Supplemental information for

Feasibility of controlled nitric oxide generation via ascorbate induced chemical reduction of nitrite ions

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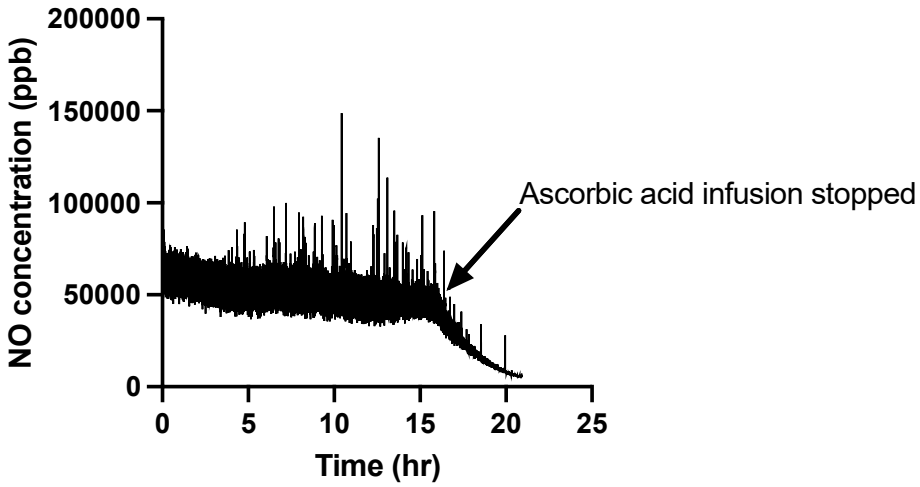


Figure S1. NO generation with ascorbic acid infused into electrolyte is sluggish. Infusion of 1 mL of 0.28 M ascorbic acid infused at 1 μL/min into 5 mL of electrolyte containing 1 M $NaNO_2$.

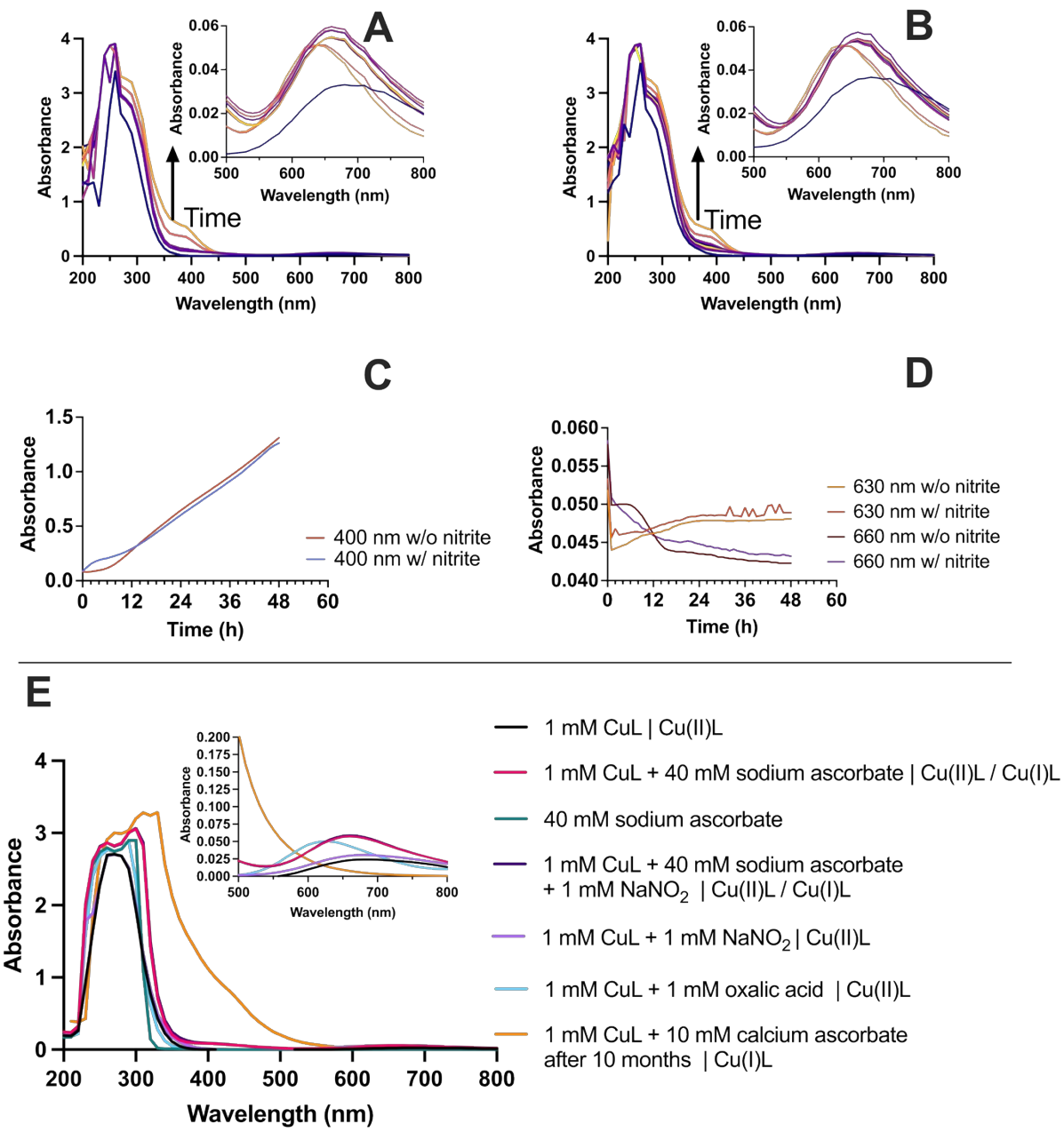
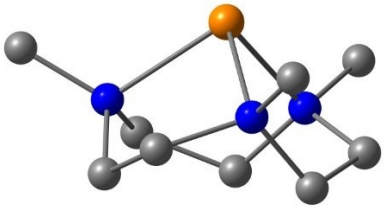
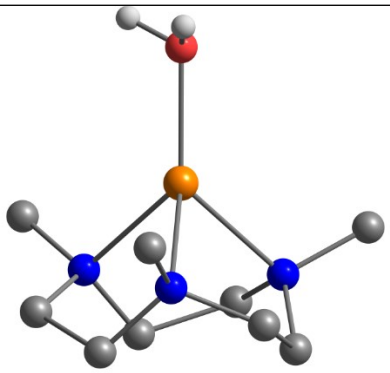
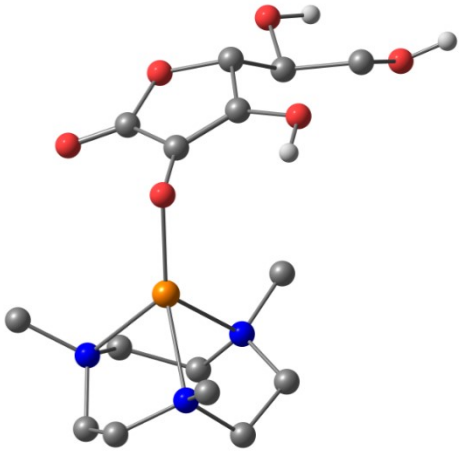
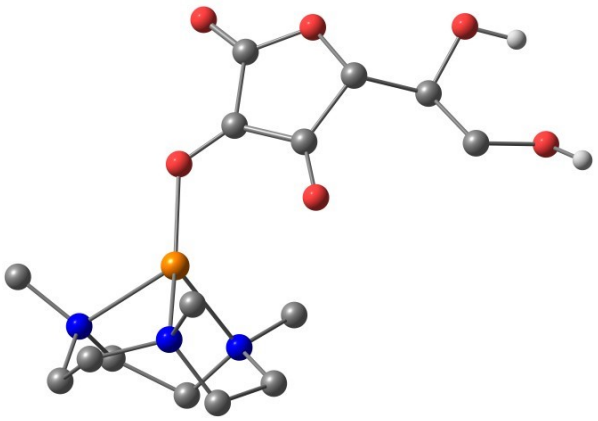
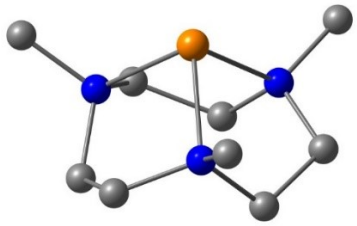
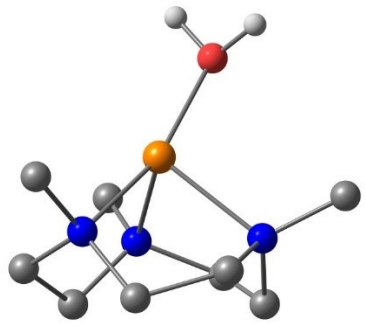
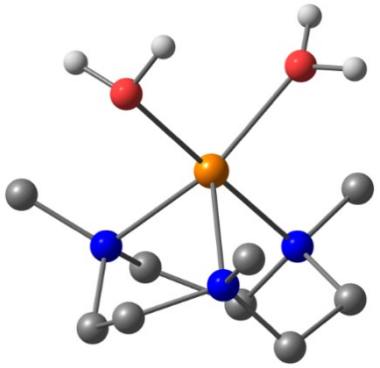
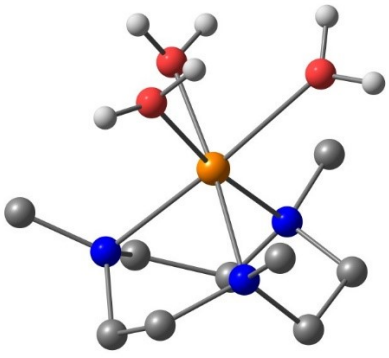


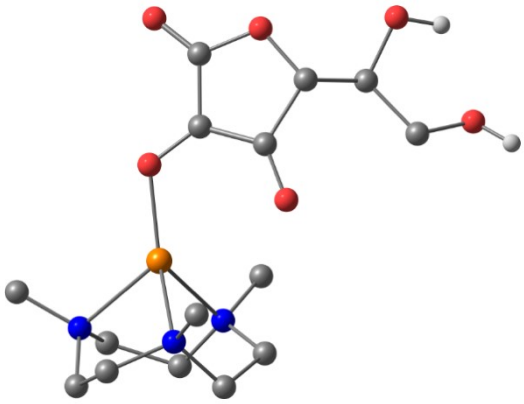
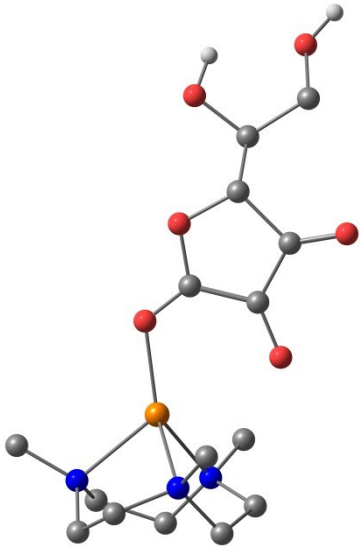
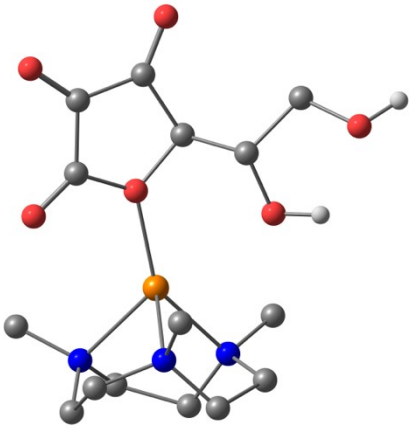
Figure S2. UV-vis spectra of deoxygenated electrolyte before and after addition of ascorbate over time (0 min, 10 min, 20 min, 30 min, 1 h, 2 h, 3 h, 4 h, 24 h, 48 h) (A) in the absence and (B) presence of nitrite ions. Insets show the visible (500-800 nm) range. Absorbance change of the electrolyte at (C) 400 nm and (D) 630 nm and 660 nm with and without nitrite. (E) UV-vis spectra of different electrolyte compositions in 0.5 M MES pH 5.8, exposed to air. Legend shows the individual components of electrolyte, where CuL represents Cu(II)L; the composition may change after mixing the components, as noted.

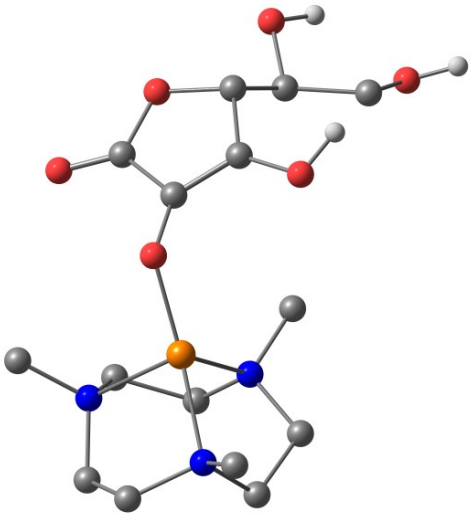
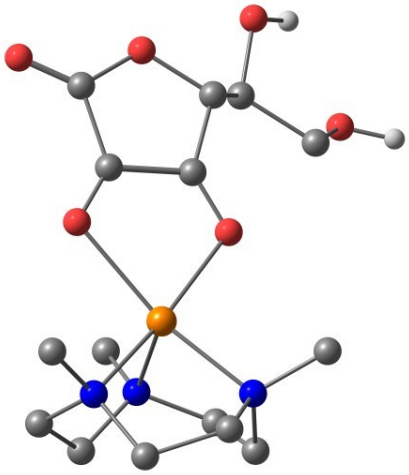
Table S1. The structures of the investigated complexes at ωB97X-D/def2SVP level.

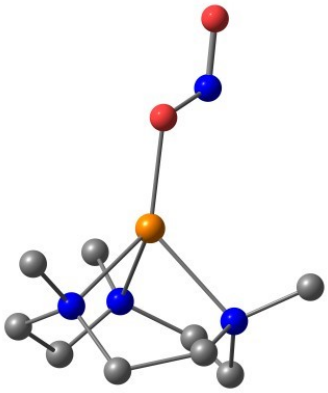
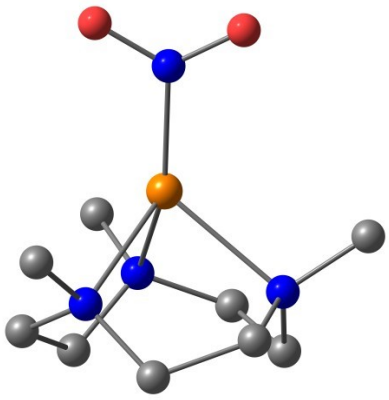
Name	Structure
$[Cu(I)L]^+$ Selected wavelengths: 376.14 nm (f = 0.01) 228.44 nm (f = 0.01) 228.39 nm (f = 0.01) 216.66 nm (f = 0.04)	
$[Cu(I)L(H_2O)]^+$ Selected wavelengths: 207.38 nm (f = 0.01) 202.54 nm (f = 0.01) 200.37 nm (f = 0.01) 199.78 nm (f = 0.01) 198.94 nm (f = 0.01)	
$[Cu(I)LHAsc]^+$ Selected wavelengths: 344.97 nm (f = 0.01) 303.59 nm (f = 0.05) 274.26 nm (f = 0.03) 258.64 nm (f = 0.01) 235.47 nm (f = 0.04)	

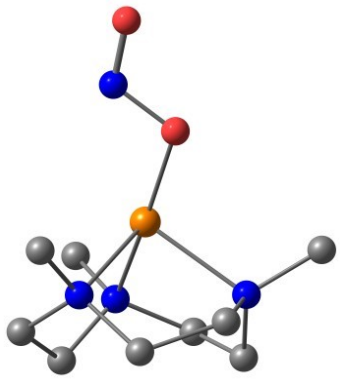
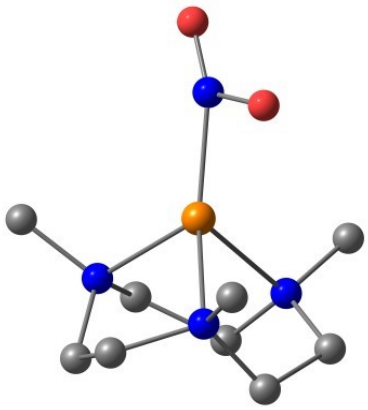
[Cu(I)LDHA]$^{+}$ Selected wavelengths: 828.59 nm (f = 0.01) 686.54 nm (f = 0.15) 566.75 nm (f = 0.06) 402.51 nm (f = 0.01) 367.25 nm (f = 0.02) 318.00 nm (f = 0.01) 299.75 nm (f = 0.02) 279.60 nm (f = 0.01) 271.87 nm (f = 0.06)	
[Cu(II)L]$^{2+}$ Selected wavelengths: 529.57 nm (f = 0.03) 425.46 nm (f = 0.06) 347.12 nm (f = 0.02) 304.90 nm (f = 0.01) 295.01 nm (f = 0.01) 282.31 nm (f = 0.01) 280.25 nm (f = 0.01) 229.70 nm (f = 0.01) 222.94 nm (f = 0.01) 229.70 nm (f = 0.01) 213.74 nm (f = 0.04) 212.48 nm (f = 0.01) 202.02 nm (f = 0.01)	

$[Cu(II)L(H_2O)]^{2+}$ Selected wavelengths: 439.70 nm (f = 0.06) 407.11 nm (f = 0.03) 335.46 nm (f = 0.04) 260.56 nm (f = 0.01) 258.23 nm (f = 0.01) 257.29 nm (f = 0.01) 211.92 nm (f = 0.01) 204.42 nm (f = 0.01) 176.54 nm (f = 0.02)	
$[Cu(II)L(H_2O)_2]^{2+}$ Selected wavelengths: 432.28 nm (f = 0.01) 368.88 nm (f = 0.07) 319.14 nm (f = 0.07) 244.88 nm (f = 0.01) 240.91 nm (f = 0.01) 233.5 nm (f = 0.01) 193.64 nm (f = 0.01) 189.86 nm (f = 0.01) 176.29 nm (f = 0.01)	
$[Cu(II)L(H_2O)_3]^{2+}$ Selected wavelengths: 348.80 nm (f = 0.09) 310.91 nm (f = 0.08) 221.37 nm (f = 0.01) 214.29 nm (f = 0.01)	

[Cu(II)LAsc], conformer 1 Selected wavelengths: 745.35 nm (f = 0.01) 656.06 nm (f = 0.05) 340.35 nm (f = 0.01) 317.40 nm (f = 0.03) 262.51 nm (f = 0.01) 260.31 nm (f = 0.01)	
[Cu(II)LAsc], conformer 2 Selected wavelengths: 595.80 nm (f = 0.01) 365.97 nm (f = 0.07) 298.34 nm (f = 0.01) 285.00 nm (f = 0.01) 272.68 nm (f = 0.08) 268.98 nm (f = 0.04) 261.93 nm (f = 0.01)	
[Cu(II)LAsc], conformer 3 Selected wavelengths: 676.81 nm (f = 0.01) 468.92 nm (f = 0.07) 382.59 nm (f = 0.01) 378.17 nm (f = 0.07) 345.49 nm (f = 0.01) 294.52 nm (f = 0.01) 267.27 nm (f = 0.04)	

[Cu(II)LHAsc]$^{+}$ Selected wavelengths: 650.41 nm (f = 0.08) 617.40 nm (f = 0.10) 372.38 nm (f = 0.01) 365.17 nm (f = 0.02) 324.70 nm (f = 0.03) 309.37 nm (f = 0.03) 280.62 nm (f = 0.02) 235.81 nm (f = 0.19) 226.49 nm (f = 0.02) 215.51 nm (f = 0.01)	
[Cu(II)LDHA]$^{2+}$ Selected wavelengths: 895.07 nm (f = 0.02) 441.38 nm (f = 0.03) 414.81 nm (f = 0.01) 381.71 nm (f = 0.01) 374.04 nm (f = 0.01) 366.14 nm (f = 0.04) 342.66 nm (f = 0.04) 335.37 nm (f = 0.08)	

[Cu(I)LNO$_2$], conformer 1 Selected wavelengths: 349.13 nm (f = 0.05) 231.61 nm (f = 0.01) 230.53 nm (f = 0.01) 223.11 nm (f = 0.01) 222.95 nm (f = 0.01) 219.04 nm (f = 0.01) 204.38 nm (f = 0.01) 203.65 nm (f = 0.01) 199.87 nm (f = 0.02)	
[Cu(I)LNO$_2$], conformer 2 Selected wavelengths: 391.78 nm (f = 0.01) 300.27 nm (f = 0.05) 286.20 nm (f = 0.02) 273.82 nm (f = 0.01) 268.92 nm (f = 0.01) 263.55 nm (f = 0.01) 227.21 nm (f = 0.01) 205.44 nm (f = 0.01) 197.05 nm (f = 0.01) 193.49 nm (f = 0.01) 188.52 nm (f = 0.01) 186.66 nm (f = 0.01)	

$[Cu(II)LNO_2]^+$, conformer 1 Selected wavelengths: 837.18 nm (f = 0.02) 387.70 nm (f = 0.11) 363.02 nm (f = 0.03) 361.24 nm (f = 0.02) 360.00 nm (f = 0.03) 333.54 nm (f = 0.01) 255.88 nm (f = 0.01) 222.77 nm (f = 0.01) 220.82 nm (f = 0.01)	
$[Cu(II)LNO_2]^+$, conformer 2 Selected wavelengths: 562.20 nm (f = 0.01) 542.95 nm (f = 0.01) 430.29 nm (f = 0.11) 356.42 nm (f = 0.01) 341.30 nm (f = 0.03) 330.81 nm (f = 0.01) 309.31 nm (f = 0.01) 305.02 nm (f = 0.02) 302.61 nm (f = 0.02) 259.66 nm (f = 0.01) 257.34 nm (f = 0.01) 208.38 nm (f = 0.01)	

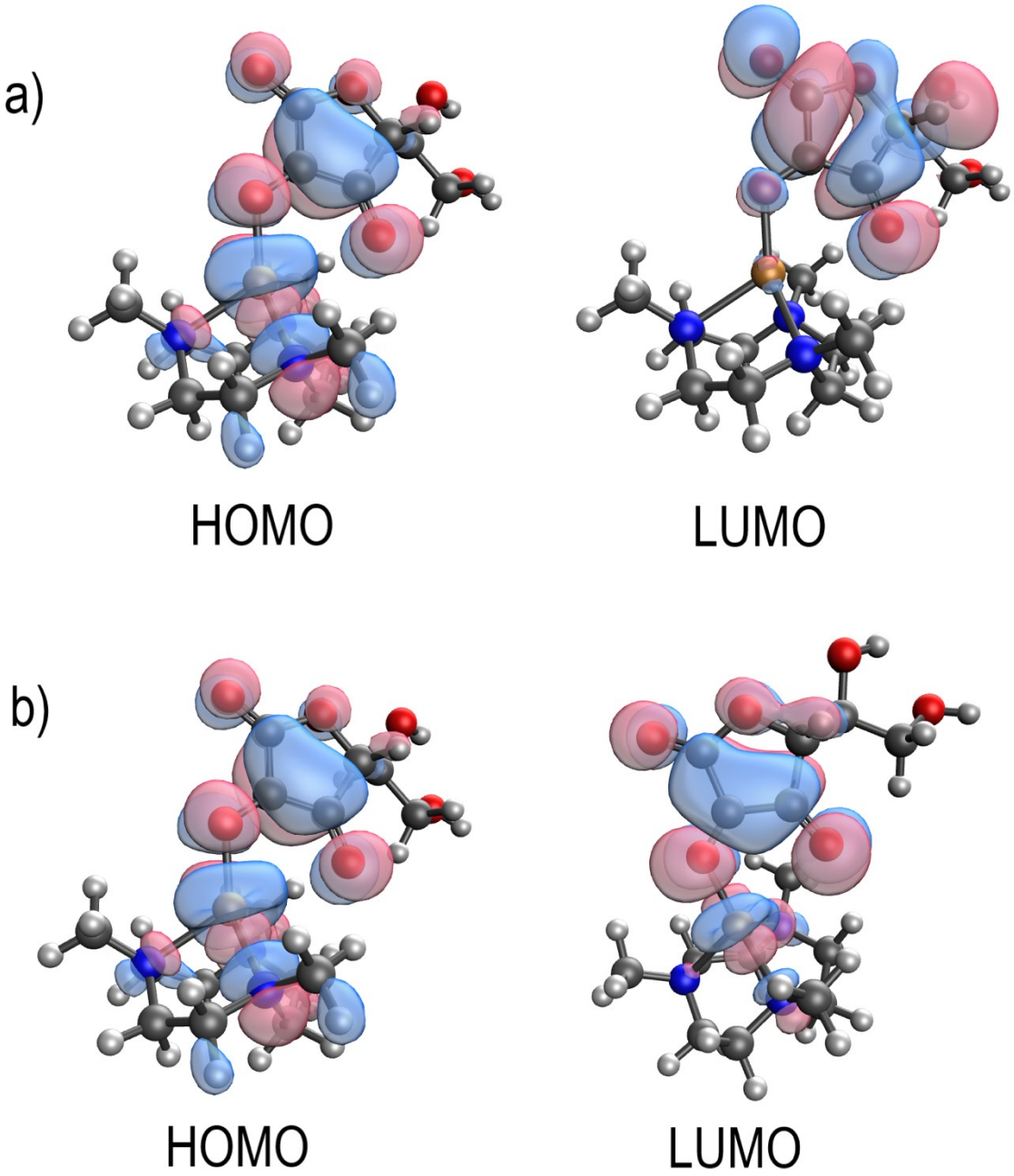


Figure S3. The HOMO and the LUMO of the a) [Cu(II)L(Asc)], conformer 1, b) $[Cu(I)L(DHA)]^+$ at ωB97X-D/def2SVP level, isovalue = 0.050.

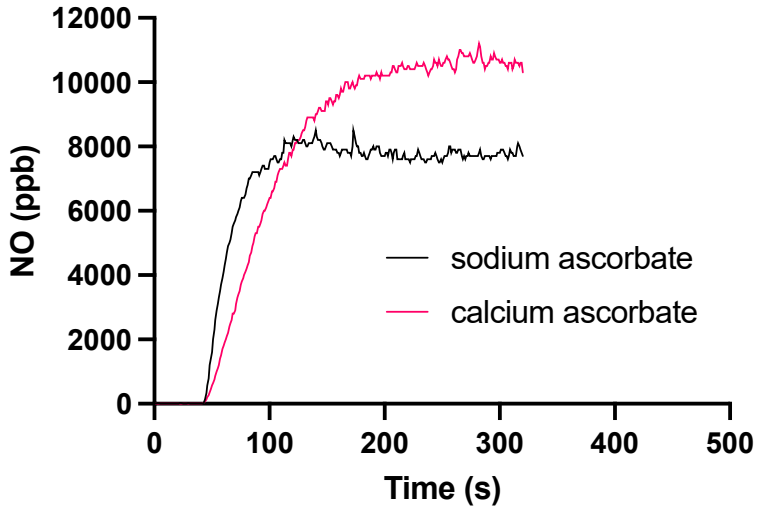


Figure S4: NO generation of electrolyte containing sodium ascorbate (280 mM) and calcium ascorbate (140 mM) infused with 15 μL/min 10 mM sodium nitrite).

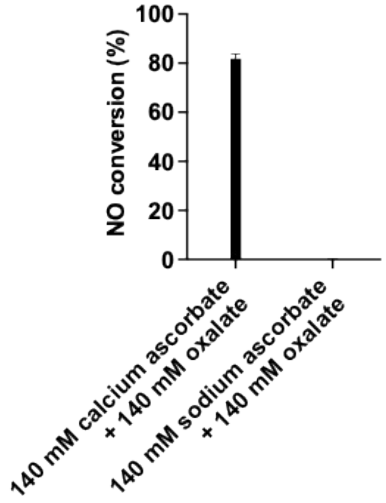


Figure S5. Oxalate present at a high initial concentration in the electrolyte stops nitrite conversion. The presence of 140 mM sodium oxalate dissolved into solution along with 140 mM sodium ascorbate prevents any nitrite conversion to NO from the bolus injection of 2 μL of 10 mM sodium nitrite, as compared to the control with no added sodium oxalate.

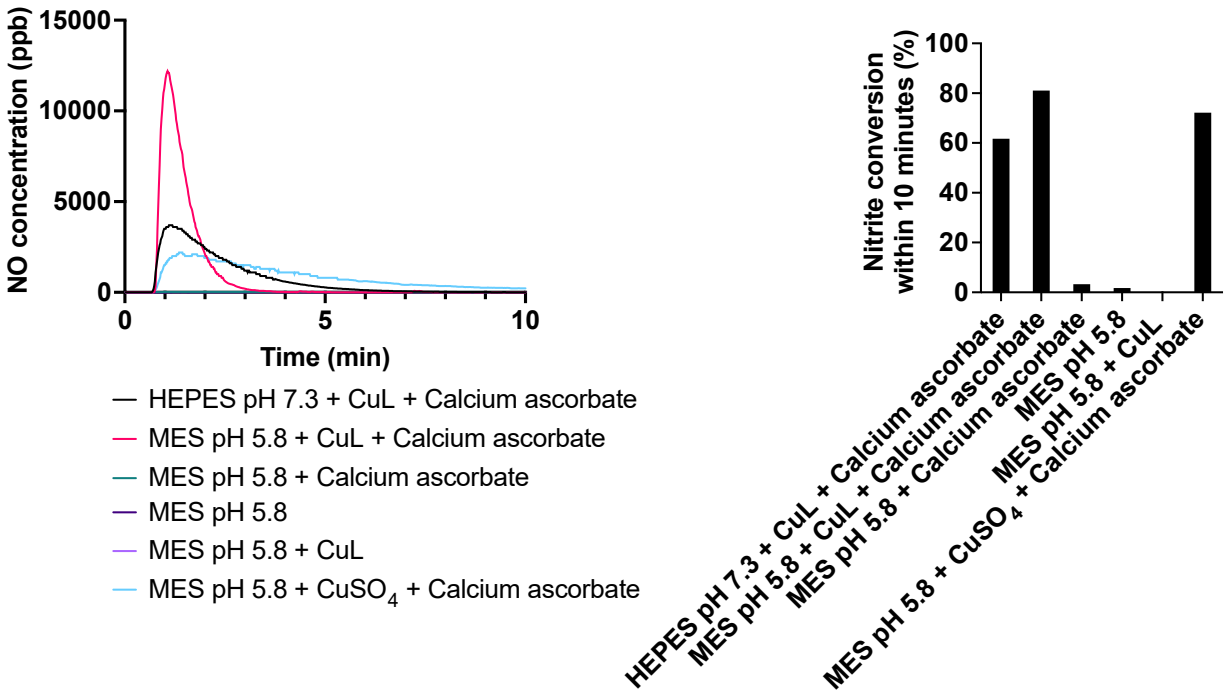


Figure S6. Generated NO concentrations (left) and nitrite conversion to NO (right) from different electrolyte compositions. 10 μL of 10 mM sodium nitrite was injected into 5 mL of the specified electrolyte composition (when present, concentrations of the components are 7 mM CuL, 140 mM calcium ascorbate, and 7 mM copper sulfate).

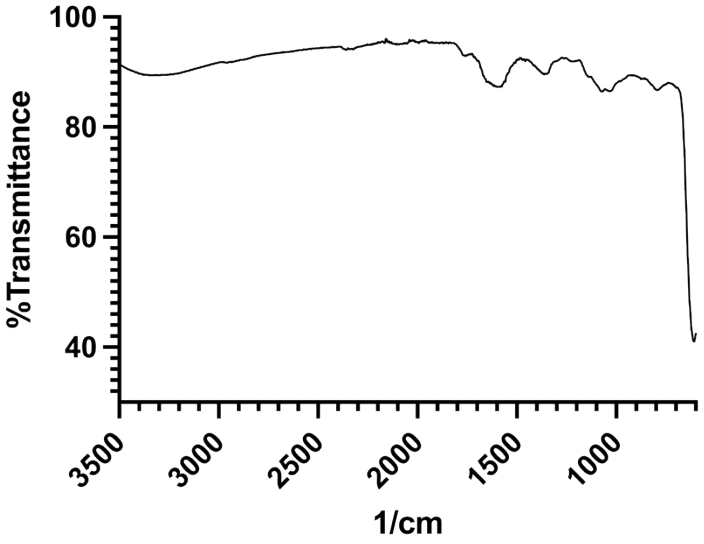


Figure S7. FT-IR ATR spectrum of the freeze dried yellow precipitate formed after mixing $CuSO_4$ and calcium ascorbate.

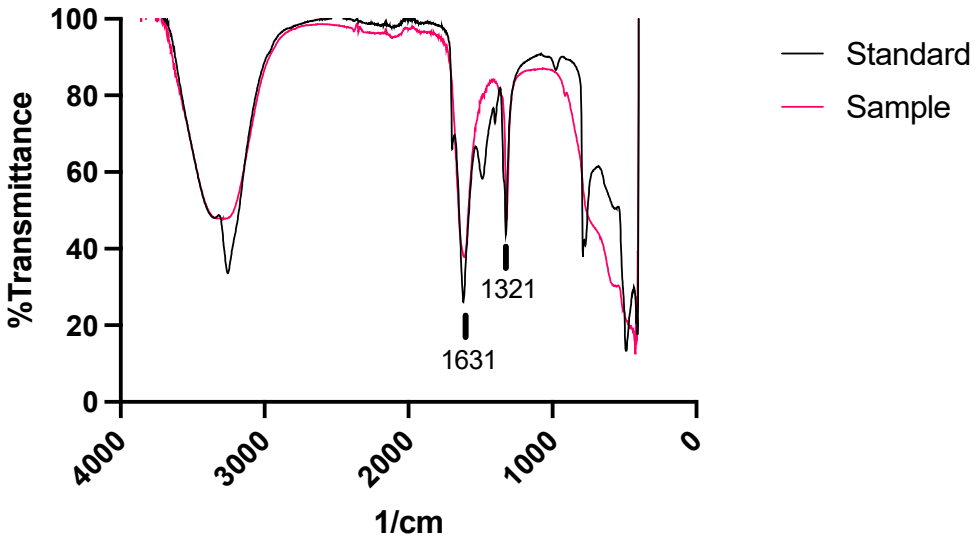


Figure S8. FT-IR ATR spectra of calcium oxalate standard (Standard) and the precipitate (Sample) formed with Ca^{2+} during the storage of the electrolyte. The asymmetric stretching (v_a), symmetric stretching (v_s) oxalate fundamental vibrations assigned to the bands at 1631 and 1321 cm^{-1}, respectively.

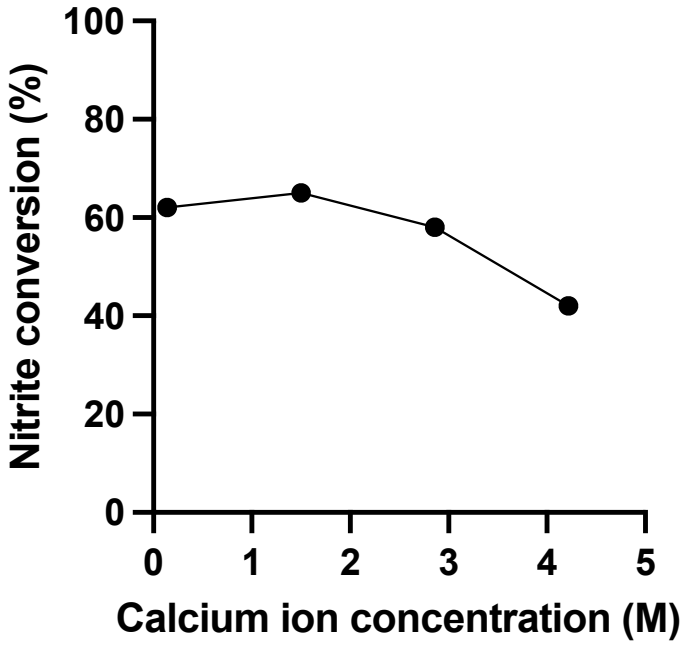


Figure S9. Very high concentrations of calcium ions will eventually deplete nitrite conversion to NO. 15 μL/min of nitrite was infused to 5 mL of electrolyte containing 140 mM calcium ascorbate. One gram of calcium chloride was added by removing one mL of electrolyte from the reaction cell and dissolving the calcium chloride in it, then adding it back to the reaction cell. This was done once a plateau from the previous addition was reached.

Table S2. Summary of electrolyte optimization process.

Initial electrolyte components in reaction chamber	**NO generating addition**	**Major issue(s)**	**Expected source of the issues**	**Improvement**
TACN, $CuSO_4$, nitrite, HEPES pH 7.4	Ascorbic acid	Slow return to baseline	Cu(I) accumulation	
TACN, $CuSO_4$, sodium ascorbate, HEPES pH 7.4	Nitrite	Short shelf life, slow and incomplete NO conversion	Oxalate accumulation due to high pH	Infusing Nitrite greatly improved return to baseline
TACN, $CuSO_4$, sodium ascorbate, MES pH 5.8	Nitrite	Short shelf life	Oxalate accumulation	Optimizing pH improved response time and conversion rate without proton mechanism
TACN, $CuSO_4$, calcium ascorbate, MES pH 5.8	Nitrite			Added calcium ions to remove oxalate from solution
TACN, $CuSO_4$, glutathione, MES pH 5.8	Nitrite	Slow and incomplete NO conversion	Thiolate cluster formation	None
TACN, $CuSO_4$, cysteine, MES pH 5.8	Nitrite	Slow and incomplete NO conversion	Thiolate cluster formation	None
$CuSO_4$, calcium ascorbate, MES pH 5.8	Nitrite	NO was not produced	Copper ions precipitate	None

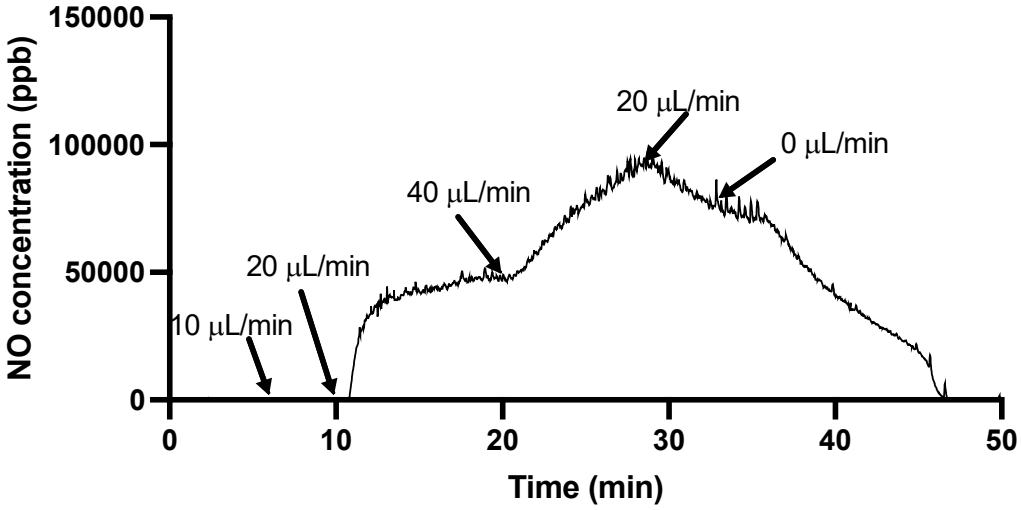


Figure S10. 10 mM calcium ascorbate infused into optimized electrolyte and 140 mM sodium nitrite results in sluggish NO generation and slow responsiveness.

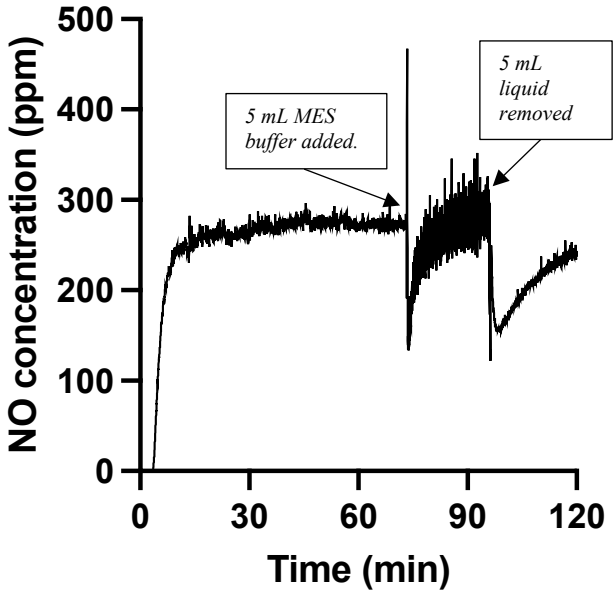


Figure S11. Noisier signal from increased water column. Nitrite (242 mM) was infused at 15 μL/min. There is a part of the reaction cell where the needle is inserted via a septum that, as the water level rises within the cell, can trap NO until sufficient pressure builds up to release the NO. This results in higher spikes and lower dips as more pressure is needed to release the bubble. Additionally, there is likely some variation in the size of the N_2 bubbles sparging the solution over time as a result of the increasing reaction chamber volume. This effect could have been responsible for the increase in NO signal noise observed with time.

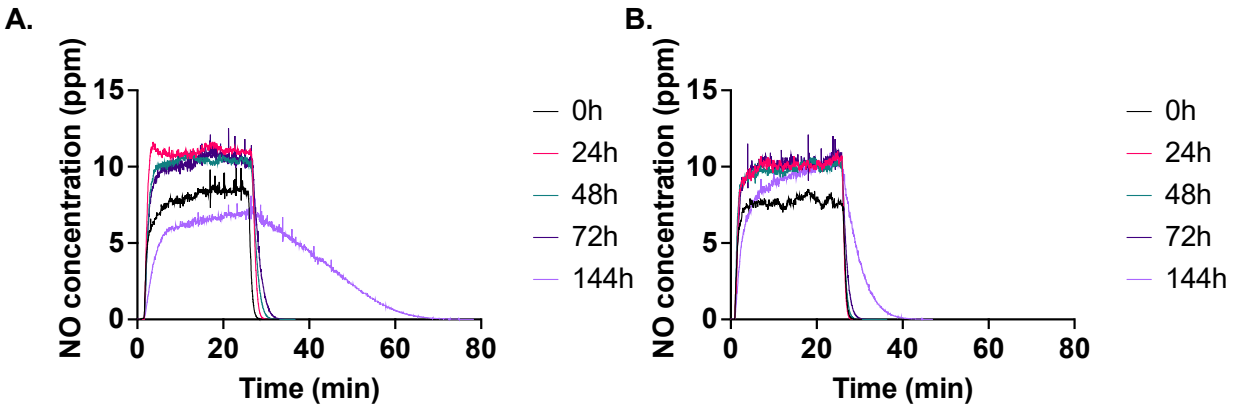


Figure S12: Storage stability of TACN-copper complex with calcium ascorbate concentration of 7 mM (A) and 35 mM (B) over six days. A total of 250 μL of 10 mM $NaNO_2$ was infused at 10 μL/min. The N_2 sparging rate was 0.15 L/min.

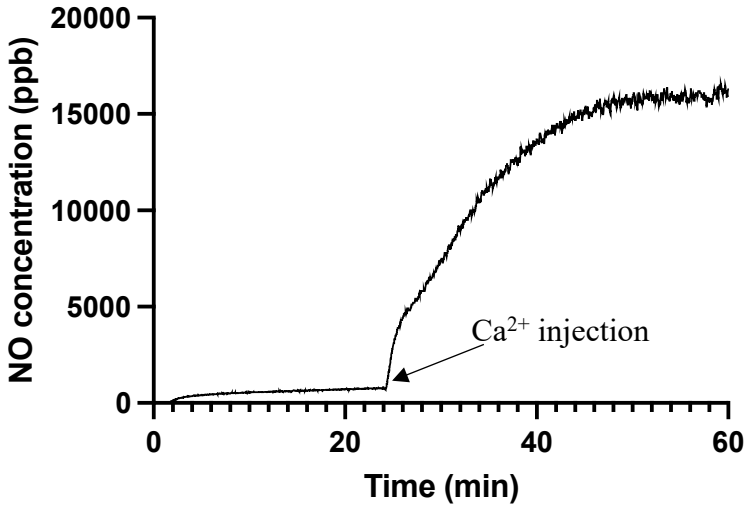


Figure S13: NO generation from continuous nitrite infusion (15 μL/min 10 mM) into electrolyte (1 mL, 1 M ascorbate, MES pH 5.8, 7 mM CuL) stored for 9 months. Electrolyte was stored at RT without light protection, without deoxygenation and without calcium ions. NO generation (flow rate: 200 mL/min) was restored with the addition of calcium ions (100 mL 192 mM $CaCl_2$).

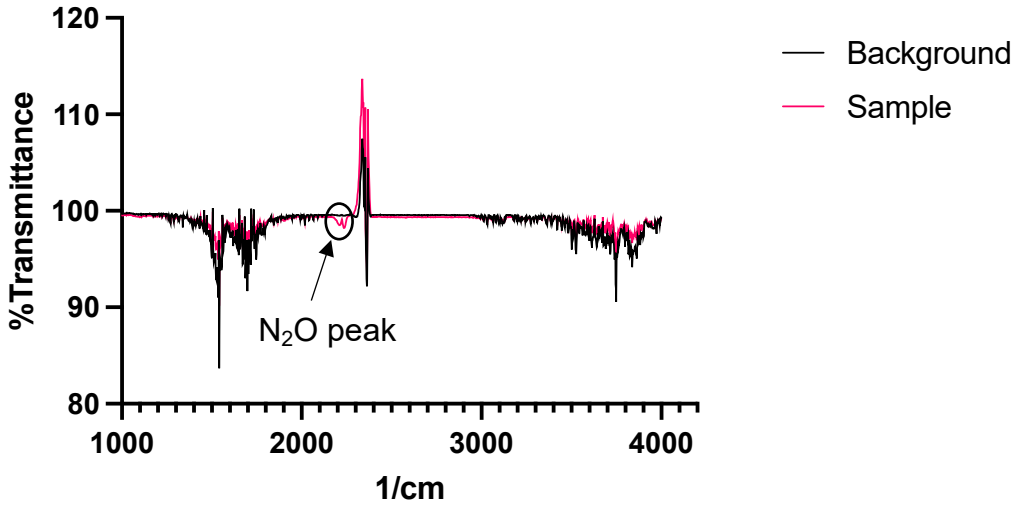


Figure S14. FT-IR spectra of the generated gas from the reaction cell containing 25 mL of 7 mM $[Cu(II)L]^{2+}$, 3.5 mM calcium ascorbate and 14 mM $CaCl_2$ before (black) and after (pink) the addition of 1 mL of 10 mM $NaNO_2$.

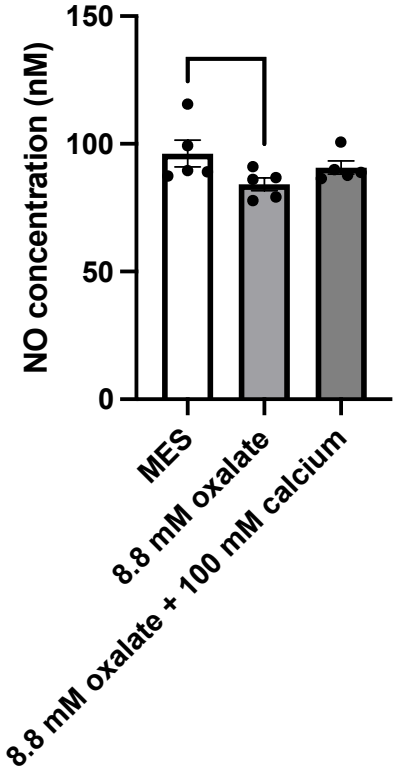


Figure S15. The presence of oxalate in a buffered solution scavenges injected NO gas. 10 mL of DI water was deoxygenated by vigorous sparging with N_2 gas, then 50 ppm of 50 mL/min NO(g) in N_2 was sparged through this deoxygenated water. 200 μL of the NO solution was injected through a Hamilton syringe into a glass reaction cell containing 5 mL of the specified buffered salts.

Time dependent DFT calculations (at B3LYP/def2SVP//ωB97X-D/def2SVP level)

[Cu(I)L]$^+$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4449 eV 507.11 nm f=0.0002 <S**2>=0.000
62 -> 63 0.69792
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2159.51927131
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.4455 eV 506.99 nm f=0.0002 <S**2>=0.000
61 -> 63 0.69792

Excited State 3: Singlet-A 3.1802 eV 389.86 nm f=0.0018 <S**2>=0.000
60 -> 63 0.70034

Excited State 4: Singlet-A 3.1804 eV 389.84 nm f=0.0018 <S**2>=0.000
59 -> 63 0.70034

Excited State 5: Singlet-A 3.2962 eV 376.14 nm f=0.0062 <S**2>=0.000
58 -> 63 0.70307

Excited State 6: Singlet-A 5.4275 eV 228.44 nm f=0.0110 <S**2>=0.000
56 -> 63 0.68167

Excited State 7: Singlet-A 5.4286 eV 228.39 nm f=0.0110 <S**2>=0.000
55 -> 63 0.68162

Excited State 8: Singlet-A 5.7225 eV 216.66 nm f=0.0426 <S**2>=0.000
57 -> 63 0.69094

Excited State 9: Singlet-A 5.7731 eV 214.76 nm f=0.0009 <S**2>=0.000
61 -> 65 -0.32167
61 -> 66 0.36616
62 -> 65 0.37680
62 -> 66 0.32913

Excited State 10: Singlet-A 5.7916 eV 214.08 nm f=0.0017 <S**2>=0.000
61 -> 65 0.28455
62 -> 64 0.57040
62 -> 66 0.27330

Excited State 11: Singlet-A 5.7929 eV 214.03 nm f=0.0017 <S**2>=0.000
61 -> 64 0.56756
61 -> 66 -0.28963
62 -> 65 0.27343

Excited State 12: Singlet-A 5.8163 eV 213.17 nm f=0.0103 <S**2>=0.000
61 -> 64 -0.39410
61 -> 66 -0.40076
62 -> 65 0.40606

Excited State 13: Singlet-A 5.8170 eV 213.14 nm f=0.0103 <S**2>=0.000
61 -> 65 0.40405
62 -> 64 -0.39015
62 -> 66 0.40629

Excited State 14: Singlet-A 5.8878 eV 210.58 nm f=0.0025 <S**2>=0.000
57 -> 63 0.12317
61 -> 65 0.36700
61 -> 66 0.32594
62 -> 65 0.32314
62 -> 66 -0.36445

Excited State 15: Singlet-A 6.0909 eV 203.56 nm f=0.0021 <S**2>=0.000
62 -> 67 0.70071

Excited State 16: Singlet-A 6.0915 eV 203.54 nm f=0.0021 <S**2>=0.000
61 -> 67 0.70072

Excited State 17: Singlet-A 6.7342 eV 184.11 nm f=0.0000 <S**2>=0.000
60 -> 66 0.39403

Excited State 18: Singlet-A 6.7715 eV 183.10 nm f=0.0042 <S**2>=0.000
59 -> 65 -0.29933
59 -> 66 0.39518
60 -> 65 -0.38846
60 -> 66 -0.29065

Excited State 19: Singlet-A 6.7795 eV 182.88 nm f=0.0067 <S**2>=0.000
59 -> 66 0.47627
60 -> 65 0.48105

Excited State 20: Singlet-A 6.7796 eV 182.88 nm f=0.0068 <S**2>=0.000
59 -> 65 -0.47805
60 -> 66 0.48323

Excited State 21: Singlet-A 6.8107 eV 182.04 nm f=0.0003 <S**2>=0.000

58 -> 65 -0.12487
60 -> 64 0.67932

Excited State 22: Singlet-A 6.8110 eV 182.04 nm f=0.0004 <S**2>=0.000
58 -> 66 0.13262
59 -> 64 0.67535

Excited State 23: Singlet-A 6.8407 eV 181.25 nm f=0.0028 <S**2>=0.000
58 -> 65 0.51764
58 -> 66 -0.42618
59 -> 64 0.13575

Excited State 24: Singlet-A 6.8408 eV 181.24 nm f=0.0027 <S**2>=0.000
58 -> 65 0.42802
58 -> 66 0.51789
60 -> 64 0.13137

Excited State 25: Singlet-A 6.8901 eV 179.94 nm f=0.0002 <S**2>=0.000
58 -> 64 0.69698

Excited State 26: Singlet-A 6.8980 eV 179.74 nm f=0.0000 <S**2>=0.000
62 -> 68 0.69960

Excited State 27: Singlet-A 6.8986 eV 179.72 nm f=0.0000 <S**2>=0.000
61 -> 68 0.69963

Excited State 28: Singlet-A 7.0983 eV 174.67 nm f=0.0002 <S**2>=0.000
60 -> 67 0.69594

Excited State 29: Singlet-A 7.0984 eV 174.66 nm f=0.0002 <S**2>=0.000
59 -> 67 0.69596

Excited State 30: Singlet-A 7.1853 eV 172.55 nm f=0.0042 <S**2>=0.000
61 -> 69 -0.30214
61 -> 70 0.36875
62 -> 69 0.40703
62 -> 70 0.29885

[Cu(I)L(H2O)]$^{+}$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2049 eV 386.86 nm f=0.0002 <S**2>=0.000
67 -> 68 0.69927
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2235.89219535
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2666 eV 379.56 nm f=0.0000 <S**2>=0.000
66 -> 68 0.69984

Excited State 3: Singlet-A 3.9432 eV 314.42 nm f=0.0000 <S**2>=0.000
64 -> 68 0.33270
65 -> 68 0.61562

Excited State 4: Singlet-A 3.9936 eV 310.46 nm f=0.0001 <S**2>=0.000
63 -> 68 0.15547
64 -> 68 0.60471
65 -> 68 -0.31655

Excited State 5: Singlet-A 4.0079 eV 309.35 nm f=0.0004 <S**2>=0.000
63 -> 68 0.68075
64 -> 68 -0.11507
65 -> 68 0.11478

Excited State 6: Singlet-A 5.3413 eV 232.12 nm f=0.0015 <S**2>=0.000
67 -> 69 0.69536

Excited State 7: Singlet-A 5.4217 eV 228.68 nm f=0.0009 <S**2>=0.000
66 -> 69 0.68342

Excited State 8: Singlet-A 5.5641 eV 222.83 nm f=0.0000 <S**2>=0.000
66 -> 69 0.11245
66 -> 71 0.11067
67 -> 70 0.48195
67 -> 71 -0.46365

Excited State 9: Singlet-A 5.6142 eV 220.84 nm f=0.0017 <S**2>=0.000
66 -> 70 -0.35440
66 -> 71 0.57620

Excited State 10: Singlet-A 5.6729 eV 218.56 nm f=0.0044 <S**2>=0.000
67 -> 70 0.49154
67 -> 71 0.49519

Excited State 11: Singlet-A 5.7204 eV 216.74 nm f=0.0037 <S**2>=0.000
66 -> 70 0.60130
66 -> 71 0.35710

Excited State 12: Singlet-A 5.8596 eV 211.59 nm f=0.0012 <S**2>=0.000
60 -> 68 -0.14550
62 -> 68 0.33001
67 -> 71 0.12228

67 -> 72 0.50802
67 -> 74 -0.25606

Excited State 13: Singlet-A 5.8974 eV 210.24 nm f=0.0004 <S**2>=0.000
60 -> 68 0.16246
61 -> 68 -0.39306
65 -> 69 0.21436
66 -> 71 0.10787
66 -> 72 0.40278
66 -> 74 -0.26076

Excited State 14: Singlet-A 5.9127 eV 209.69 nm f=0.0013 <S**2>=0.000
60 -> 68 -0.18456
61 -> 68 -0.15236
62 -> 68 0.45814
67 -> 72 -0.45307
67 -> 74 -0.10061

Excited State 15: Singlet-A 5.9515 eV 208.32 nm f=0.0006 <S**2>=0.000
61 -> 68 0.27810
65 -> 69 -0.34493
66 -> 72 0.53172

Excited State 16: Singlet-A 5.9785 eV 207.38 nm f=0.0109 <S**2>=0.000
60 -> 68 -0.12515
61 -> 68 0.35069
65 -> 69 0.56243
66 -> 72 0.15628

Excited State 17: Singlet-A 6.1213 eV 202.54 nm f=0.0115 <S**2>=0.000
60 -> 68 0.58125
61 -> 68 0.17491
62 -> 68 0.32579

Excited State 18: Singlet-A 6.1878 eV 200.37 nm f=0.0091 <S**2>=0.000
62 -> 68 0.13959
63 -> 69 -0.16109
64 -> 69 -0.13456
65 -> 70 -0.34880
65 -> 71 0.50585
67 -> 74 0.19753

Excited State 19: Singlet-A 6.2062 eV 199.78 nm f=0.0067 <S**2>=0.000
64 -> 69 0.67170

Excited State 20: Singlet-A 6.2322 eV 198.94 nm f=0.0080 <S**2>=0.000

62 -> 68 0.14856
63 -> 69 0.59100
67 -> 74 0.30609

Excited State 21: Singlet-A 6.2731 eV 197.64 nm f=0.0029 <S**2>=0.000
60 -> 68 -0.16787
63 -> 69 -0.32089
65 -> 70 0.21819
65 -> 71 -0.19742
67 -> 72 0.11473
67 -> 74 0.47900

Excited State 22: Singlet-A 6.3131 eV 196.39 nm f=0.0040 <S**2>=0.000
61 -> 68 -0.22930
66 -> 72 0.15760
66 -> 74 0.60883

Excited State 23: Singlet-A 6.3319 eV 195.81 nm f=0.0011 <S**2>=0.000
65 -> 70 0.55296
65 -> 71 0.42135

Excited State 24: Singlet-A 6.4257 eV 192.95 nm f=0.0046 <S**2>=0.000
64 -> 70 -0.40417
64 -> 71 0.53868
64 -> 74 0.11276

Excited State 25: Singlet-A 6.4371 eV 192.61 nm f=0.0026 <S**2>=0.000
63 -> 70 -0.37960
63 -> 71 0.53395
63 -> 74 0.12150
67 -> 73 -0.15212

Excited State 26: Singlet-A 6.4514 eV 192.18 nm f=0.0021 <S**2>=0.000
63 -> 71 0.11704
67 -> 73 0.68264

Excited State 27: Singlet-A 6.5228 eV 190.08 nm f=0.0017 <S**2>=0.000
65 -> 72 0.58259
65 -> 74 -0.15561
66 -> 73 -0.33223

Excited State 28: Singlet-A 6.5386 eV 189.62 nm f=0.0007 <S**2>=0.000
65 -> 72 0.33051
66 -> 73 0.61025

Excited State 29: Singlet-A 6.5911 eV 188.11 nm f=0.0011 <S**2>=0.000

64 -> 70 0.54542
64 -> 71 0.42744
64 -> 72 0.11364

Excited State 30: Singlet-A 6.6195 eV 187.30 nm f=0.0000 <S**2>=0.000
63 -> 70 0.55521
63 -> 71 0.41605
63 -> 72 0.11998

[Cu(I)L($C_6H_7O_6$)]$^+$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.5941 eV 344.97 nm f=0.0097 <S**2>=0.000
107 ->109 0.26177
108 ->109 0.62471
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2843.36149466
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6998 eV 335.11 nm f=0.0008 <S**2>=0.000
107 ->109 0.62167
108 ->109 -0.25788

Excited State 3: Singlet-A 4.0082 eV 309.33 nm f=0.0024 <S**2>=0.000
107 ->110 0.67937
108 ->110 0.11815

Excited State 4: Singlet-A 4.0436 eV 306.62 nm f=0.0020 <S**2>=0.000
106 ->109 0.64736
108 ->110 -0.16534

Excited State 5: Singlet-A 4.0839 eV 303.59 nm f=0.0520 <S**2>=0.000
106 ->109 0.12123
106 ->110 0.19987
107 ->110 -0.11587
108 ->109 -0.11226
108 ->110 0.62745

Excited State 6: Singlet-A 4.3205 eV 286.97 nm f=0.0016 <S**2>=0.000
106 ->111 0.10242
108 ->109 -0.10207
108 ->111 0.66973
108 ->112 -0.13798

Excited State 7: Singlet-A 4.3906 eV 282.38 nm f=0.0032 <S**2>=0.000
108 ->111 0.13755

108 ->112 0.66537

Excited State 8: Singlet-A 4.4394 eV 279.28 nm f=0.0015 <S**2>=0.000
107 ->109 -0.10229
107 ->111 0.68660

Excited State 9: Singlet-A 4.5058 eV 275.17 nm f=0.0022 <S**2>=0.000
104 ->109 -0.10861
105 ->109 0.13773
107 ->112 0.65790

Excited State 10: Singlet-A 4.5208 eV 274.26 nm f=0.0278 <S**2>=0.000
104 ->109 0.10916
105 ->109 0.11498
106 ->110 0.63676
108 ->110 -0.15170

Excited State 11: Singlet-A 4.5378 eV 273.23 nm f=0.0025 <S**2>=0.000
103 ->109 0.11218
104 ->109 -0.28043
105 ->109 0.56396
107 ->112 -0.18388

Excited State 12: Singlet-A 4.6209 eV 268.31 nm f=0.0018 <S**2>=0.000
103 ->109 0.53468
104 ->109 0.37734

Excited State 13: Singlet-A 4.6648 eV 265.79 nm f=0.0030 <S**2>=0.000
103 ->109 -0.16028
108 ->114 0.65100

Excited State 14: Singlet-A 4.7937 eV 258.64 nm f=0.0075 <S**2>=0.000
103 ->109 -0.27279
104 ->109 0.31824
105 ->109 0.22594
106 ->111 0.16089
106 ->112 -0.27718
108 ->113 -0.28768
108 ->115 0.17105

Excited State 15: Singlet-A 4.8110 eV 257.71 nm f=0.0009 <S**2>=0.000
106 ->111 0.47115
107 ->114 0.35927
108 ->113 0.31589

Excited State 16: Singlet-A 4.8171 eV 257.38 nm f=0.0016 <S**2>=0.000

106 ->111 -0.38330
107 ->114 0.54001

Excited State 17: Singlet-A 4.8295 eV 256.72 nm f=0.0023 <S**2>=0.000
103 ->109 -0.11865
104 ->109 0.13715
106 ->111 -0.26033
106 ->112 -0.15748
108 ->113 0.53437
108 ->114 -0.16062
108 ->115 0.11626

Excited State 18: Singlet-A 4.8881 eV 253.64 nm f=0.0022 <S**2>=0.000
102 ->110 -0.13781
103 ->109 -0.11866
104 ->109 0.13766
104 ->110 0.18417
105 ->109 0.16379
105 ->110 -0.31947
106 ->112 0.48423

Excited State 19: Singlet-A 4.9129 eV 252.36 nm f=0.0020 <S**2>=0.000
102 ->110 0.18204
104 ->109 0.13585
104 ->110 -0.25868
105 ->110 0.42906
106 ->112 0.33190
108 ->115 0.21941

Excited State 20: Singlet-A 4.9614 eV 249.90 nm f=0.0045 <S**2>=0.000
103 ->109 0.10035
104 ->109 -0.17235
105 ->109 -0.12573
105 ->110 -0.14568
106 ->115 0.10135
108 ->115 0.59798

Excited State 21: Singlet-A 5.0582 eV 245.11 nm f=0.0014 <S**2>=0.000
103 ->110 0.40971
104 ->110 0.37223
105 ->110 0.23214
107 ->115 -0.32671

Excited State 22: Singlet-A 5.0736 eV 244.37 nm f=0.0026 <S**2>=0.000
103 ->110 0.25433
104 ->110 0.21977

107 ->114 -0.14423
107 ->115 0.56034

Excited State 23: Singlet-A 5.1649 eV 240.05 nm f=0.0001 <S**2>=0.000
107 ->113 0.68643

Excited State 24: Singlet-A 5.1764 eV 239.52 nm f=0.0041 <S**2>=0.000
103 ->110 0.21197
104 ->110 -0.16147
106 ->114 0.56748
106 ->115 0.10326

Excited State 25: Singlet-A 5.2210 eV 237.47 nm f=0.0032 <S**2>=0.000
100 ->110 -0.10205
102 ->109 -0.19477
102 ->110 0.49233
103 ->110 -0.19244
104 ->110 0.30348
106 ->114 0.19541

Excited State 26: Singlet-A 5.2654 eV 235.47 nm f=0.0381 <S**2>=0.000
102 ->110 0.31138
103 ->110 0.39482
104 ->110 -0.21714
105 ->110 -0.30499
106 ->114 -0.17033
108 ->118 -0.10579

Excited State 27: Singlet-A 5.3508 eV 231.71 nm f=0.0005 <S**2>=0.000
104 ->111 -0.24353
105 ->109 -0.11246
105 ->111 0.62818

Excited State 28: Singlet-A 5.3770 eV 230.58 nm f=0.0047 <S**2>=0.000
104 ->111 -0.23112
105 ->112 0.22400
106 ->114 -0.19066
106 ->115 0.37895
108 ->118 0.38538

Excited State 29: Singlet-A 5.4155 eV 228.95 nm f=0.0010 <S**2>=0.000
103 ->111 0.36841
104 ->111 0.50908
105 ->111 0.17975
106 ->115 0.17259

Excited State 30: Singlet-A 5.4212 eV 228.70 nm f=0.0032 <S**2>=0.000
104 ->112 -0.36107
105 ->112 0.51319
106 ->115 -0.23077

[Cu(I)LDHA]$^{+}$

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 0.7816 eV 1586.26 nm f=0.0017 <S**2>=0.000
106 ->108 0.47647
107 ->108 0.51538
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.73322556
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.4963 eV 828.59 nm f=0.0072 <S**2>=0.000
104 ->108 0.12193
105 ->108 0.66017
106 ->108 -0.13376
107 ->108 0.14141

Excited State 3: Singlet-A 1.8059 eV 686.54 nm f=0.1494 <S**2>=0.000
101 ->108 -0.11422
102 ->108 0.14475
103 ->108 0.21182
105 ->108 0.18543
106 ->108 0.47488
107 ->108 -0.43450
106 <-108 -0.13374
107 <-108 0.13786

Excited State 4: Singlet-A 2.1011 eV 590.09 nm f=0.0034 <S**2>=0.000
100 ->108 0.29916
101 ->108 0.37952
103 ->108 0.46886
104 ->108 -0.15865

Excited State 5: Singlet-A 2.1876 eV 566.75 nm f=0.0617 <S**2>=0.000
100 ->108 0.29112
101 ->108 0.36776
102 ->108 -0.14983
103 ->108 -0.35448
104 ->108 0.22134
106 ->108 0.19261
107 ->108 -0.21018

Excited State 6: Singlet-A 2.2147 eV 559.82 nm f=0.0013 <S**2>=0.000
99 ->108 -0.14126
100 ->108 0.16563
102 ->108 0.52354
104 ->108 0.37492
105 ->108 -0.13893

Excited State 7: Singlet-A 2.8357 eV 437.22 nm f=0.0003 <S**2>=0.000
100 ->108 -0.12031
102 ->108 -0.33911
103 ->108 0.32284
104 ->108 0.50933

Excited State 8: Singlet-A 3.0803 eV 402.51 nm f=0.0074 <S**2>=0.000
98 ->108 -0.28772
99 ->108 0.59264
100 ->108 -0.13733
102 ->108 0.17007

Excited State 9: Singlet-A 3.1176 eV 397.69 nm f=0.0021 <S**2>=0.000
99 ->108 0.17296
100 ->108 0.49842
101 ->108 -0.43256
102 ->108 -0.14558

Excited State 10: Singlet-A 3.3760 eV 367.25 nm f=0.0222 <S**2>=0.000
98 ->108 0.63208
99 ->108 0.28842

Excited State 11: Singlet-A 3.6187 eV 342.62 nm f=0.0010 <S**2>=0.000
95 ->108 0.60633
96 ->108 -0.29070
97 ->108 0.13613

Excited State 12: Singlet-A 3.8988 eV 318.00 nm f=0.0054 <S**2>=0.000
95 ->108 0.30997
96 ->108 0.62378

Excited State 13: Singlet-A 4.1363 eV 299.75 nm f=0.0202 <S**2>=0.000
96 ->108 0.12861
97 ->108 0.66281

Excited State 14: Singlet-A 4.4343 eV 279.60 nm f=0.0087 <S**2>=0.000
106 ->109 0.30160
107 ->109 0.62688

Excited State 15: Singlet-A 4.5603 eV 271.87 nm f=0.0576 <S**2>=0.000
106 ->109 0.62288
107 ->109 -0.30226

Excited State 16: Singlet-A 4.7642 eV 260.24 nm f=0.0045 <S**2>=0.000
85 ->108 -0.23019
93 ->108 0.53265
94 ->108 0.36455

Excited State 17: Singlet-A 4.7810 eV 259.33 nm f=0.0002 <S**2>=0.000
93 ->108 -0.42377
94 ->108 0.55876

Excited State 18: Singlet-A 4.8164 eV 257.42 nm f=0.0040 <S**2>=0.000
92 ->108 0.69936

Excited State 19: Singlet-A 4.8584 eV 255.20 nm f=0.0026 <S**2>=0.000
85 ->108 0.51974
86 ->108 0.14524
89 ->108 -0.15673
91 ->108 0.12653
93 ->108 0.17540
94 ->108 0.21788
105 ->109 -0.19030

Excited State 20: Singlet-A 5.0881 eV 243.67 nm f=0.0011 <S**2>=0.000
90 ->108 -0.43466
91 ->108 0.19085
102 ->109 -0.11189
105 ->109 0.46805

Excited State 21: Singlet-A 5.1083 eV 242.71 nm f=0.0012 <S**2>=0.000
85 ->108 0.13834
90 ->108 0.54667
91 ->108 0.18041
105 ->109 0.34444

Excited State 22: Singlet-A 5.1588 eV 240.34 nm f=0.0010 <S**2>=0.000
85 ->108 -0.17587
91 ->108 0.63904
105 ->109 -0.19540

Excited State 23: Singlet-A 5.4023 eV 229.50 nm f=0.0019 <S**2>=0.000
86 ->108 0.17444
88 ->108 0.60669
89 ->108 0.29721

Excited State 24: Singlet-A 5.4127 eV 229.06 nm f=0.0037 <S**2>=0.000
89 ->108 0.11707
106 ->110 0.15275
107 ->110 0.66438

Excited State 25: Singlet-A 5.4331 eV 228.20 nm f=0.0037 <S**2>=0.000
85 ->108 0.18850
88 ->108 -0.29638
89 ->108 0.59348
107 ->110 -0.10018

Excited State 26: Singlet-A 5.4511 eV 227.45 nm f=0.0043 <S**2>=0.000
86 ->108 -0.17721
87 ->108 0.66732
88 ->108 0.12062

Excited State 27: Singlet-A 5.5172 eV 224.72 nm f=0.0011 <S**2>=0.000
106 ->110 0.66845
107 ->110 -0.16794

Excited State 28: Singlet-A 5.5375 eV 223.90 nm f=0.0006 <S**2>=0.000
85 ->108 -0.18011
86 ->108 0.63090
87 ->108 0.20784
88 ->108 -0.15046

Excited State 29: Singlet-A 5.8102 eV 213.39 nm f=0.0003 <S**2>=0.000
100 ->109 0.14885
102 ->109 0.30204
103 ->109 -0.16060
104 ->109 0.52665
105 ->109 0.23452

Excited State 30: Singlet-A 5.9584 eV 208.08 nm f=0.0027 <S**2>=0.000
100 ->109 -0.10947
102 ->109 -0.32993
103 ->109 0.43766
104 ->109 0.40855

M06 method:
Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 0.8774 eV 1413.15 nm f=0.0018 <S**2>=0.000
98 ->108 0.11947
106 ->108 0.53180

107 ->108 0.44791
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2841.90336117
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.5459 eV 802.04 nm f=0.0114 <S**2>=0.000
105 ->108 0.65800
106 ->108 -0.12905
107 ->108 0.18656

Excited State 3: Singlet-A 1.8032 eV 687.59 nm f=0.1491 <S**2>=0.000
102 ->108 -0.15848
103 ->108 -0.11922
105 ->108 -0.21948
106 ->108 -0.42925
107 ->108 0.49647
107 <-108 -0.13318

Excited State 4: Singlet-A 2.1687 eV 571.70 nm f=0.0010 <S**2>=0.000
100 ->108 -0.17334
101 ->108 0.49765
102 ->108 -0.14056
103 ->108 0.44026

Excited State 5: Singlet-A 2.2483 eV 551.45 nm f=0.0406 <S**2>=0.000
101 ->108 -0.23296
102 ->108 0.40445
103 ->108 0.44038
104 ->108 -0.17414
106 ->108 -0.12617
107 ->108 0.18006

Excited State 6: Singlet-A 2.2921 eV 540.93 nm f=0.0005 <S**2>=0.000
99 ->108 -0.36818
101 ->108 0.17743
102 ->108 0.37444
104 ->108 0.40256

Excited State 7: Singlet-A 3.0918 eV 401.00 nm f=0.0008 <S**2>=0.000
101 ->108 -0.30684
102 ->108 -0.25767
103 ->108 0.26518
104 ->108 0.50544

Excited State 8: Singlet-A 3.1589 eV 392.49 nm f=0.0063 <S**2>=0.000
98 ->108 0.30239

99 ->108 0.49016
100 ->108 -0.21458
102 ->108 0.24381
103 ->108 -0.10325
104 ->108 0.17348

Excited State 9: Singlet-A 3.3598 eV 369.02 nm f=0.0059 <S**2>=0.000
95 ->108 -0.10538
98 ->108 0.24416
100 ->108 0.60600
101 ->108 0.21338

Excited State 10: Singlet-A 3.4159 eV 362.96 nm f=0.0129 <S**2>=0.000
98 ->108 0.56477
99 ->108 -0.32708
100 ->108 -0.16105
102 ->108 -0.12879

Excited State 11: Singlet-A 3.7936 eV 326.82 nm f=0.0009 <S**2>=0.000
95 ->108 0.59227
96 ->108 -0.24516
97 ->108 0.14327
100 ->108 0.11722

Excited State 12: Singlet-A 4.1061 eV 301.95 nm f=0.0207 <S**2>=0.000
95 ->108 -0.14656
97 ->108 0.66815

Excited State 13: Singlet-A 4.1533 eV 298.52 nm f=0.0068 <S**2>=0.000
95 ->108 0.24793
96 ->108 0.65140

Excited State 14: Singlet-A 4.6655 eV 265.75 nm f=0.0299 <S**2>=0.000
85 ->108 0.10228
107 ->109 0.68018

Excited State 15: Singlet-A 4.7468 eV 261.19 nm f=0.0286 <S**2>=0.000
85 ->108 0.11844
106 ->109 0.66199
107 ->109 -0.12004

Excited State 16: Singlet-A 4.7557 eV 260.71 nm f=0.0022 <S**2>=0.000
93 ->108 0.68343

Excited State 17: Singlet-A 4.7725 eV 259.79 nm f=0.0003 <S**2>=0.000
94 ->108 0.69247

Excited State 18: Singlet-A 4.9484 eV 250.55 nm f=0.0024 <S**2>=0.000
82 ->108 0.15800
83 ->108 -0.12075
85 ->108 0.54939
92 ->108 -0.10988
105 ->109 -0.13857
106 ->109 -0.18311

Excited State 19: Singlet-A 5.0820 eV 243.97 nm f=0.0012 <S**2>=0.000
92 ->108 0.68721

Excited State 20: Singlet-A 5.1013 eV 243.04 nm f=0.0049 <S**2>=0.000
91 ->108 0.69462

Excited State 21: Singlet-A 5.2093 eV 238.00 nm f=0.0044 <S**2>=0.000
106 ->110 0.13148
107 ->110 0.67091

Excited State 22: Singlet-A 5.3006 eV 233.91 nm f=0.0006 <S**2>=0.000
85 ->108 0.11621
99 ->109 0.17276
104 ->109 -0.10176
105 ->109 0.44039
106 ->110 -0.43367

Excited State 23: Singlet-A 5.3140 eV 233.32 nm f=0.0009 <S**2>=0.000
85 ->108 0.11463
99 ->109 0.13739
105 ->109 0.35132
106 ->110 0.51409
107 ->110 -0.14325

Excited State 24: Singlet-A 5.3981 eV 229.68 nm f=0.0011 <S**2>=0.000
86 ->108 -0.32198
87 ->108 -0.10901
88 ->108 0.54717
89 ->108 0.22199
90 ->108 -0.14786

Excited State 25: Singlet-A 5.4311 eV 228.29 nm f=0.0029 <S**2>=0.000
86 ->108 0.10240
89 ->108 0.42222
90 ->108 0.54679

Excited State 26: Singlet-A 5.4484 eV 227.56 nm f=0.0041 <S**2>=0.000

86 ->108 0.28285
87 ->108 0.58543
88 ->108 0.22520
90 ->108 -0.13213

Excited State 27: Singlet-A 5.4564 eV 227.23 nm f=0.0011 <S**2>=0.000
85 ->108 0.13597
88 ->108 -0.29275
89 ->108 0.49153
90 ->108 -0.36066

Excited State 28: Singlet-A 5.5232 eV 224.48 nm f=0.0006 <S**2>=0.000
86 ->108 0.53862
87 ->108 -0.36768
88 ->108 0.23714

Excited State 29: Singlet-A 6.0499 eV 204.94 nm f=0.0003 <S**2>=0.000
77 ->108 0.15929
99 ->109 -0.24536
101 ->109 0.23993
102 ->109 0.17684
104 ->109 0.43917
105 ->109 0.31696

Excited State 30: Singlet-A 6.1211 eV 202.55 nm f=0.0010 <S**2>=0.000
83 ->108 0.23743
84 ->108 0.65670

[Cu(II)L]$^{2+}$

Excitation energies and oscillator strengths:

Excited State 1: 2.003-A 0.1803 eV 6874.70 nm f=0.0005 <S**2>=0.753
52B -> 62B -0.20922
56B -> 62B -0.11044
61B -> 62B 0.96758
61B <- 62B -0.15981
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2159.20092213
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.005-A 1.9122 eV 648.38 nm f=0.0011 <S**2>=0.755
45B -> 62B -0.10634
51B -> 62B -0.12445
53B -> 62B 0.14232
55B -> 62B 0.92407
57B -> 62B 0.16497

58B -> 62B 0.13027
59B -> 62B -0.10999
60B -> 62B 0.11186

Excited State 3: 2.004-A 1.9396 eV 639.23 nm f=0.0011 <S**2>=0.754
48B -> 62B -0.15099
49B -> 62B -0.11071
51B -> 62B 0.16563
53B -> 62B -0.11568
54B -> 62B 0.91806
56B -> 62B -0.11247
58B -> 62B 0.11491
60B -> 62B 0.13200

Excited State 4: 2.004-A 2.1276 eV 582.74 nm f=0.0019 <S**2>=0.754
48B -> 62B 0.91122
52B -> 62B 0.22553
54B -> 62B 0.17101
56B -> 62B -0.11801
60B -> 62B -0.12648

Excited State 5: 2.007-A 2.3412 eV 529.57 nm f=0.0263 <S**2>=0.757
48B -> 62B 0.11244
51B -> 62B 0.15704
52B -> 62B 0.29275
54B -> 62B -0.13865
55B -> 62B -0.10463
56B -> 62B 0.15656
58B -> 62B 0.10630
60B -> 62B 0.86429
61B -> 62B 0.18532

Excited State 6: 2.007-A 2.9141 eV 425.46 nm f=0.0626 <S**2>=0.757
48B -> 62B -0.13377
50B -> 62B 0.14694
51B -> 62B 0.27085
52B -> 62B 0.59007
53B -> 62B 0.20396
56B -> 62B 0.34871
58B -> 62B 0.32324
60B -> 62B -0.43442
61B -> 62B 0.22878

Excited State 7: 3.450-A 3.2680 eV 379.39 nm f=0.0004 <S**2>=2.725
62A -> 63A -0.62995
61B -> 63B 0.75695

Excited State 8: 2.011-A 3.5718 eV 347.12 nm f=0.0214 <S**2>=0.761
60A -> 63A -0.10368
62A -> 63A -0.25570
57B -> 62B 0.15628
59B -> 62B 0.90810
61B -> 63B -0.19032

Excited State 9: 2.008-A 3.6045 eV 343.97 nm f=0.0030 <S**2>=0.758
48B -> 62B 0.14168
51B -> 62B -0.11644
52B -> 62B -0.31520
57B -> 62B -0.26344
58B -> 62B 0.87711

Excited State 10: 2.008-A 3.6222 eV 342.29 nm f=0.0025 <S**2>=0.758
62A -> 63A 0.10070
53B -> 62B -0.17415
55B -> 62B -0.16184
56B -> 62B -0.10181
57B -> 62B 0.91372
58B -> 62B 0.22609
59B -> 62B -0.11992

Excited State 11: 2.030-A 3.7829 eV 327.75 nm f=0.0077 <S**2>=0.781
62A -> 63A 0.70840
59B -> 62B 0.31578
61B -> 63B 0.59689

Excited State 12: 2.008-A 3.9531 eV 313.64 nm f=0.0008 <S**2>=0.758
52B -> 62B -0.13834
53B -> 62B 0.87597
55B -> 62B -0.14401
56B -> 62B -0.39957

Excited State 13: 2.008-A 4.0663 eV 304.90 nm f=0.0108 <S**2>=0.758
48B -> 62B 0.15251
52B -> 62B -0.43260
53B -> 62B 0.26247
54B -> 62B 0.21070
55B -> 62B -0.13485
56B -> 62B 0.78771
57B -> 62B 0.11064

Excited State 14: 2.009-A 4.2028 eV 295.01 nm f=0.0069 <S**2>=0.760
61A -> 63A -0.14275

48B -> 62B 0.10691
51B -> 62B 0.88299
52B -> 62B -0.34418
54B -> 62B -0.13311
55B -> 62B 0.14933

Excited State 15: 2.063-A 4.3102 eV 287.65 nm f=0.0002 <S**2>=0.814
61A -> 63A 0.91631
50B -> 62B -0.30336
51B -> 62B 0.16402

Excited State 16: 2.013-A 4.3917 eV 282.31 nm f=0.0147 <S**2>=0.763
61A -> 63A 0.26886
49B -> 62B -0.40738
50B -> 62B 0.83449
52B -> 62B -0.10737
53B -> 62B -0.12116

Excited State 17: 2.011-A 4.4241 eV 280.25 nm f=0.0144 <S**2>=0.761
61A -> 63A 0.18862
49B -> 62B 0.88937
50B -> 62B 0.37096

Excited State 18: 2.009-A 4.8896 eV 253.57 nm f=0.0016 <S**2>=0.759
45B -> 62B 0.11861
46B -> 62B -0.22275
47B -> 62B 0.95065

Excited State 19: 2.009-A 5.0463 eV 245.69 nm f=0.0039 <S**2>=0.759
44B -> 62B -0.20535
46B -> 62B 0.93931
47B -> 62B 0.21532

Excited State 20: 3.321-A 5.2638 eV 235.54 nm f=0.0045 <S**2>=2.508
60A -> 63A -0.53217
45B -> 62B 0.27257
60B -> 63B 0.76509

Excited State 21: 2.138-A 5.2813 eV 234.76 nm f=0.0023 <S**2>=0.893
44B -> 62B -0.25551
45B -> 62B 0.89083
47B -> 62B -0.12632
52B -> 62B -0.10675
60B -> 63B -0.26332

Excited State 22: 2.012-A 5.3976 eV 229.70 nm f=0.0123 <S**2>=0.762

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   44B -> 62B       0.92639
   45B -> 62B       0.27375
   46B -> 62B       0.17882

Excited State  23:  2.010-A     5.5612 eV  222.94 nm  f=0.0102  <S**2>=0.760
   43B -> 62B       0.98357

Excited State  24:  3.132-A     5.7668 eV  214.99 nm  f=0.0024  <S**2>=2.203
   54A -> 63A      -0.27489
   55A -> 63A      -0.10126
   60A -> 63A      -0.13132
   54B -> 63B       0.17003
   55B -> 63B       0.62278
   58B -> 63B       0.17276
   59B -> 63B      -0.60900
   60B -> 63B      -0.15650

Excited State  25:  2.252-A     5.8006 eV  213.74 nm  f=0.0364  <S**2>=1.018
   52A -> 63A      -0.11485
   60A -> 63A       0.68817
   42B -> 62B      -0.11245
   54B -> 63B      -0.26088
   59B -> 62B       0.14305
   59B -> 63B      -0.29213
   60B -> 63B       0.49065

Excited State  26:  3.141-A     5.8352 eV  212.48 nm  f=0.0089  <S**2>=2.216
   51A -> 63A       0.10575
   53A -> 63A       0.27081
   54A -> 63A      -0.26437
   60A -> 63A       0.27931
   54B -> 63B       0.51296
   55B -> 63B       0.31848
   59B -> 63B       0.57578
   60B -> 63B       0.11686

Excited State  27:  3.295-A     5.8714 eV  211.17 nm  f=0.0037  <S**2>=2.464
   52A -> 63A       0.20930
   53A -> 63A       0.32081
   54A -> 63A       0.11760
   55A -> 63A       0.15672
   51B -> 63B       0.16046
   53B -> 63B      -0.14992
   54B -> 63B       0.54142
   55B -> 63B      -0.42188
   56B -> 63B      -0.18049
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57B -> 63B -0.18706
59B -> 63B -0.38848

Excited State 28: 2.200-A 6.1372 eV 202.02 nm f=0.0050 <S**2>=0.960
52A -> 63A 0.29730
54A -> 63A 0.67015
55A -> 63A 0.36727
56A -> 63A -0.10239
58A -> 63A 0.21355
59A -> 63A 0.11011
55B -> 63B 0.43138
57B -> 63B 0.11419

Excited State 29: 2.592-A 6.2033 eV 199.87 nm f=0.0047 <S**2>=1.429
50A -> 63A -0.18627
51A -> 63A 0.17408
52A -> 63A 0.32907
53A -> 63A 0.46390
54A -> 63A -0.20569
55A -> 63A 0.11897
59A -> 63A -0.33927
52B -> 63B 0.25643
53B -> 63B 0.13497
54B -> 63B -0.42990
56B -> 63B 0.24110
58B -> 63B 0.15928

Excited State 30: 2.994-A 6.2227 eV 199.25 nm f=0.0033 <S**2>=1.992
50A -> 63A 0.11245
51A -> 63A 0.14775
53A -> 63A 0.49972
54A -> 63A -0.10431
57A -> 63A 0.12692
59A -> 63A 0.11894
60A -> 63A -0.10374
42B -> 62B 0.23906
50B -> 63B -0.13054
51B -> 63B -0.21915
52B -> 63B -0.43311
53B -> 63B -0.12080
54B -> 63B -0.18475
56B -> 63B -0.24455
58B -> 63B -0.42864

[Cu(II)L(H_2O)]$^{2+}$

Excitation energies and oscillator strengths:

Excited State 1: 2.008-A 0.5645 eV 2196.26 nm f=0.0042 <S**2>=0.758
55B -> 67B 0.10170
58B -> 67B 0.21313
59B -> 67B 0.19350
66B -> 67B 0.94580
66B <- 67B -0.10174
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2235.61503936
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.003-A 2.0013 eV 619.53 nm f=0.0001 <S**2>=0.753
48B -> 67B -0.20780
50B -> 67B -0.12082
54B -> 67B -0.14627
58B -> 67B -0.10474
60B -> 67B 0.60730
61B -> 67B -0.60079
62B -> 67B -0.19084
63B -> 67B 0.19827
64B -> 67B 0.25189

Excited State 3: 2.003-A 2.0752 eV 597.46 nm f=0.0013 <S**2>=0.753
50B -> 67B -0.11633
58B -> 67B -0.10783
59B -> 67B -0.10952
60B -> 67B 0.63050
61B -> 67B 0.53468
62B -> 67B 0.48306
63B -> 67B -0.12004

Excited State 4: 2.003-A 2.1909 eV 565.91 nm f=0.0001 <S**2>=0.753
49B -> 67B -0.11507
54B -> 67B 0.37595
55B -> 67B -0.35971
56B -> 67B 0.60556
57B -> 67B 0.51271
58B -> 67B 0.20745
63B -> 67B 0.13809

Excited State 5: 2.011-A 2.8197 eV 439.70 nm f=0.0618 <S**2>=0.761
61B -> 67B -0.10920
64B -> 67B -0.14948
65B -> 67B 0.97175

Excited State 6: 2.027-A 3.0454 eV 407.11 nm f=0.0278 <S**2>=0.777

54B -> 67B -0.17825
55B -> 67B 0.23227
57B -> 67B 0.10795
58B -> 67B 0.59670
59B -> 67B 0.55351
60B -> 67B 0.15029
63B -> 67B -0.25671
66B -> 67B -0.33278

Excited State 7: 2.006-A 3.6960 eV 335.46 nm f=0.0373 <S**2>=0.756
60B -> 67B -0.18603
61B -> 67B 0.13434
64B -> 67B 0.94142
65B -> 67B 0.16058

Excited State 8: 2.014-A 4.0731 eV 304.40 nm f=0.0022 <S**2>=0.765
55B -> 67B 0.10540
56B -> 67B -0.13414
58B -> 67B 0.16922
59B -> 67B 0.18194
61B -> 67B 0.12151
62B -> 67B 0.24734
63B -> 67B 0.90583

Excited State 9: 2.013-A 4.1066 eV 301.92 nm f=0.0031 <S**2>=0.763
60B -> 67B -0.20788
61B -> 67B -0.51579
62B -> 67B 0.81242
63B -> 67B -0.14520

Excited State 10: 2.013-A 4.4104 eV 281.12 nm f=0.0002 <S**2>=0.763
54B -> 67B 0.13627
55B -> 67B -0.10240
58B -> 67B -0.62766
59B -> 67B 0.74801

Excited State 11: 2.026-A 4.6932 eV 264.18 nm f=0.0007 <S**2>=0.776
54B -> 67B -0.13960
55B -> 67B 0.42351
56B -> 67B -0.26955
57B -> 67B 0.80045
58B -> 67B -0.20283
59B -> 67B -0.16807

Excited State 12: 2.080-A 4.7584 eV 260.56 nm f=0.0106 <S**2>=0.831
54B -> 67B -0.57644

55B -> 67B 0.26879
56B -> 67B 0.66542
57B -> 67B -0.11248
58B -> 67B -0.21306
60B -> 67B -0.20366
66B -> 68B 0.17670

Excited State 13: 2.394-A 4.8013 eV 258.23 nm f=0.0128 <S**2>=1.183
67A -> 68A 0.16797
53B -> 67B -0.12208
54B -> 67B 0.59178
55B -> 67B 0.53529
56B -> 67B 0.12628
57B -> 67B -0.20253
66B -> 68B 0.47076

Excited State 14: 2.895-A 4.8188 eV 257.29 nm f=0.0066 <S**2>=1.846
67A -> 68A 0.25767
54B -> 67B -0.19985
55B -> 67B -0.47374
56B -> 67B -0.21884
66B -> 68B 0.76722

Excited State 15: 2.025-A 4.9364 eV 251.17 nm f=0.0014 <S**2>=0.775
53B -> 67B 0.97947

Excited State 16: 2.307-A 5.1466 eV 240.90 nm f=0.0002 <S**2>=1.081
67A -> 68A 0.93097
66B -> 68B -0.33155

Excited State 17: 2.156-A 5.2481 eV 236.25 nm f=0.0016 <S**2>=0.912
66A -> 68A 0.97808

Excited State 18: 2.015-A 5.3772 eV 230.58 nm f=0.0024 <S**2>=0.765
48B -> 67B 0.21475
50B -> 67B 0.27557
52B -> 67B 0.91541

Excited State 19: 2.015-A 5.4748 eV 226.46 nm f=0.0031 <S**2>=0.765
47B -> 67B 0.11605
48B -> 67B -0.50059
50B -> 67B -0.26741
51B -> 67B 0.72379
52B -> 67B 0.27892
60B -> 67B -0.17811

Excited State 20: 2.015-A 5.5508 eV 223.36 nm f=0.0020 <S**2>=0.765
47B -> 67B -0.13334
48B -> 67B 0.43683
49B -> 67B 0.27701
50B -> 67B 0.45710
51B -> 67B 0.64555
52B -> 67B -0.22886
60B -> 67B 0.12323

Excited State 21: 2.015-A 5.8505 eV 211.92 nm f=0.0062 <S**2>=0.765
47B -> 67B 0.10769
48B -> 67B -0.34490
49B -> 67B -0.60412
50B -> 67B 0.68488
52B -> 67B -0.12294

Excited State 22: 2.016-A 5.8765 eV 210.98 nm f=0.0038 <S**2>=0.766
48B -> 67B -0.54571
49B -> 67B 0.71159
50B -> 67B 0.36497
51B -> 67B -0.19859

Excited State 23: 2.015-A 6.0651 eV 204.42 nm f=0.0105 <S**2>=0.765
47B -> 67B 0.96466
48B -> 67B 0.17354
49B -> 67B 0.15183

Excited State 24: 3.221-A 6.5163 eV 190.27 nm f=0.0034 <S**2>=2.344
65A -> 68A -0.31791
64B -> 68B 0.10046
65B -> 68B 0.90628
66B -> 70B 0.14669

Excited State 25: 2.056-A 6.7475 eV 183.75 nm f=0.0008 <S**2>=0.806
65A -> 68A -0.18844
46B -> 67B 0.95354

Excited State 26: 2.230-A 6.7721 eV 183.08 nm f=0.0018 <S**2>=0.994
65A -> 68A -0.46029
45B -> 67B 0.80147
46B -> 67B -0.18286
64B -> 68B -0.19781
65B -> 68B -0.18792

Excited State 27: 2.496-A 6.8809 eV 180.19 nm f=0.0047 <S**2>=1.308
65A -> 68A 0.50994

44B -> 67B 0.48452
45B -> 67B 0.49237
64B -> 68B 0.42698
65B -> 68B 0.13564

Excited State 28: 2.262-A 6.9135 eV 179.34 nm f=0.0029 <S**2>=1.029
65A -> 68A -0.28059
44B -> 67B 0.82762
45B -> 67B -0.24834
46B -> 67B -0.13816
61B -> 68B 0.12461
64B -> 68B -0.22145
66B -> 69B 0.19788

Excited State 29: 3.015-A 6.9545 eV 178.28 nm f=0.0009 <S**2>=2.022
67A -> 69A 0.12034
44B -> 67B -0.16165
58B -> 68B -0.11870
66B -> 69B 0.91704

Excited State 30: 2.826-A 7.0232 eV 176.54 nm f=0.0193 <S**2>=1.747
61A -> 68A 0.18243
62A -> 68A 0.21487
65A -> 68A -0.43575
45B -> 67B -0.15346
61B -> 68B -0.36045
62B -> 68B -0.20112
63B -> 68B 0.13141
64B -> 68B 0.57350
65B -> 68B -0.25296
66B -> 70B 0.19099

[Cu(II)L(H_2O)$_2$]$^{2+}$

Excitation energies and oscillator strengths:

Excited State 1: 2.003-A 0.6904 eV 1795.93 nm f=0.0012 <S**2>=0.753
61B -> 72B -0.12038
64B -> 72B -0.23894
66B -> 72B -0.22811
71B -> 72B 0.91872
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2312.01230810
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.002-A 2.1200 eV 584.84 nm f=0.0006 <S**2>=0.752
52B -> 72B -0.14601

54B -> 72B -0.13936
57B -> 72B 0.14078
59B -> 72B 0.12191
60B -> 72B -0.15642
64B -> 72B 0.24184
65B -> 72B 0.70117
66B -> 72B -0.43080
67B -> 72B -0.22575
68B -> 72B -0.19197
69B -> 72B 0.15596

Excited State 3: 2.002-A 2.1600 eV 574.00 nm f=0.0006 <S**2>=0.752
62B -> 72B -0.13769
63B -> 72B -0.10743
64B -> 72B -0.48940
65B -> 72B 0.52056
66B -> 72B 0.62764
67B -> 72B -0.11289
69B -> 72B 0.10434

Excited State 4: 2.002-A 2.2583 eV 549.01 nm f=0.0006 <S**2>=0.752
53B -> 72B -0.11504
54B -> 72B 0.22226
57B -> 72B 0.31058
58B -> 72B 0.52322
60B -> 72B 0.33957
61B -> 72B 0.49639
62B -> 72B -0.34173
63B -> 72B -0.13392
66B -> 72B -0.12724
68B -> 72B -0.12499

Excited State 5: 2.005-A 2.8681 eV 432.28 nm f=0.0096 <S**2>=0.755
61B -> 72B 0.15585
62B -> 72B 0.12889
64B -> 72B 0.42208
65B -> 72B 0.12923
66B -> 72B 0.35436
68B -> 72B -0.17675
70B -> 72B 0.67798
71B -> 72B 0.33914

Excited State 6: 2.006-A 3.3611 eV 368.88 nm f=0.0679 <S**2>=0.756
61B -> 72B -0.22244
62B -> 72B -0.11867
64B -> 72B -0.45401

66B -> 72B -0.35805
68B -> 72B 0.17357
69B -> 72B 0.10532
70B -> 72B 0.70065
71B -> 72B -0.20039

Excited State 7: 2.006-A 3.8849 eV 319.14 nm f=0.0653 <S**2>=0.756
65B -> 72B -0.17541
69B -> 72B 0.95923
70B -> 72B -0.10814

Excited State 8: 2.006-A 4.4589 eV 278.06 nm f=0.0014 <S**2>=0.756
61B -> 72B 0.10027
64B -> 72B 0.27023
65B -> 72B 0.19426
67B -> 72B 0.19880
68B -> 72B 0.90690

Excited State 9: 2.006-A 4.5106 eV 274.88 nm f=0.0015 <S**2>=0.756
63B -> 72B -0.13182
64B -> 72B -0.12751
65B -> 72B 0.18621
67B -> 72B 0.93155
68B -> 72B -0.19691

Excited State 10: 2.007-A 4.8493 eV 255.67 nm f=0.0007 <S**2>=0.757
62B -> 72B -0.25121
63B -> 72B 0.94220
65B -> 72B 0.14219

Excited State 11: 3.275-A 4.9732 eV 249.30 nm f=0.0002 <S**2>=2.431
72A -> 73A -0.36873
71B -> 73B 0.91421

Excited State 12: 2.010-A 5.0632 eV 244.88 nm f=0.0062 <S**2>=0.760
57B -> 72B -0.16935
59B -> 72B -0.20249
60B -> 72B 0.21215
61B -> 72B 0.45841
62B -> 72B 0.70102
64B -> 72B -0.25283
65B -> 72B 0.19856
66B -> 72B -0.22745

Excited State 13: 2.011-A 5.1466 eV 240.91 nm f=0.0060 <S**2>=0.761
57B -> 72B -0.26452

58B -> 72B -0.40198
59B -> 72B -0.16904
60B -> 72B -0.39272
61B -> 72B 0.59463
62B -> 72B -0.41743
63B -> 72B -0.14406

Excited State 14: 2.278-A 5.1506 eV 240.72 nm f=0.0004 <S**2>=1.047
72A -> 73A 0.90054
60B -> 72B -0.14320
61B -> 72B 0.11593
71B -> 73B 0.35871

Excited State 15: 2.013-A 5.1925 eV 238.77 nm f=0.0043 <S**2>=0.763
72A -> 73A 0.16739
57B -> 72B -0.34378
58B -> 72B -0.23979
59B -> 72B -0.38602
60B -> 72B 0.67767
61B -> 72B -0.15547
62B -> 72B -0.27844
63B -> 72B -0.10403
64B -> 72B 0.20743

Excited State 16: 2.007-A 5.3098 eV 233.50 nm f=0.0100 <S**2>=0.757
54B -> 72B -0.11084
57B -> 72B 0.16362
58B -> 72B -0.50308
59B -> 72B 0.69983
60B -> 72B 0.38718
61B -> 72B 0.11488
64B -> 72B -0.17337

Excited State 17: 2.007-A 5.4966 eV 225.56 nm f=0.0003 <S**2>=0.757
56B -> 72B 0.11091
57B -> 72B 0.76089
58B -> 72B -0.37212
59B -> 72B -0.48879

Excited State 18: 2.218-A 5.7127 eV 217.03 nm f=0.0004 <S**2>=0.980
71A -> 73A 0.98002

Excited State 19: 2.009-A 5.8146 eV 213.23 nm f=0.0009 <S**2>=0.759
52B -> 72B -0.15977
54B -> 72B -0.32326
56B -> 72B 0.89023

57B -> 72B -0.11211
58B -> 72B 0.13609

Excited State 20: 2.010-A 5.8573 eV 211.67 nm f=0.0026 <S**2>=0.760
52B -> 72B 0.26823
53B -> 72B -0.16205
54B -> 72B 0.54977
55B -> 72B 0.61178
56B -> 72B 0.34743
57B -> 72B -0.10473
58B -> 72B -0.18622
59B -> 72B 0.10531

Excited State 21: 2.008-A 5.9539 eV 208.24 nm f=0.0011 <S**2>=0.758
53B -> 72B 0.19725
54B -> 72B -0.57338
55B -> 72B 0.74916
56B -> 72B -0.16612
58B -> 72B 0.14073

Excited State 22: 2.007-A 6.2903 eV 197.10 nm f=0.0014 <S**2>=0.757
53B -> 72B 0.93971
54B -> 72B 0.24183
56B -> 72B 0.16458

Excited State 23: 2.009-A 6.4029 eV 193.64 nm f=0.0073 <S**2>=0.759
51B -> 72B -0.21389
52B -> 72B 0.89693
54B -> 72B -0.31309
55B -> 72B -0.16374

Excited State 24: 3.221-A 6.4815 eV 191.29 nm f=0.0014 <S**2>=2.343
70A -> 73A -0.10930
72A -> 74A -0.25787
72A -> 75A -0.13766
70B -> 73B 0.24455
71B -> 74B 0.86602
71B -> 75B 0.23211

Excited State 25: 2.008-A 6.5305 eV 189.86 nm f=0.0061 <S**2>=0.758
51B -> 72B 0.96604
52B -> 72B 0.22759

Excited State 26: 2.366-A 6.6524 eV 186.37 nm f=0.0010 <S**2>=1.150
70A -> 73A 0.10594
72A -> 74A 0.85911

72A -> 75A 0.15693
70B -> 73B -0.14445
71B -> 74B 0.39827
71B -> 75B -0.16446

Excited State 27: 3.267-A 6.7592 eV 183.43 nm f=0.0022 <S**2>=2.419
70A -> 73A -0.18173
72A -> 74A 0.40658
72A -> 75A -0.20314
70B -> 73B 0.64153
71B -> 74B -0.27567
71B -> 75B 0.48413

Excited State 28: 3.035-A 6.8952 eV 179.81 nm f=0.0031 <S**2>=2.053
72A -> 75A -0.21405
69B -> 73B 0.11114
70B -> 73B -0.66606
71B -> 75B 0.68055

Excited State 29: 2.337-A 7.0160 eV 176.72 nm f=0.0033 <S**2>=1.115
70A -> 73A 0.31515
72A -> 75A 0.73404
69B -> 73B -0.37086
70B -> 73B 0.10071
71B -> 75B 0.41548

Excited State 30: 2.818-A 7.0330 eV 176.29 nm f=0.0054 <S**2>=1.736
72A -> 75A 0.37751
69B -> 73B 0.89469

[Cu(II)L(H_2O)$_3$]$^{2+}$
Excitation energies and oscillator strengths:

Excited State 1: 2.002-A 0.4848 eV 2557.55 nm f=0.0005 <S**2>=0.752
71B -> 77B 0.27131
73B -> 77B -0.27159
75B -> 77B -0.18163
76B -> 77B 0.88887
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2388.65843567
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.001-A 1.8872 eV 656.97 nm f=0.0002 <S**2>=0.751
60B -> 77B 0.16389
64B -> 77B 0.10618
65B -> 77B -0.21165

68B -> 77B 0.26414
70B -> 77B 0.37971
71B -> 77B -0.29477
72B -> 77B 0.75256
75B -> 77B -0.12869

Excited State 3: 2.001-A 1.9231 eV 644.72 nm f=0.0001 <S**2>=0.751
67B -> 77B -0.14107
69B -> 77B 0.58953
70B -> 77B 0.30308
71B -> 77B 0.55440
72B -> 77B 0.16433
73B -> 77B 0.41616

Excited State 4: 2.002-A 2.1001 eV 590.38 nm f=0.0004 <S**2>=0.752
60B -> 77B 0.39961
61B -> 77B 0.11304
62B -> 77B 0.38362
63B -> 77B -0.18840
64B -> 77B -0.24455
65B -> 77B 0.19459
66B -> 77B -0.25487
67B -> 77B 0.57731
68B -> 77B -0.14046
70B -> 77B 0.28916
72B -> 77B -0.11905

Excited State 5: 2.004-A 2.9002 eV 427.50 nm f=0.0013 <S**2>=0.754
71B -> 77B -0.43893
73B -> 77B 0.39468
75B -> 77B 0.65236
76B -> 77B 0.42667

Excited State 6: 2.005-A 3.5546 eV 348.80 nm f=0.0860 <S**2>=0.755
67B -> 77B 0.15784
71B -> 77B 0.34288
72B -> 77B 0.16344
73B -> 77B -0.52191
75B -> 77B 0.70859
76B -> 77B -0.16633

Excited State 7: 2.004-A 3.9878 eV 310.91 nm f=0.0818 <S**2>=0.754
74B -> 77B 0.98187

Excited State 8: 2.005-A 4.5862 eV 270.34 nm f=0.0007 <S**2>=0.755
67B -> 77B 0.16817

69B -> 77B -0.47639
70B -> 77B -0.47593
71B -> 77B 0.31375
72B -> 77B 0.40842
73B -> 77B 0.49608

Excited State 9: 2.006-A 4.7669 eV 260.09 nm f=0.0006 <S**2>=0.756
62B -> 77B -0.10202
63B -> 77B 0.12384
64B -> 77B 0.19463
65B -> 77B -0.30229
66B -> 77B 0.16751
68B -> 77B 0.31025
69B -> 77B -0.44793
70B -> 77B 0.51193
71B -> 77B 0.27066
72B -> 77B -0.37140
73B -> 77B 0.17618

Excited State 10: 2.006-A 4.9417 eV 250.89 nm f=0.0019 <S**2>=0.756
60B -> 77B 0.12345
62B -> 77B 0.10086
66B -> 77B -0.12436
67B -> 77B 0.13335
68B -> 77B 0.85564
69B -> 77B 0.28008
70B -> 77B -0.31207
72B -> 77B -0.14530

Excited State 11: 2.007-A 5.0592 eV 245.07 nm f=0.0020 <S**2>=0.757
64B -> 77B 0.21479
65B -> 77B -0.54324
66B -> 77B 0.25778
67B -> 77B 0.55946
68B -> 77B -0.20880
69B -> 77B 0.35290
70B -> 77B -0.19726
71B -> 77B -0.15548
73B -> 77B 0.14716

Excited State 12: 2.006-A 5.2659 eV 235.45 nm f=0.0010 <S**2>=0.756
60B -> 77B 0.14515
62B -> 77B 0.17929
63B -> 77B -0.11240
64B -> 77B -0.14080
65B -> 77B 0.30894

66B -> 77B 0.89603

Excited State 13: 2.008-A 5.3865 eV 230.18 nm f=0.0035 <S**2>=0.758
60B -> 77B 0.49673
61B -> 77B 0.12145
62B -> 77B 0.44078
65B -> 77B -0.48233
67B -> 77B -0.47903
68B -> 77B -0.12336
70B -> 77B -0.17047
72B -> 77B -0.12210

Excited State 14: 3.036-A 5.5774 eV 222.30 nm f=0.0002 <S**2>=2.054
77A -> 78A -0.16046
76B -> 78B 0.97132

Excited State 15: 2.009-A 5.6007 eV 221.37 nm f=0.0118 <S**2>=0.759
62B -> 77B 0.10012
63B -> 77B -0.64331
64B -> 77B 0.72332
65B -> 77B 0.17341

Excited State 16: 2.018-A 5.6093 eV 221.03 nm f=0.0030 <S**2>=0.768
60B -> 77B 0.19649
62B -> 77B 0.21730
63B -> 77B 0.70094
64B -> 77B 0.51687
65B -> 77B 0.35817
76B -> 78B -0.10563

Excited State 17: 2.594-A 5.7707 eV 214.85 nm f=0.0006 <S**2>=1.432
77A -> 78A 0.97939
76B -> 78B 0.16516

Excited State 18: 2.007-A 5.7859 eV 214.29 nm f=0.0069 <S**2>=0.757
60B -> 77B -0.63973
61B -> 77B -0.14615
62B -> 77B 0.72898

Excited State 19: 2.006-A 5.8382 eV 212.37 nm f=0.0014 <S**2>=0.756
60B -> 77B -0.21887
61B -> 77B 0.96232

Excited State 20: 2.006-A 6.2919 eV 197.05 nm f=0.0003 <S**2>=0.756
57B -> 77B -0.12762
58B -> 77B 0.24664

59B -> 77B 0.95016

Excited State 21: 2.008-A 6.3402 eV 195.55 nm f=0.0005 <S**2>=0.758
56B -> 77B 0.14402
58B -> 77B 0.94726
59B -> 77B -0.23397

Excited State 22: 2.254-A 6.4115 eV 193.38 nm f=0.0004 <S**2>=1.021
76A -> 78A 0.98878

Excited State 23: 3.023-A 6.6628 eV 186.08 nm f=0.0009 <S**2>=2.034
77A -> 79A -0.13835
76B -> 79B 0.97517

Excited State 24: 2.009-A 6.7197 eV 184.51 nm f=0.0044 <S**2>=0.759
54B -> 77B 0.13353
55B -> 77B 0.11239
57B -> 77B 0.96313
59B -> 77B 0.14364

Excited State 25: 2.016-A 6.7882 eV 182.65 nm f=0.0046 <S**2>=0.766
55B -> 77B 0.12214
56B -> 77B 0.96818
58B -> 77B -0.12217

Excited State 26: 2.928-A 6.8276 eV 181.59 nm f=0.0010 <S**2>=1.894
77A -> 79A 0.33717
76B -> 80B 0.90943
76B -> 81B -0.11152

Excited State 27: 2.718-A 6.8557 eV 180.85 nm f=0.0011 <S**2>=1.596
77A -> 79A 0.91094
77A -> 80A 0.14873
76B -> 79B 0.14664
76B -> 80B -0.32464

Excited State 28: 2.007-A 6.9105 eV 179.41 nm f=0.0048 <S**2>=0.757
54B -> 77B 0.18147
55B -> 77B 0.96082
56B -> 77B -0.10302
57B -> 77B -0.13895

Excited State 29: 2.641-A 7.0182 eV 176.66 nm f=0.0006 <S**2>=1.494
77A -> 80A 0.93645
77A -> 81A -0.15596
76B -> 80B 0.16645

76B -> 81B 0.18310

Excited State 30: 3.013-A 7.0706 eV 175.35 nm f=0.0046 <S**2>=2.020
77A -> 80A -0.21947
77A -> 81A -0.11735
76B -> 81B 0.95036
76B -> 82B -0.10832

[Cu(II)LAsc], conformer 1

TD-B3LYP method:
Excitation energies and oscillator strengths:

Excited State 1: 2.015-A 1.5764 eV 786.50 nm f=0.0002 <S**2>=0.765
102B ->108B 0.11665
105B ->108B 0.42276
106B ->108B 0.87275
107B ->108B 0.15093
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.84036663
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.012-A 1.6634 eV 745.35 nm f=0.0123 <S**2>=0.762
105B ->108B 0.70490
106B ->108B -0.22858
107B ->108B -0.66320

Excited State 3: 2.013-A 1.8898 eV 656.06 nm f=0.0484 <S**2>=0.763
105B ->108B 0.54676
106B ->108B -0.40440
107B ->108B 0.71793

Excited State 4: 2.030-A 2.3111 eV 536.46 nm f=0.0011 <S**2>=0.780
102B ->108B -0.60064
103B ->108B -0.29000
104B ->108B 0.70325
105B ->108B 0.11393
106B ->108B 0.10188

Excited State 5: 2.013-A 2.4365 eV 508.86 nm f=0.0009 <S**2>=0.763
102B ->108B 0.72936
103B ->108B -0.53616
104B ->108B 0.41667

Excited State 6: 2.013-A 2.4638 eV 503.22 nm f=0.0044 <S**2>=0.763
102B ->108B 0.26879

103B ->108B 0.78726
104B ->108B 0.54755

Excited State 7: 2.146-A 3.3016 eV 375.52 nm f=0.0002 <S**2>=0.901
99B ->108B 0.14548
100B ->108B 0.53178
101B ->108B 0.76646
102B ->112B -0.12491
104B ->112B 0.11625

Excited State 8: 2.082-A 3.6428 eV 340.35 nm f=0.0128 <S**2>=0.834
106A ->110A -0.10589
108A ->109A -0.39508
108A ->110A 0.59243
93B ->108B 0.10102
94B ->108B 0.10057
99B ->108B -0.39166
100B ->108B 0.42926
101B ->108B -0.23960
107B ->112B 0.12035

Excited State 9: 2.075-A 3.9063 eV 317.40 nm f=0.0269 <S**2>=0.826
99A ->110A -0.10306
108A ->109A 0.52808
108A ->110A -0.33368
93B ->108B -0.13404
94B ->108B -0.10890
99B ->108B -0.37560
100B ->108B 0.52677
101B ->108B -0.30147

Excited State 10: 2.376-A 3.9471 eV 314.12 nm f=0.0029 <S**2>=1.162
106A ->109A 0.13786
108A ->109A 0.61067
108A ->110A 0.59772
108A ->111A 0.24411
108A ->115A 0.15093
99B ->108B 0.11645
100B ->108B -0.16244
107B ->109B 0.19325

Excited State 11: 2.092-A 4.0991 eV 302.46 nm f=0.0007 <S**2>=0.844
93B ->108B -0.20716
94B ->108B 0.41363
95B ->108B -0.41621
96B ->108B 0.13818

98B ->108B -0.22054
99B ->108B 0.52268
100B ->108B 0.24419
101B ->108B -0.38212

Excited State 12: 2.847-A 4.1543 eV 298.44 nm f=0.0008 <S**2>=1.777
108A ->109A -0.19179
108A ->110A -0.17458
99B ->108B -0.16014
107B ->109B 0.83693
107B ->110B 0.29128
107B ->115B 0.18112

Excited State 13: 2.096-A 4.1906 eV 295.86 nm f=0.0008 <S**2>=0.849
93B ->108B 0.27039
94B ->108B -0.36689
95B ->108B 0.43396
96B ->108B -0.12239
98B ->108B 0.20358
99B ->108B 0.55774
100B ->108B 0.32136
101B ->108B -0.24556
107B ->109B 0.15361

Excited State 14: 3.426-A 4.2845 eV 289.38 nm f=0.0001 <S**2>=2.685
107A ->109A -0.47810
107A ->110A -0.25919
107A ->111A -0.19845
107A ->115A -0.13507
106B ->109B 0.68257
106B ->110B 0.25246
106B ->115B 0.16701

Excited State 15: 2.099-A 4.4134 eV 280.92 nm f=0.0006 <S**2>=0.851
107A ->109A 0.64257
107A ->110A 0.31075
107A ->111A 0.21974
107A ->115A 0.12886
106B ->109B 0.56774
106B ->110B 0.16823

Excited State 16: 2.327-A 4.4864 eV 276.36 nm f=0.0001 <S**2>=1.103
106A ->109A 0.12929
106A ->111A 0.19851
107A ->109A 0.10521
108A ->109A -0.25024

108A ->110A -0.14983
108A ->111A 0.85957
105B ->109B -0.17249
107B ->109B -0.12073

Excited State 17: 2.963-A 4.4955 eV 275.80 nm f=0.0002 <S**2>=1.946
102A ->109A -0.22309
102A ->110A 0.39444
104A ->110A -0.16575
105A ->109A -0.26622
105A ->110A 0.32719
106A ->109A -0.28415
106A ->110A 0.30348
107A ->109A -0.22276
107A ->110A 0.47987
108A ->111A 0.19173

Excited State 18: 3.206-A 4.5204 eV 274.27 nm f=0.0005 <S**2>=2.319
102A ->109A 0.13233
105A ->109A -0.20585
105A ->110A -0.20635
105A ->111A -0.15028
105A ->115A -0.10654
106A ->109A -0.35237
106A ->110A -0.29444
106A ->111A -0.13285
106A ->115A -0.12527
107A ->110A -0.15080
108A ->111A 0.27194
105B ->109B 0.55849
105B ->110B 0.23213
105B ->115B 0.17262
107B ->109B 0.14397

Excited State 19: 2.187-A 4.6286 eV 267.86 nm f=0.0035 <S**2>=0.946
105A ->109A 0.12479
106A ->112A 0.11507
108A ->112A 0.94504

Excited State 20: 2.896-A 4.6628 eV 265.90 nm f=0.0017 <S**2>=1.847
102A ->110A -0.11738
105A ->110A -0.17506
106A ->109A 0.36324
106A ->110A -0.40779
107A ->109A -0.32935
107A ->110A 0.62173

108A ->110A -0.14002
93B ->108B 0.15105
98B ->108B -0.13042
105B ->109B 0.10974

Excited State 21: 2.776-A 4.6763 eV 265.13 nm f=0.0017 <S**2>=1.677
105A ->109A -0.12072
106A ->109A 0.16230
106A ->110A 0.15425
108A ->112A 0.11892
105B ->109B 0.23509
107B ->109B -0.36025
107B ->110B 0.80041

Excited State 22: 2.487-A 4.7231 eV 262.51 nm f=0.0105 <S**2>=1.297
105A ->109A -0.19073
106A ->109A 0.41147
106A ->110A 0.26160
106A ->111A 0.11418
107A ->110A -0.20008
108A ->110A -0.10292
93B ->108B 0.21047
94B ->108B 0.11437
95B ->108B 0.17067
96B ->108B 0.14774
97B ->108B 0.28561
98B ->108B -0.29391
105B ->109B 0.28859
106B ->109B 0.11770
107B ->110B -0.39910
107B ->112B -0.16778

Excited State 23: 2.434-A 4.7630 eV 260.31 nm f=0.0082 <S**2>=1.231
105A ->109A 0.38330
105A ->110A 0.29464
105A ->111A 0.16388
105A ->115A 0.12063
106A ->109A -0.31866
106A ->110A -0.21501
107A ->109A 0.13059
108A ->109A 0.15975
108A ->112A -0.17102
93B ->108B 0.30779
94B ->108B 0.19391
95B ->108B 0.21383
96B ->108B 0.10178

97B ->108B 0.11272
98B ->108B -0.37237
107B ->110B 0.18315
107B ->112B -0.16624

Excited State 24: 2.743-A 4.8079 eV 257.88 nm f=0.0003 <S**2>=1.631
102A ->110A -0.14162
105A ->109A 0.45178
105A ->110A -0.24830
106A ->109A -0.17327
106A ->110A 0.33212
107A ->109A -0.14885
107A ->110A 0.20713
108A ->110A 0.16319
93B ->108B -0.18086
94B ->108B -0.12115
96B ->108B 0.11054
97B ->108B 0.45343
98B ->108B 0.11727
105B ->109B 0.19474
107B ->112B -0.27387

Excited State 25: 3.177-A 4.8504 eV 255.61 nm f=0.0001 <S**2>=2.273
105A ->110A -0.13305
106A ->110A 0.12615
107A ->110A 0.11650
107A ->111A -0.24609
106B ->109B -0.32499
106B ->110B 0.83661
107B ->112B -0.11739

Excited State 26: 2.708-A 4.8508 eV 255.59 nm f=0.0020 <S**2>=1.584
105A ->109A 0.15342
105A ->110A 0.42838
105A ->111A 0.10820
106A ->109A 0.21585
106A ->110A -0.23297
93B ->108B -0.18782
94B ->108B -0.13774
95B ->108B -0.17331
97B ->108B 0.44940
98B ->108B 0.17287
105B ->109B 0.22893
106B ->110B 0.20441
107B ->112B 0.40643

Excited State 27: 2.206-A 4.8631 eV 254.95 nm f=0.0008 <S**2>=0.967
105A ->109A -0.28918
105A ->110A -0.23515
105A ->111A -0.11005
106A ->109A -0.17212
96B ->108B -0.22571
97B ->108B 0.59699
98B ->108B -0.12297
105B ->109B -0.36027
107B ->111B 0.41353

Excited State 28: 2.754-A 4.8846 eV 253.83 nm f=0.0021 <S**2>=1.646
105A ->109A 0.18568
106A ->110A 0.15286
108A ->113A 0.16864
108A ->114A -0.14076
96B ->108B 0.14806
97B ->108B -0.20463
105B ->109B 0.14655
107B ->111B 0.83579
107B ->112B 0.20541

Excited State 29: 2.345-A 4.8987 eV 253.10 nm f=0.0008 <S**2>=1.125
107A ->109A -0.23447
107A ->110A -0.16999
107A ->111A 0.81421
108A ->113A 0.24010
108A ->114A -0.20435
106B ->110B 0.29601

Excited State 30: 2.201-A 4.9123 eV 252.40 nm f=0.0007 <S**2>=0.961
107A ->111A -0.33227
108A ->113A 0.66063
108A ->114A -0.54669
108A ->115A -0.11527
96B ->108B -0.14921
97B ->108B 0.11070
107B ->111B -0.14061

M06 method:
Excitation energies and oscillator strengths:

Excited State 1: 2.018-A 1.7276 eV 717.67 nm f=0.0000 <S**2>=0.768
104B ->108B -0.24819
105B ->108B 0.61040
106B ->108B 0.73147

This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.01564230
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.013-A 1.9289 eV 642.79 nm f=0.0125 <S**2>=0.763
105B ->108B -0.54725
106B ->108B 0.39419
107B ->108B 0.72458

Excited State 3: 2.014-A 2.1342 eV 580.95 nm f=0.0396 <S**2>=0.764
105B ->108B 0.52330
106B ->108B -0.50935
107B ->108B 0.66529

Excited State 4: 2.029-A 2.4779 eV 500.37 nm f=0.0020 <S**2>=0.779
100B ->108B -0.10550
104B ->108B 0.93723
105B ->108B 0.18130
106B ->108B 0.17687
107B ->108B 0.11755

Excited State 5: 2.013-A 2.7642 eV 448.53 nm f=0.0008 <S**2>=0.763
103B ->108B 0.99172

Excited State 6: 2.013-A 2.8155 eV 440.37 nm f=0.0031 <S**2>=0.763
102B ->108B 0.99132

Excited State 7: 2.145-A 3.4477 eV 359.61 nm f=0.0001 <S**2>=0.900
94B ->108B -0.10092
96B ->108B 0.10491
99B ->108B 0.12411
100B ->108B 0.66927
101B ->108B -0.63069
104B ->108B 0.15215
104B ->112B 0.16659
104B ->113B -0.10723

Excited State 8: 2.044-A 3.7497 eV 330.65 nm f=0.0270 <S**2>=0.794
106A ->110A 0.13559
108A ->109A -0.19692
108A ->110A 0.82099
93B ->108B -0.16592
99B ->108B -0.30011
100B ->108B 0.21870
101B ->108B 0.19980

Excited State 9: 2.316-A 3.8981 eV 318.06 nm f=0.0003 <S**2>=1.091
106A ->109A -0.18407
108A ->109A 0.89915
108A ->110A 0.15937
108A ->111A 0.13925
108A ->115A 0.14089
107B ->109B 0.12345

Excited State 10: 2.086-A 4.1040 eV 302.11 nm f=0.0255 <S**2>=0.838
99A ->110A 0.12729
108A ->110A 0.40073
93B ->108B -0.14186
99B ->108B 0.55188
100B ->108B -0.51443
101B ->108B -0.43435

Excited State 11: 2.109-A 4.2015 eV 295.10 nm f=0.0006 <S**2>=0.862
93B ->108B -0.19965
94B ->108B 0.72555
95B ->108B 0.38136
96B ->108B -0.12895
98B ->108B 0.31141
99B ->108B -0.14672
101B ->108B -0.22834
107B ->109B 0.13513

Excited State 12: 3.135-A 4.2331 eV 292.89 nm f=0.0002 <S**2>=2.207
107A ->109A -0.34409
108A ->109A -0.17530
106B ->109B 0.28156
107B ->109B 0.75228
107B ->110B 0.14956
107B ->115B 0.14166
107B ->122B 0.10003

Excited State 13: 3.220-A 4.3280 eV 286.47 nm f=0.0001 <S**2>=2.342
106A ->109A -0.12523
107A ->109A 0.53989
107A ->111A 0.10581
107A ->115A 0.10911
105B ->109B 0.12984
106B ->109B -0.53341
106B ->110B -0.10998
106B ->115B -0.11152
107B ->109B 0.46896

Excited State 14: 2.047-A 4.4227 eV 280.34 nm f=0.0010 <S**2>=0.798
93B ->108B -0.15284
94B ->108B 0.15433
95B ->108B 0.13273
99B ->108B 0.69720
100B ->108B 0.38616
101B ->108B 0.52134

Excited State 15: 2.102-A 4.4663 eV 277.60 nm f=0.0008 <S**2>=0.855
107A ->109A 0.63573
107A ->111A 0.10857
107A ->115A 0.10092
106B ->109B 0.68090
106B ->110B 0.12019
106B ->115B 0.10728

Excited State 16: 3.331-A 4.5958 eV 269.78 nm f=0.0002 <S**2>=2.524
104A ->109A -0.14017
105A ->109A -0.39406
105A ->115A -0.11026
106A ->109A 0.38086
107A ->109A -0.13915
104B ->109B 0.17016
105B ->109B 0.62399
105B ->110B 0.13768
105B ->115B 0.15189
105B ->119B -0.10876
105B ->122B 0.10543

Excited State 17: 2.922-A 4.7142 eV 263.00 nm f=0.0000 <S**2>=1.885
103A ->110A 0.17126
104A ->110A -0.50159
105A ->110A 0.54457
106A ->109A 0.25718
106A ->110A -0.28915
107A ->110A 0.40172
105B ->109B -0.12722

Excited State 18: 2.606-A 4.7283 eV 262.22 nm f=0.0007 <S**2>=1.447
104A ->110A 0.19079
105A ->109A 0.35827
105A ->110A -0.17779
106A ->109A 0.68248
106A ->110A 0.12842
106A ->111A 0.14188
106A ->115A 0.11047

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  107A ->110A       -0.15767
  108A ->109A        0.20910
  108A ->111A       -0.16879
  108A ->112A        0.13855
  105B ->109B       -0.15313
  106B ->109B       -0.11348
  107B ->109B        0.15552

Excited State  19:  2.089-A     4.8118 eV  257.67 nm  f=0.0267  <S**2>=0.841
  105A ->109A       -0.24783
  106A ->109A        0.13711
  108A ->110A        0.20668
  108A ->111A        0.23231
  108A ->112A       -0.32323
   92B ->108B        0.13196
   93B ->108B        0.49290
   94B ->108B        0.15167
   95B ->108B       -0.28091
   97B ->108B       -0.11400
   98B ->108B        0.41194
   99B ->108B        0.10743
  105B ->109B       -0.21693

Excited State  20:  2.215-A     4.8364 eV  256.35 nm  f=0.0029  <S**2>=0.977
  105A ->109A        0.11707
  106A ->109A        0.22233
  106A ->111A       -0.16146
  108A ->111A        0.90186
   93B ->108B       -0.16318
   98B ->108B       -0.12093

Excited State  21:  2.183-A     4.9046 eV  252.79 nm  f=0.0029  <S**2>=0.942
  105A ->109A       -0.16552
  106A ->112A       -0.13786
  108A ->109A       -0.10820
  108A ->112A        0.88012
   93B ->108B        0.11852
   95B ->108B       -0.10222
   98B ->108B        0.17962
  105B ->109B       -0.11890

Excited State  22:  2.094-A     4.9503 eV  250.46 nm  f=0.0060  <S**2>=0.846
  104A ->109A        0.12154
  105A ->109A        0.51022
  106A ->109A       -0.12607
  106A ->110A       -0.13735
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108A ->110A 0.16948
93B ->108B 0.36504
94B ->108B 0.11701
96B ->108B 0.16342
97B ->108B 0.38227
105B ->109B 0.45171

Excited State 23: 2.088-A 5.0088 eV 247.53 nm f=0.0011 <S**2>=0.840
103A ->109A -0.11236
105A ->109A -0.27898
106A ->109A 0.13908
106A ->110A -0.11265
107A ->110A -0.14151
97B ->108B 0.79856
98B ->108B -0.25809
105B ->109B -0.26520

Excited State 24: 2.900-A 5.0513 eV 245.45 nm f=0.0029 <S**2>=1.852
100A ->110A 0.10737
105A ->110A -0.23701
106A ->110A 0.41949
107A ->110A 0.75916
95B ->108B -0.17202
96B ->108B -0.10642
97B ->108B 0.22176

Excited State 25: 3.433-A 5.0781 eV 244.15 nm f=0.0000 <S**2>=2.697
102A ->109A 0.12103
103A ->109A -0.51762
103A ->111A -0.12113
103A ->115A -0.14297
103A ->119A 0.10186
103A ->122A -0.10541
104A ->109A -0.16869
103B ->109B 0.64942
103B ->110B 0.15585
103B ->115B 0.16986
103B ->119B -0.11849
103B ->122B 0.11690

Excited State 26: 3.432-A 5.0822 eV 243.96 nm f=0.0001 <S**2>=2.695
102A ->109A -0.55138
102A ->111A -0.12970
102A ->115A -0.15307
102A ->119A 0.10690
102A ->122A -0.11237

103A ->109A -0.10559
104A ->109A -0.11464
102B ->109B 0.62975
102B ->110B 0.15157
102B ->115B 0.16670
102B ->119B -0.11491
102B ->122B 0.11496

Excited State 27: 2.524-A 5.1382 eV 241.30 nm f=0.0002 <S**2>=1.343
105A ->109A -0.10688
105A ->110A -0.17377
106A ->109A 0.10020
106A ->110A -0.18165
107A ->110A 0.20141
108A ->113A 0.22985
108A ->114A 0.42385
95B ->108B 0.24414
96B ->108B 0.41081
98B ->108B -0.11887
103B ->109B -0.11509
107B ->109B -0.12063
107B ->110B 0.50278

Excited State 28: 2.660-A 5.1470 eV 240.89 nm f=0.0006 <S**2>=1.519
105A ->110A 0.11884
106A ->110A 0.15213
107A ->110A -0.13936
93B ->108B -0.10249
95B ->108B -0.22387
96B ->108B -0.41508
98B ->108B 0.10031
107B ->109B -0.17810
107B ->110B 0.77324

Excited State 29: 2.244-A 5.1657 eV 240.01 nm f=0.0003 <S**2>=1.009
105A ->110A 0.13589
106A ->110A 0.20875
107A ->110A -0.13386
108A ->113A 0.51283
108A ->114A 0.63049
108A ->118A 0.10167
95B ->108B -0.13471
96B ->108B -0.27786
107B ->110B -0.23118

Excited State 30: 2.819-A 5.2092 eV 238.01 nm f=0.0041 <S**2>=1.737

103A ->109A -0.13615
104A ->110A -0.13722
105A ->110A 0.32063
106A ->110A 0.60444
107A ->110A -0.19920
93B ->108B 0.10435
94B ->108B 0.12152
96B ->108B 0.47010
98B ->108B -0.11316
107B ->111B -0.28484
107B ->112B 0.11491
107B ->113B -0.15447

[Cu(II)LAsc], conformer 2

Excitation energies and oscillator strengths:

Excited State 1: 2.025-A 1.5942 eV 777.72 nm f=0.0000 <S**2>=0.775
101B ->108B -0.12179
104B ->108B 0.63764
105B ->108B 0.16356
106B ->108B -0.28767
107B ->108B 0.67243
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.83659604
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.036-A 2.0810 eV 595.80 nm f=0.0114 <S**2>=0.786
104B ->108B -0.18192
105B ->108B -0.10902
106B ->108B 0.80465
107B ->108B 0.54459

Excited State 3: 2.040-A 2.1714 eV 570.98 nm f=0.0008 <S**2>=0.791
104B ->108B 0.63262
105B ->108B 0.32532
106B ->108B 0.50626
107B ->108B -0.46608

Excited State 4: 2.034-A 2.4320 eV 509.80 nm f=0.0002 <S**2>=0.784
104B ->108B -0.36006
105B ->108B 0.91790
107B ->108B 0.11465

Excited State 5: 2.030-A 2.8462 eV 435.62 nm f=0.0001 <S**2>=0.780
102B ->108B 0.12693
103B ->108B 0.98605

Excited State 6: 2.030-A 2.8576 eV 433.88 nm f=0.0016 <S**2>=0.780
102B ->108B 0.98680
103B ->108B -0.12843

Excited State 7: 2.189-A 3.1693 eV 391.20 nm f=0.0000 <S**2>=0.948
104A ->109A -0.13598
100B ->108B 0.34025
101B ->108B 0.85778
104B ->110B -0.22336
107B ->108B 0.11064

Excited State 8: 2.045-A 3.3878 eV 365.97 nm f=0.0750 <S**2>=0.796
108A ->109A 0.94528
96B ->108B 0.17367
99B ->108B -0.17641

Excited State 9: 2.723-A 3.8223 eV 324.37 nm f=0.0001 <S**2>=1.603
106A ->110A -0.37355
106A ->111A -0.10481
107A ->110A -0.15798
108A ->110A 0.80653
108A ->111A 0.14850
106B ->109B 0.20439
107B ->109B 0.16812

Excited State 10: 3.403-A 3.9292 eV 315.55 nm f=0.0000 <S**2>=2.645
106A ->110A 0.12618
107A ->109A 0.17178
107A ->110A -0.56847
107A ->111A -0.15391
107A ->115A 0.11942
108A ->110A -0.16221
106B ->109B -0.17895
107B ->109B 0.62834
107B ->111B 0.16494
107B ->115B -0.12518

Excited State 11: 2.966-A 3.9572 eV 313.31 nm f=0.0002 <S**2>=1.950
104A ->109A 0.47233
105A ->109A 0.15182
107A ->109A 0.80656
107A ->110A 0.10130
101B ->108B 0.13738
107B ->109B -0.14498

Excited State 12: 2.855-A 4.0004 eV 309.93 nm f=0.0004 <S**2>=1.788
106A ->110A -0.18486
107A ->110A 0.17846
108A ->110A -0.37587
106B ->109B 0.73217
106B ->111B 0.18999
106B ->114B 0.10102
106B ->115B -0.14263
107B ->109B 0.32436

Excited State 13: 2.046-A 4.0764 eV 304.15 nm f=0.0004 <S**2>=0.796
107A ->110A 0.67756
107A ->111A 0.14923
108A ->110A 0.10847
106B ->109B -0.34668
107B ->109B 0.54423
107B ->111B 0.11363

Excited State 14: 3.031-A 4.1558 eV 298.34 nm f=0.0086 <S**2>=2.046
104A ->109A -0.13993
106A ->109A 0.90443
107A ->109A 0.21437
105B ->109B -0.12090
106B ->109B -0.10000
106B ->110B 0.15723

Excited State 15: 2.267-A 4.2160 eV 294.08 nm f=0.0010 <S**2>=1.035
106A ->110A 0.78183
106A ->111A 0.18815
106A ->115A -0.12345
108A ->110A 0.33671
105B ->109B 0.15912
106B ->109B 0.33707

Excited State 16: 2.919-A 4.2600 eV 291.05 nm f=0.0001 <S**2>=1.880
104A ->109A 0.65160
105A ->109A 0.36163
106A ->109A 0.25168
107A ->109A -0.49838
101B ->108B 0.16112
104B ->110B 0.17101
107B ->110B 0.15165

Excited State 17: 3.414-A 4.2825 eV 289.51 nm f=0.0002 <S**2>=2.664
105A ->110A 0.61365
105A ->111A 0.19236

105A ->114A 0.10651
105A ->115A -0.16533
106A ->109A -0.12554
106A ->110A 0.18032
104B ->109B 0.11789
105B ->109B -0.57077
105B ->111B -0.18087
105B ->114B -0.10024
105B ->115B 0.15447

Excited State 18: 2.032-A 4.3503 eV 285.00 nm f=0.0139 <S**2>=0.783
108A ->109A -0.10314
99B ->108B -0.10545
100B ->108B 0.90790
101B ->108B -0.34953

Excited State 19: 2.259-A 4.4736 eV 277.15 nm f=0.0002 <S**2>=1.026
106A ->110A 0.16042
106A ->111A -0.22944
108A ->110A -0.14154
108A ->111A 0.93645

Excited State 20: 2.736-A 4.4836 eV 276.53 nm f=0.0001 <S**2>=1.622
105A ->109A 0.67463
104B ->110B -0.31347
105B ->110B -0.10040
106B ->110B 0.22515
107B ->110B -0.56867

Excited State 21: 2.774-A 4.5028 eV 275.35 nm f=0.0013 <S**2>=1.674
104A ->109A -0.47123
105A ->109A 0.59256
104B ->110B 0.20855
105B ->110B 0.11814
106B ->110B -0.14940
107B ->110B 0.51762

Excited State 22: 2.126-A 4.5469 eV 272.68 nm f=0.0767 <S**2>=0.880
106A ->109A -0.10072
108A ->109A -0.19459
108A ->112A 0.57442
94B ->108B -0.23948
96B ->108B 0.40082
99B ->108B -0.50582
100B ->108B -0.13979
107B ->110B -0.12700

Excited State 23: 2.367-A 4.6094 eV 268.98 nm f=0.0418 <S**2>=1.150
105A ->110A 0.13791
106A ->112A -0.20833
108A ->109A 0.10244
108A ->112A 0.67851
94B ->108B 0.17253
96B ->108B -0.23732
99B ->108B 0.36090
105B ->109B 0.18974
106B ->110B 0.32304
107B ->110B 0.16512

Excited State 24: 2.268-A 4.6180 eV 268.48 nm f=0.0000 <S**2>=1.036
105A ->110A 0.38615
106A ->109A -0.10646
106A ->112A 0.10577
108A ->112A -0.31837
94B ->108B -0.17271
96B ->108B 0.18722
98B ->108B -0.10831
99B ->108B -0.13468
105B ->109B 0.41396
106B ->110B 0.57061
107B ->110B 0.19519

Excited State 25: 3.206-A 4.6653 eV 265.76 nm f=0.0002 <S**2>=2.320
107A ->110A 0.12856
107A ->111A -0.29710
107B ->109B -0.27148
107B ->111B 0.87251

Excited State 26: 3.459-A 4.6804 eV 264.90 nm f=0.0001 <S**2>=2.741
103A ->110A 0.61894
103A ->111A 0.19749
103A ->114A 0.10744
103A ->115A -0.16404
103B ->109B -0.60261
103B ->111B -0.19403
103B ->114B -0.10582
103B ->115B 0.16187

Excited State 27: 3.456-A 4.6911 eV 264.30 nm f=0.0000 <S**2>=2.736
102A ->110A -0.59472
102A ->111A -0.19040
102A ->114A -0.10428

102A ->115A 0.15949
102B ->109B 0.62517
102B ->111B 0.19967
102B ->114B 0.10842
102B ->115B -0.16556

Excited State 28: 2.747-A 4.7042 eV 263.56 nm f=0.0018 <S**2>=1.637
106A ->111A -0.10918
107A ->110A -0.22373
107A ->111A 0.77511
106B ->109B -0.14466
106B ->111B 0.41700
107B ->111B 0.25438

Excited State 29: 2.564-A 4.7229 eV 262.52 nm f=0.0016 <S**2>=1.394
107A ->111A -0.41505
106B ->109B -0.23801
106B ->111B 0.80070
107B ->111B -0.21819

Excited State 30: 2.272-A 4.7336 eV 261.93 nm f=0.0067 <S**2>=1.041
103A ->110A -0.17773
105A ->110A -0.46759
106A ->109A -0.15858
108A ->112A -0.11888
103B ->109B -0.23415
105B ->109B -0.43740
106B ->110B 0.47432
106B ->111B 0.20294
107B ->110B 0.26743

[Cu(II)LAsc], conformer 3

Excitation energies and oscillator strengths:

Excited State 1: 2.024-A 1.6708 eV 742.07 nm f=0.0008 <S**2>=0.774
102B ->108B 0.59646
105B ->108B 0.24979
107B ->108B 0.74872
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.85251361
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.025-A 1.7957 eV 690.44 nm f=0.0017 <S**2>=0.775
102B ->108B -0.40235
105B ->108B -0.17466
106B ->108B 0.77605

107B ->108B 0.43756

Excited State 3: 2.025-A 1.8319 eV 676.81 nm f=0.0055 <S**2>=0.776
102B ->108B 0.53955
105B ->108B 0.23229
106B ->108B 0.62573
107B ->108B -0.49338

Excited State 4: 2.028-A 2.4726 eV 501.44 nm f=0.0001 <S**2>=0.778
102B ->108B -0.38049
105B ->108B 0.92074

Excited State 5: 2.029-A 2.6440 eV 468.92 nm f=0.0054 <S**2>=0.779
104B ->108B 0.99053

Excited State 6: 2.027-A 2.6654 eV 465.15 nm f=0.0002 <S**2>=0.778
103B ->108B 0.99386

Excited State 7: 2.238-A 3.2406 eV 382.59 nm f=0.0070 <S**2>=1.002
102A ->109A -0.15226
108A ->109A 0.32003
96B ->108B 0.17525
98B ->108B -0.15226
99B ->108B 0.66401
100B ->108B -0.50792
102B ->109B 0.22755

Excited State 8: 2.098-A 3.2785 eV 378.17 nm f=0.0679 <S**2>=0.851
106A ->109A -0.34936
107A ->109A 0.23335
108A ->109A 0.81087
94B ->108B 0.15108
99B ->108B -0.23074
100B ->108B 0.18462

Excited State 9: 2.828-A 3.4854 eV 355.72 nm f=0.0028 <S**2>=1.750
106A ->109A -0.14654
107A ->109A 0.92892
108A ->109A -0.30632

Excited State 10: 2.858-A 3.5886 eV 345.49 nm f=0.0081 <S**2>=1.792
106A ->109A 0.89044
107A ->109A 0.26212
108A ->109A 0.33715

Excited State 11: 3.443-A 3.7116 eV 334.05 nm f=0.0001 <S**2>=2.713

106A ->110A 0.30777
107A ->110A -0.27332
108A ->110A 0.50887
106B ->110B -0.32160
107B ->109B -0.15269
107B ->110B 0.55502

Excited State 12: 3.444-A 3.8316 eV 323.58 nm f=0.0001 <S**2>=2.716
106A ->110A 0.27419
107A ->110A 0.57704
108A ->110A 0.14176
106B ->109B 0.16156
106B ->110B -0.56179
107B ->109B 0.12380
107B ->110B -0.32485

Excited State 13: 2.269-A 4.0285 eV 307.77 nm f=0.0003 <S**2>=1.037
102A ->109A 0.16792
105A ->109A 0.16268
106A ->110A 0.13679
107A ->110A 0.61250
106B ->109B -0.19022
106B ->110B 0.32526
107B ->109B -0.46111
107B ->110B 0.36055

Excited State 14: 2.772-A 4.0578 eV 305.55 nm f=0.0005 <S**2>=1.670
102A ->109A 0.51627
105A ->109A 0.55022
106A ->110A -0.10572
107A ->110A -0.25000
95B ->108B -0.22113
99B ->108B 0.13262
102B ->109B -0.14737
106B ->109B 0.18317
106B ->110B -0.21235
107B ->109B -0.28878
107B ->110B -0.22258

Excited State 15: 2.787-A 4.0934 eV 302.89 nm f=0.0029 <S**2>=1.691
102A ->109A 0.28249
105A ->109A 0.42142
106A ->110A 0.12343
108A ->110A 0.17114
106B ->109B -0.26480
106B ->110B 0.18156

107B ->109B 0.74020
107B ->110B 0.13850

Excited State 16: 2.614-A 4.1387 eV 299.57 nm f=0.0034 <S**2>=1.458
106A ->110A -0.12846
107A ->110A 0.14361
108A ->110A -0.29331
106B ->109B 0.78731
107B ->109B 0.23904
107B ->110B 0.40071

Excited State 17: 2.239-A 4.2096 eV 294.52 nm f=0.0081 <S**2>=1.003
104A ->109A -0.10272
105A ->110A 0.11703
106A ->110A 0.22750
108A ->110A 0.50587
106B ->109B 0.42926
106B ->110B 0.53590
107B ->110B -0.34247

Excited State 18: 2.775-A 4.2370 eV 292.62 nm f=0.0001 <S**2>=1.676
102A ->109A -0.43495
105A ->109A 0.63136
95B ->108B 0.46663
95B ->109B -0.11825
97B ->108B 0.10456
102B ->109B 0.22975
107B ->109B -0.18279

Excited State 19: 2.335-A 4.3738 eV 283.47 nm f=0.0002 <S**2>=1.113
102A ->109A 0.54210
103A ->109A 0.18896
104A ->109A 0.20905
105A ->109A -0.25306
95B ->108B 0.61028
95B ->109B -0.13509
96B ->108B -0.13269
97B ->108B 0.14427
98B ->108B -0.17498
100B ->108B -0.19366
102B ->109B 0.16771

Excited State 20: 2.840-A 4.3992 eV 281.83 nm f=0.0018 <S**2>=1.766
102A ->109A -0.20831
103A ->109A 0.33145
104A ->109A 0.86967

95B ->108B -0.12906
101B ->108B 0.10762

Excited State 21: 2.845-A 4.4118 eV 281.03 nm f=0.0001 <S**2>=1.773
102A ->109A -0.11527
103A ->109A 0.90232
104A ->109A -0.39748

Excited State 22: 3.437-A 4.4371 eV 279.43 nm f=0.0000 <S**2>=2.703
105A ->110A 0.63879
105A ->115A 0.10259
102B ->110B 0.10097
105B ->109B 0.19250
105B ->110B -0.62731
105B ->115B -0.10784

Excited State 23: 2.047-A 4.4811 eV 276.68 nm f=0.0018 <S**2>=0.797
101B ->108B 0.98122

Excited State 24: 2.696-A 4.5142 eV 274.66 nm f=0.0018 <S**2>=1.567
103A ->110A -0.29114
104A ->110A -0.33400
106A ->110A 0.63546
107A ->110A -0.17313
108A ->110A -0.41830
104B ->110B 0.31306

Excited State 25: 2.035-A 4.5758 eV 270.96 nm f=0.0022 <S**2>=0.785
94B ->108B 0.13358
95B ->108B 0.13469
98B ->108B -0.16254
99B ->108B 0.54589
100B ->108B 0.77740

Excited State 26: 3.452-A 4.5900 eV 270.12 nm f=0.0000 <S**2>=2.728
103A ->110A 0.47282
104A ->110A -0.44387
103B ->109B -0.16437
103B ->110B 0.63326
103B ->115B 0.11293

Excited State 27: 2.104-A 4.6389 eV 267.27 nm f=0.0410 <S**2>=0.857
106A ->109A 0.11820
106A ->122A 0.11905
108A ->109A -0.11144
108A ->122A -0.12388

94B ->108B 0.75653
96B ->108B 0.41448
97B ->108B 0.16716
99B ->108B -0.14213
100B ->108B -0.11649

Excited State 28: 2.909-A 4.6522 eV 266.51 nm f=0.0009 <S**2>=1.865
103A ->110A -0.24034
104A ->110A -0.23450
105A ->110A -0.15961
106A ->110A -0.41820
107A ->110A 0.11673
108A ->110A 0.27660
103B ->110B -0.10262
104B ->109B -0.19070
104B ->110B 0.64329
104B ->115B 0.10308
105B ->109B 0.12076
105B ->110B -0.15679

Excited State 29: 2.626-A 4.6857 eV 264.60 nm f=0.0022 <S**2>=1.474
102A ->109A 0.12360
105A ->110A -0.21380
106A ->110A 0.10151
95B ->108B -0.18494
97B ->108B -0.15041
98B ->108B 0.16873
99B ->108B -0.14466
102B ->109B 0.41623
105B ->109B 0.77016

Excited State 30: 2.054-A 4.7551 eV 260.74 nm f=0.0013 <S**2>=0.804
103A ->110A -0.14092
105A ->110A 0.38522
106A ->110A -0.14324
95B ->108B 0.10948
98B ->108B 0.73926
99B ->108B 0.15202
102B ->109B 0.15041
105B ->110B 0.37794

[Cu(II)LHAsc]$^{+}$

Excited State 1: 2.009-A 0.8135 eV 1524.17 nm f=0.0031 <S**2>=0.759
85B ->108B 0.10397
92B ->108B 0.16526
93B ->108B 0.34975

95B ->108B 0.13350
96B ->108B -0.12554
97B ->108B 0.18261
106B ->108B 0.83092
107B ->108B 0.19056
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2843.02524431
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.009-A 1.4749 eV 840.63 nm f=0.0029 <S**2>=0.759
84B ->108B 0.10090
85B ->108B 0.14046
87B ->108B 0.24844
88B ->108B -0.20399
89B ->108B 0.23946
91B ->108B -0.13057
92B ->108B 0.16194
93B ->108B -0.19125
97B ->108B -0.14140
98B ->108B 0.29906
100B ->108B -0.42193
102B ->108B -0.10283
105B ->108B 0.59164
107B ->108B -0.13454

Excited State 3: 2.008-A 1.8832 eV 658.36 nm f=0.0026 <S**2>=0.758
84B ->108B -0.17206
89B ->108B 0.17081
92B ->108B -0.34941
93B ->108B 0.45283
95B ->108B 0.14866
96B ->108B 0.22604
97B ->108B -0.29847
98B ->108B 0.55824
99B ->108B 0.16632
105B ->108B -0.10380
107B ->108B -0.11931

Excited State 4: 2.029-A 1.9063 eV 650.41 nm f=0.0786 <S**2>=0.779
89B ->108B 0.16503
93B ->108B 0.11002
94B ->108B -0.20692
95B ->108B 0.15609
97B ->108B -0.47005
98B ->108B -0.40364
99B ->108B 0.11274

106B ->108B -0.11019
107B ->108B 0.64622

Excited State 5: 2.037-A 2.0082 eV 617.40 nm f=0.0965 <S**2>=0.788
93B ->108B -0.11196
94B ->108B 0.15585
95B ->108B -0.15046
97B ->108B 0.38037
98B ->108B 0.50590
106B ->108B -0.13989
107B ->108B 0.69032

Excited State 6: 2.178-A 3.3295 eV 372.38 nm f=0.0055 <S**2>=0.936
108A ->109A -0.23773
84B ->108B -0.20985
85B ->108B -0.23088
87B ->108B -0.30837
88B ->108B 0.24216
89B ->108B -0.24560
91B ->108B 0.12606
92B ->108B -0.19420
93B ->108B 0.12526
98B ->108B -0.16712
102B ->108B 0.11257
105B ->108B 0.64285
107B ->109B -0.19077

Excited State 7: 3.149-A 3.3952 eV 365.17 nm f=0.0227 <S**2>=2.228
106A ->109A -0.13564
108A ->109A 0.67737
84B ->108B -0.11323
85B ->108B -0.10223
105B ->108B 0.22969
107B ->108B 0.10398
107B ->109B 0.58197

Excited State 8: 2.030-A 3.8184 eV 324.70 nm f=0.0267 <S**2>=0.780
84B ->108B 0.10607
85B ->108B 0.14529
87B ->108B 0.10219
92B ->108B 0.18589
93B ->108B 0.63706
95B ->108B 0.21915
96B ->108B -0.18236
97B ->108B 0.28318
102B ->108B 0.14307

105B ->108B 0.10514
106B ->108B -0.50312

Excited State 9: 2.024-A 4.0076 eV 309.37 nm f=0.0344 <S**2>=0.774
93B ->108B -0.12354
99B ->108B 0.19886
101B ->108B -0.14453
102B ->108B 0.93158

Excited State 10: 2.038-A 4.4182 eV 280.62 nm f=0.0225 <S**2>=0.789
97B ->108B 0.12917
99B ->108B 0.90116
101B ->108B -0.21262
102B ->108B -0.19125
107B ->109B -0.12825

Excited State 11: 2.405-A 4.9484 eV 250.55 nm f=0.0019 <S**2>=1.196
101A ->109A -0.11585
105A ->109A -0.27960
84B ->108B 0.10822
85B ->108B 0.10145
87B ->108B 0.10713
100B ->108B 0.73031
100B ->109B 0.16477
101B ->108B 0.16503
104B ->108B -0.17690
105B ->108B 0.29575
105B ->109B 0.25440

Excited State 12: 3.177-A 5.0324 eV 246.37 nm f=0.0009 <S**2>=2.273
101A ->109A 0.18987
104A ->109A -0.10522
105A ->109A 0.62048
106A ->109A -0.22393
107A ->109A -0.20487
100B ->108B 0.37248
100B ->109B -0.11505
105B ->108B 0.19072
105B ->109B -0.42922
106B ->109B -0.11826

Excited State 13: 2.080-A 5.2578 eV 235.81 nm f=0.1888 <S**2>=0.832
108A ->109A -0.60151
105B ->109B -0.18989
107B ->109B 0.71201

Excited State 14: 2.060-A 5.4278 eV 228.43 nm f=0.0013 <S**2>=0.811

105A ->109A	-0.11345
89B ->108B	0.17377
96B ->108B	0.10214
97B ->108B	0.11217
99B ->108B	-0.15030
100B ->108B	0.22808
101B ->108B	-0.56139
103B ->108B	-0.13897
104B ->108B	0.65090
105B ->109B	-0.15951

Excited State 15: 2.062-A 5.4741 eV 226.49 nm f=0.0209 <S**2>=0.813

101A ->109A	0.11759
105A ->109A	0.45929
106A ->109A	-0.15686
107A ->109A	-0.16607
108A ->109A	-0.16931
100B ->109B	0.17901
101B ->108B	-0.19286
104B ->108B	0.11573
105B ->109B	0.68323
106B ->109B	0.20274
107B ->109B	0.18763

Excited State 16: 2.177-A 5.6025 eV 221.30 nm f=0.0013 <S**2>=0.935

102A ->109A	-0.17212
84B ->108B	0.12697
89B ->108B	-0.13515
96B ->108B	-0.10195
99B ->108B	0.10779
101B ->108B	0.56847
101B ->109B	0.12568
102B ->108B	0.11176
104B ->108B	0.68204
104B ->109B	-0.12843

Excited State 17: 2.836-A 5.7532 eV 215.51 nm f=0.0088 <S**2>=1.760

99A ->109A	-0.12069
102A ->109A	0.42020
108A ->109A	-0.10786
84B ->108B	-0.14852
89B ->108B	0.30690
95B ->108B	-0.26658
96B ->109B	0.10474
97B ->108B	0.17082

98B ->108B -0.11527
100B ->109B 0.11475
101B ->108B 0.32058
101B ->109B -0.41073
103B ->108B 0.27806
104B ->108B 0.10419

Excited State 18: 2.804-A 5.8098 eV 213.41 nm f=0.0007 <S**2>=1.716
108A ->110A 0.86619
108A ->111A 0.22519
107B ->110B 0.25593

Excited State 19: 2.683-A 5.8589 eV 211.62 nm f=0.0049 <S**2>=1.549
99A ->109A -0.11705
102A ->109A 0.41148
108A ->110A -0.21879
84B ->108B 0.16244
87B ->108B -0.10089
89B ->108B -0.34596
94B ->108B 0.14137
95B ->108B 0.39555
96B ->108B -0.10639
96B ->109B 0.10549
97B ->108B -0.19391
98B ->108B 0.12917
101B ->109B -0.35083
103B ->108B -0.24703

Excited State 20: 2.603-A 5.9585 eV 208.08 nm f=0.0042 <S**2>=1.444
108A ->110A -0.23905
95B ->108B -0.14332
107B ->110B 0.89320
107B ->111B 0.14205
107B ->116B 0.10878

Excited State 21: 2.053-A 5.9806 eV 207.31 nm f=0.0015 <S**2>=0.804
89B ->108B 0.17675
92B ->108B -0.30283
93B ->108B -0.25760
95B ->108B 0.64289
96B ->108B -0.13058
97B ->108B 0.23539
103B ->108B 0.50998
107B ->110B 0.10109

Excited State 22: 2.031-A 6.0108 eV 206.27 nm f=0.0011 <S**2>=0.781

92B ->108B 0.11021
94B ->108B 0.84634
96B ->108B 0.27510
97B ->108B -0.26364
103B ->108B 0.27609

Excited State 23: 2.053-A 6.1428 eV 201.84 nm f=0.0035 <S**2>=0.804
84B ->108B 0.15275
86B ->108B -0.12447
89B ->108B -0.38280
93B ->108B 0.11055
94B ->108B -0.30146
95B ->108B -0.19654
97B ->108B -0.13731
98B ->108B 0.14369
100B ->108B 0.15668
101B ->108B -0.25469
103B ->108B 0.67072

Excited State 24: 3.321-A 6.2671 eV 197.83 nm f=0.0002 <S**2>=2.508
101A ->109A 0.58254
104A ->109A -0.10362
105A ->109A -0.13057
107A ->109A 0.33535
90B ->108B -0.20220
92B ->108B 0.14634
100B ->109B -0.42891
106B ->109B 0.28877
106B ->110B 0.10409

Excited State 25: 2.120-A 6.3116 eV 196.44 nm f=0.0016 <S**2>=0.873
101A ->109A 0.15993
84B ->108B -0.20315
87B ->108B 0.12583
89B ->108B -0.14957
90B ->108B 0.91070

Excited State 26: 2.718-A 6.4661 eV 191.74 nm f=0.0005 <S**2>=1.597
101A ->109A -0.40535
107A ->109A -0.21506
107A ->110A 0.16282
93B ->110B 0.10707
100B ->109B -0.27624
106B ->109B 0.38022
106B ->110B 0.58913
106B ->116B 0.10563

106B ->118B -0.11880

Excited State 27: 2.536-A 6.5126 eV 190.38 nm f=0.0002 <S**2>=1.358
101A ->109A -0.24654
107A ->109A -0.20046
107A ->110A -0.23038
86B ->108B 0.11592
88B ->108B 0.45810
90B ->108B 0.11320
91B ->108B -0.11416
92B ->108B 0.26567
93B ->108B -0.12397
97B ->108B -0.12077
100B ->109B -0.32779
106B ->109B 0.12119
106B ->110B -0.43733

Excited State 28: 2.272-A 6.5843 eV 188.30 nm f=0.0022 <S**2>=1.041
101A ->109A 0.13184
107A ->109A 0.11613
107A ->110A 0.13733
84B ->108B 0.14894
85B ->108B 0.11035
88B ->108B 0.73420
89B ->108B 0.14926
92B ->108B 0.10184
94B ->108B -0.10560
100B ->109B 0.32059
106B ->109B -0.20110
106B ->110B 0.28566

Excited State 29: 2.049-A 6.6238 eV 187.18 nm f=0.0044 <S**2>=0.799
87B ->108B 0.81722
88B ->108B 0.18603
89B ->108B -0.30498
90B ->108B -0.21466
92B ->108B -0.27711
106B ->109B 0.11371

Excited State 30: 2.147-A 6.7074 eV 184.85 nm f=0.0044 <S**2>=0.902
75B ->108B 0.11577
84B ->108B -0.27136
85B ->108B -0.23418
86B ->108B 0.61131
88B ->108B -0.18586
89B ->108B -0.17383

91B ->108B -0.12183
92B ->108B 0.40670
95B ->108B 0.12554
96B ->108B -0.16017
97B ->108B -0.12184
100B ->109B 0.17723
106B ->109B -0.21458
106B ->110B 0.12368

[Cu(II)LDHA]$^{2+}$

Excitation energies and oscillator strengths:

Excited State 1: 2.002-A 0.5597 eV 2215.33 nm f=0.0015 <S**2>=0.752
92B ->108B -0.26035
98B ->108B -0.13993
99B ->108B -0.11025
106B ->108B 0.92616
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2842.53931966
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.368-A 1.1111 eV 1115.84 nm f=0.0034 <S**2>=2.586
103A ->108A -0.19299
107A ->108A -0.44243
103B ->107B 0.24310
106B ->107B 0.82809

Excited State 3: 2.287-A 1.3852 eV 895.07 nm f=0.0230 <S**2>=1.057
103A ->108A 0.33220
106A ->108A 0.12891
107A ->108A 0.75751
106B ->107B 0.52889

Excited State 4: 3.352-A 1.5672 eV 791.14 nm f=0.0008 <S**2>=2.558
103A ->108A -0.45015
106A ->108A -0.21490
107A ->108A 0.43126
102B ->107B -0.14321
103B ->107B 0.62441
105B ->107B 0.32559
106B ->107B -0.12791

Excited State 5: 2.037-A 1.8327 eV 676.51 nm f=0.0027 <S**2>=0.787
103A ->108A 0.37732
105A ->108A 0.27851
106A ->108A 0.60425

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  107A ->108A       -0.15326
  103B ->107B        0.31578
  105B ->107B        0.51579

Excited State   6:  2.279-A      1.8709 eV  662.69 nm  f=0.0002  <S**2>=1.048
  104A ->108A        0.15345
  105A ->108A        0.89277
  106A ->108A       -0.37833

Excited State   7:  3.397-A      1.9342 eV  641.00 nm  f=0.0000  <S**2>=2.636
  103A ->108A        0.28852
  105A ->108A       -0.23089
  106A ->108A       -0.52227
  103B ->107B       -0.29381
  105B ->107B        0.69557

Excited State   8:  2.007-A      2.0041 eV  618.66 nm  f=0.0019  <S**2>=0.757
  105A ->108A       -0.10051
   94B ->108B        0.75836
   96B ->108B        0.49414
   97B ->108B        0.18807
   98B ->108B        0.10786
  100B ->108B        0.12272
  103B ->108B       -0.19454

Excited State   9:  2.018-A      2.0359 eV  608.99 nm  f=0.0029  <S**2>=0.768
  103A ->108A        0.59737
  106A ->108A       -0.36400
  107A ->108A       -0.10711
   93B ->108B        0.20261
   95B ->108B        0.10137
  103B ->107B        0.51912
  105B ->107B       -0.34596

Excited State  10:  2.009-A      2.0572 eV  602.68 nm  f=0.0006  <S**2>=0.760
  103A ->108A       -0.17419
  105A ->108A        0.12579
   86B ->108B        0.17668
   91B ->108B        0.32020
   93B ->108B        0.70026
   94B ->108B        0.23518
   95B ->108B        0.33388
   98B ->108B       -0.14518
  101B ->108B        0.11816
  103B ->107B       -0.13727
  103B ->108B        0.20283
```

Excited State 11: 3.436-A 2.1330 eV 581.26 nm f=0.0000 <S**2>=2.701
104A ->108A 0.78852
104B ->107B -0.59710

Excited State 12: 2.043-A 2.1467 eV 577.54 nm f=0.0012 <S**2>=0.794
104A ->108A 0.59029
104B ->107B 0.79456

Excited State 13: 2.004-A 2.1817 eV 568.29 nm f=0.0000 <S**2>=0.754
86B ->108B 0.76948
87B ->108B -0.13192
88B ->108B 0.13500
90B ->108B -0.19393
91B ->108B -0.18173
92B ->108B 0.32939
93B ->108B -0.21956
94B ->108B 0.10933
98B ->108B -0.12560
99B ->108B -0.14086
103B ->108B 0.18404

Excited State 14: 2.007-A 2.6183 eV 473.54 nm f=0.0031 <S**2>=0.757
86B ->108B -0.13959
103B ->108B 0.16329
105B ->108B 0.96461

Excited State 15: 2.007-A 2.7718 eV 447.30 nm f=0.0008 <S**2>=0.757
103B ->108B -0.10079
104B ->108B 0.98999

Excited State 16: 2.008-A 2.8090 eV 441.38 nm f=0.0326 <S**2>=0.758
86B ->108B -0.13602
92B ->108B 0.18520
96B ->108B 0.10894
98B ->108B 0.16372
99B ->108B 0.13467
102B ->108B 0.57320
103B ->108B 0.66390
104B ->108B 0.13334
105B ->108B -0.20518
106B ->108B 0.17683

Excited State 17: 3.462-A 2.8309 eV 437.96 nm f=0.0000 <S**2>=2.746
99A ->108A 0.17485
100A ->108A -0.16211

101A ->108A -0.58157
102A ->108A -0.29392
98B ->107B -0.17293
99B ->107B 0.13307
100B ->107B -0.17059
101B ->107B 0.61321
102B ->107B 0.13629

Excited State 18: 2.987-A 2.9635 eV 418.37 nm f=0.0019 <S**2>=1.980
101A ->108A 0.13363
99B ->107B -0.10329
102B ->107B 0.93128
103B ->107B 0.17290

Excited State 19: 2.008-A 2.9890 eV 414.81 nm f=0.0058 <S**2>=0.758
86B ->108B -0.11706
88B ->108B -0.12730
90B ->108B 0.12839
92B ->108B -0.41060
93B ->108B -0.25589
94B ->108B 0.16716
97B ->108B 0.10047
98B ->108B -0.21218
99B ->108B -0.18401
102B ->108B -0.40959
103B ->108B 0.57687
105B ->108B -0.10341
106B ->108B -0.25992

Excited State 20: 3.112-A 3.1553 eV 392.93 nm f=0.0006 <S**2>=2.170
96A ->108A 0.24893
99A ->108A 0.14164
100A ->108A 0.15214
101A ->108A 0.15721
102A ->108A -0.21934
103A ->109A -0.10144
92B ->107B 0.11799
94B ->107B 0.11729
95B ->107B 0.15243
98B ->107B -0.15593
99B ->107B -0.18869
100B ->107B 0.71527
101B ->107B 0.26521
102B ->107B -0.20884
103B ->109B 0.10297

Excited State 21: 2.546-A 3.2481 eV 381.71 nm f=0.0062 <S**2>=1.371
96A ->108A -0.25196
99A ->108A -0.15075
100A ->108A -0.10580
102A ->108A 0.73316
100B ->107B 0.29140
101B ->107B 0.46509

Excited State 22: 2.193-A 3.3148 eV 374.04 nm f=0.0133 <S**2>=0.952
101A ->108A 0.68528
98B ->107B -0.10411
100B ->107B -0.48485
101B ->107B 0.48305

Excited State 23: 2.067-A 3.3862 eV 366.14 nm f=0.0425 <S**2>=0.819
102A ->108A 0.10016
86B ->108B 0.18206
88B ->108B -0.10361
92B ->108B -0.45214
93B ->108B -0.13204
94B ->108B 0.11081
98B ->108B -0.23891
99B ->108B -0.19161
102B ->108B 0.66541
103B ->108B -0.22591
106B ->108B -0.19750

Excited State 24: 3.184-A 3.4087 eV 363.73 nm f=0.0021 <S**2>=2.285
96A ->108A 0.32802
98A ->108A -0.10124
99A ->108A 0.20270
100A ->108A 0.18372
101A ->108A -0.26159
102A ->108A 0.51195
92B ->107B 0.12170
92B ->108B 0.10054
95B ->107B 0.23708
96B ->107B -0.14649
98B ->107B -0.29338
99B ->107B -0.30097
100B ->107B -0.26857
101B ->107B -0.10931
102B ->108B -0.12894

Excited State 25: 2.104-A 3.6182 eV 342.66 nm f=0.0372 <S**2>=0.857
96A ->108A 0.39287

98A ->108A -0.14669
99A ->108A 0.28014
100A ->108A 0.26564
93B ->107B 0.15465
95B ->107B -0.21881
96B ->107B 0.14679
98B ->107B 0.36288
99B ->107B 0.36051
100B ->108B 0.45978
101B ->108B 0.17389

Excited State 26: 2.188-A 3.6970 eV 335.37 nm f=0.0757 <S**2>=0.947
96A ->108A -0.24779
99A ->108A -0.13078
100A ->108A -0.13705
102A ->108A -0.11537
92B ->107B 0.12285
93B ->107B 0.16375
94B ->107B -0.21866
94B ->108B -0.10012
95B ->107B 0.20383
96B ->107B -0.27868
97B ->107B -0.18872
98B ->107B -0.18952
99B ->107B -0.11043
100B ->108B 0.65566
101B ->108B 0.26455

Excited State 27: 3.324-A 3.7769 eV 328.27 nm f=0.0027 <S**2>=2.512
80A ->108A 0.10997
81A ->108A 0.10746
93A ->108A 0.10903
94A ->108A 0.12720
97A ->108A -0.11061
99A ->108A 0.40128
100A ->108A -0.25605
101A ->108A 0.18254
102A ->108A 0.11492
79B ->107B -0.12979
93B ->107B -0.14631
94B ->107B -0.38635
95B ->107B -0.25139
96B ->107B -0.16253
97B ->107B -0.24010
98B ->107B -0.26245
99B ->107B 0.27468

100B ->107B 0.12751
100B ->108B -0.14382
101B ->107B -0.13394

Excited State 28: 3.176-A 3.8655 eV 320.75 nm f=0.0017 <S**2>=2.271
94A ->108A -0.14296
96A ->108A -0.11398
98A ->108A 0.10095
99A ->108A 0.26110
100A ->108A -0.29830
101A ->108A 0.14016
92B ->107B 0.15497
94B ->107B 0.56255
96B ->107B 0.42863
98B ->107B -0.30601
99B ->107B 0.17621
100B ->108B 0.14142
101B ->107B -0.20240

Excited State 29: 2.798-A 3.9954 eV 310.32 nm f=0.0001 <S**2>=1.707
77A ->108A -0.18942
87A ->108A 0.37395
88A ->108A -0.22838
94A ->108A 0.60675
95A ->108A 0.12545
96A ->108A 0.21166
100A ->108A -0.12078
82B ->107B 0.15769
85B ->107B 0.12731
94B ->107B 0.19486
96B ->107B 0.19401
97B ->107B 0.15967
101B ->108B 0.18285

Excited State 30: 3.112-A 4.0116 eV 309.06 nm f=0.0007 <S**2>=2.171
90A ->108A -0.14197
96A ->108A 0.17821
97A ->108A 0.13295
100A ->108A -0.15487
91B ->107B 0.24084
92B ->107B -0.21052
93B ->107B 0.54017
95B ->107B 0.39105
96B ->107B -0.16902
97B ->107B -0.17671
99B ->107B 0.26572

101B ->108B -0.32513

[Cu(I)LNO$_2$], conformer 1

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1993 eV 387.54 nm f=0.0016 <S**2>=0.000
69 -> 75 0.23265
71 -> 75 -0.12148
72 -> 75 -0.32726
73 -> 75 0.56224
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2364.69119569
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5133 eV 352.90 nm f=0.0008 <S**2>=0.000
69 -> 75 -0.15758
72 -> 75 0.54258
73 -> 75 0.39703
74 -> 75 -0.11137

Excited State 3: Singlet-A 3.5512 eV 349.13 nm f=0.0525 <S**2>=0.000
74 -> 75 0.68299

Excited State 4: Singlet-A 3.7381 eV 331.68 nm f=0.0007 <S**2>=0.000
69 -> 75 0.49371
70 -> 75 0.20120
71 -> 75 -0.32235
72 -> 75 0.29009
73 -> 75 -0.12746

Excited State 5: Singlet-A 4.1250 eV 300.56 nm f=0.0003 <S**2>=0.000
74 -> 76 0.68731

Excited State 6: Singlet-A 4.1574 eV 298.23 nm f=0.0011 <S**2>=0.000
70 -> 75 -0.35094
71 -> 75 -0.22446
73 -> 76 0.55220

Excited State 7: Singlet-A 4.1959 eV 295.49 nm f=0.0049 <S**2>=0.000
70 -> 75 0.48516
71 -> 75 0.28640
72 -> 76 0.13022
73 -> 76 0.39179

Excited State 8: Singlet-A 4.2265 eV 293.35 nm f=0.0011 <S**2>=0.000
69 -> 75 0.41428

70 -> 75 -0.29839
71 -> 75 0.48449

Excited State 9: Singlet-A 4.6550 eV 266.35 nm f=0.0010 <S**2>=0.000
72 -> 76 0.66127
73 -> 76 -0.11732

Excited State 10: Singlet-A 4.9139 eV 252.32 nm f=0.0002 <S**2>=0.000
70 -> 76 0.55629
71 -> 76 0.39848

Excited State 11: Singlet-A 4.9618 eV 249.88 nm f=0.0001 <S**2>=0.000
69 -> 76 0.19134
70 -> 76 -0.38290
71 -> 76 0.52389

Excited State 12: Singlet-A 5.1881 eV 238.98 nm f=0.0001 <S**2>=0.000
73 -> 77 0.14613
74 -> 77 0.61544
74 -> 78 0.28030
74 -> 79 -0.10639

Excited State 13: Singlet-A 5.2119 eV 237.89 nm f=0.0005 <S**2>=0.000
73 -> 77 -0.24785
73 -> 78 -0.17086
74 -> 77 -0.22152
74 -> 78 0.58400

Excited State 14: Singlet-A 5.2249 eV 237.30 nm f=0.0012 <S**2>=0.000
73 -> 77 -0.45913
73 -> 78 0.50874
74 -> 77 0.13134

Excited State 15: Singlet-A 5.2649 eV 235.49 nm f=0.0001 <S**2>=0.000
73 -> 77 0.41204
73 -> 78 0.43455
73 -> 79 -0.14042
74 -> 77 -0.19086
74 -> 78 0.24634

Excited State 16: Singlet-A 5.3532 eV 231.61 nm f=0.0051 <S**2>=0.000
74 -> 79 0.68417

Excited State 17: Singlet-A 5.3783 eV 230.53 nm f=0.0051 <S**2>=0.000
73 -> 77 0.14745
73 -> 79 0.67092

Excited State 18: Singlet-A 5.4531 eV 227.37 nm f=0.0002 <S**2>=0.000
64 -> 75 -0.44398
67 -> 75 0.51393
72 -> 78 0.12293

Excited State 19: Singlet-A 5.5571 eV 223.11 nm f=0.0056 <S**2>=0.000
67 -> 75 0.11909
72 -> 77 0.47896
72 -> 78 -0.47871

Excited State 20: Singlet-A 5.5610 eV 222.95 nm f=0.0079 <S**2>=0.000
72 -> 77 0.48779
72 -> 78 0.48374
72 -> 79 -0.10527

Excited State 21: Singlet-A 5.6605 eV 219.04 nm f=0.0113 <S**2>=0.000
69 -> 76 0.65285
70 -> 76 0.10947
71 -> 76 -0.17182

Excited State 22: Singlet-A 5.7472 eV 215.73 nm f=0.0019 <S**2>=0.000
72 -> 79 0.68179

Excited State 23: Singlet-A 5.7685 eV 214.93 nm f=0.0032 <S**2>=0.000
74 -> 80 0.67167
74 -> 83 -0.12355

Excited State 24: Singlet-A 5.7949 eV 213.95 nm f=0.0035 <S**2>=0.000
73 -> 80 0.66712
73 -> 83 -0.11385

Excited State 25: Singlet-A 6.0370 eV 205.37 nm f=0.0002 <S**2>=0.000
70 -> 77 0.49881
71 -> 77 0.27154
71 -> 78 0.37435

Excited State 26: Singlet-A 6.0581 eV 204.66 nm f=0.0046 <S**2>=0.000
69 -> 77 0.12047
70 -> 77 -0.18640
70 -> 78 -0.29000
71 -> 77 0.56644
71 -> 78 -0.13420

Excited State 27: Singlet-A 6.0663 eV 204.38 nm f=0.0054 <S**2>=0.000
70 -> 77 -0.41493

70 -> 78 0.33738
71 -> 77 0.11453
71 -> 78 0.41998

Excited State 28: Singlet-A 6.0881 eV 203.65 nm f=0.0131 <S**2>=0.000
69 -> 78 -0.13622
70 -> 77 0.10932
70 -> 78 0.51986
71 -> 77 0.22619
71 -> 78 -0.36015

Excited State 29: Singlet-A 6.2033 eV 199.87 nm f=0.0151 <S**2>=0.000
68 -> 75 -0.29101
72 -> 80 0.61017

Excited State 30: Singlet-A 6.2435 eV 198.58 nm f=0.0009 <S**2>=0.000
70 -> 79 0.47286
71 -> 79 0.47647

[Cu(I)LNO$_2$], conformer 2

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.1646 eV 391.78 nm f=0.0062 <S**2>=0.000
72 -> 75 0.27007
74 -> 75 0.64354
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2364.69537862
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6469 eV 339.97 nm f=0.0020 <S**2>=0.000
72 -> 75 0.20475
73 -> 75 0.65662

Excited State 3: Singlet-A 4.1290 eV 300.27 nm f=0.0492 <S**2>=0.000
68 -> 75 -0.11005
70 -> 75 -0.13610
71 -> 75 0.29469
72 -> 75 0.51216
73 -> 75 -0.23466
74 -> 75 -0.20847

Excited State 4: Singlet-A 4.3320 eV 286.20 nm f=0.0241 <S**2>=0.000
68 -> 75 -0.14654
69 -> 75 -0.33007
70 -> 75 0.11742
71 -> 75 0.49375

72 -> 75 -0.27476
74 -> 75 0.14364

Excited State 5: Singlet-A 4.5279 eV 273.82 nm f=0.0138 <S**2>=0.000
69 -> 75 0.18203
70 -> 75 0.65373
72 -> 75 0.10648
74 -> 76 0.11431

Excited State 6: Singlet-A 4.6104 eV 268.92 nm f=0.0062 <S**2>=0.000
69 -> 75 -0.32641
71 -> 75 -0.17468
72 -> 76 -0.10259
74 -> 76 0.57895

Excited State 7: Singlet-A 4.7044 eV 263.55 nm f=0.0113 <S**2>=0.000
68 -> 75 0.29716
69 -> 75 0.37402
70 -> 75 -0.15102
71 -> 75 0.33445
73 -> 76 -0.16723
74 -> 76 0.27438

Excited State 8: Singlet-A 4.7773 eV 259.53 nm f=0.0033 <S**2>=0.000
68 -> 75 0.55013
69 -> 75 -0.23197
72 -> 76 0.13828
73 -> 76 0.29971

Excited State 9: Singlet-A 4.7870 eV 259.00 nm f=0.0038 <S**2>=0.000
68 -> 75 -0.19519
69 -> 75 0.15659
72 -> 76 -0.14395
73 -> 76 0.59322
74 -> 76 0.15636

Excited State 10: Singlet-A 5.1018 eV 243.02 nm f=0.0025 <S**2>=0.000
68 -> 75 -0.13319
72 -> 76 0.64693
74 -> 76 0.17027

Excited State 11: Singlet-A 5.4568 eV 227.21 nm f=0.0084 <S**2>=0.000
74 -> 77 0.55450
74 -> 78 -0.41375

Excited State 12: Singlet-A 5.5009 eV 225.39 nm f=0.0041 <S**2>=0.000

74 -> 77 0.39693
74 -> 78 0.54020
74 -> 79 -0.18908

Excited State 13: Singlet-A 5.6169 eV 220.74 nm f=0.0034 <S**2>=0.000
70 -> 76 0.10762
74 -> 77 0.12799
74 -> 78 0.12952
74 -> 79 0.66151

Excited State 14: Singlet-A 5.6307 eV 220.19 nm f=0.0035 <S**2>=0.000
71 -> 76 0.66070

Excited State 15: Singlet-A 5.6384 eV 219.89 nm f=0.0008 <S**2>=0.000
70 -> 76 0.67034
74 -> 79 -0.10077

Excited State 16: Singlet-A 5.7111 eV 217.09 nm f=0.0007 <S**2>=0.000
73 -> 77 0.68460

Excited State 17: Singlet-A 5.7312 eV 216.33 nm f=0.0007 <S**2>=0.000
73 -> 78 0.68958

Excited State 18: Singlet-A 5.8474 eV 212.03 nm f=0.0032 <S**2>=0.000
73 -> 79 0.69480

Excited State 19: Singlet-A 5.9972 eV 206.74 nm f=0.0020 <S**2>=0.000
72 -> 77 0.51152
72 -> 78 -0.46517

Excited State 20: Singlet-A 6.0351 eV 205.44 nm f=0.0069 <S**2>=0.000
72 -> 77 0.45360
72 -> 78 0.49311
72 -> 79 -0.15057

Excited State 21: Singlet-A 6.1020 eV 203.19 nm f=0.0027 <S**2>=0.000
72 -> 80 -0.12364
74 -> 80 0.66677

Excited State 22: Singlet-A 6.1805 eV 200.61 nm f=0.0032 <S**2>=0.000
72 -> 78 0.10503
72 -> 79 0.67475

Excited State 23: Singlet-A 6.2919 eV 197.05 nm f=0.0055 <S**2>=0.000
66 -> 75 0.16062
73 -> 80 0.63876

73 -> 83 -0.13932

Excited State 24: Singlet-A 6.3176 eV 196.25 nm f=0.0008 <S**2>=0.000
65 -> 75 -0.34599
66 -> 75 0.57739
73 -> 80 -0.16296

Excited State 25: Singlet-A 6.3624 eV 194.87 nm f=0.0024 <S**2>=0.000
64 -> 75 0.12287
65 -> 75 -0.31653
66 -> 75 -0.19044
68 -> 76 -0.19064
69 -> 76 0.51068
74 -> 83 0.10650

Excited State 26: Singlet-A 6.4076 eV 193.49 nm f=0.0051 <S**2>=0.000
65 -> 75 0.21946
66 -> 75 0.12700
67 -> 75 0.10550
68 -> 76 0.47316
69 -> 76 0.38560

Excited State 27: Singlet-A 6.5486 eV 189.33 nm f=0.0039 <S**2>=0.000
65 -> 75 0.27688
66 -> 75 0.14761
68 -> 76 -0.17719
72 -> 80 0.36338
74 -> 81 -0.10310
74 -> 83 0.37780
74 -> 86 -0.13954

Excited State 28: Singlet-A 6.5768 eV 188.52 nm f=0.0062 <S**2>=0.000
64 -> 75 0.18915
65 -> 75 0.32550
66 -> 75 0.20703
68 -> 76 -0.30985
69 -> 76 0.15515
74 -> 80 -0.13164
74 -> 81 0.13733
74 -> 83 -0.29676

Excited State 29: Singlet-A 6.6337 eV 186.90 nm f=0.0017 <S**2>=0.000
70 -> 77 -0.39033
70 -> 78 0.45541
71 -> 77 -0.18788
72 -> 80 -0.14142

74 -> 81 -0.22176

Excited State 30: Singlet-A 6.6423 eV 186.66 nm f=0.0069 <S**2>=0.000
70 -> 77 -0.26363
70 -> 78 0.20074
71 -> 77 0.10256
71 -> 78 -0.19819
72 -> 80 0.31283
74 -> 81 0.44188

[Cu(II)LNO$_2$]$^+$, conformer 1

Excitation energies and oscillator strengths:

Excited State 1: 2.006-A 0.8305 eV 1492.95 nm f=0.0043 <S**2>=0.756
63B -> 74B 0.10818
65B -> 74B 0.16504
66B -> 74B 0.29718
72B -> 74B 0.92075
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2364.61652613
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.023-A 1.4810 eV 837.18 nm f=0.0201 <S**2>=0.773
63B -> 74B 0.16677
70B -> 74B 0.12939
73B -> 74B 0.95382

Excited State 3: 2.008-A 1.8697 eV 663.13 nm f=0.0004 <S**2>=0.758
61B -> 74B 0.36960
62B -> 74B 0.46409
64B -> 74B -0.12912
65B -> 74B 0.17443
70B -> 74B 0.63012
71B -> 74B -0.35827
73B -> 74B -0.19353

Excited State 4: 2.002-A 2.1153 eV 586.12 nm f=0.0010 <S**2>=0.752
63B -> 74B -0.10128
68B -> 74B 0.97638

Excited State 5: 2.121-A 2.2108 eV 560.81 nm f=0.0001 <S**2>=0.875
74A -> 75A 0.17024
61B -> 74B 0.11653
62B -> 74B -0.12560
63B -> 74B 0.70788
65B -> 74B -0.48406

67B -> 74B 0.14654
70B -> 74B -0.10493
71B -> 74B -0.26504
73B -> 74B -0.17468
73B -> 75B -0.18008

Excited State 6: 3.355-A 2.3028 eV 538.40 nm f=0.0005 <S**2>=2.564
73A -> 75A -0.10914
74A -> 75A 0.68655
63B -> 74B -0.17704
65B -> 74B 0.11430
73B -> 74B 0.11602
73B -> 75B -0.67660

Excited State 7: 2.010-A 3.1980 eV 387.70 nm f=0.1072 <S**2>=0.760
63B -> 74B 0.20225
65B -> 74B -0.13695
69B -> 74B -0.26741
70B -> 74B 0.39350
71B -> 74B 0.82522

Excited State 8: 2.018-A 3.4153 eV 363.02 nm f=0.0306 <S**2>=0.768
74A -> 75A -0.10562
63B -> 74B 0.15013
64B -> 74B -0.19426
65B -> 74B 0.39017
66B -> 74B 0.55234
69B -> 74B -0.51151
70B -> 74B -0.25821
72B -> 74B -0.29957
73B -> 75B -0.10276

Excited State 9: 2.009-A 3.4322 eV 361.24 nm f=0.0203 <S**2>=0.759
74A -> 75A 0.52205
63B -> 74B 0.17997
65B -> 74B 0.15810
66B -> 74B 0.34145
69B -> 74B 0.44270
72B -> 74B -0.18080
73B -> 75B 0.53012

Excited State 10: 2.012-A 3.4440 eV 360.00 nm f=0.0346 <S**2>=0.762
74A -> 75A -0.43672
62B -> 74B -0.14520
63B -> 74B 0.16216
66B -> 74B 0.29399

69B -> 74B 0.59599
70B -> 74B 0.20591
71B -> 74B 0.11251
72B -> 74B -0.14732
73B -> 75B -0.45822

Excited State 11: 2.021-A 3.7173 eV 333.54 nm f=0.0084 <S**2>=0.771
59B -> 74B 0.12134
61B -> 74B -0.42839
62B -> 74B -0.52755
63B -> 74B -0.10126
66B -> 74B 0.15427
69B -> 74B -0.27176
70B -> 74B 0.54631
71B -> 74B -0.26661

Excited State 12: 3.414-A 4.0223 eV 308.24 nm f=0.0004 <S**2>=2.663
70A -> 75A 0.38303
71A -> 75A -0.50555
72A -> 75A 0.14408
73A -> 75A 0.24152
62B -> 75B -0.10550
70B -> 75B 0.64929
72B -> 75B -0.23108
70B <- 75B 0.10307

Excited State 13: 2.017-A 4.4456 eV 278.89 nm f=0.0025 <S**2>=0.767
63B -> 74B -0.11738
67B -> 74B 0.95299
69B -> 74B 0.13865

Excited State 14: 2.740-A 4.5447 eV 272.81 nm f=0.0007 <S**2>=1.627
69A -> 75A -0.20900
70A -> 75A 0.29209
71A -> 75A 0.37460
72A -> 75A -0.13991
73A -> 75A 0.74606
74A -> 75A 0.12644
67B -> 75B -0.12192
71B -> 75B 0.29000

Excited State 15: 2.800-A 4.8453 eV 255.88 nm f=0.0052 <S**2>=1.710
71A -> 75A -0.12590
70B -> 75B 0.16518
72B -> 75B 0.96359

Excited State 16: 2.014-A 4.9060 eV 252.72 nm f=0.0017 <S**2>=0.764
62B -> 74B -0.22273
63B -> 74B 0.43754
64B -> 74B -0.11266
65B -> 74B 0.62489
66B -> 74B -0.58468

Excited State 17: 2.014-A 4.9292 eV 251.53 nm f=0.0022 <S**2>=0.764
64B -> 74B 0.94374
65B -> 74B 0.26955

Excited State 18: 2.886-A 5.1693 eV 239.85 nm f=0.0044 <S**2>=1.833
70A -> 75A -0.10126
71A -> 75A 0.12117
72A -> 75A 0.91823
73A -> 75A 0.22775
70B -> 75B -0.14522
71B -> 75B -0.19623

Excited State 19: 2.811-A 5.1919 eV 238.80 nm f=0.0005 <S**2>=1.725
72A -> 75A 0.30995
73A -> 75A -0.34413
67B -> 75B -0.29750
70B -> 75B 0.11058
71B -> 75B 0.80309

Excited State 20: 2.015-A 5.2282 eV 237.14 nm f=0.0004 <S**2>=0.765
61B -> 74B 0.77654
62B -> 74B -0.57176
63B -> 74B -0.22023

Excited State 21: 2.062-A 5.5180 eV 224.69 nm f=0.0007 <S**2>=0.813
74A -> 76A 0.16820
60B -> 74B 0.96351

Excited State 22: 3.149-A 5.5528 eV 223.28 nm f=0.0018 <S**2>=2.228
74A -> 76A 0.85608
60B -> 74B -0.18275
73B -> 76B -0.42846

Excited State 23: 2.027-A 5.5655 eV 222.77 nm f=0.0080 <S**2>=0.777
58B -> 74B -0.18950
59B -> 74B 0.95012
62B -> 74B 0.18946

Excited State 24: 2.019-A 5.6146 eV 220.82 nm f=0.0120 <S**2>=0.769

58B -> 74B 0.96471
59B -> 74B 0.18926
60B -> 74B 0.11878

Excited State 25: 2.024-A 5.7340 eV 216.22 nm f=0.0007 <S**2>=0.774
57B -> 74B 0.98032
73B -> 76B 0.10694

Excited State 26: 2.339-A 5.7504 eV 215.61 nm f=0.0033 <S**2>=1.117
71A -> 75A -0.17074
73A -> 76A 0.25636
74A -> 76A 0.38079
57B -> 74B -0.11758
70B -> 75B -0.11829
73B -> 76B 0.82483

Excited State 27: 2.385-A 5.8073 eV 213.50 nm f=0.0026 <S**2>=1.172
69A -> 75A -0.30126
70A -> 75A 0.65782
71A -> 75A 0.39002
73A -> 75A -0.41775
73A -> 76A 0.14131
71B -> 75B -0.27359
73B -> 76B 0.13733

Excited State 28: 3.257-A 5.8897 eV 210.51 nm f=0.0010 <S**2>=2.402
72A -> 76A -0.34311
72B -> 76B 0.90286

Excited State 29: 2.212-A 6.0797 eV 203.93 nm f=0.0018 <S**2>=0.974
73A -> 76A 0.92715
74A -> 76A -0.18105
72B -> 76B 0.10317
73B -> 76B -0.21400

Excited State 30: 2.300-A 6.1670 eV 201.04 nm f=0.0006 <S**2>=1.073
72A -> 76A 0.91137
72B -> 76B 0.35251

[Cu(II)LNO$_2$]$^+$, conformer 2

Excitation energies and oscillator strengths:

Excited State 1: 2.003-A 1.0746 eV 1153.79 nm f=0.0015 <S**2>=0.753
63B -> 74B -0.10886
64B -> 74B -0.10847
65B -> 74B -0.22487

66B -> 74B 0.15249
68B -> 74B 0.13461
70B -> 74B -0.13571
73B -> 74B 0.91857
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2364.61051790
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.003-A 2.2054 eV 562.20 nm f=0.0105 <S**2>=0.753
62B -> 74B 0.24370
63B -> 74B 0.21046
64B -> 74B 0.12542
65B -> 74B 0.17531
66B -> 74B 0.16641
67B -> 74B -0.34274
68B -> 74B 0.51570
69B -> 74B 0.32554
70B -> 74B -0.21913
71B -> 74B -0.25044
72B -> 74B -0.46034

Excited State 3: 2.003-A 2.2835 eV 542.95 nm f=0.0131 <S**2>=0.753
64B -> 74B 0.12381
65B -> 74B 0.22808
66B -> 74B 0.38096
67B -> 74B 0.58627
69B -> 74B 0.44489
70B -> 74B -0.23669
71B -> 74B -0.24421
72B -> 74B 0.32959

Excited State 4: 2.004-A 2.4194 eV 512.46 nm f=0.0023 <S**2>=0.754
62B -> 74B 0.66791
63B -> 74B 0.19674
66B -> 74B -0.41409
67B -> 74B 0.33659
69B -> 74B -0.36907
71B -> 74B -0.22964

Excited State 5: 2.826-A 2.6224 eV 472.78 nm f=0.0003 <S**2>=1.747
72A -> 75A -0.39253
73A -> 75A 0.17280
74A -> 75A 0.80168
72B -> 75B -0.38474

Excited State 6: 2.006-A 2.8814 eV 430.29 nm f=0.1054 <S**2>=0.756

62B -> 74B 0.13142
67B -> 74B -0.43798
68B -> 74B 0.32136
72B -> 74B 0.79758

Excited State 7: 2.013-A 3.4786 eV 356.42 nm f=0.0106 <S**2>=0.763
62B -> 74B -0.12183
63B -> 74B 0.14305
64B -> 74B 0.14375
65B -> 74B 0.30613
66B -> 74B -0.27736
67B -> 74B -0.17386
68B -> 74B -0.21262
69B -> 74B 0.19003
70B -> 74B 0.54054
71B -> 74B -0.49149
73B -> 74B 0.31997

Excited State 8: 2.694-A 3.5967 eV 344.72 nm f=0.0032 <S**2>=1.565
69A -> 75A 0.22795
73A -> 75A 0.23991
74A -> 75A 0.34182
69B -> 74B 0.12072
69B -> 75B 0.19963
70B -> 75B 0.16836
71B -> 74B 0.15923
71B -> 75B 0.14339
72B -> 75B 0.68966
73B -> 75B -0.36487

Excited State 9: 2.408-A 3.6327 eV 341.30 nm f=0.0345 <S**2>=1.199
69A -> 75A 0.23994
70A -> 75A -0.22923
73A -> 75A 0.14102
74A -> 75A -0.19536
62B -> 74B 0.24553
63B -> 74B 0.19021
64B -> 74B 0.16279
65B -> 74B 0.19662
69B -> 74B 0.24606
69B -> 75B 0.17109
70B -> 74B 0.24747
71B -> 74B 0.57829
72B -> 75B -0.32771
73B -> 74B 0.12355

Excited State 10: 3.085-A 3.7479 eV 330.81 nm f=0.0139 <S**2>=2.129

69A -> 75A	0.33255
70A -> 75A	-0.28602
73A -> 75A	0.22587
74A -> 75A	-0.13563
62B -> 74B	-0.12301
63B -> 74B	-0.10196
65B -> 75B	-0.13958
66B -> 74B	0.12477
66B -> 75B	-0.15438
68B -> 75B	-0.10478
69B -> 74B	-0.21420
69B -> 75B	0.46168
71B -> 74B	-0.40173
72B -> 75B	-0.24811
73B -> 75B	-0.33244

Excited State 11: 2.521-A 4.0085 eV 309.31 nm f=0.0085 <S**2>=1.339

70A -> 75A	0.24158
72A -> 75A	0.15705
73A -> 75A	0.45465
74A -> 75A	-0.11076
65B -> 74B	-0.15255
66B -> 74B	-0.45476
67B -> 74B	-0.11457
68B -> 74B	-0.21779
69B -> 74B	0.34479
70B -> 74B	-0.41601
72B -> 75B	-0.20845
73B -> 75B	-0.15854

Excited State 12: 2.144-A 4.0648 eV 305.02 nm f=0.0218 <S**2>=0.899

69A -> 75A	0.13707
73A -> 75A	0.49659
62B -> 74B	0.13025
65B -> 74B	-0.19400
66B -> 74B	0.16200
70B -> 74B	0.17040
71B -> 74B	-0.15822
72B -> 75B	0.19773
73B -> 75B	0.71542

Excited State 13: 2.556-A 4.0971 eV 302.61 nm f=0.0217 <S**2>=1.384

70A -> 75A	0.20607
73A -> 75A	0.19172
62B -> 74B	0.17350

63B -> 74B -0.12142
64B -> 74B -0.13553
65B -> 74B -0.33523
65B -> 75B 0.10648
66B -> 74B 0.22243
67B -> 74B 0.15604
68B -> 74B 0.22859
69B -> 74B 0.14195
69B -> 75B -0.23982
70B -> 74B 0.53855
72B -> 75B -0.17230
73B -> 74B -0.11063
73B -> 75B -0.37054

Excited State 14: 2.612-A 4.1421 eV 299.32 nm f=0.0035 <S**2>=1.456
69A -> 75A -0.18958
70A -> 75A 0.11971
73A -> 75A 0.53327
74A -> 75A -0.13550
62B -> 74B -0.11715
63B -> 74B 0.15321
64B -> 74B 0.17311
65B -> 74B 0.44994
66B -> 74B 0.24217
69B -> 74B -0.45772
69B -> 75B -0.20634
73B -> 75B -0.13861

Excited State 15: 2.753-A 4.4087 eV 281.23 nm f=0.0013 <S**2>=1.645
69A -> 75A 0.32297
70A -> 75A 0.27326
71A -> 75A 0.13604
72A -> 75A 0.65876
73A -> 75A -0.12709
74A -> 75A 0.26982
62B -> 74B -0.10422
65B -> 74B 0.18252
68B -> 74B 0.11333
69B -> 74B -0.18385
70B -> 75B 0.12594
71B -> 75B 0.23084
72B -> 75B -0.20209

Excited State 16: 2.522-A 4.7749 eV 259.66 nm f=0.0059 <S**2>=1.340
69A -> 75A -0.12092
72A -> 75A 0.23619

73A -> 75A 0.15599
62B -> 74B -0.30950
62B -> 75B -0.11905
66B -> 74B -0.31891
66B -> 75B -0.13168
67B -> 74B 0.26241
68B -> 74B 0.47434
68B -> 75B 0.16145
70B -> 75B -0.24231
71B -> 75B -0.46230
72B -> 75B 0.11520

Excited State 17: 2.523-A 4.8179 eV 257.34 nm f=0.0075 <S**2>=1.341
72A -> 75A -0.38092
74A -> 75A -0.19423
62B -> 74B -0.25283
66B -> 74B -0.24882
66B -> 75B 0.11867
67B -> 74B 0.22385
67B -> 75B -0.13721
68B -> 74B 0.39777
68B -> 75B -0.11593
69B -> 75B 0.16380
70B -> 75B 0.29162
71B -> 75B 0.49156
73B -> 75B 0.16936

Excited State 18: 2.009-A 5.2825 eV 234.71 nm f=0.0009 <S**2>=0.759
62B -> 74B -0.28733
63B -> 74B 0.49443
64B -> 74B 0.60860
65B -> 74B -0.53005

Excited State 19: 2.036-A 5.3019 eV 233.85 nm f=0.0009 <S**2>=0.786
69A -> 75A -0.14160
70A -> 75A -0.14256
71A -> 75A -0.12058
72A -> 75A 0.10656
62B -> 74B -0.11647
63B -> 74B 0.69832
64B -> 74B -0.62877

Excited State 20: 2.316-A 5.3149 eV 233.28 nm f=0.0005 <S**2>=1.091
69A -> 75A 0.45106
70A -> 75A 0.48436
71A -> 75A 0.41292

72A -> 75A -0.35937
73A -> 75A -0.10269
74A -> 75A -0.15713
63B -> 74B 0.16819
64B -> 74B -0.23509
70B -> 75B -0.12603
71B -> 75B -0.28156

Excited State 21: 2.007-A 5.6015 eV 221.34 nm f=0.0006 <S**2>=0.757
61B -> 74B 0.98266
62B -> 74B 0.10386

Excited State 22: 2.008-A 5.9191 eV 209.46 nm f=0.0028 <S**2>=0.758
59B -> 74B 0.33833
60B -> 74B 0.92677

Excited State 23: 2.017-A 5.9499 eV 208.38 nm f=0.0054 <S**2>=0.767
58B -> 74B -0.15021
59B -> 74B 0.91780
60B -> 74B -0.32662

Excited State 24: 3.179-A 5.9854 eV 207.15 nm f=0.0001 <S**2>=2.276
71A -> 75A -0.25949
58B -> 74B 0.10364
68B -> 75B -0.12532
70B -> 75B 0.77634
71B -> 75B -0.49080
73B -> 76B -0.10342

Excited State 25: 2.031-A 5.9986 eV 206.69 nm f=0.0048 <S**2>=0.781
74A -> 76A 0.14588
57B -> 74B 0.11459
58B -> 74B 0.95172
59B -> 74B 0.16204

Excited State 26: 2.409-A 6.0422 eV 205.20 nm f=0.0003 <S**2>=1.201
69A -> 75A -0.22897
70A -> 75A -0.39112
71A -> 75A 0.80136
72A -> 75A 0.10615
68B -> 75B -0.13405
70B -> 75B 0.25955
71B -> 75B -0.14367

Excited State 27: 2.099-A 6.0791 eV 203.95 nm f=0.0002 <S**2>=0.851
74A -> 76A -0.47095

57B -> 74B 0.85199

Excited State 28: 2.335-A 6.0863 eV 203.71 nm f=0.0047 <S**2>=1.113
71A -> 75A -0.10020
74A -> 76A 0.76958
57B -> 74B 0.48276
58B -> 74B -0.18659
69B -> 75B -0.10500
73B -> 76B 0.21538

Excited State 29: 3.059-A 6.1695 eV 200.96 nm f=0.0035 <S**2>=2.089
68A -> 75A 0.15948
65B -> 75B 0.12845
66B -> 75B 0.23439
67B -> 75B -0.24318
68B -> 75B 0.73912
69B -> 75B 0.31684
70B -> 75B 0.14800
72B -> 75B -0.12233
73B -> 76B 0.31198

Excited State 30: 3.156-A 6.2277 eV 199.09 nm f=0.0016 <S**2>=2.240
71A -> 75A -0.12427
73A -> 76A -0.42450
74A -> 76A -0.21069
68B -> 75B -0.29892
73B -> 76B 0.76003

Geometries (at ωB97X-D/def2SVP level)

[Cu(I)L]$^+$

E = -2159.556594

C	1.378462	-1.099257	1.093671
N	1.713247	-0.057661	0.102478
Cu	0.015975	0.012599	-1.181040
N	-0.790125	1.508469	0.101443
C	0.264069	1.731374	1.110625
C	1.660545	1.310171	0.641202
C	0.316199	-2.090295	0.606556
N	-0.894573	-1.443062	0.078015
C	-1.628772	-0.648078	1.082148
C	-1.956279	0.774705	0.617115
C	2.977581	-0.330449	-0.577033
C	-1.175840	2.745609	-0.573508
C	-1.763583	-2.390448	-0.616175

H	1.046010	-0.621019	2.024452
H	2.278526	-1.672391	1.369478
H	0.736732	-2.702334	-0.205902
H	0.075471	-2.780773	1.438802
H	-1.047619	-0.613377	2.013057
H	-2.574923	-1.145219	1.351047
H	-2.695387	0.728783	-0.197201
H	-2.435302	1.314953	1.457333
H	0.001731	1.197818	2.033739
H	0.307017	2.795333	1.394856
H	1.992208	1.986795	-0.161047
H	2.366501	1.440274	1.485027
H	-2.620250	-1.856454	-1.049399
H	-1.212186	-2.872309	-1.435162
H	-2.146346	-3.176536	0.062323
H	-0.284581	3.227590	-0.997885
H	-1.867765	2.521918	-1.396996
H	-1.666298	3.458950	0.115965
H	3.129712	0.394782	-1.388118
H	3.840493	-0.274135	0.113621
H	2.949793	-1.335750	-1.018954

[Cu(I)L(H_2O)]$^+$

E = -2235.936986

C	-0.013207	0.018276	0.024023
N	-0.000509	0.002027	1.483152
C	1.363249	0.002719	2.022125
C	1.414228	0.280615	3.525820
N	0.662846	1.485071	3.912443
C	1.538662	2.630657	4.135906
C	-0.858818	-1.060418	2.030893
C	-2.209003	-0.541252	2.529006
N	-2.084311	0.596889	3.444238
C	-3.362735	1.259934	3.677032
Cu	-0.746972	1.891630	2.294213
O	-1.167869	3.632182	1.382051
C	-1.384932	0.283830	4.700111
C	-0.267713	1.277261	5.026605
H	-0.331182	-1.572254	2.846642
H	-1.045544	-1.840455	1.273939
H	-2.805645	-0.202406	1.667969
H	-2.763148	-1.382324	2.992179
H	-0.976978	-0.734452	4.647463
H	-2.091383	0.267715	5.546964
H	-0.712511	2.255853	5.265076
H	0.257162	0.932753	5.940313

H	1.027997	-0.585270	4.079980
H	2.471852	0.366657	3.826360
H	1.922716	0.787800	1.490240
H	1.884115	-0.954943	1.820546
H	-0.722380	4.399233	1.762800
H	-2.104593	3.865361	1.384187
H	-3.210009	2.150674	4.302325
H	-3.793180	1.588367	2.720486
H	-4.092878	0.598209	4.183041
H	2.172756	2.790314	3.252729
H	0.936684	3.537515	4.289058
H	2.195443	2.490557	5.016779
H	0.533052	0.897366	-0.345548
H	0.448462	-0.890983	-0.408592
H	-1.048921	0.086323	-0.336748

[Cu(I)LHasc]$^{+}$

E = -2843.211234

C	3.442881	-0.728644	-0.652674
C	2.272996	-0.155239	-1.381780
C	1.186118	-0.957768	-1.286596
C	1.598364	-2.071027	-0.401707
O	2.912074	-1.927108	-0.081260
O	2.334801	1.011355	-2.053330
O	0.011555	-0.787986	-1.826467
Cu	-1.365892	-0.151049	-0.632563
N	-3.237505	0.977768	-0.737762
C	-4.216173	-0.040255	-0.344680
C	-3.846619	-0.744534	0.962970
N	-2.471900	-1.251997	0.954982
C	-1.674966	-0.887910	2.126163
C	-1.482771	0.623466	2.280933
N	-0.958051	1.257631	1.067469
C	-1.703144	2.426728	0.607903
C	-3.142413	2.100754	0.208349
O	0.958982	-3.004496	0.027269
C	4.037985	0.120683	0.464724
O	5.108946	-0.590770	1.027876
C	-2.405885	-2.678215	0.661265
C	4.538504	1.477639	-0.020080
O	5.241743	2.034319	1.069622
C	0.473262	1.505508	1.138884
C	-3.444297	1.437203	-2.107190
H	-3.983403	-0.058421	1.809679
H	-4.569046	-1.561164	1.133990
H	-4.256655	-0.784002	-1.155618

H	-5.235100	0.386467	-0.248121
H	-3.734375	1.873867	1.105040
H	-3.600116	3.009697	-0.217607
H	-1.168662	2.828173	-0.267598
H	-1.722035	3.234884	1.368088
H	-2.434441	1.095827	2.560849
H	-0.811408	0.799932	3.139049
H	-0.690103	-1.365986	2.002924
H	-2.112386	-1.286401	3.065115
H	4.263368	-1.016111	-1.334442
H	3.242374	0.289930	1.218032
H	5.202542	1.331757	-0.891484
H	3.695389	2.112805	-0.334912
H	5.817405	2.734337	0.748863
H	5.637163	0.079745	1.484481
H	-1.360666	-2.973078	0.494170
H	-2.835795	-3.294068	1.477343
H	-2.968344	-2.889906	-0.259657
H	0.989736	0.582744	1.437469
H	0.854479	1.789624	0.147143
H	0.733550	2.302170	1.864813
H	-2.647523	2.140752	-2.386319
H	-3.399088	0.584410	-2.798818
H	-4.420988	1.944738	-2.236173
H	1.449310	1.151063	-2.423353

[Cu(I)LDHA]$^{+}$

E = -2842.433679

C	-1.255477	1.487085	-0.378745
C	-2.342253	2.500541	-0.124314
O	-3.516763	1.887855	-0.322966
C	-3.418575	0.500253	-0.704159
C	-1.933192	0.201183	-0.719411
O	-2.225677	3.645818	0.194410
C	-4.233845	-0.351258	0.263244
O	-5.551505	0.112237	0.218569
O	-1.371259	-0.841242	-0.946368
Cu	1.274978	0.310872	-0.246598
N	1.351287	-1.049906	1.385653
C	1.404777	-2.318333	0.638712
C	2.455697	-2.297829	-0.469793
N	2.350145	-1.100535	-1.335932
C	3.642147	-0.421923	-1.547910
C	4.218397	0.171107	-0.260721
N	3.239244	0.993757	0.467809
C	3.114526	0.665812	1.891600

C	2.590207	-0.750340	2.134303
O	-0.049357	1.679016	-0.345710
C	-4.199409	-1.834421	-0.102728
O	-5.158216	-2.438912	0.732255
C	1.691405	-1.413881	-2.608545
C	3.433814	2.422856	0.241160
C	0.167963	-0.968859	2.241866
H	4.582990	-0.630629	0.394960
H	5.111729	0.762115	-0.520537
H	3.467322	0.384623	-2.275890
H	4.383607	-1.109011	-1.997099
H	3.463325	-2.342863	-0.037377
H	2.352700	-3.215289	-1.069925
H	0.409512	-2.475590	0.198110
H	1.606159	-3.174557	1.309761
H	3.359268	-1.486889	1.868067
H	2.424572	-0.879469	3.215639
H	2.415048	1.393051	2.331749
H	4.077047	0.781192	2.426952
H	-3.832948	0.404288	-1.720892
H	-3.803248	-0.226566	1.277852
H	-4.462234	-1.951701	-1.169443
H	-3.192229	-2.254345	0.052186
H	-5.405821	-3.292473	0.364779
H	-6.083132	-0.619828	0.565211
H	2.599349	2.987586	0.679860
H	4.379993	2.789196	0.682483
H	3.451109	2.627019	-0.838400
H	0.112532	0.025546	2.705907
H	-0.739820	-1.122873	1.643426
H	0.188482	-1.730213	3.042937
H	0.716206	-1.877198	-2.411965
H	1.523803	-0.489853	-3.178320
H	2.300712	-2.103920	-3.220271

[Cu(II)L]$^{2+}$

E = -2159.359233

C	1.401557	-1.106547	1.104777
N	1.722945	-0.061646	0.100417
Cu	-0.037957	-0.002382	-1.076019
N	-0.810437	1.427108	0.109193
C	0.259319	1.701893	1.113459
C	1.662306	1.311103	0.644031
C	0.320941	-2.071710	0.616763
N	-0.888368	-1.373558	0.107748
C	-1.649187	-0.640290	1.161268

C	-2.001820	0.760612	0.692806
C	3.001856	-0.319929	-0.577813
C	-1.169913	2.634964	-0.656242
C	-1.757829	-2.268886	-0.680191
H	1.101486	-0.632825	2.048015
H	2.298103	-1.695834	1.344579
H	0.709377	-2.684482	-0.209264
H	0.036134	-2.760071	1.428870
H	-1.046532	-0.615227	2.076152
H	-2.564597	-1.193935	1.410763
H	-2.771483	0.721128	-0.090295
H	-2.407479	1.357646	1.525380
H	0.007501	1.176795	2.041399
H	0.255135	2.772809	1.359560
H	2.001009	1.991348	-0.151088
H	2.353827	1.438404	1.494765
H	-2.624763	-1.707205	-1.048904
H	-1.202330	-2.682399	-1.531458
H	-2.108028	-3.099637	-0.047658
H	-0.265447	3.080800	-1.089241
H	-1.867069	2.374568	-1.462637
H	-1.646702	3.370417	0.010547
H	3.147831	0.413462	-1.381164
H	3.845887	-0.253012	0.128724
H	2.985173	-1.322905	-1.022705

[Cu(II)L(H_2O)]$^{2+}$

E = -2235.756523

C	1.732132	0.750197	-1.237677
N	1.494238	-0.538368	-0.541347
Cu	0.016665	-0.143377	0.898535
O	0.160269	-1.735772	2.044272
C	1.299651	1.920033	-0.365822
N	-0.065561	1.696787	0.180611
C	-1.125310	1.757820	-0.869891
C	-2.139108	0.633687	-0.718775
N	-1.466017	-0.666092	-0.523820
C	-0.669327	-1.096993	-1.699506
C	0.756443	-1.531981	-1.347563
C	2.731093	-1.105344	0.014948
C	-2.403927	-1.710015	-0.090333
C	-0.362767	2.612584	1.300915
H	1.194615	0.751699	-2.193885
H	2.795933	0.859937	-1.492113
H	1.980892	2.026121	0.490175
H	1.331447	2.865788	-0.930335

H	-0.642404	1.716654	-1.852285
H	-1.634670	2.730209	-0.821572
H	-2.776313	0.809224	0.159865
H	-2.800229	0.616692	-1.602271
H	-0.649415	-0.289045	-2.440791
H	-1.166439	-1.941431	-2.198391
H	0.728964	-2.462197	-0.761194
H	1.297038	-1.753550	-2.283634
H	-0.624548	-2.100559	2.476854
H	0.877181	-1.783110	2.692841
H	-1.373024	2.413906	1.680843
H	0.365948	2.465842	2.108822
H	-0.308400	3.657900	0.958643
H	-1.856278	-2.643154	0.096165
H	-2.904077	-1.400703	0.836519
H	-3.169834	-1.898599	-0.860908
H	2.493168	-1.990904	0.617905
H	3.423482	-1.400073	-0.790464
H	3.222917	-0.362769	0.656006

$[Cu(II)L(H_2O)_2]^{2+}$

E = -2312.136702

C	-1.137224	0.297023	-1.996693
N	-0.323754	1.229386	-1.192983
Cu	-0.071007	0.231381	0.763005
O	-1.604339	0.885753	1.986958
C	-1.929351	-0.669010	-1.118785
N	-1.086440	-1.333821	-0.094306
C	-0.086152	-2.261377	-0.692368
C	1.284634	-2.059128	-0.075550
N	1.635651	-0.621168	-0.041477
C	1.812295	-0.040133	-1.402799
C	1.090661	1.290778	-1.587899
O	0.919879	1.758345	1.677442
C	-0.913221	2.568345	-1.120684
C	2.834965	-0.399560	0.783328
C	-1.923439	-2.040206	0.893794
H	-0.492115	-0.255666	-2.691845
H	-1.847086	0.845394	-2.634185
H	-2.722074	-0.128146	-0.583307
H	-2.427141	-1.427411	-1.745929
H	-0.053670	-2.100160	-1.775750
H	-0.406775	-3.302966	-0.551775
H	1.297254	-2.426234	0.960807
H	2.042784	-2.632955	-0.634789
H	1.469087	-0.767717	-2.147296

H	2.883135	0.106254	-1.602845
H	1.567164	2.060508	-0.963007
H	1.209087	1.607409	-2.640232
H	0.289953	2.269768	2.205584
H	1.683214	1.608292	2.251129
H	-1.748539	0.496695	2.860167
H	-2.433099	1.313924	1.736365
H	-1.286707	-2.491430	1.665681
H	-2.611778	-1.334273	1.370088
H	-2.506613	-2.833141	0.399889
H	3.102395	0.664519	0.769086
H	2.649350	-0.722227	1.816629
H	3.685733	-0.973924	0.383125
H	-0.370876	3.172455	-0.380527
H	-0.873237	3.083416	-2.096813
H	-1.964233	2.499943	-0.810300

[Cu(II)L(H_2O)$_3$]$^{2+}$

E = -2388.50488020

Cu -0.366972 0.070410 -0.553719
O -2.692359 0.232090 -0.950191
H -3.043606 0.943007 -1.500937
H -3.463835 -0.123008 -0.492404
N 1.879963 -0.022525 -0.304048
C 2.610340 -0.118930 -1.566717
N -0.358876 -1.505741 0.794601
C -1.460520 -2.445315 0.527162
N -0.311041 1.294222 1.111879
C -1.012669 2.563583 0.868341
O -0.212728 1.591532 -1.947775
O -0.669593 -1.050183 -2.270318
C 2.119738 -1.177167 0.575727
C 0.950422 -2.159597 0.564302
C 2.081330 1.280857 0.337226
C 1.109898 1.527926 1.487055
C -0.482978 -0.931406 2.161412
C -1.041610 0.478192 2.105979
H 2.322565 -0.832760 1.598317
H 3.026331 -1.722779 0.271069
H 0.892566 -2.661113 -0.412155
H 1.115862 -2.947246 1.319052
H 0.498571 -0.944344 2.648751
H -1.134316 -1.563590 2.781212
H -2.096137 0.456714 1.796456
H -1.001208 0.946005 3.104376
H 1.360510 0.891705 2.343688

H 1.231950 2.561999 1.840116
H 1.935631 2.047752 -0.437719
H 3.111565 1.397884 0.721817
H -0.285084 1.223081 -2.839406
H -0.687856 2.432022 -1.961066
H -1.622222 -1.158846 -2.408337
H -0.226310 -1.820672 -2.646302
H -0.428366 3.179908 0.173752
H -2.002430 2.361924 0.439853
H -1.134300 3.125454 1.808451
H -2.421337 -1.960392 0.737345
H -1.441167 -2.759309 -0.522100
H -1.370749 -3.336174 1.168994
H 2.279025 0.677205 -2.246747
H 3.701559 -0.027274 -1.417912
H 2.408383 -1.087094 -2.043988

[Cu(II)LAsc], conformer 1
E = -2842.60944767
C 1.327592 1.549608 0.248253
C 2.433026 2.496354 0.011908
O 3.609347 1.875401 0.280199
C 3.409352 0.517589 0.684499
C 1.898707 0.314865 0.687844
O 2.398822 3.646504 -0.353492
C 4.163912 -0.404545 -0.263143
O 5.524327 -0.061377 -0.223110
O 1.323543 -0.732219 1.006314
O 0.095929 1.837554 0.092875
Cu -1.245051 0.458215 0.141678
N -1.352100 -1.262271 -1.218828
C -1.311090 -2.343657 -0.230986
C -2.341154 -2.163773 0.885237
N -2.289127 -0.828845 1.508535
C -3.599519 -0.179343 1.617511
C -4.226519 0.126031 0.254594
N -3.308553 0.832659 -0.645767
C -3.193990 0.246611 -1.981345
C -2.610609 -1.168454 -1.969485
C 4.009240 -1.878181 0.100302
O 4.915738 -2.569561 -0.732468
C -1.575575 -0.853161 2.783117
C -3.560902 2.266311 -0.685916
C -0.182879 -1.262670 -2.089198
H -4.560444 -0.806522 -0.219937
H -5.147007 0.711907 0.419306

H -3.450710 0.762971 2.167099
H -4.310763 -0.788549 2.210510
H -3.352769 -2.343808 0.497242
H -2.176400 -2.949981 1.640899
H -0.302988 -2.333583 0.206880
H -1.466529 -3.336556 -0.699895
H -3.342024 -1.871003 -1.547342
H -2.468754 -1.492878 -3.014535
H -2.531171 0.902734 -2.567091
H -4.169399 0.223867 -2.509087
H 3.820008 0.403054 1.701819
H 3.750830 -0.249547 -1.282122
H 4.261678 -2.016692 1.167373
H 2.969948 -2.209129 -0.050348
H 5.076470 -3.443662 -0.365888
H 5.983036 -0.840363 -0.569740
H -2.762432 2.770983 -1.248189
H -4.533358 2.511245 -1.157729
H -3.561060 2.672416 0.335523
H -0.206472 -0.379604 -2.743616
H 0.728938 -1.210267 -1.479024
H -0.134154 -2.167776 -2.726683
H -0.566516 -1.255521 2.625244
H -1.471167 0.170687 3.169327
H -2.101072 -1.465396 3.542075

[Cu(II)LAsc], conformer 2
E = -2842.60131571
C -1.455652 0.545630 -0.423827
O -2.613280 1.132222 -0.740860
C -3.683713 0.173439 -0.746408
C -3.035573 -1.165249 -0.390503
C -1.626823 -0.893381 -0.186817
C -4.767544 0.639038 0.213256
C -5.964143 -0.306306 0.245956
O -6.942237 0.351625 1.022410
O -3.639306 -2.231958 -0.309153
O -0.699659 -1.681237 0.127030
Cu 1.338112 0.372161 -0.018585
O -0.426056 1.214717 -0.367286
N 3.236542 1.533843 0.043405
C 2.976556 2.921825 -0.313303
C 4.165477 0.883791 -0.889684
C 3.456818 0.006503 -1.925619
N 2.520001 -0.941646 -1.324262
C 1.623622 -1.549264 -2.299084

C 3.589119 1.376137 1.455003
C 3.549988 -0.080504 1.923844
N 2.291265 -0.756212 1.583773
C 1.379280 -0.845566 2.718549
C 2.460336 -2.050876 0.916621
C 3.148223 -1.937657 -0.445822
O -5.197268 1.912624 -0.191439
H 4.889243 0.281023 -0.324694
H 4.771577 1.633776 -1.426483
H 2.877629 0.649607 -2.606529
H 4.225361 -0.502656 -2.542782
H 4.210107 -1.688713 -0.313502
H 3.142254 -2.934635 -0.919152
H 1.452296 -2.464013 0.773858
H 3.033822 -2.762259 1.545579
H 4.392592 -0.635366 1.489084
H 3.723717 -0.098594 3.013300
H 2.861084 1.960820 2.038947
H 4.591023 1.795528 1.680712
H -4.092100 0.144846 -1.770124
H -4.325064 0.681144 1.230424
H -6.320301 -0.473146 -0.786933
H -5.678230 -1.281018 0.670448
H -7.799978 -0.047658 0.851684
H -6.062045 2.024560 0.229074
H 2.179053 3.329671 0.323883
H 3.875212 3.561548 -0.204339
H 2.636310 2.979534 -1.356916
H 1.223975 0.153679 3.149822
H 0.408632 -1.224835 2.371288
H 1.766202 -1.511803 3.515697
H 0.872760 -2.153954 -1.772749
H 1.088852 -0.763282 -2.852028
H 2.162715 -2.187657 -3.027600

[Cu(II)LAsc], conformer 3

E = -2842.59815556
C -2.343345 0.048532 -0.721149
O -1.195504 -0.735809 -0.360978
C -1.557515 -1.981652 0.115830
C -3.017558 -2.142818 -0.025936
C -3.529698 -0.901150 -0.567126
O -0.713817 -2.725874 0.550540
Cu 0.731279 -0.076632 -0.308772
N 2.059919 1.555337 -0.777263
C 2.100935 2.236279 0.523371
C 2.416731 1.296291 1.691277

N 1.553096 0.111340 1.720959
C 0.450617 0.240729 2.661906
O -3.647597 -3.180891 0.286524
O -4.688276 -0.594063 -0.845905
C -2.405590 1.265940 0.187893
C -3.560483 2.197530 -0.155818
O -3.368315 3.344855 0.642386
N 2.513918 -1.319479 -0.659621
C 2.145734 -2.616234 -1.215632
O -1.194860 1.972597 0.070618
C 2.254541 -1.167742 1.830654
C 3.182003 -1.447296 0.645018
C 3.236284 -0.485528 -1.621866
C 3.351599 0.973753 -1.178204
C 1.495424 2.411998 -1.817326
H 3.468279 0.981481 1.648367
H 2.326004 1.872534 2.628240
H 1.108607 2.680854 0.681255
H 2.838280 3.064243 0.523067
H 4.062723 1.054572 -0.345232
H 3.802085 1.554009 -2.000669
H 2.682678 -0.530938 -2.572582
H 4.254383 -0.875583 -1.825327
H 4.047936 -0.772037 0.679320
H 3.601602 -2.460286 0.768168
H 1.482983 -1.951415 1.869721
H 2.847969 -1.238568 2.765417
H -2.214561 0.365195 -1.768587
H -2.532125 0.905076 1.228530
H -3.515925 2.445263 -1.231692
H -4.523804 1.702677 0.042291
H -3.873264 4.075092 0.273223
H -1.384215 2.860727 0.409052
H -0.227459 -0.618351 2.556680
H 0.794263 0.290739 3.714455
H -0.121657 1.150752 2.431893
H 1.507914 -3.152375 -0.501088
H 1.564640 -2.473868 -2.138106
H 3.032722 -3.236926 -1.452708
H 1.457646 1.861396 -2.767796
H 0.469536 2.689096 -1.542023
H 2.095999 3.330272 -1.970829

[Cu(II)LHAsc]$^{+}$

E = -2843.055138

C	-1.156377	1.048626	-0.984238
C	-1.786950	2.157942	-0.233600

O	-3.119152	1.934412	-0.155501
C	-3.453303	0.673544	-0.733758
C	-2.147648	0.176172	-1.291667
O	-1.274368	3.133746	0.254662
C	-4.094075	-0.187402	0.355443
O	-5.295495	0.429591	0.722689
O	-1.979784	-0.966722	-1.963686
O	0.113360	1.039165	-1.288371
Cu	1.497846	0.017549	-0.653205
N	0.946665	-1.234289	1.006317
C	1.770273	-2.423395	0.726574
C	3.201657	-2.047240	0.368233
N	3.256405	-0.971618	-0.657891
C	4.236159	0.089141	-0.317926
C	3.793001	0.892471	0.901660
N	2.389330	1.330865	0.766201
C	1.534807	1.030488	1.926372
C	1.385600	-0.469369	2.195249
C	-4.375682	-1.624574	-0.074684
O	-5.136271	-2.185249	0.967724
C	3.509277	-1.527191	-1.999129
C	2.272841	2.733022	0.352659
C	-0.475535	-1.573521	1.072107
H	3.908670	0.301923	1.819654
H	4.461178	1.758757	1.020372
H	4.309258	0.753448	-1.191517
H	5.236416	-0.345265	-0.150742
H	3.743780	-1.713196	1.260609
H	3.735947	-2.938546	0.008410
H	1.299391	-2.954373	-0.114161
H	1.780883	-3.119918	1.584374
H	2.331078	-0.884411	2.567008
H	0.665052	-0.600245	3.016645
H	0.548490	1.470631	1.712300
H	1.917503	1.516219	2.842190
H	-4.200231	0.848461	-1.527224
H	-3.388231	-0.215048	1.210749
H	-4.944115	-1.621063	-1.023431
H	-3.433279	-2.177590	-0.229445
H	-5.589141	-2.969997	0.645269
H	-5.802166	-0.257777	1.178841
H	1.221680	2.958103	0.130144
H	2.639391	3.411289	1.143197
H	2.867067	2.897051	-0.556429
H	-1.058750	-0.663093	1.260463
H	-0.800577	-1.998913	0.113329

H	-0.681292	-2.296687	1.880455
H	2.750648	-2.286121	-2.231475
H	3.452806	-0.729412	-2.751607
H	4.507209	-1.992953	-2.047876
H	-2.813604	-1.306726	-2.309450

[Cu(II)LDHA]$^{2+}$, conformer 3

E = -2842.239742

C	-1.244612	1.769617	-0.176433
C	-2.524352	2.591307	-0.081645
O	-3.525914	1.755236	-0.378550
C	-3.162732	0.393210	-0.707422
C	-1.676446	0.372998	-0.558219
O	-2.640317	3.739886	0.199004
C	-3.941316	-0.587692	0.171819
O	-5.291980	-0.367813	-0.087900
O	-0.852706	-0.506052	-0.671291
Cu	1.126145	0.185556	-0.296764
N	1.422871	-0.658223	1.674971
C	1.491762	-2.080381	1.293416
C	2.386429	-2.327268	0.079642
N	2.081094	-1.438119	-1.077560
C	3.294150	-0.833264	-1.677106
C	3.943901	0.131394	-0.702487
N	2.930655	1.054712	-0.115230
C	3.053495	1.201673	1.357976
C	2.721319	-0.088626	2.103386
O	-0.087933	2.039983	0.009303
C	-3.576380	-2.040664	-0.137221
O	-4.520240	-2.803167	0.570626
C	1.271005	-2.133800	-2.093541
C	2.949398	2.365542	-0.795088
C	0.362437	-0.414907	2.659956
H	4.445584	-0.405545	0.110177
H	4.724674	0.711018	-1.213609
H	2.981607	-0.306823	-2.589951
H	4.009741	-1.616107	-1.977706
H	3.440985	-2.202863	0.350958
H	2.277800	-3.376212	-0.229709
H	0.464686	-2.410787	1.077596
H	1.860366	-2.706359	2.125012
H	3.515767	-0.832997	1.964309
H	2.711299	0.129784	3.181127
H	2.362168	2.001204	1.660941
H	4.070822	1.538044	1.616334
H	-3.426553	0.222427	-1.765421

H	-3.696758	-0.375579	1.231189
H	-3.650307	-2.212345	-1.225645
H	-2.543306	-2.264513	0.179895
H	-4.562882	-3.687377	0.194023
H	-5.738067	-1.178621	0.200437
H	2.142421	3.000089	-0.411244
H	3.914412	2.864776	-0.616413
H	2.813916	2.222621	-1.874581
H	0.294155	0.658935	2.878272
H	-0.605098	-0.753967	2.264036
H	0.557439	-0.954341	3.602579
H	0.380776	-2.568457	-1.623980
H	0.956385	-1.426245	-2.870921
H	1.861803	-2.938878	-2.558530

[Cu(I)LNO$_2$], conformer 1

E = -2364.621904

N	0.033728	-0.090553	-0.083193
C	0.023260	-0.139858	1.379273
C	1.425311	-0.067490	1.987780
N	2.352771	-1.046227	1.401999
C	3.632537	-0.477557	0.971796
C	3.482977	0.544955	-0.157212
N	2.687410	0.037877	-1.282259
C	1.617963	0.936218	-1.719814
C	0.551427	1.163136	-0.645419
Cu	1.512235	-1.671027	-0.526281
O	1.242151	-3.437808	-1.284645
N	0.877614	-3.465852	-2.509234
O	0.724439	-4.580018	-2.969509
C	-1.246709	-0.473777	-0.663325
C	3.517914	-0.421936	-2.387805
C	2.527086	-2.217017	2.253772
H	1.834681	0.944047	1.864139
H	1.339584	-0.212670	3.078061
H	-0.445787	-1.093142	1.669076
H	-0.596894	0.668749	1.817094
H	0.961201	1.784590	0.162220
H	-0.263356	1.762901	-1.085927
H	1.147495	0.475743	-2.602582
H	2.011416	1.921226	-2.044027
H	3.024666	1.465207	0.229533
H	4.491572	0.843163	-0.491134
H	4.257196	-1.313465	0.620238
H	4.176357	-0.002306	1.813303
H	3.121340	-2.976952	1.727109

H	3.033950	-1.971421	3.208080
H	1.546659	-2.656810	2.484416
H	-2.062584	0.222431	-0.384228
H	-1.166500	-0.491657	-1.759344
H	-1.518470	-1.485959	-0.331383
H	4.070318	0.406511	-2.874429
H	4.247500	-1.158021	-2.021621
H	2.892032	-0.918844	-3.142461

[Cu(I)LNO$_2$], conformer 2

E = -2364.626131

C	0.040252	0.014928	-0.007617
C	0.046083	0.072608	1.520276
N	1.396037	0.023749	2.080652
C	2.125412	-1.223907	1.823809
C	3.527740	-0.980575	1.258257
N	3.528938	-0.091938	0.097234
C	2.811072	-0.603339	-1.073241
C	1.830521	0.423118	-1.646545
N	0.947534	1.002840	-0.624053
Cu	2.341039	1.618233	0.880821
N	3.184416	3.115115	1.758175
O	4.395890	3.329889	1.630878
O	2.547993	3.807242	2.562391
C	0.214024	2.158461	-1.139330
C	4.856281	0.415446	-0.225177
C	1.439685	0.425841	3.480462
H	0.318034	-0.992828	-0.343396
H	-0.993179	0.164190	-0.361334
H	-0.408350	1.020511	1.848690
H	-0.597431	-0.742257	1.909492
H	1.546338	-1.851683	1.132861
H	2.220027	-1.821629	2.746457
H	4.148136	-0.501119	2.031841
H	3.997114	-1.960030	1.033250
H	2.275965	-1.523981	-0.804250
H	3.511834	-0.899425	-1.872690
H	2.396721	1.254234	-2.094452
H	1.249140	-0.048031	-2.463562
H	0.920904	2.921394	-1.493149
H	-0.458749	1.883298	-1.974612
H	-0.389954	2.601625	-0.335780
H	0.834791	-0.236706	4.130337
H	2.479571	0.405476	3.835874
H	1.078765	1.459146	3.580466
H	5.573483	-0.395165	-0.462509

H	4.790822	1.084799	-1.094731
H	5.236502	1.014762	0.613648

[Cu(II)LNO$_2$]$^+$, conformer 1

E = -2364.460202

N	0.022808	-0.015126	-0.048235
C	0.001744	-0.033506	1.436597
C	1.414733	-0.076084	2.008905
N	2.220088	-1.129235	1.351153
C	3.528004	-0.671739	0.848112
C	3.420832	0.380886	-0.259173
N	2.530856	-0.020674	-1.373693
C	1.544811	1.012457	-1.738253
C	0.562827	1.259648	-0.600429
Cu	1.271354	-1.503421	-0.507621
O	2.063491	-3.164890	-0.929389
N	1.761287	-3.444691	-2.164170
O	2.070786	-4.544678	-2.516397
C	-1.306212	-0.318328	-0.614224
C	3.287123	-0.501639	-2.533397
C	2.345553	-2.338289	2.172382
H	1.913773	0.894266	1.890975
H	1.357811	-0.251337	3.093209
H	-0.550612	-0.934815	1.741005
H	-0.549970	0.838427	1.825034
H	1.044419	1.817827	0.210591
H	-0.263805	1.892518	-0.953327
H	1.009266	0.654388	-2.629861
H	2.034465	1.963036	-2.014133
H	3.074267	1.335020	0.156882
H	4.434073	0.577926	-0.639868
H	4.049646	-1.560458	0.463127
H	4.145078	-0.259040	1.665568
H	2.807798	-3.137071	1.578066
H	2.959734	-2.148663	3.069177
H	1.348660	-2.674138	2.486697
H	-2.045086	0.429430	-0.284675
H	-1.250558	-0.305356	-1.710621
H	-1.636592	-1.313008	-0.287016
H	3.874547	0.312433	-2.991132
H	3.969559	-1.301433	-2.218071
H	2.597931	-0.914256	-3.281738

[Cu(II)LNO$_2$]$^+$, conformer 2

E =-2364.463565

C	0.044050	0.026833	0.015260

C	0.051659	0.084734	1.541031
N	1.412480	0.049964	2.092727
C	2.140500	-1.205093	1.830326
C	3.532676	-0.954917	1.249323
N	3.511066	-0.030077	0.093117
C	2.801659	-0.583480	-1.090727
C	1.813540	0.423794	-1.666715
N	0.969741	1.012868	-0.602429
Cu	2.383502	1.522797	0.779418
N	3.348297	2.907822	1.772741
O	4.256355	3.455385	2.319804
O	2.212419	3.429471	1.631493
C	0.249578	2.206888	-1.072655
C	4.865647	0.433563	-0.251235
C	1.448858	0.435124	3.503675
H	0.315048	-0.978590	-0.329003
H	-0.980340	0.198785	-0.346500
H	-0.411956	1.024487	1.877712
H	-0.573885	-0.739737	1.930204
H	1.552051	-1.838582	1.153831
H	2.253393	-1.792926	2.754671
H	4.176622	-0.496749	2.014444
H	3.996411	-1.915153	0.965195
H	2.288670	-1.508021	-0.800328
H	3.524929	-0.871581	-1.867180
H	2.359157	1.249953	-2.145392
H	1.195389	-0.055901	-2.444829
H	0.965921	2.959573	-1.427354
H	-0.440093	1.951523	-1.894051
H	-0.326696	2.636735	-0.243178
H	0.872523	-0.263534	4.136268
H	2.489473	0.450171	3.855522
H	1.034480	1.445774	3.622971
H	5.511793	-0.416389	-0.525243
H	4.811563	1.129101	-1.098716
H	5.306922	0.959679	0.605243