.70255883691849	14.69378834162087	17.64282552114329
H	5.70426589938910	14.40313862009468	17.93660693850259
C	0.76986566391651	12.02203955652308	17.39859584781304
H	-0.30699159855868	12.11395180773954	17.55712696387391
H	1.21811363880615	11.64782048127236	18.32257134240561
H	1.17135337261528	13.01385409877117	17.20090358689364
C	0.46053790816251	9.67605362358627	16.58482891011151
H	0.67603901005110	8.93211863948191	15.81835888791541
H	0.87158577417115	9.31180146128900	17.52776004391071
H	-0.62270052052629	9.74632169774968	16.69990724017442
C	6.42729700320097	14.40698691235620	11.43415619707955
H	7.42652036423933	14.34731989927354	11.86929777793884
H	6.53522195756702	14.58125816806427	10.36117781455093
H	5.91522760003109	15.26556847916694	11.86773734925885
C	6.33396775308644	11.94461212966318	10.95250245784498
H	7.38030978826087	11.86443772431905	11.25583259830443
H	5.85122982563249	10.98985068911684	11.16358861997201
H	6.30472259260534	12.11250667278747	9.87372563150033

$[7]^{2+}$ - D^{ox} (S = 1)

Eh = -3167.568410546929

Cu	1.22440749596925	3.93544545656942	5.02034908236390
N	1.35224552819468	5.50869348940592	6.20900197584010
N	1.38671921060532	4.57120104565888	8.32127611579639
N	2.82711691922565	6.34159424374430	7.86721782309343
N	0.94973470289243	5.30658398895533	3.61018976530094
N	0.22469203467625	2.34295044393482	4.41002479182167
N	-1.70758929312306	3.24526642423872	3.51905674196574
N	-0.67152524785922	1.49838635467475	2.38425205976157
N	2.44404374941236	2.58442769381977	5.81528910669425
C	1.85508052960524	5.49485426446888	7.45898302980316
C	0.07576938185341	3.95480143393252	8.12897063326870
H	-0.54370135100437	4.60434090890021	7.51723643217873
H	-0.38960478464556	3.82159742906204	9.10667072267398
H	0.16929288429917	2.97569541901144	7.64918042211546
C	2.19810704809334	3.98777279517398	9.39016101267765
H	2.14207184249121	2.90035277689425	9.30842996682582
H	1.83079335811951	4.28316064686842	10.37487541111080
H	3.23382586593977	4.29702382479319	9.28061587212081
C	2.89978740382314	6.86656562522939	9.23450712296437
H	2.94163629700132	7.95680757121767	9.17981070744290
H	3.79274859859654	6.51111151889224	9.75230016725205
H	2.01228404037739	6.57584750525591	9.79015881070774
C	3.77398787189310	6.93245948042892	6.92298994218304
H	3.75203780113485	6.38313446960390	5.98468862867813
H	4.77379409102593	6.87161377816519	7.35672850352482
H	3.53628177088851	7.98068720777308	6.72750641767206
C	1.10882852713808	6.70712597903678	5.52438018073997
C	0.96282334096042	7.96701418871643	6.07979595894046
H	1.06030867949253	8.10444377431097	7.14882182077595
C	0.66801825816966	9.08438348472081	5.27361430127793
H	0.56453165440748	10.05222364872734	5.74827823456500
C	0.51788524018466	8.97102949346875	3.91292041989736
H	0.31448639307824	9.83883441640074	3.29837543174491
C	0.62320797760274	7.69766977521975	3.30902124993621
C	0.89416397326400	6.57003886036072	4.12805104363960
C	0.47975819129516	7.46894623823667	1.92285981189202
H	0.28787203997035	8.30727976975297	1.26308755523215
C	0.58777503358421	6.19255177858804	1.42028105040001
H	0.49855272498171	5.99515377149515	0.36029073781455
C	0.80670009599494	5.12755742694533	2.30433408746826
H	0.86693014970019	4.10724329153713	1.94567184110404
C	-0.71133128016713	2.34107928323139	3.44095993688720
C	-2.07732452321357	3.85075636922394	4.79652359731974
H	-1.60882940412633	4.83257040115676	4.91559685656336
H	-1.76999251885706	3.19814889357855	5.60871246210019
H	-3.16088565939820	3.97525223910735	4.81870130084530
C	-2.36004825151164	3.82106370720306	2.34270428329706
H	-1.82748433260667	3.52612897521776	1.44274821671308
H	-2.33022166773438	4.90889227282045	2.43235673080517
H	-3.40240144577590	3.50473775718160	2.27054760953689
C	-1.88063488388589	0.95024166872257	1.76174461190242
H	-1.99646630450117	1.30165023523650	0.73456578219483
H	-2.75476788349629	1.22627503860824	2.34527777655209
H	-1.79397341335354	-0.13872116248343	1.74726236536650
C	0.58770925914956	0.93617063183593	1.89983993224178

H	0.59974536569525	1.00864491073290	0.81073375916294
H	0.68848768992544	-0.11344267347961	2.18555987353994
H	1.42452649219463	1.49687316137178	2.30957509328367
C	0.78041389073273	1.15348366141238	4.90128997582286
C	0.23939438211018	-0.11758716991295	4.80844907312416
H	-0.69905236197343	-0.27278297319861	4.29224645844639
C	0.88515491053846	-1.22424006176114	5.39485136204794
H	0.42851642009769	-2.20128908491945	5.29674451859709
C	2.07125433624282	-1.08935086705124	6.07430303665165
H	2.57212975390752	-1.94902907630701	6.50116057399993
C	2.64083105194092	0.19531992144755	6.22349618749474
C	1.97298876350562	1.31182382416128	5.65473443030217
C	3.85183931601245	0.44582387017281	6.90511616760933
H	4.39894260945193	-0.38343453931752	7.33865707471813
C	4.32988949036508	1.73167848363675	7.01040102665926
H	5.26411240757911	1.94566849891580	7.51234364187793
C	3.58281125486644	2.78388924620705	6.46441829047259
H	3.91569750697482	3.81047886305753	6.55661200259662

[7]^{0} - D^{red} (S = 1)

Eh = -3167.985283039161

Cu	6.97031030106683	8.70152569522433	5.45816671595473
N	8.52824446149057	9.88947639315182	6.22453259481482
N	9.41463796639483	9.73552242580987	8.43137418798875
N	7.51792448218780	11.01255375590983	7.97547735174714
N	8.43709111422870	7.96761780828678	4.35940913533669
N	5.44383457174601	9.58889082526539	4.28550187034403
N	6.55381491538365	10.21861295222879	2.35938260839148
N	4.76879628273099	8.73292575807604	2.16654234606010
N	5.45618539977243	8.31371493814017	6.64829657903314
C	8.51642083249437	10.20314984758303	7.49641101052872
C	9.95070312141406	10.59695200101081	9.47158976427417
H	11.01786876393845	10.78187754839716	9.29585253053708
H	9.83938343867384	10.13772583734373	10.45959612614032
H	9.42142711340744	11.54721707691807	9.45960859035645
C	10.12327846955586	8.48719187486116	8.20861092650811
H	9.55623045562793	7.87167128078839	7.51243850777395
H	10.20747284718035	7.96136060228346	9.16456151606383
H	11.12561415648330	8.64615493567910	7.79705896244875
C	6.83152541667963	10.69198282697263	9.22441648993033
H	7.41642812701291	9.96720876058159	9.78513460271342
H	5.84912249039002	10.25770344366007	9.01322955564932
H	6.70047230758344	11.59423516462144	9.82818505463894
C	6.70313569357213	11.73355896955194	7.00560549002119
H	7.34535934591183	12.12705766424891	6.22094828318858
H	6.20671207248440	12.55727735482806	7.52339091257799
H	5.95079044895538	11.08577965502440	6.54438198098717
C	9.70850831542803	9.61560667707933	5.53295711491901
C	10.90302638257223	10.31913522823814	5.70891893399889
H	10.95066397048692	11.10109889863549	6.45811756802785
C	12.01528242535920	10.03780820664043	4.91248944076120
H	12.93041121365514	10.59930963458928	5.06481739909483
C	11.96317954961486	9.06211091576801	3.93107110012745
H	12.83161405579188	8.84672019681515	3.31875371260045
C	10.77149595283052	8.33829488709440	3.70902244883235
C	9.63268342851662	8.62267997611796	4.51920422777745
C	10.63248579445596	7.33351390236577	2.71871392053729

H	11.47627669259335	7.08805325033874	2.08434778445216
C	9.41704384761215	6.67859829488226	2.58137309595837
H	9.28169813431003	5.90402566705839	1.83587930517523
C	8.35267656728484	7.01677840884643	3.40975015902746
H	7.39311260666056	6.52274113927741	3.31700899073116
C	5.55481117591938	9.51861179742684	2.98133310676964
C	7.34598051584407	9.61553509486019	1.29088311949713
H	6.87898126517431	8.68867310970138	0.96880323101109
H	8.35134804082447	9.38770162205986	1.65696716930066
H	7.42435266885497	10.29799367352169	0.43944558847972
C	7.25063597789736	11.24424606802954	3.12415834818542
H	6.53489272173020	11.76957247404479	3.75181741089524
H	7.70999945011391	11.94290240960697	2.42095688527176
H	8.02541474794992	10.81292159192589	3.76532054651352
C	4.29728150631518	9.20178655083424	0.87487893134630
H	4.76736447360531	10.15536932438440	0.64512164621627
H	3.20893081224044	9.33850996179989	0.89805862669373
H	4.53727522754220	8.48484618510943	0.08243563463611
C	4.10653722466654	7.55509421889202	2.69846350464221
H	4.62519589300449	7.22752465789827	3.59749953291301
H	4.15447182456823	6.76038713041943	1.94752848294592
H	3.05830258325977	7.74759958805146	2.95043376664688
C	4.22249835127698	9.44934639376305	4.94104463291728
C	3.01634224276415	9.97889919435689	4.47615056740683
H	2.99895394049722	10.49532522995043	3.52328079903851
C	1.85002517761889	9.86822333044129	5.23751403574487
H	0.92666737953289	10.28844596917742	4.85448151249688
C	1.85977341683318	9.24091044165802	6.47074945676813
H	0.95167235429053	9.15704372810346	7.05700692105254
C	3.06046568516798	8.70721063485255	6.98734487895768
C	4.25228804493430	8.81151723422482	6.21152122158255
C	3.15466343820232	8.06554753563668	8.24738779115085
H	2.26918138701055	7.96756886557544	8.86464657558065
C	4.37973615180753	7.57168439230582	8.66753863718374
H	4.48336605640485	7.07446717296101	9.62461489575663
C	5.49686017393422	7.70962201770133	7.84968375955851
H	6.46479255667364	7.33344272053054	8.15823888680899

[7]$^{+}$ - S_0 (S = 0)

Eh = -3167.861333071082

Cu	6.98204807999777	8.77702420433037	5.42054279144505
N	8.55448159944739	9.83412401318067	6.25512388560640
N	9.42985685515834	9.78338028085413	8.46448159558611
N	7.54596084172646	11.04303779717849	7.94064925465305
N	8.46256494169819	7.94085102611855	4.36439018873945
N	5.42695749704109	9.49907401640230	4.25780292473643
N	6.49604022177409	10.22179836571847	2.34761118560978
N	4.70614523813092	8.75651566336561	2.11578127426915
N	5.47966698593964	8.26753996256326	6.63668227951428
C	8.54010100062123	10.21474727398424	7.52124248242171
C	9.89616691109943	10.64541145740486	9.54433890974250
H	10.98297522083306	10.75507882908385	9.47331802726068
H	9.65561377442635	10.22396370029976	10.52440807712657
H	9.43727125257940	11.62663177542666	9.45230682543058
C	10.13636522243784	8.51990333304079	8.31357636419526
H	9.60254487990205	7.88655962051477	7.60805783397463
H	10.16929592555623	8.02425095864981	9.28678379451508

H	11.15970891900667	8.66351060791476	7.95379563665144
C	6.89199182046841	10.86614573536084	9.23516583544854
H	7.37335524281765	10.05960876593425	9.78198540550004
H	5.84219386837990	10.60366078829259	9.07711491200790
H	6.93922923446565	11.78298629115116	9.82737648123977
C	6.77218652948408	11.77348687838344	6.94458239995526
H	7.43429749730451	12.11789267048498	6.15414205255768
H	6.30963330782244	12.63198192548218	7.43342407480978
H	5.99468235654498	11.14360441923102	6.49970313756237
C	9.73686121235023	9.55776932156325	5.57894541871320
C	10.93845298689458	10.22587182808392	5.75941961215606
H	11.00649638182558	10.99989696174728	6.51446803904560
C	12.06117261094215	9.93045550614498	4.96592047349290
H	12.98081566139877	10.47675747282597	5.13801956545473
C	12.00746346678918	8.97638323151556	3.97757657155409
H	12.87464705314889	8.75424894273430	3.36791024037419
C	10.79942838902519	8.28099790663541	3.74505589472115
C	9.66275824656240	8.57415782933685	4.54630055521934
C	10.65086366661390	7.29490519790458	2.74194033162649
H	11.49716785897358	7.04615181959699	2.11203725669053
C	9.44155483553721	6.66596173407777	2.58062342392751
H	9.29995101498133	5.90258882734958	1.82641796783791
C	8.36825183558513	7.02006073603647	3.41487322848660
H	7.40261648546136	6.54035960256010	3.30592515832173
C	5.51006293850067	9.49531532613087	2.93796186344645
C	7.23700957199450	9.72344433364391	1.19125976631831
H	6.84280201800566	8.75613611050517	0.89070298364019
H	8.28885570444251	9.60160764102995	1.46375985324775
H	7.17071233716133	10.41868805677057	0.35098651400276
C	7.17186019652587	11.25371449161196	3.12395995790211
H	6.45040198879365	11.75092683476772	3.76707782635374
H	7.60421058576160	11.97654488458468	2.43051064858174
H	7.96390747085055	10.82898885523424	3.74898433568739
C	4.27521185835501	9.24309722893065	0.80976659772487
H	4.68239392640417	10.23628130106413	0.63785999826617
H	3.18228870143009	9.30078822653054	0.79065849726961
H	4.59968279469484	8.57526089221638	0.00697189385814
C	4.03242652711063	7.55914971196985	2.59484161786427
H	4.53167410709768	7.19317623704746	3.48944020640675
H	4.08644916402894	6.79554395880908	1.81501539471906
H	2.98131598423562	7.75012377951974	2.83146646477708
C	4.21713812798534	9.36591349650096	4.92675619825951
C	3.00056305833124	9.87135738329433	4.49279910533819
H	2.94813288343467	10.37795169876768	3.53645936663958
C	1.84165481294127	9.75594528298906	5.28037274043181
H	0.91131528963424	10.16445332360082	4.90439872058545
C	1.87318627946212	9.14752187081974	6.51268247068725
H	0.97824538121535	9.06160894740719	7.11660966716504
C	3.09381943093168	8.63341331207116	7.00520892913767
C	4.26762257106751	8.74383033943974	6.21149408664103
C	3.21761589138379	8.00437487973530	8.26591116250233
H	2.34234522004676	7.90273979619008	8.89715750948515
C	4.43976270716251	7.52947001480675	8.67170803287258
H	4.56397752295381	7.03804850056888	9.62808136829349
C	5.54974535133456	7.68209874186478	7.82454361949622
H	6.52577866596798	7.31709826311106	8.12221023421641

$[7]^{+}$ - T_1 (S = 2)

Eh = -3167.806918989192

Cu	1.27232345398881	3.93542090397898	4.98846740100057
N	1.33399801887553	5.50483574534404	6.21253736201948
N	1.41838527505007	4.53377352004630	8.30766956109701
N	2.81387713828310	6.34190259494080	7.86510531515319
N	0.94191148667175	5.28443280626525	3.62397772446634
N	0.21458570052004	2.34522660865410	4.42286456969454
N	-1.68461465707781	3.28177096359400	3.49761728483940
N	-0.67654945397106	1.49850564606174	2.39550054465705
N	2.41990070937905	2.60604177505838	5.82673667755585
C	1.85264034019000	5.47840649855069	7.44171447642263
C	0.14028764806089	3.86255763020337	8.09769618468178
H	-0.51485961294875	4.51227982227406	7.52398381860984
H	-0.30612598774402	3.65903581879008	9.07309733314830
H	0.27358368453277	2.91691142676459	7.56428345457904
C	2.28652165792986	3.92391338903988	9.31068127763622
H	2.29250986307255	2.84270931939440	9.15748600904078
H	1.93284451099046	4.13810239374267	10.32224410017889
H	3.30033123498599	4.29572506971365	9.19264020403532
C	2.85924086915513	6.86152252584381	9.22868482189534
H	2.83029361389093	7.95416259389052	9.19077298624761
H	3.77415564717552	6.55685057909069	9.74324922165725
H	1.99576480032213	6.50562669303311	9.78490377439150
C	3.73947824520452	6.95787753132761	6.92133658195006
H	3.72420739498630	6.40698143543365	5.98386551644422
H	4.74441358909740	6.91947232969262	7.34804570453478
H	3.47320154404168	7.99893567409305	6.72146474910813
C	1.07858538345835	6.70363602344212	5.52676415703692
C	0.91246807322136	7.96302626984014	6.10190745244666
H	1.00433766974958	8.08845711918057	7.17305484267072
C	0.60339117902048	9.06716793645545	5.29966591883671
H	0.48056431976108	10.03627598806192	5.76796174529145
C	0.45809398273504	8.94492824700486	3.93070696199315
H	0.24195240059656	9.81152272456940	3.31795161704095
C	0.58048464969318	7.68061700010092	3.31680097059488
C	0.86807933784089	6.55635403356348	4.13758466017594
C	0.43973848544851	7.45159937098262	1.92510085552416
H	0.23770717643685	8.28529643346671	1.26414940929665
C	0.57528951866148	6.16366070350144	1.42618191478210
H	0.49250638067590	5.96617008349138	0.36500401530210
C	0.81296187218974	5.10619256586388	2.29397817497469
H	0.90304394878486	4.08849267046147	1.93581099315531
C	-0.69770231515685	2.35743545718191	3.44923183120645
C	-2.02304916326675	3.94355905891125	4.75321969932214
H	-1.48869243727000	4.89247669284681	4.85520125451970
H	-1.76419421281681	3.29142253676705	5.58284902590795
H	-3.09712022750680	4.13881201960742	4.76034855476952
C	-2.25945477946176	3.88611055029345	2.29931539665218
H	-1.73099866529139	3.53000111294521	1.41951748632473
H	-2.13913232266394	4.96970305259851	2.36247491104632
H	-3.32255197301717	3.65009837130501	2.20862777105566
C	-1.89324567834916	0.95489176126871	1.79953506987141
H	-2.00389215365730	1.26569559265573	0.75740742481626
H	-2.75884795123548	1.28422350043320	2.36883664827207
H	-1.84323318038192	-0.13718397655575	1.83145611794245
C	0.57460713034865	0.91395008373377	1.92763868135234

H	0.59540913799807	0.96752253427368	0.83663897091646
H	0.66895886110007	-0.12974177781786	2.23825582337399
H	1.41266437517492	1.47595021893276	2.33300333504527
C	0.76648129929000	1.15497003586159	4.92529032437438
C	0.20281497954271	-0.11744174489953	4.83682252491810
H	-0.73726932091857	-0.26129404530605	4.32013576470281
C	0.83869246667726	-1.21116141594546	5.43484762295853
H	0.38300811487711	-2.19048131378702	5.35196225286885
C	2.03039469633992	-1.06607954306692	6.11962527243335
H	2.52449981639813	-1.92475566582727	6.55746743086877
C	2.61208446672621	0.21096536084672	6.26384515366409
C	1.94964781457551	1.32417103050250	5.67855575162044
C	3.82474476436864	0.46334129117924	6.95286051294002
H	4.36874354851838	-0.36121556583414	7.39660509507121
C	4.30599673455522	1.76211687438404	7.03823508583895
H	5.24040195505320	1.97721234747400	7.54084144831589
C	3.58216782271101	2.80696542551346	6.47987432025357
H	3.92346630380207	3.83202767471527	6.54871209260829

[8]$^{2+}$ - D^{ox} (S = 1)

Eh = -3246.253599860859

Cu	10.30962323189138	2.54381380549217	6.88398390284297
C	7.94583733926882	2.01014313318413	8.65413416231655
N	8.43690994883481	2.08950837721227	7.40298261227537
C	9.49159794120540	0.17823425691855	9.16717864735049
H	9.27690719225051	-0.08866651030694	8.13698610422637
H	9.28365962332267	-0.67398292195409	9.81726971189116
H	10.54643539178531	0.44406803339218	9.26566920606471
N	8.63259582993007	1.29086030344854	9.56534138616484
C	8.66883976539137	1.62820978717770	10.98717666980004
H	9.71400773325217	1.67116744337474	11.30092538737859
H	8.15444155009707	0.87875512296122	11.59204075797680
H	8.21155639559631	2.60043323241227	11.14854073284791
N	6.81505290486301	2.64091224705649	9.04377285032085
N	9.45149921275980	3.08953733073777	5.16958107239286
C	5.90411802958360	2.07736395687120	10.04453828816854
H	4.89912977014635	2.05740013929696	9.61705999541165
H	5.88157994543624	2.68248228699569	10.95308666606206
H	6.20329275565865	1.06134753402515	10.28736386400025
C	6.32356182145727	3.84504509970491	8.37785062648718
H	7.09563133509789	4.25941543633238	7.73626785850853
H	6.05715802736735	4.57730797264519	9.14255650366383
H	5.43984801153632	3.62483722086292	7.77464101390549
C	7.58530005244573	2.12544682867995	6.29024914102302
C	6.30026926011675	1.60982735801789	6.22431036867318
H	5.85767695231672	1.14755779093682	7.09734507303628
C	5.55948517717910	1.66227052653297	5.02920158240178
H	4.55938533999354	1.24734706914401	5.01845791405760
C	6.07717996075158	2.23437694692198	3.89119310875516
H	5.49279514968844	2.29841172546324	2.98207645297449
C	8.01637696833077	3.36560353043821	2.80317092279350
H	7.46970891734646	3.46630380952397	1.87257676231874
C	8.15018299258810	2.65984677809750	5.10473928860374
C	7.39327321869575	2.74572619769626	3.91067735410135
C	10.01176924047106	3.68849555097975	4.12206050936128
C	9.29376463494351	3.84991472102021	2.91693783677285
H	9.77164341750266	4.35674769549486	2.08822940215214

C	11.40777935315339	4.21124556604755	4.25142885818354
H	12.08047837714164	3.71720210359044	3.54651318750703
H	11.78017940659474	4.06641901494445	5.26486049636711
H	11.42890689079749	5.27883214307642	4.02040481342330
C	12.37951202927925	1.09946351132429	5.27077990034905
N	11.96595411774500	1.51186434560885	6.48392435876319
C	10.36483515630479	-0.27454108771581	5.05069893581835
H	9.43485277349001	0.28908983435699	4.94582541028381
H	10.55847257518357	-0.46803065456639	6.10134003060361
H	10.26275260506736	-1.22147323832939	4.51754765470195
N	11.49249745147915	0.45994728603941	4.48097546152176
C	11.49706541130308	0.56274288104461	3.02259457868485
H	11.74935317418003	-0.39083673723307	2.55462781769861
H	12.20902881945634	1.31987103752543	2.70636053487925
H	10.49712361942016	0.85707146189336	2.69654212266842
N	11.31517713926333	3.07885444794693	8.51825715148094
N	13.62840853825930	1.32060675046581	4.80266215446540
C	14.45515496156340	2.42596985512655	5.28159067150495
H	14.88808183045400	2.93328931953585	4.41725622020009
H	15.26270446304481	2.05972846069527	5.91935829187427
H	13.84799885970054	3.12738004744801	5.84585164809311
C	14.31467491005319	0.37940798288244	3.91260395873012
H	14.47350432967417	0.80802468957187	2.92099916067836
H	13.73830649427123	-0.53790584512399	3.82861896812255
H	15.28882718963377	0.14706233783935	4.34850569139384
C	12.81850709981750	1.47988593881799	7.59570118119623
C	13.91130687256820	0.64440777788810	7.76572014394067
H	14.18983620885686	-0.04773686741007	6.98138561219667
C	14.66146969885884	0.66738674356961	8.95583145648769
H	15.50763561059727	-0.00151874364881	9.05077504206858
C	14.34553399537324	1.52335479290259	9.98434368930235
H	14.94256328028766	1.55715076434745	10.88683262836437
C	13.22222553837906	2.37010476450493	9.86041653522054
C	12.44740679988129	2.32094488469995	8.67561078043309
C	12.81512994248843	3.29319357068806	10.85100990196592
H	13.38563174664453	3.37511382641847	11.76905420654233
C	11.71779479414985	4.08703915124496	10.63933293111672
H	11.41236538329778	4.82056885479412	11.37462543043612
C	10.96128628190132	3.95566276541326	9.45414809301074
C	9.76699959802090	4.82394338539499	9.21369393116377
H	10.07697003123386	5.87047044509702	9.15210893564994
H	9.05124564590112	4.74972754960451	10.03514841686595
H	9.27553595612521	4.55353706488844	8.27998626895813

[8]^{0} - D^{red} (S = 1)

Eh = -3246.66924432558

Cu	10.32196996400212	2.61341176949332	6.90212070923884
C	7.93945224957391	1.82577252685379	8.54811110918450
N	8.40878501560998	1.78193997471553	7.32718533871388
C	9.54251639157184	0.10615404481664	9.15137799475990
H	9.18039263565385	-0.39745887024855	8.25860201331074
H	9.63021454359449	-0.60904547717760	9.97290211790336
H	10.52755156087050	0.52879128159534	8.93603014898414
N	8.58373167965454	1.13198951502761	9.54013565500062
C	8.84100093408141	1.74418619677296	10.84031709905334
H	9.88686626654265	2.06105191780188	10.90858409994214
H	8.63347609292632	1.03123378528151	11.64292495208077

H	8.20375552550092	2.61611211333289	10.96449989956272
N	6.85273472508641	2.57524308418348	8.95051958193869
N	9.38536592431786	3.16421294412311	5.24534918263144
C	5.88706411875098	2.05923322355389	9.90642226976376
H	4.92546658941523	1.87884123484415	9.40964962773654
H	5.72339191115275	2.76951561646853	10.72375106814106
H	6.25245997666895	1.12120051745267	10.31800945042407
C	6.42221277960776	3.73334495103567	8.18542046309006
H	7.24903252712680	4.09534858445788	7.57876105849976
H	6.12280613757193	4.51934938907861	8.88554977075183
H	5.58066207876793	3.50106089120523	7.52474427574522
C	7.58194367332628	1.92961636285541	6.21340058609837
C	6.31650403102937	1.34797268204692	6.09665391225165
H	5.92014512100709	0.77546216978947	6.92745526057507
C	5.57811300406239	1.48293156113299	4.91856030446119
H	4.60005736018528	1.01965594909224	4.85088828828216
C	6.07867479450624	2.19421839955975	3.84235361842904
H	5.49864993478431	2.30508230440625	2.93317766003627
C	7.94936021730383	3.52106722166559	2.85938548299862
H	7.40291810184704	3.66119097982722	1.93389140629760
C	8.12323939883811	2.63780260600606	5.10818448047511
C	7.36167161550658	2.78179883956955	3.91327420999560
C	9.91476870034518	3.86638575998959	4.22160637120463
C	9.21376003036359	4.06310451146109	3.03097629071788
H	9.67763797972287	4.64059070201482	2.23974084208470
C	11.30089020355351	4.40071254192975	4.41443807082285
H	12.05031555424114	3.63908250397481	4.17785965174867
H	11.44786424680455	4.68261476432274	5.46109922368449
H	11.48475128002350	5.26288891501675	3.77045014387124
C	12.30012331461178	0.93306285982116	5.41306762409890
N	11.89566035416308	1.21106078556148	6.62653028806269
C	10.27632821372145	-0.36861727360283	5.12201825501473
H	9.45884356628017	0.33593578476109	5.29641741883259
H	10.54902999153151	-0.82376146614577	6.07104412136625
H	9.94373717042726	-1.13970593589050	4.42285109545883
N	11.44747055119680	0.28653293494011	4.55509363957889
C	11.28184445125711	0.73846401013701	3.17671469493664
H	11.27285865677050	-0.11571269882371	2.49396088210557
H	12.10132676475919	1.40058665706404	2.90865485938035
H	10.34023356492457	1.28646085730940	3.07105351812580
N	11.42692102692675	3.11727381727798	8.45976002706889
N	13.52378535678629	1.28930525949859	4.88564642378285
C	14.28966454862850	2.38678706563645	5.45175645403094
H	14.74734974244861	2.94960648824402	4.63226160040561
H	15.07565294395079	2.03447159935659	6.12768650592456
H	13.62644310709299	3.04568147042273	6.00716356891262
C	14.26327020101887	0.39642857232914	4.00907844616672
H	14.55465901150273	0.90410806510620	3.08344008589693
H	13.64468411610384	-0.46369665996667	3.76326275446373
H	15.17420471661605	0.04779159446464	4.51133608097932
C	12.78278904860962	1.30059145985971	7.69880633663891
C	13.84950585468051	0.42121582454840	7.90159060019936
H	14.03578523957411	-0.35864315015385	7.17208550737943
C	14.65216918300300	0.52874682473925	9.03976182436666
H	15.47264707946631	-0.16669246638629	9.17751320300789
C	14.41136743610220	1.50497388486317	9.99041643269795
H	15.04046484174011	1.59031121615826	10.86921881590294

C	13.33081826121212	2.40186219169530	9.83206527298077
C	12.50500696456424	2.29187889056424	8.67631062636271
C	13.00892453187417	3.42106175960839	10.75964678023485
H	13.61310651451903	3.54423660542759	11.65097798558322
C	11.92606098948266	4.25145227671648	10.51019316751466
H	11.66681914359121	5.04263559162802	11.20398339464713
C	11.14929364165898	4.08001626230474	9.36419287015346
C	9.95337647407212	4.93658619521625	9.08198873287394
H	9.94067549330755	5.82220792196954	9.71989355968592
H	9.02802634577352	4.37867135960879	9.25260959884623
H	9.95006671054721	5.24374757480082	8.03161025583634

$[8]^{+}$ - S_0 (S = 0)

Eh = -3246.548912529476

Cu	10.30478626022288	2.55543541708676	6.88300838303230
C	7.91441862127392	1.83063929000179	8.57201879406081
N	8.38374396865405	1.86463382402458	7.33772316227555
C	9.50741884059974	0.06152939500486	9.06883349806516
H	9.14793229491089	-0.36847292267945	8.13822742799966
H	9.54960094453114	-0.71032995027654	9.83974614508691
H	10.51166228973897	0.46281200942703	8.90634138589611
N	8.58085616023587	1.09729886634195	9.50514542302424
C	8.78060062018599	1.57912333177647	10.86832265855232
H	9.84811522813254	1.74513688610350	11.04070277517706
H	8.41713448460469	0.85319986469082	11.59985629085537
H	8.25467948866777	2.52013505156087	11.00679830861800
N	6.81984994032356	2.52732176505794	9.00503639993327
N	9.36979701102383	3.20140659800533	5.23547327552664
C	5.90977485778690	1.99382175208212	10.01212152108575
H	4.90732510783717	1.90767435332870	9.58075382421468
H	5.85300885971677	2.64876861529785	10.88637062961784
H	6.24472324280779	1.00758649675479	10.32323789602541
C	6.35736816916608	3.72484450516223	8.32101518322525
H	7.15190362792750	4.11926908908190	7.69319660379613
H	6.09018455752576	4.47282349211543	9.07200289171892
H	5.48304663449678	3.52228782340362	7.69489544417697
C	7.54853451512109	2.01971011061247	6.23652202160448
C	6.27493310902200	1.48233931423427	6.11621431718850
H	5.85452284527378	0.92721707320938	6.94637926910779
C	5.53145667433656	1.62809089414891	4.93238682453397
H	4.54111067099605	1.19203374244021	4.87898309358055
C	6.04291415795279	2.30275541396194	3.84873324226322
H	5.46736919521935	2.41546483312967	2.93806782028884
C	7.95553421116433	3.54980851976167	2.85364132151631
H	7.41202016689456	3.68547172413120	1.92549453636977
C	8.09849476422567	2.70351558820005	5.11159125229846
C	7.34350773620465	2.84952835617332	3.92020697952645
C	9.91732995914609	3.86164073070361	4.21998835607767
C	9.22005236369827	4.05322067209939	3.00604276947684
H	9.70013059775089	4.60057241426155	2.20420811048772
C	11.31073930376466	4.38145107495727	4.40060513827380
H	12.03129436749608	3.73755918898886	3.88683317563991
H	11.56079991508676	4.39377231164347	5.46290000191670
H	11.41400721620754	5.38595934631482	3.98562369998447
C	12.36010039602352	0.95366889826838	5.37943585836175
N	11.94193671156783	1.30607949577439	6.58164430086185
C	10.32586319262931	-0.35131108504243	5.12004218260777

H	9.48637423709591	0.34283305705038	5.21842150801821
H	10.57535391949241	-0.73954533945333	6.10367401432326
H	10.03708727314164	-1.17327950085112	4.46243840847908
N	11.49820344152094	0.30102607536009	4.55250729165522
C	11.41830839558160	0.60064688010834	3.12623624359081
H	11.55554259133436	-0.30222252775241	2.52606101769951
H	12.18315749791573	1.32548110869632	2.85979603491450
H	10.43632378442735	1.02581837412560	2.89898664205798
N	11.41370606700248	3.17102996614540	8.43407649667674
N	13.59731390706844	1.24442363540133	4.87315535847361
C	14.38762323209964	2.35365356197881	5.38447088931861
H	14.85001982220145	2.86966023594175	4.53913488655952
H	15.17374817113844	2.01245279578509	6.06488144558076
H	13.74217707353943	3.04855705168414	5.91587662360281
C	14.30528611946628	0.32769363494166	3.98641912979776
H	14.52302323331813	0.79320531588368	3.02089562820918
H	13.70501658128555	-0.56471006102900	3.82815279158437
H	15.25334870842811	0.03894578910516	4.45113667236823
C	12.80359062196621	1.38132331498578	7.66985485090527
C	13.86864337524144	0.52324017686624	7.90316916457993
H	14.09573256881785	-0.24647771082609	7.17514927010444
C	14.64053421968958	0.62220079344538	9.07309907469742
H	15.46260181640061	-0.06818919291845	9.21912050823549
C	14.36375372081991	1.57046749236763	10.03019538982876
H	14.96106870523704	1.64677180199052	10.93052461066111
C	13.27751981451801	2.45364115127095	9.84163326007219
C	12.49245688690717	2.35519632322267	8.66476491515576
C	12.91218738551310	3.45364833051135	10.77473651611791
H	13.48559460275222	3.56354949138527	11.68818406652491
C	11.84628559300601	4.27185109052168	10.51259975638789
H	11.55923593408987	5.04959743654643	11.20971478946372
C	11.10177340143332	4.10928943719177	9.32165689529576
C	9.93531826973847	5.00030940258471	9.01922050769129
H	10.25885185438978	6.04173514972308	8.93801130411959
H	9.18769878317207	4.95471255116376	9.81547353927639
H	9.47812511009542	4.69656073552015	8.07622530403965

$[8]^+$ - T_1 (S = 2)

Eh = -3246.485773029048

Cu	10.31939386379718	2.59712057893128	6.88720183641506
C	7.96303459006977	1.99140167418036	8.64565182997308
N	8.44747541263532	2.04785716597923	7.40571590242867
C	9.56258593364414	0.22634088965129	9.21215476205577
H	9.34544637913433	-0.08293105012692	8.19407344575058
H	9.40936430991101	-0.61305920973755	9.89476380158556
H	10.60363245452646	0.54942684493561	9.27746567865379
N	8.65160935028553	1.30253759206238	9.58548351954943
C	8.70454956055197	1.70963366921167	10.98549150093350
H	9.75053464295416	1.83960086459952	11.27281869556037
H	8.25074442349934	0.95803780355701	11.63638940531591
H	8.18609581082699	2.65627371990026	11.11326705144897
N	6.82121868347343	2.62302026987976	9.03331162117792
N	9.46747002195892	3.06442812033233	5.19197589855337
C	5.89888826835658	2.04134888287828	10.00428811566649
H	4.91411465889021	1.94334067058958	9.53832059965264
H	5.80087220998023	2.67282633501871	10.89103429834577
H	6.24792521377117	1.05507798012916	10.29916002800612

C	6.32485879289344	3.80338625130318	8.33422598247786
H	7.11208330447963	4.22150179017206	7.71322460787984
H	6.02029169342838	4.54253021849104	9.07895326660621
H	5.46956273706906	3.55714198766899	7.70017447813303
C	7.59752962226584	2.08192288253107	6.28773686649230
C	6.31523953674853	1.53461092309689	6.22630108656952
H	5.89092911892635	1.05281569825032	7.09827993697884
C	5.58132523727947	1.59236815170562	5.03716855011894
H	4.58850817020301	1.15980656971423	5.01096659543930
C	6.09663539079097	2.19802976583524	3.90635938065776
H	5.50868640358029	2.26819900548960	2.99940287183012
C	8.01481014880184	3.38289252620911	2.82420116213763
H	7.46669390977866	3.50101555482771	1.89764235490122
C	8.16232220838575	2.63362287022978	5.11821691805118
C	7.40300726513221	2.73178350846298	3.92224061309035
C	10.02160389378827	3.70673752050094	4.13611387402398
C	9.29909494394057	3.88932322642718	2.95871620816855
H	9.76523187640253	4.42752152234593	2.14258786102576
C	11.42464680144077	4.20952016289409	4.28447909995164
H	12.15720287144514	3.45155475709826	3.99389617003678
H	11.62555325809477	4.48575781229346	5.32308436205006
H	11.58749749696883	5.08216429002475	3.65117122737246
C	12.34666352900450	1.08502767759480	5.28652312694980
N	11.94320422365099	1.47079818340945	6.49674892749785
C	10.30137268199524	-0.22907853606126	5.02362640852858
H	9.39915240793285	0.38335521366356	4.96219537829922
H	10.49965553424446	-0.47658398267034	6.06238779505873
H	10.14559753502960	-1.14547652388853	4.44986616658222
N	11.45812446857166	0.46899283381588	4.47241987218018
C	11.44341795076495	0.66097020506352	3.02564016759441
H	11.63508129655134	-0.27689966425882	2.49840677443206
H	12.19514106892848	1.39324572996193	2.74328945863801
H	10.46082675469518	1.03709572050699	2.73188365173987
N	11.30735816920251	3.05899561754666	8.50840461828904
N	13.60097081115551	1.30433954093850	4.80756673342976
C	14.43433948889306	2.38996259778294	5.31158284472274
H	14.88673699890557	2.90387284811344	4.46008747081894
H	15.22420566412846	2.01013464750872	5.96416795708646
H	13.82338847350609	3.09107369683732	5.87282282773123
C	14.27682356384862	0.35451438920330	3.92834916027626
H	14.47837942956763	0.78896480406207	2.94580286945934
H	13.66496301583676	-0.53642795584785	3.81178803622006
H	15.23016850547750	0.07302814276029	4.38414756560545
C	12.80322847565549	1.44202027062463	7.60591207565920
C	13.88845857034031	0.58024257645072	7.76747104596679
H	14.13889476261347	-0.12592670923134	6.98568139241512
C	14.64312164492272	0.61242955095304	8.94461197436466
H	15.48037894063091	-0.06663621669633	9.05098397571023
C	14.34475994127775	1.49897846267132	9.96232466912495
H	14.95391263289553	1.53960062277469	10.85701584735303
C	13.23449154863691	2.36264938444800	9.84640184358425
C	12.44428022457846	2.29894412120247	8.66809502182980
C	12.85509291569400	3.31407874478070	10.82357517844074
H	13.43946059267096	3.41407912678775	11.72989510649996
C	11.75736887513444	4.12983671257302	10.59320289287602
H	11.48069398061502	4.89283336363177	11.31029049895442
C	10.98195817115718	3.98175064830517	9.44448342945813

C	9.77051927082900	4.82751524345390	9.19866037687819
H	9.86168048321227	5.78527130853321	9.71177672460910
H	8.86094115450158	4.34413978430961	9.56531388452229
H	9.64008577263025	5.01239002084040	8.12891178554550

$[9]^{2+}$ - D^{ox} (S = 1)

Eh = -3403.577411117799

Cu	10.31452058367590	2.83701333261377	6.83991753237119
C	7.98573621809186	1.83982010260959	8.57107216856986
N	8.50616553678646	2.09630143319981	7.35454379091974
C	9.73362124402458	0.18204050384901	9.05351758539343
H	9.78704557402975	0.15782202635907	7.97138915827508
H	9.46142831764856	-0.80539118316209	9.43506810500921
H	10.70769241468843	0.45694363434146	9.45887414881176
N	8.72406181276394	1.15154030523916	9.46644805232983
C	8.59362244309674	1.30299709646164	10.91477305054276
H	9.58733330126633	1.49440574795946	11.32585893129820
H	8.19653394425455	0.39504719899942	11.37393118687921
H	7.94770682822366	2.14236365978454	11.14897063082456
N	6.75687518152279	2.27383047081228	8.94289823470972
N	9.42371625721941	3.29196629330280	5.10756863679608
C	5.86817294222531	1.49250061462526	9.80742609065159
H	4.91701333012806	1.35916619275002	9.28611487543162
H	5.67517849636704	2.00580970716873	10.75155655674949
H	6.30109428293839	0.51541725899814	10.00320817761792
C	6.13409762626609	3.44580311657297	8.33184916907119
H	6.87930190374677	4.01911303627625	7.78895431804759
H	5.70997698424680	4.06305624005202	9.12596808220551
H	5.33742759009067	3.14997722022148	7.64552896675386
C	7.69167690957427	2.04448880149359	6.21734226860634
C	6.50938586572935	1.32240863172397	6.11929799998109
H	6.15121980436496	0.76558629362282	6.97516054756489
C	5.77084383150701	1.28033356304161	4.92660355021405
H	4.85321790501943	0.70619528907279	4.89756092372373
C	6.19374985339302	1.96434861942299	3.81264781129685
H	5.61258213506680	1.96560072788369	2.89920035603983
C	7.91786868975043	3.39770957029004	2.75552342822300
H	7.34404471879661	3.44075578912247	1.83689921742007
C	8.18376305356591	2.68569764473823	5.04835938172098
C	7.41305135477539	2.67246973420894	3.85735497059412
C	9.88118037830141	3.96735646189895	4.05279189802783
C	9.11201360172069	4.04995567922011	2.86692306215866
H	9.49784333597594	4.64092043833835	2.04614480055799
C	12.25998267184473	1.05869774562929	5.26868066351667
N	11.84973494505753	1.58940300524658	6.43696294815465
C	10.11744641006765	-0.10142024807783	4.93710948248051
H	9.25731453952349	0.32000451469406	4.41706715181672
H	10.02391065921474	0.08900375193213	5.99995370609141
H	10.14545535537675	-1.17857519796415	4.75183061179723
N	11.34587913858326	0.51022278071982	4.44022175700557
C	11.50663885693594	0.44168335846119	2.98884316155217
H	11.64192971889015	-0.58846131518485	2.65173182500508
H	12.35539499167294	1.04007615321180	2.67476669245545
H	10.60035149405429	0.84027001819570	2.52786174198434
N	11.33534100173953	3.27088545545819	8.50675288073470
N	13.55576333119771	1.07904881911265	4.87025791692878

C	14.50013702983590	2.09009842446166	5.33915994858715
H	15.06085512248844	2.46148137436247	4.47932833997905
H	15.19862971361739	1.66544928230628	6.06377035003136
H	13.96460780280094	2.91392319519540	5.79974264533862
C	14.17267738607526	-0.02960458612971	4.13611932004461
H	14.50274380910037	0.28273782114043	3.14339373544911
H	13.47267740246608	-0.85560770872157	4.04655866972656
H	15.04580548493229	-0.36700150066993	4.70020324320685
C	12.64178930271129	1.46641232155177	7.58431872973262
C	13.58368859585850	0.46698538826451	7.79224473598711
H	13.75105877463943	-0.27594649937679	7.02344843500722
C	14.31780609400153	0.38400138535939	8.98516304315328
H	15.04258954318066	-0.41202446685876	9.10150894413622
C	14.13260867189160	1.30378286354542	9.98849775037960
H	14.71898097727933	1.26962664428250	10.89800256053445
C	13.15142632545023	2.30568895527799	9.83579473286411
C	12.37292559698321	2.36755128799035	8.65121129670090
C	12.90211093379949	3.28395400175530	10.82279616330272
H	13.49808220973553	3.29266007511885	11.72819885121005
C	11.92497432831575	4.21479104630122	10.61815569421369
H	11.73933261206783	4.99150950544907	11.34904457198171
C	11.11471948120164	4.18114505390554	9.45695336642220
C	11.20696916139749	4.70248062916718	4.02820319307578
H	10.95814678739787	5.67862869857838	3.59622828556707
C	12.19175450047706	4.02910945085071	3.05616350459751
C	11.86875083909828	4.95464170937992	5.37365130365296
H	11.20612870194958	5.48461519193180	6.05276304102471
H	12.18480934404883	4.02462628181091	5.85120731450650
H	12.76003112684820	5.56826604874840	5.23118651694257
H	12.53945790443293	3.08056483893529	3.46628962255596
H	13.05861513734117	4.67526100949472	2.91058368979140
H	11.74154084732552	3.84053405224632	2.08093515556537
C	10.00692878473887	5.21872158181125	9.41746976893101
H	10.47464717316718	6.12128005413878	9.82440345840735
C	8.88467374392786	4.83152007136302	10.39734339573649
C	9.43445310596355	5.58680204574387	8.05550135507134
H	10.16880228748537	6.10275990560852	7.44091428063770
H	9.06322987449322	4.71468778795303	7.50903148049017
H	8.58957918300591	6.26420715118783	8.19237782872894
H	9.27817137560752	4.56024676723664	11.37789331735545
H	8.31483479036610	3.98927651019345	10.00707523950112
H	8.20526751849126	5.67548392856038	10.52465878095831

[9]^{0} - D^{red} (S = 1)

Eh = -3403.989357382413

Cu	10.33022331612197	2.73827796983568	6.98551347652745
C	7.87617154399871	1.63198148632575	8.47125943800258
N	8.46241033150720	1.88068017675540	7.32067770450273
C	9.73240147624045	0.17235215166137	9.12628485546980
H	9.82017522837567	0.08534278259583	8.04945205530820
H	9.66471778902770	-0.81723528139520	9.58971420879460
H	10.62631796791817	0.67746972825187	9.50045109730320
N	8.53729303958589	0.93584813784285	9.44326122272380
C	8.32258852668432	1.17015139289336	10.86248912212135
H	9.26404341788238	1.48379550844161	11.32348463620564
H	7.97964416680574	0.25835785418402	11.36269938868698
H	7.58509766904002	1.95562680614642	11.00080704850907

N	6.61743057545796	2.08646881010704	8.82013939756303
N	9.44974819363775	3.38755202804111	5.24587064309116
C	5.64068649063551	1.20619354219022	9.44026571487342
H	4.83133512675299	0.98655751857771	8.73249091966583
H	5.20244965328517	1.66736956419059	10.33150845099991
H	6.11739965201718	0.27050235072153	9.72439345584147
C	6.07040842681502	3.28448243454895	8.20553481350717
H	6.88137138507514	3.88720472003176	7.80401946387166
H	5.54457196089923	3.85947267885849	8.97383308097914
H	5.37669152597343	3.04564893807602	7.39300818593406
C	7.70282056141286	1.98183459931975	6.15445094489283
C	6.53402346160751	1.23595405486524	5.94506644654384
H	6.20996230267971	0.54837076359629	6.71674815046198
C	5.80239132428304	1.35224958059630	4.76574073113888
H	4.90120834552860	0.76327842950766	4.63620726774335
C	6.21898105763841	2.21522858258803	3.76944072130580
H	5.64491470434028	2.33523462910891	2.85767541591623
C	7.90688051233507	3.81404393382728	2.91867147344887
H	7.32159334474445	3.98240144219200	2.02190819566257
C	8.20932325138297	2.79364157260226	5.09905322156591
C	7.42389750329500	2.93603915499545	3.91397368894161
C	9.89705385423633	4.18227017173847	4.24823804665809
C	9.12399364382593	4.43333433151661	3.10802852993332
H	9.52219260296015	5.10425307348984	2.35484024903015
C	12.27930819548725	0.82413225873700	5.57931201672910
N	11.84467161506013	1.29393973078885	6.72693741112807
C	10.17764622117107	-0.36893728801376	5.29917835669367
H	9.40321498016689	0.39939521684348	5.35668858121871
H	10.36146606847694	-0.76201317291965	6.29585292398203
H	9.83101590040799	-1.17724676144727	4.65085737006207
N	11.42372592329763	0.14520667957036	4.75333683079006
C	11.41400447316306	0.34805425505895	3.30961562376983
H	11.35323812644444	-0.61557933991906	2.79586670837680
H	12.32081539901663	0.86000764414214	3.00165576510147
H	10.55016848089555	0.95570155314558	3.01919189456450
N	11.46370830408270	3.30884192792347	8.57007675242332
N	13.56577247678992	0.97582049027800	5.10024804372189
C	14.41584284559114	2.06076064664322	5.55913209526138
H	14.96543166344356	2.45852562863077	4.70071484451217
H	15.12713954150427	1.72625681596237	6.32113316459679
H	13.80160059310086	2.85091660917156	5.98156891813754
C	14.26014365531909	-0.11235376526482	4.43247298291317
H	14.66003101445449	0.20887380868421	3.46478286864294
H	13.57334652796363	-0.94112529670568	4.27648379042359
H	15.09704379969730	-0.45616803870035	5.05322676081535
C	12.71196031922388	1.37800660802553	7.81954681457605
C	13.68918596010494	0.40664798621544	8.06946525717477
H	13.77289742416186	-0.43421654789929	7.39106837090703
C	14.53820748608431	0.50292076185591	9.17024244777441
H	15.28662060688418	-0.26374617087087	9.33702813719309
C	14.43091659044481	1.57060534204739	10.04120711637640
H	15.09996848268431	1.66935845542642	10.88855646174782
C	13.42523440759904	2.54389106804376	9.85306373181257
C	12.52202245953991	2.43667987663518	8.75118173854964
C	13.26160966600987	3.64553237056310	10.72122494542451
H	13.94704359426310	3.78251812888791	11.54970049474670
C	12.21707153026782	4.52187757328098	10.50200150186470

H	12.05969777310069	5.36641869109949	11.16315926524862
C	11.31414849499351	4.32468317855424	9.45224807900991
C	11.30441753597897	4.75904625862348	4.21924320207775
H	11.21730741593733	5.69078640829938	3.64909739396212
C	12.21786925583167	3.82622274760251	3.40746241201437
C	11.94966355233521	5.09819033374274	5.55482925003010
H	11.41949724697490	5.90413810681414	6.05658317168395
H	11.96042407512117	4.23796034391456	6.23029519832710
H	12.98197002864628	5.42033016693060	5.39126890465431
H	12.34853869519286	2.88085447519571	3.93244840912888
H	13.20339418270143	4.28177284130717	3.27325909670920
H	11.79394776586383	3.61646557361599	2.42315306657460
C	10.08457492442449	5.21526532560677	9.43669937213043
H	10.34460226647376	6.07736582465563	10.05945872669610
C	8.92387018267840	4.48746363558096	10.12754115480704
C	9.64119655025386	5.74495401028023	8.07631061321152
H	10.38171928871027	6.42918155087876	7.66223742855892
H	9.48683676916151	4.92922042641381	7.36353659848561
H	8.69876652219460	6.28987480383305	8.18207753848832
H	8.63032001681303	3.62264697004966	9.53437432997961
H	8.05804951024356	5.14898920163722	10.22477905454589
H	9.21261317955720	4.14199745171641	11.12240654793726

[9]$^{+}$ - S_0 (S = 0)

Eh = -3403.872121873042

Cu	10.33037625280999	2.71465291691518	6.98509220536361
C	7.85692910850407	1.68262769346185	8.49295905514838
N	8.44739407899479	1.95191983150282	7.33679293260944
C	9.68230693190569	0.16689505793657	9.10501342747619
H	9.81834973910921	0.17673779517489	8.02976058805624
H	9.53128411286735	-0.85478172952221	9.46529269240428
H	10.58039684613269	0.57622671245930	9.57358112791623
N	8.52510093562418	0.98120666318168	9.44399655089390
C	8.29044553230240	1.14908671220257	10.87267475249071
H	9.24172556288101	1.38118498916117	11.35837309127608
H	7.88899440492237	0.23496063579169	11.31893424230532
H	7.59892070300674	1.96880095636156	11.04272875456966
N	6.61135965896322	2.14419936149190	8.83579992728504
N	9.44807073610376	3.39303237800780	5.22212674458368
C	5.63845955755619	1.30179126644859	9.52339300898114
H	4.78114276367373	1.13023640839411	8.86348301836972
H	5.27867631229864	1.77657383474088	10.44003984432036
H	6.08530471460546	0.34162106034023	9.76877873094848
C	6.05985689611230	3.34186830980534	8.21885548099038
H	6.86543040644909	3.94058981291744	7.80134405087974
H	5.54539375585409	3.92077613236491	8.98960764527326
H	5.35051999398480	3.09614829552895	7.42288721209339
C	7.69747261869375	2.01327615997030	6.16778236504774
C	6.53504666590141	1.27824462881962	5.95911351040947
H	6.18276272717217	0.62507543960036	6.74767868625307
C	5.81568817452821	1.35065303069308	4.75874394326868
H	4.91090319676232	0.76522778344549	4.64766765597365
C	6.25060593971228	2.15643390412394	3.73528164591174
H	5.69602922157928	2.23943400339571	2.80854078727488
C	7.96822460468351	3.69307065517452	2.84925182131151
H	7.40248095732391	3.81169214317746	1.93206288533605
C	8.21519962188900	2.78562228172596	5.08027173070404

C	7.45822492294541	2.87170881282707	3.87965644375009
C	9.91388245897334	4.12875913500030	4.21633338594178
C	9.16482842726623	4.31964995485056	3.02752963977256
H	9.57647327092166	4.95835605936260	2.25538506325608
C	12.31003426528447	0.86126607385849	5.54890406837959
N	11.87771858624508	1.34905440139919	6.70188726542592
C	10.23278342620268	-0.38380655268009	5.32707855089143
H	9.43299357806594	0.35626415807819	5.40072634435537
H	10.45374747012610	-0.77115313180241	6.31820884837602
H	9.90273171455196	-1.20436743748047	4.68771995055176
N	11.44494572537490	0.17971101047413	4.75034906060148
C	11.42885542282755	0.31866434432500	3.29772036714367
H	11.44056371049179	-0.66372102967656	2.81969532196976
H	12.29196932409286	0.88731262901403	2.96655382122385
H	10.52094401575660	0.84790269027595	2.99093371056970
N	11.47076569235981	3.31686052504080	8.58858364811974
N	13.58423081094827	1.01993164976022	5.07132596785953
C	14.44609381335502	2.09673319306565	5.53422960980669
H	14.98537950879888	2.50238324571319	4.67491828669776
H	15.16928376712039	1.74416198690630	6.27567701263963
H	13.84272377847756	2.88352887226647	5.97762271514455
C	14.26263914773105	-0.03084691475439	4.32045396593636
H	14.57401661431489	0.32339287547173	3.33380148801591
H	13.60091317101715	-0.88530353763709	4.20364638028695
H	15.15517583902290	-0.34510386069450	4.87134495673935
C	12.72757406313233	1.40335574000281	7.80237157844242
C	13.70119708108284	0.44472055220023	8.05512925333600
H	13.81582380027050	-0.37651530757448	7.35781210440316
C	14.53042853555168	0.51080093795317	9.18345071374316
H	15.28008187856178	-0.25617899696949	9.33634256498949
C	14.39665399988809	1.53864163975651	10.08446362490713
H	15.04080184611575	1.61394732203031	10.95208503097330
C	13.38702729250288	2.50660384127818	9.89296646604035
C	12.51970506077220	2.43674069751393	8.76805971063922
C	13.18959956392857	3.57278035980180	10.79777597137512
H	13.84847138801883	3.67652393196434	11.65246434005022
C	12.16851404268928	4.45167266783209	10.58305355167739
H	11.99417975734980	5.27623505318435	11.26325093646955
C	11.29302773238534	4.29000313062891	9.48092463600314
C	11.30018507031599	4.74984094872173	4.20011327420432
H	11.17714140593549	5.70299959920348	3.67427601257002
C	12.22296571866480	3.87756535448716	3.33073512464666
C	11.94763896733664	5.04234697490286	5.54367364384785
H	11.40041285718434	5.80661389713453	6.08896879981360
H	11.99404362486578	4.15025499311984	6.17359797632156
H	12.96615494417134	5.40414089120103	5.38422760647021
H	12.40909983871882	2.92305117514454	3.82258711868130
H	13.18087829254099	4.38112283410017	3.18423760511856
H	11.78516181775495	3.67970668028630	2.35043744366839
C	10.08534024286898	5.21064285643512	9.45735640888679
H	10.38256211106226	6.09494348890925	10.02892494752525
C	8.94351180511676	4.53275912829426	10.23038205257127
C	9.60728775772607	5.68322757943818	8.08998214385321
H	10.33314808980071	6.35396419096388	7.63178329962132
H	9.43510763757835	4.84269247600591	7.41129918785773
H	8.66929345161649	6.23194955521480	8.20251509700434
H	8.61327438328020	3.64720373890281	9.69070405874353

H	8.09694614238704	5.21597693146529	10.32747673727960
H	9.26190210364212	4.23238985870777	11.23066598908190

[9]$^{+}$ - T_1 (S = 2)

Eh = -3403.805693065654

Cu	10.31875850953606	2.88993475972451	6.85172824449710
C	8.00193127690695	1.84329958743233	8.57101559131739
N	8.50637432394055	2.11396916784490	7.36590700407270
C	9.81960539183248	0.26937902167953	9.08072587937303
H	9.93086752433265	0.30073006135721	8.00295757739356
H	9.57177714368246	-0.74582108126640	9.40549072023345
H	10.76171341538948	0.56641775434911	9.54128137390327
N	8.75608436557728	1.18140954742519	9.48001272281671
C	8.61077926735376	1.34707406540455	10.92117859937369
H	9.58522492818203	1.61179946544704	11.33878081473165
H	8.26956179013540	0.42103080221218	11.39207272123523
H	7.90610003422873	2.14346270077788	11.13724976023783
N	6.75161181982851	2.23344789369455	8.95424679894654
N	9.45724638192383	3.27763001291455	5.12881452010457
C	5.87643105920333	1.38233682950913	9.75411082397566
H	4.96508063213372	1.17827624798690	9.18345007829110
H	5.59505263656242	1.86821373278717	10.69189601591122
H	6.37103625508705	0.43898014122163	9.97055889003674
C	6.10438398559209	3.39466240265040	8.35642139152103
H	6.84392717577914	3.99642046222845	7.83627510492623
H	5.65170130312255	3.98838768540515	9.15412948252949
H	5.33096369856635	3.09227087596057	7.64568105469233
C	7.69508759834818	2.06094896926058	6.22273426723760
C	6.51168175572108	1.32176625396193	6.12928834053951
H	6.16047875717028	0.76355669319187	6.98688241889598
C	5.79287825578946	1.26890513362761	4.93453858876545
H	4.87890924461593	0.68878101629960	4.89265485431369
C	6.23285065650360	1.94815621420345	3.81562135112100
H	5.66414776913739	1.93215684401570	2.89398560789222
C	7.97930374480083	3.35121292258133	2.74239623547779
H	7.42287424249773	3.37963976891187	1.81359554969062
C	8.20479809021539	2.68875795817177	5.06141802536872
C	7.44968895808611	2.65902753685694	3.85546618418838
C	9.93836873536382	3.93981542354873	4.04669555215201
C	9.19251402918857	3.99669018132015	2.86572105036614
H	9.59363795579524	4.56662719265611	2.03627011102204
C	12.20608110387216	1.04891483980486	5.28719624738348
N	11.81795359124822	1.55652855892613	6.45817428451139
C	10.05042354581008	-0.08551205770418	4.95111213249784
H	9.18051436837174	0.43725312229200	4.55384207052487
H	10.03665971019105	-0.02668693350295	6.03345667070483
H	10.00693205678721	-1.13212972607579	4.63464940642664
N	11.28116766973264	0.51355087014969	4.45407416539170
C	11.38813586959168	0.55601150733187	3.00080534857648
H	11.42141094323199	-0.45298330182954	2.58077246109047
H	12.28040665459598	1.09788549644769	2.70549233160153
H	10.51204945433027	1.07437057257958	2.60253250004099
N	11.31960555062098	3.26335682154115	8.49895812222710
N	13.50159442175835	1.05227227074037	4.85866149426315
C	14.46869809549316	2.03741120050621	5.32583572722075
H	15.01907802822265	2.42038085135245	4.46293073707059
H	15.17145279926364	1.59196060271997	6.03440338856586

H	13.95358982876087	2.85889176506447	5.81331055855103
C	14.07863437838400	-0.06809686168486	4.12194947210278
H	14.43996347874973	0.24474522166276	3.13871138053724
H	13.33720269494080	-0.85348915771076	4.00041637182042
H	14.92509273319104	-0.46484355972270	4.69066684118797
C	12.63636605615394	1.45939943455868	7.59338790919425
C	13.58497311757143	0.45037528602856	7.78993829212973
H	13.72766735776488	-0.30369446088120	7.02672348335635
C	14.33115664942357	0.38958324360627	8.96670550800014
H	15.05840137618489	-0.40344023241465	9.09248471109771
C	14.15464856393259	1.33197931696451	9.96103640104030
H	14.75445277878849	1.30925972953235	10.86267560387674
C	13.17121948402996	2.33251055435735	9.82037094883104
C	12.37414943183299	2.37356477412110	8.64199466692487
C	12.92785665342044	3.31892792168396	10.80234600189605
H	13.53440257810096	3.34494882064102	11.69929730847031
C	11.92854754973939	4.24742785266855	10.59096048950142
H	11.74800420477196	5.03012423782458	11.31805748874032
C	11.10894021506148	4.20140947872712	9.46013635770514
C	11.26204119658120	4.68717479808469	4.04656509810195
H	11.02046016235703	5.66543941339455	3.61500574738273
C	12.28336844422759	4.03274209133622	3.10243681287782
C	11.89157246620726	4.94354912059026	5.40729781154220
H	11.20924891371547	5.46763318463436	6.07124424564352
H	12.20010493607739	4.01548738029871	5.89493538204366
H	12.78536025073866	5.56021893611021	5.28985007746930
H	12.62934785091240	3.08421717733146	3.51401292321665
H	13.15045014537672	4.68659402376688	2.98250409224630
H	11.85775184692067	3.84506337175784	2.11580200143890
C	9.98527953869802	5.22566616837360	9.41648376053019
H	10.42702187357195	6.12741611562791	9.85295564763936
C	8.83195601143156	4.81626385095061	10.34684338332298
C	9.44664972715946	5.62081769892696	8.04674575819864
H	10.19913393970762	6.13940310981370	7.45602067798542
H	9.08209930396098	4.76077005353136	7.47533598477925
H	8.60114901723197	6.30113471221012	8.17181011048694
H	9.19723463307666	4.55430072936500	11.34101911013124
H	8.29806663693952	3.95979380763108	9.93817346238994
H	8.12376415005072	5.64232962460339	10.44642158835899

5. References

(1) Kovalevsky, A. Yu.; Gembicky, M.; Novozhilova, I. V.; Coppens, P. Solid-State Structure Dependence of the Molecular Distortion and Spectroscopic Properties of the Cu(I) Bis(2,9-Dimethyl-1,10-Phenanthroline) Ion. *Inorg. Chem.* **2003**, *42* (26), 8794–8802. https://doi.org/10.1021/ic0348805.

(2) Cunningham, C. T.; Moore, J. J.; Cunningham, K. L. H.; Fanwick, P. E.; McMillin, D. R. Structural and Photophysical Studies of Cu(NN)2+ Systems in the Solid State. Emission at Last from Complexes with Simple 1,10-Phenanthroline Ligands. *Inorg. Chem.* **2000**, *39* (16), 3638–3644. https://doi.org/10.1021/ic000082s.

(3) Kubiček, K.; Thekku Veedu, S.; Storozhuk, D.; Kia, R.; Techert, S. Geometric and Electronic Properties in a Series of Phosphorescent Heteroleptic Cu(I) Complexes: Crystallographic and Computational Studies. *Polyhedron* **2017**, *124*, 166–176. https://doi.org/10.1016/j.poly.2016.12.035.

(4) Smith, C. S.; Branham, C. W.; Marquardt, B. J.; Mann, K. R. Oxygen Gas Sensing by Luminescence Quenching in Crystals of Cu(Xantphos)(Phen) + Complexes. *J. Am. Chem. Soc.* **2010**, *132* (40), 14079–14085. https://doi.org/10.1021/ja103112m.

(5) Hoffmann, A.; Binder, S.; Jesser, A.; Haase, R.; Flörke, U.; Gnida, M.; Salomone Stagni, M.; Meyer-Klaucke, W.; Lebsanft, B.; Grünig, L. E.; Schneider, S.; Hashemi, M.; Goos, A.; Wetzel, A.; Rübhausen, M.; Herres-Pawlis, S. Catching an Entatic State - A Pair of Copper Complexes. *Angew. Chem. - Int. Ed.* **2014**, *53* (1), 299–304. https://doi.org/10.1002/anie.201306061.

(6) Cunningham, K. L.; McMillin, D. R. Reductive Quenching of Photoexcited Cu(Dipp)2+ and Cu(Tptap)2+ by Ferrocenes (Dipp = 2,9-Diisopropyl-1,10-Phenanthroline and Tptap = 2,3,6,7-Tetraphenyl-1,4,5,8-Tetraazaphenanthrene). *Inorg. Chem.* **1998**, *37* (16), 4114–4119. https://doi.org/10.1021/ic980213d.

(7) Heck, J.; Metz, F.; Buchenau, S.; Teubner, M.; Grimm-Lebsanft, B.; Spaniol, T. P.; Hoffmann, A.; Rübhausen, M. A.; Herres-Pawlis, S. Manipulating Electron Transfer – the Influence of Substituents on Novel Copper Guanidine Quinolinyl Complexes. *Chem. Sci.* **2022**, *13*, 8274–8288. https://doi.org/10.1039/D2SC02910C.

(8) Eggleston, M. K.; McMillin, D. R.; Koenig, K. S.; Pallenberg, A. J. Steric Effects in the Ground and Excited States of Cu(NN)2+ Systems. *Inorg. Chem.* **1997**, *36* (2), 172–176. https://doi.org/10.1021/ic960698a.

(9) Gimeno, L.; Blart, E.; Rebilly, J.; Coupeau, M.; Allain, M.; Roisnel, T.; Quarré de Verneuil, A.; Gourlaouen, C.; Daniel, C.; Pellegrin, Y. Non-Symmetrical Sterically Challenged Phenanthroline Ligands and Their Homoleptic Copper(I) Complexes with Improved Excited-State Properties. *Chem. – Eur. J.* **2020**, *26* (51), 11887–11899. https://doi.org/10.1002/chem.202001209.

(10) Neese, F. The ORCA Program System. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2* (1), 73–78. https://doi.org/10.1002/wcms.81.

(11) Neese, F. Software Update: The ORCA Program System—Version 5.0. *WIREs Comput. Mol. Sci.* **2022**, *12* (5), e1606. https://doi.org/10.1002/wcms.1606.

(12) Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. Comparative Assessment of a New Nonempirical Density Functional: Molecules and Hydrogen-Bonded Complexes. *J. Chem. Phys.* **2003**, *119* (23), 12129–12137. https://doi.org/10.1063/1.1626543.

(13) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7* (18), 3297. https://doi.org/10.1039/b508541a.

(14) Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. Efficient, Approximate and Parallel Hartree–Fock and Hybrid DFT Calculations. A 'Chain-of-Spheres' Algorithm for the Hartree–Fock Exchange. *Chem. Phys.* **2009**, *356* (1–3), 98–109. https://doi.org/10.1016/j.chemphys.2008.10.036.

(15) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132* (15), 154104. https://doi.org/10.1063/1.3382344.

(16) Baik, M.-H.; Friesner, R. A. Computing Redox Potentials in Solution: Density Functional Theory as A Tool for Rational Design of Redox Agents. *J. Phys. Chem. A* **2002**, *106* (32), 7407–7412. https://doi.org/10.1021/jp025853n.
(17) Roy, L. E.; Jakubikova, E.; Guthrie, M. G.; Batista, E. R. Calculation of One-Electron Redox Potentials Revisited. Is It Possible to Calculate Accurate Potentials with Density Functional Methods? *J. Phys. Chem. A* **2009**, *113* (24), 6745–6750. https://doi.org/10.1021/jp811388w.
(18) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113* (18), 6378–6396. https://doi.org/10.1021/jp810292n.
(19) Pascual-Ahuir, J. L.; Silla, E. GEPOL: An Improved Description of Molecular Surfaces. I. Building the Spherical Surface Set. *J. Comput. Chem.* **1990**, *11* (9), 1047–1060. https://doi.org/10.1002/jcc.540110907.
(20) Silla, E.; Tuñón, I.; Pascual-Ahuir, J. L. GEPOL: An Improved Description of Molecular Surfaces II. Computing the Molecular Area and Volume. *J. Comput. Chem.* **1991**, *12* (9), 1077–1088. https://doi.org/10.1002/jcc.540120905.
(21) Pascual-ahuir, J. L.; Silla, E.; Tuñon, I. GEPOL: An Improved Description of Molecular Surfaces. III. A New Algorithm for the Computation of a Solvent-Excluding Surface. *J. Comput. Chem.* **1994**, *15* (10), 1127–1138. https://doi.org/10.1002/jcc.540151009.
(22) Demissie, T. B.; Ruud, K.; Hansen, J. H. DFT as a Powerful Predictive Tool in Photoredox Catalysis: Redox Potentials and Mechanistic Analysis. *Organometallics* **2015**, *34* (17), 4218–4228. https://doi.org/10.1021/acs.organomet.5b00582.
(23) Sandoval-Pauker, C.; Pinter, B. Electronic Structure Analysis of Copper Photoredox Catalysts Using the Quasi-Restricted Orbital Approach. *J. Chem. Phys.* **2022**, *157* (7), 074306. https://doi.org/10.1063/5.0094380.
(24) Medina, E.; Pinter, B. Electron Density Difference Analysis on the Oxidative and Reductive Quenching Cycles of Classical Iridium and Ruthenium Photoredox Catalysts. *J. Phys. Chem. A* **2020**, *124* (21), 4223–4234. https://doi.org/10.1021/acs.jpca.9b10238.
(25) Medina, E.; Sandoval-Pauker, C.; Salvador, P.; Pinter, B. Mechanistic Insights into the Oxidative and Reductive Quenching Cycles of Transition Metal Photoredox Catalysts through Effective Oxidation State Analysis. *Inorg. Chem.* **2022**, *61* (47), 18923–18933. https://doi.org/10.1021/acs.inorgchem.2c02945.
(26) Medina, E.; Pinter, B. A DFT Study on the Redox Active Behavior of Carbene and Pyridine Ligands in the Oxidative and Reductive Quenching Cycles of Ruthenium Photoredox Catalysts. *Catalysts* **2020**, *10* (1), 80. https://doi.org/10.3390/catal10010080.
(27) Suo, B.; Shen, K.; Li, Z.; Liu, W. Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. *J. Phys. Chem. A* **2017**, *121* (20), 3929–3942. https://doi.org/10.1021/acs.jpca.7b00752.
(28) Jacquemin, D.; Mennucci, B.; Adamo, C. Excited-State Calculations with TD-DFT: From Benchmarks to Simulations in Complex Environments. *Phys. Chem. Chem. Phys.* **2011**, *13* (38), 16987–16998. https://doi.org/10.1039/c1cp22144b.
(29) Kirchhoff, J. R.; Gamache, R. E.; Blaskie, M. W.; Del Paggio, A. A.; Lengel, R. K.; McMillin, D. R. Temperature Dependence of Luminescence from Cu(NN)2+ Systems in Fluid Solution. Evidence for the Participation of Two Excited States. *Inorg. Chem.* **1983**, *22* (17), 2380–2384. https://doi.org/10.1021/ic00159a008.
(30) Kuang, S.-M.; Cuttell, D. G.; McMillin, D. R.; Fanwick, P. E.; Walton, R. A. Synthesis and Structural Characterization of Cu(I) and Ni(II) Complexes That Contain the Bis[2-(Diphenylphosphino)Phenyl]Ether Ligand. Novel Emission Properties for the Cu(I) Species. *Inorg. Chem.* **2002**, *41* (12), 3313–3322. https://doi.org/10.1021/ic0201809.
(31) Armaroli, N.; Accorsi, G.; Bergamini, G.; Ceroni, P.; Holler, M.; Moudam, O.; Duhayon, C.; Delavaux-Nicot, B.; Nierengarten, J.-F. Heteroleptic Cu(I) Complexes Containing Phenanthroline-

Type and 1,1′-Bis(Diphenylphosphino)Ferrocene Ligands: Structure and Electronic Properties. *Inorganica Chim. Acta* **2007**, *360* (3), 1032–1042. https://doi.org/10.1016/j.ica.2006.07.085.