# Reversible Modulation of the Redox Characteristics of Acid-Sensitive Molybdenum and Tungsten Scorpionate Complexes

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*# equal contribution*

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*Electrochemical studies*

Electrochemical studies were carried out for complexes **2**$^-$-**5**$^-$ with the following general procedure. Stock solutions of 0.02 M $[ML(CO)_3]^-$ and 1.0 M tetrabutylammonium hexafluorophosphate in MeCN were prepared, along with 0.1 M DPhAT in MeCN, 0.1 M $BF_3$ etherate in 90% MeCN 10% $Et_2O$, 0.1 M borane-tetrahydrofuran in 90% MeCN 10% THF, 0.1 M Cu(II)$(OTf)_2$ in MeCN, and 0.1 M Sc(III)$(OTf)_3$. The concentration of complex was held constant by adding 1 mL of the (complex + electrolyte) solution to the CV cell, and adding variable amounts of acid and solvent until a final volume of 2 mL was reached. For example, the introduction of 0.5 eq of DPhAT solution is obtained by adding (0.1 mL x N) DPhAT solution then adding (1 mL – (0.10 mL x N)) of MeCN to reach the final 2 mL volume. Through these additions, the effects of acid were tested from 0 – 5 eq of DPhAT and the varying Lewis acids (0 – 0.05 M acid vs 0.01 M **2**$^-$-**5**$^-$). All runs were performed in the presence of cobaltocenium hexafluorophosphate as an internal standard.

Nernst plots were constructed by starting with a solution of 0.002 mM **3**$^-$ or **5**$^-$ and 0.38 M 2-methoxypyridine solution in 1 mL acetonitrile. Varying amounts of 2-methoxypyridinium triflate were added to create a 6-point $\log_{10}([A]/[HA^+])$ range of -0.93 to -0.42 for **3**$^-$ and of -0.04 to 0.44 for **5**$^-$.

*Non-electrochemical infrared spectroscopy studies*

Infrared spectroscopy studies were carried out for complexes **2**$^-$-**5**$^-$. 2 mL samples of 0.05 M DPhAT, $BF_3$-etherate, and Sc(III)$(OTf)_3$ vs 0.01 M complex were prepared and drop-cast on a NaCl salt plate. A sample of MeCN drop-cast on a NaCl salt plate was used as a background.

*Determination of $pK_a$ of complexes **3**$^-$ and **5**$^-$*

The parent pyridine para resonance was determined via NMR of pyridine in DMSO to be δ 7.79. To account for natural dissociation of pyridinium in DMSO, the pyridinium para resonance was determined by adding pyridinium trifluoromethanesulfonate (24.8 mg, 0.0108 mmol) to 1 mL of $d_6$-DMSO. Using pyridinium's $pK_a^{DMSO}$ of 1.8, the mole ratio of pyridinium to pyridine in solution was calculated to be about 16.13. Using the equation

$$HA^+(\text{resonance}) = \frac{\text{Obs(resonance)} - \frac{[A]}{[HA^+]} * A(\text{resonance})}{1 - \frac{[A]}{[HA^+]}}$$

the observed para resonance of δ 8.61, and the pyridine para peak of δ 7.79, the pyridinium para resonance was calculated to be δ 8.66. Pyridinium trifluoromethanesulfonate (21 mg, 0.0916 mmol) and complex **3**$^-$ (86 mg, 0.163 mmol) were added to an NMR tube with 3 mL of $d_6$-DMSO. Rapid interconversion was observed between the pyridinium and pyridine and complex **3**$^-$ and **3H**. Relative abundance of the pyridinium and pyridine species was determined by the observed para proton resonance shift with that of the pyridine and pyridinium in $^1$H NMR. The observed resonance of δ 8.50 corresponds to a mole ratio of 4.35 pyridinium to pyridine. Using the equilibrium between complex **3**$^-$ and pyridinium

with pyridine and protonated complex **3H** the mole ratio of complex $\mathbf{3}^-$ to its conjugate acid **3H** was calculated to be 8.68. Relating various equilibria, using the equation

$$\mathrm{pK}_a(\text{complex } \mathbf{3}) = \mathrm{pK}_a(\text{pyridinium}) - \mathrm{pK}_{eq}$$

the $pK_a$ was calculated to be 1.8. This was repeated twice with 21.2 mg of pyridinium triflate (0.0925 mmol) and 93 mg of complex $\mathbf{3}^-$ (0.177 mmol) for the first trial and 19.6 mg of pyridinium triflate (0.0855 mmol) and 105 mg of complex $\mathbf{3}^-$ (0.2 mmol) to receive $pK_a$ values of 1.7 and 1.8 respectively. The mode of 1.8 was used. This experiment was repeated for complex $\mathbf{5}^-$ with 3 separate trials. Trial 1 used 20.4 mg of pyridinium trifluoromethanesulfonate (0.089 mmol) and 100 mg of complex $\mathbf{5}^-$ (0.162 mmol) to result in a $pK_a$ of 1.7. Trial 2 used 21.4 mg of pyridinium trifluoromethanesulfonate (0.0934 mmol) and 113 mg of complex $\mathbf{5}^-$ (0.184 mmol) to result in a $pK_a$ of 1.8. Trial 3 used 19.6 mg of pyridinium trifluoromethanesulfonate (0.0934 mmol) and 106 mg of complex $\mathbf{5}^-$ (0.173 mmol) to result in a $pK_a$ of 1.8. The mode of 1.8 was used.

The same method was repeated for $pK_a^{AN}$ for complexes $\mathbf{3}^-$ and $\mathbf{5}^-$, again using pyridinium as the acid with the $pK_a^{AN}$ of 12.53. The pyridinium para peak was again used at δ 8.62 now in AN with a corresponding pyridine peak of δ 7.73. For complex $\mathbf{3}^-$, trial 1 had 0.04 M $\mathbf{3}^-$ and 0.044 M pyridinium triflate, resulting in a $pK_a$ of 11.0, trial 2 had 0.04 M $\mathbf{3}^-$ and 0.048 M pyridinium triflate resulting in a $pK_a$ of 10.9, and trial 3 had 0.04 M $\mathbf{3}^-$ and 0.039 M pyridinium triflate resulting in a $pK_a$ of 11.0 The mode of 11.0 was used.. For complex $\mathbf{5}^-$, trial 1 had 0.024 M $\mathbf{5}^-$ and 0.039 M pyridinium triflate, resulting in a $pK_a$ of 11.8, trial 2 had 0.051 M $\mathbf{5}^-$ and 0.048 M pyridinium triflate resulting in a $pK_a$ of 11.9, and trial 3 had 0.031 M $\mathbf{5}^-$ and 0.039 M pyridinium triflate resulting in a $pK_a$ of 12.0 The average of 11.9 was used.

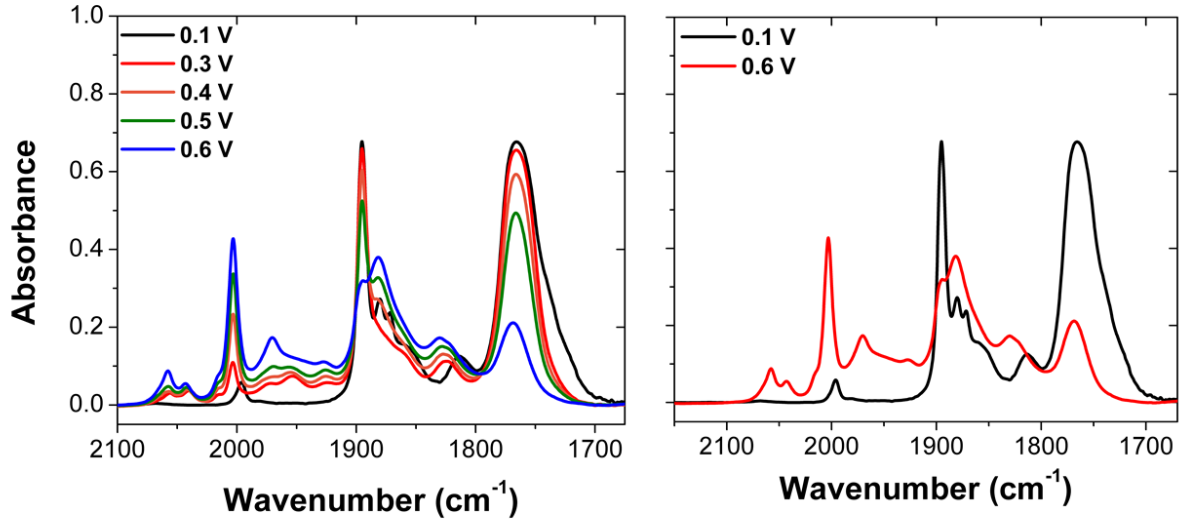



**Figure S1**. IR-SEC data from the oxidation of K[WTtz(CO)$_3$] (**5**$^-$) (0.019 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

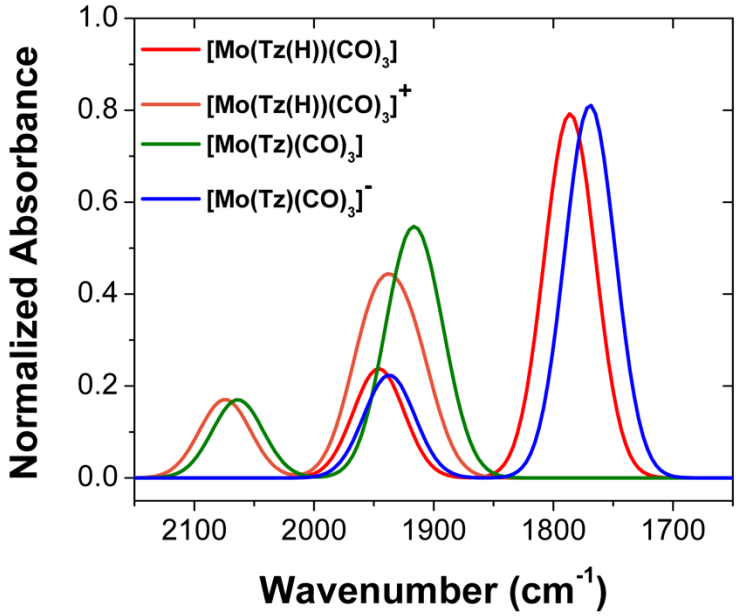



**Figure S2**. Simulated IR data from numerical frequency calculations performed on **3**$^-$, **3H**, and **3**. ORCA 4.0.0: B3LYP/G functional and ZORA-def2-TZVP basis set (def2/J and SARC/J auxiliary basis sets where necessary) with the RIJCOSX approximation, D3BJ dispersion correction, and CPCM to model the AN solvent.

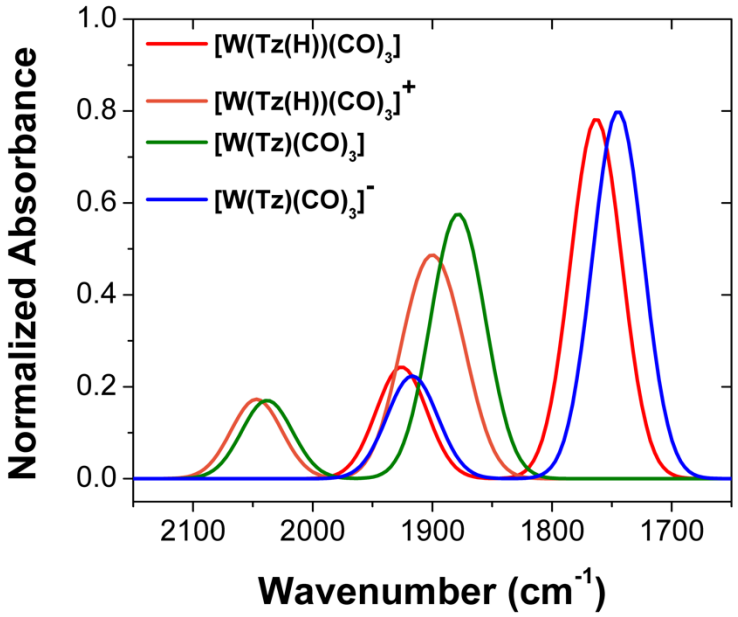



**Figure S3**. Simulated IR data from numerical frequency calculations performed on **5**$^{-}$, **5H**, **5**, **5H**$^{+}$. ORCA 4.0.0: B3LYP/G functional and ZORA-def2-TZVP basis set (def2/J and SARC/J auxiliary basis sets where necessary) with the RIJCOSX approximation, D3BJ dispersion correction, and CPCM to model the AN solvent.

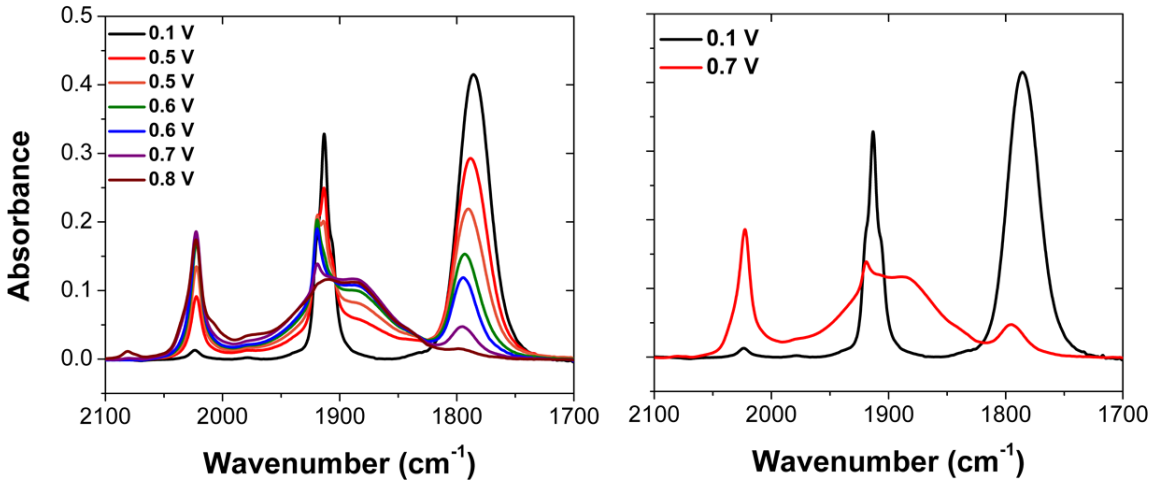



**Figure S4**. IR-SEC data showing the oxidation of K[MoTtz(CO)$_3$] (**3**$^{-}$) (0.013 M) with added 2-methoxypyridinium triflate (0.04 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

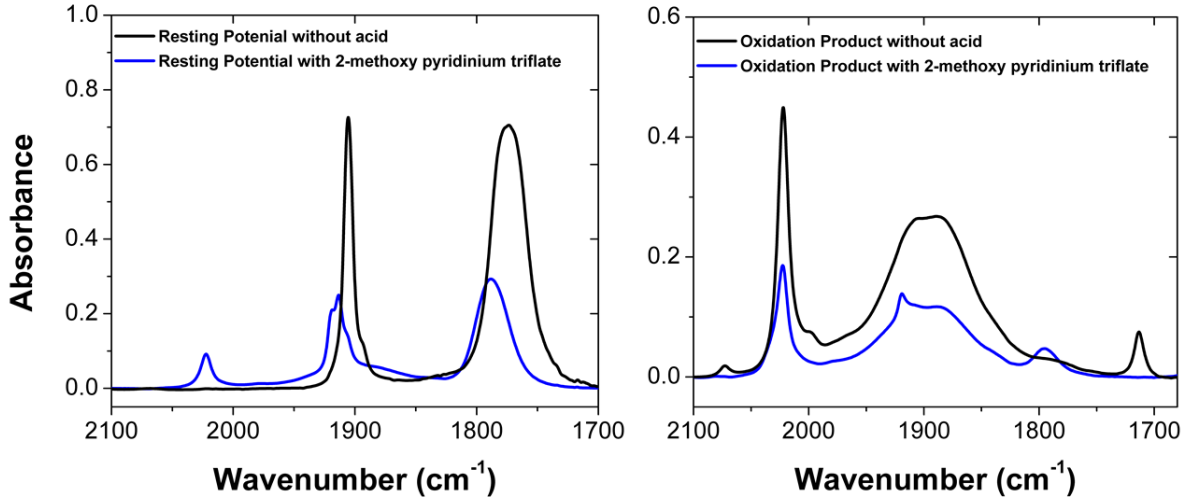



**Figure S5**. IR-SEC data comparing the species at resting potential and the oxidation products of K[MoTtz(CO)$_3$] (**3**$^-$) (0.013 M) with and without added 2-methoxypyridinium triflate (0.04 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

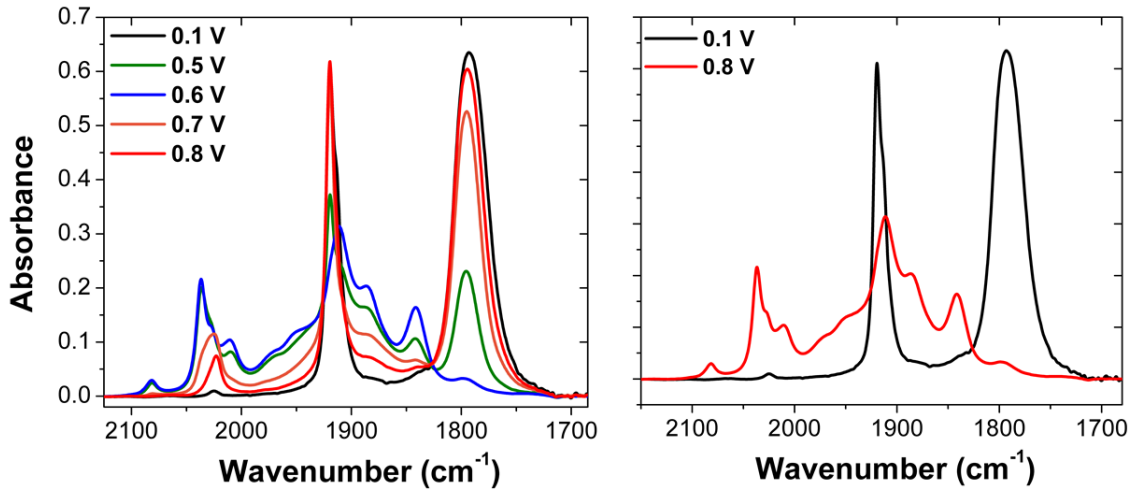



**Figure S6**. IR-SEC data showing the oxidation of K[MoTtz(CO)$_3$] (**3**$^-$) (0.013 M) with added DPhAT (0.03 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

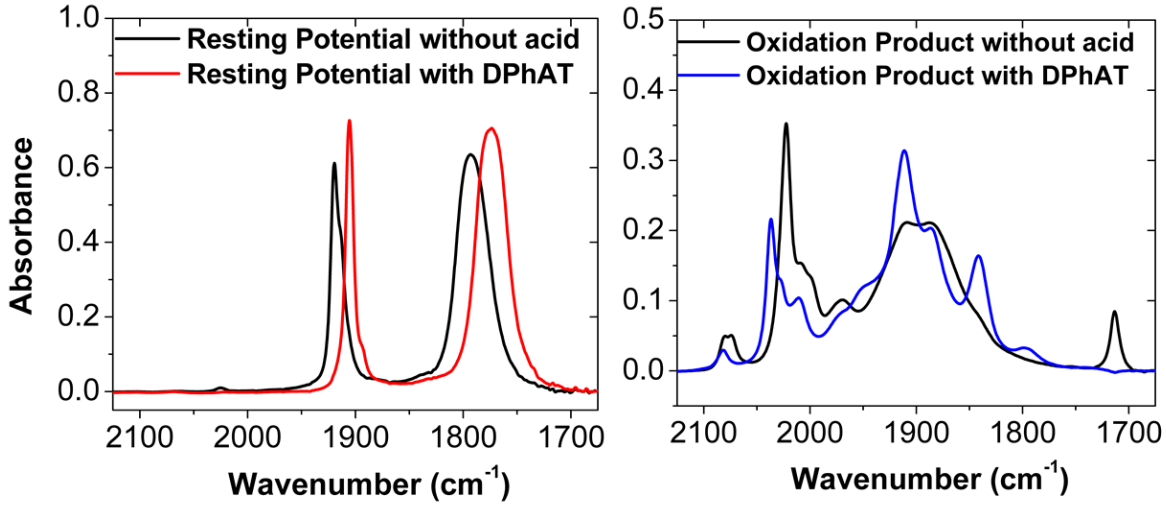



**Figure S7**. IR-SEC data comparing the species at resting potential and the oxidation products of K[MoTtz(CO)$_3$] (**3**$^-$) (0.013 M) with and without added DPhAT (0.03 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

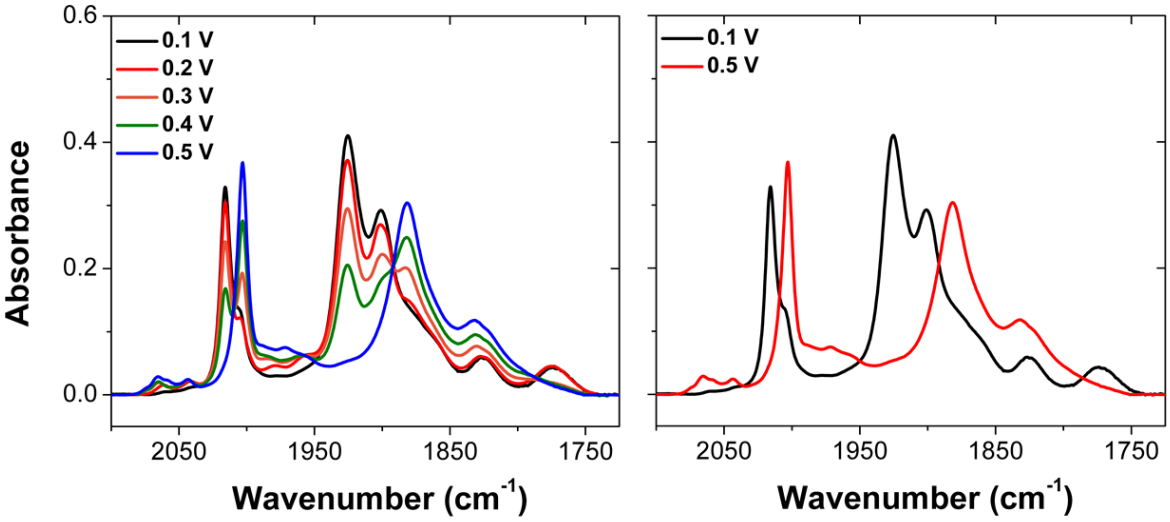



**Figure S8**. IR-SEC data from the oxidation of K[WTtz(CO)$_3$] (**5**$^-$) (0.013 M) with added 2-methoxypyridinium triflate (0.058 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

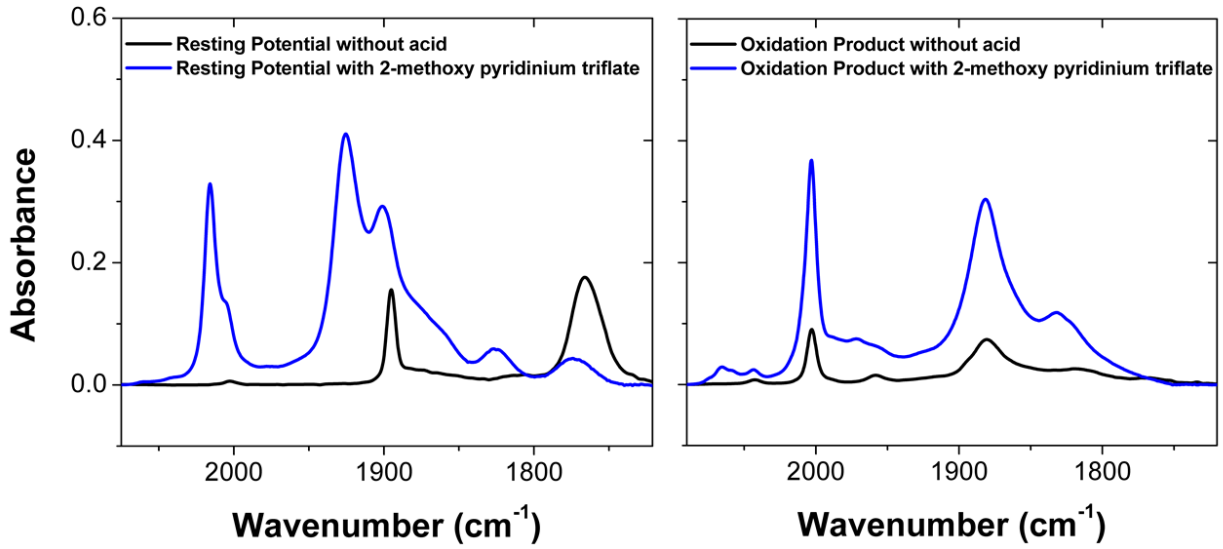



**Figure S9**. IR-SEC data comparing the species at resting potential and the oxidation products of K[WTtz(CO)$_3$] (**5**$^-$) (0.013 M) with and without added 2-methoxypyridinium triflate (0.058 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

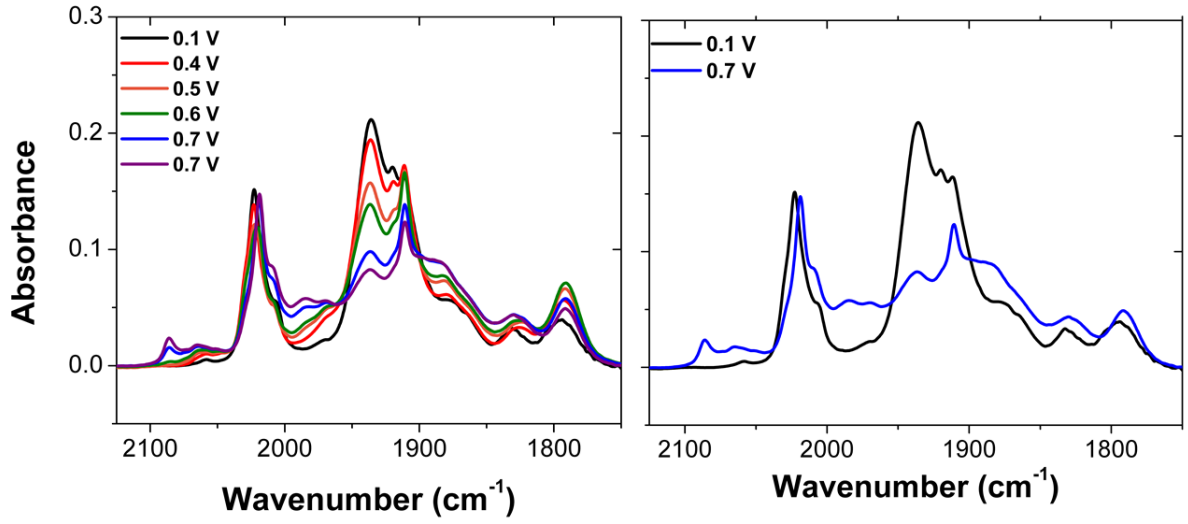



**Figure S10**. IR-SEC data from the oxidation of K[WTtz(CO)$_3$] (**5**$^-$) (0.007 M) with added DPhAT (0.019 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

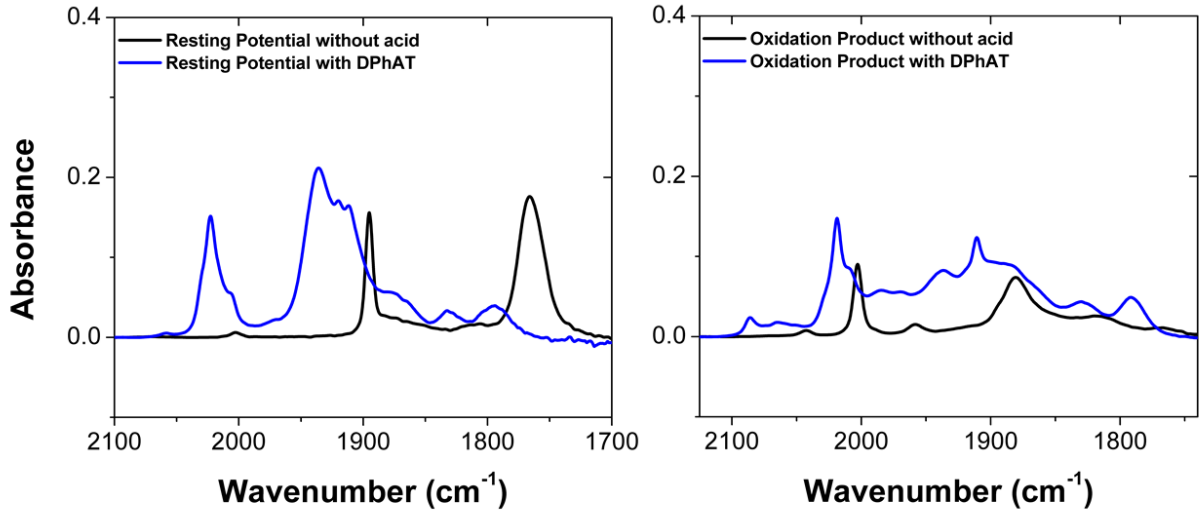



**Figure S11**. IR-SEC data comparing the species at resting potential and the oxidation products of K[WTtz(CO)$_3$] (**5**$^-$) (0.007 M) with and without added DPhAT (0.019 M). Conditions: glassy carbon working electrode, glassy carbon counter electrode, Ag bare metal pseudoreference electrode; internal ferrocene reference; referenced to NHE.

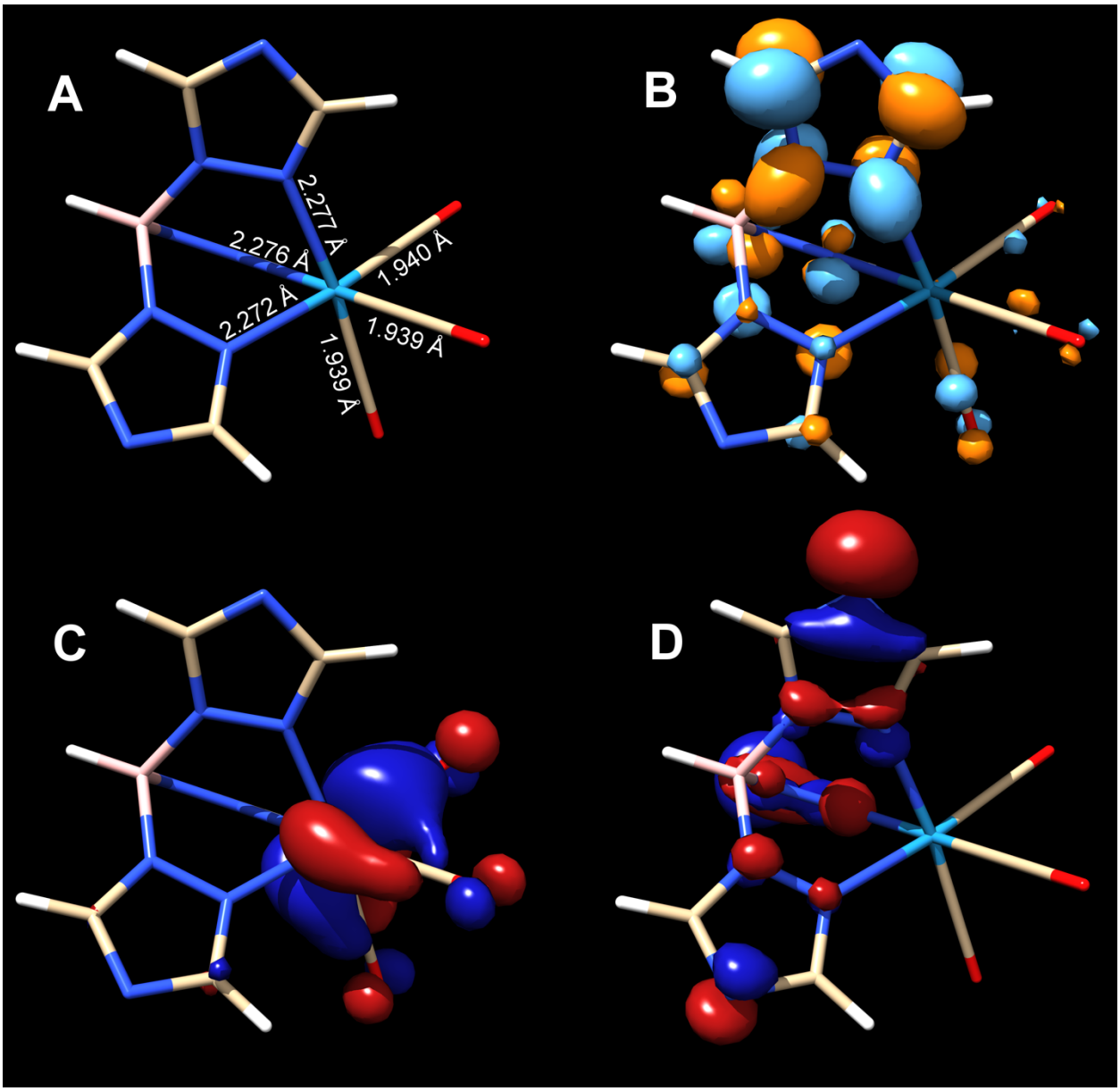



**Figure S12.** Kohn-Sham orbital representations of $[W(Ttz)(CO)_3]^-$ **5**$^-$ (A); LUMO (B); HOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

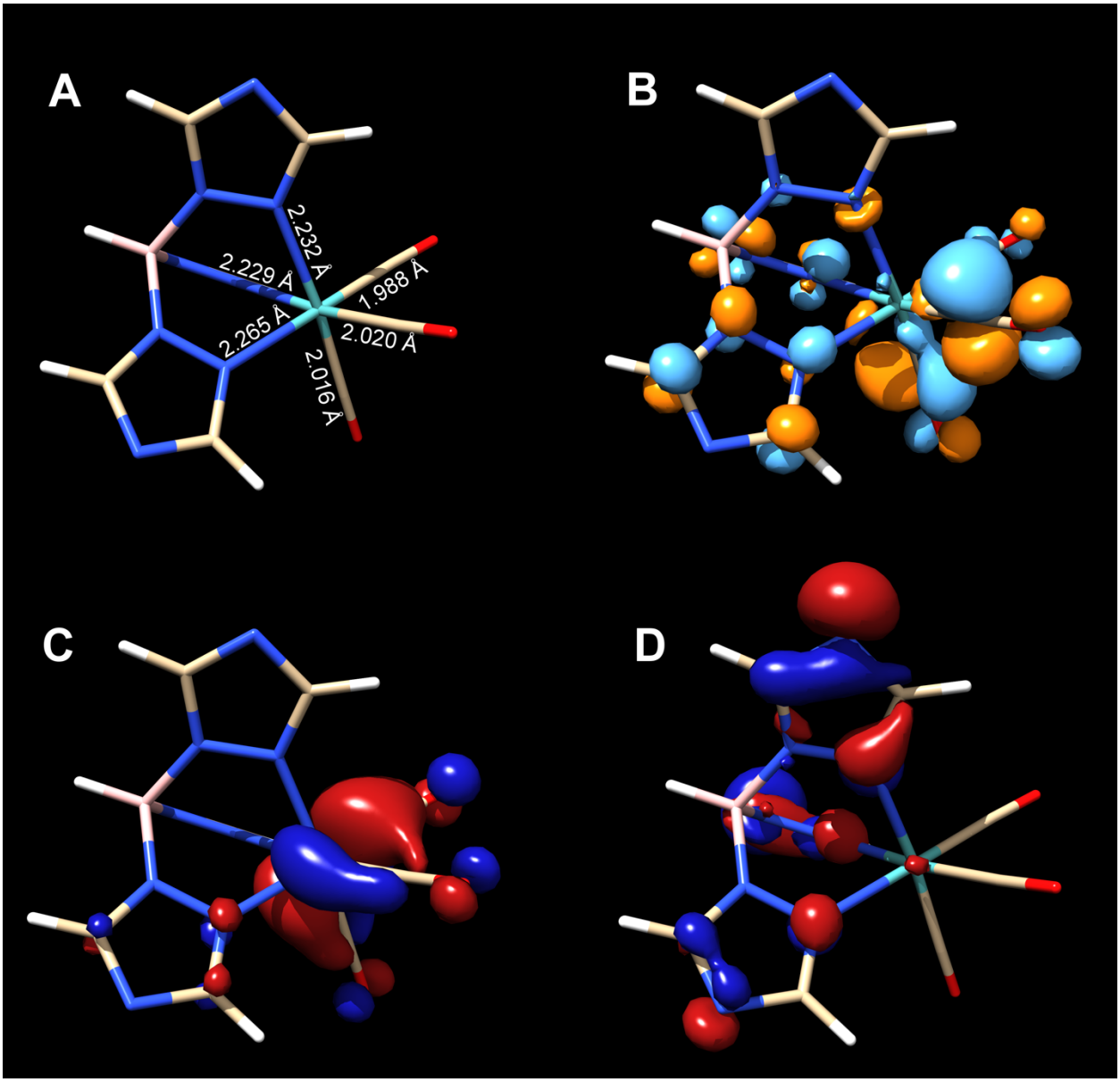



**Figure S13.** Kohn-Sham orbital representations of [Mo(Ttz)$(CO)_3$] **3** (A); LUMO (B); SOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

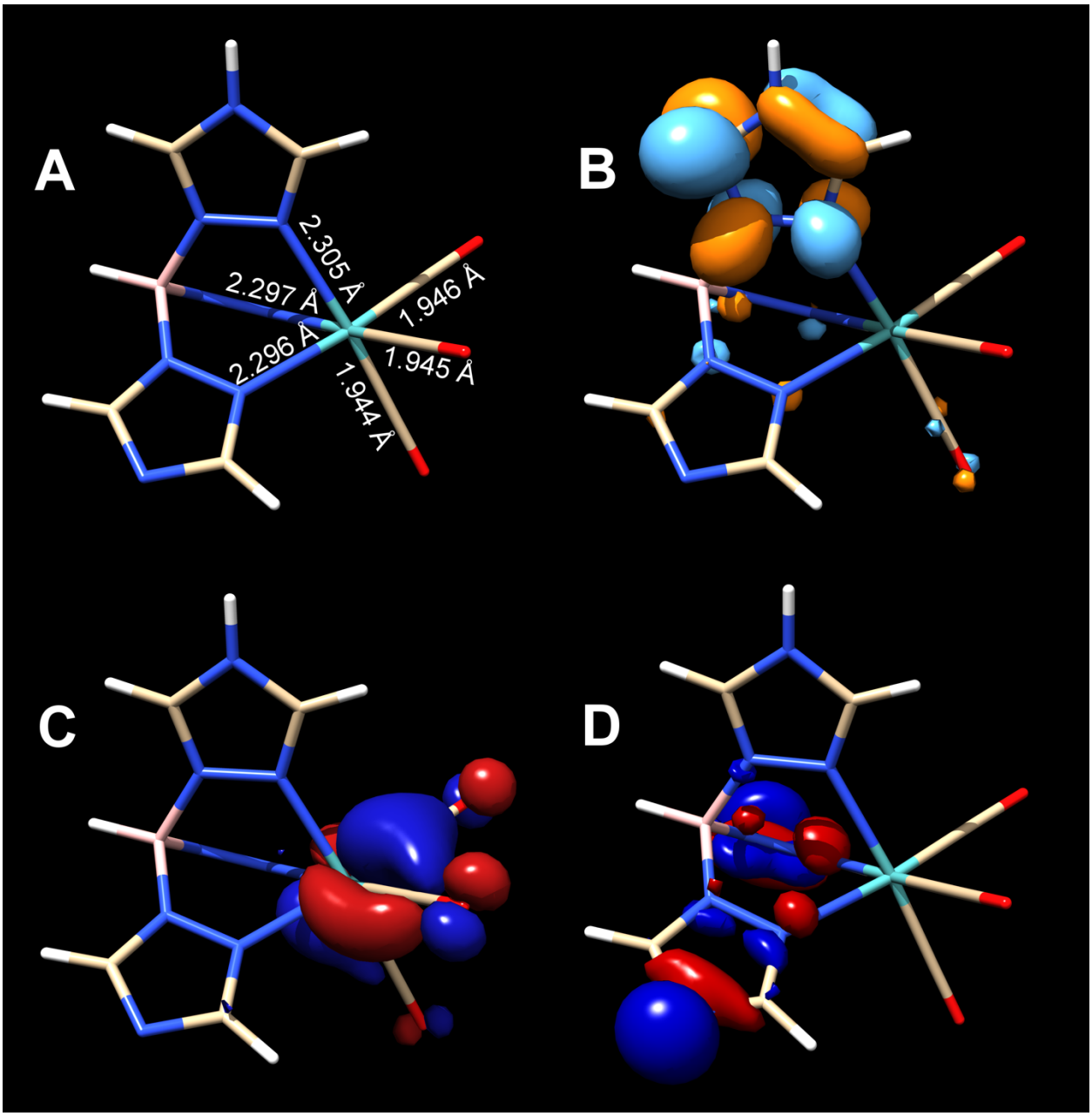



**Figure S14.** Kohn-Sham orbital representations of [Mo(HTtz)$(CO)_3$] **3H** (A); LUMO (B); HOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

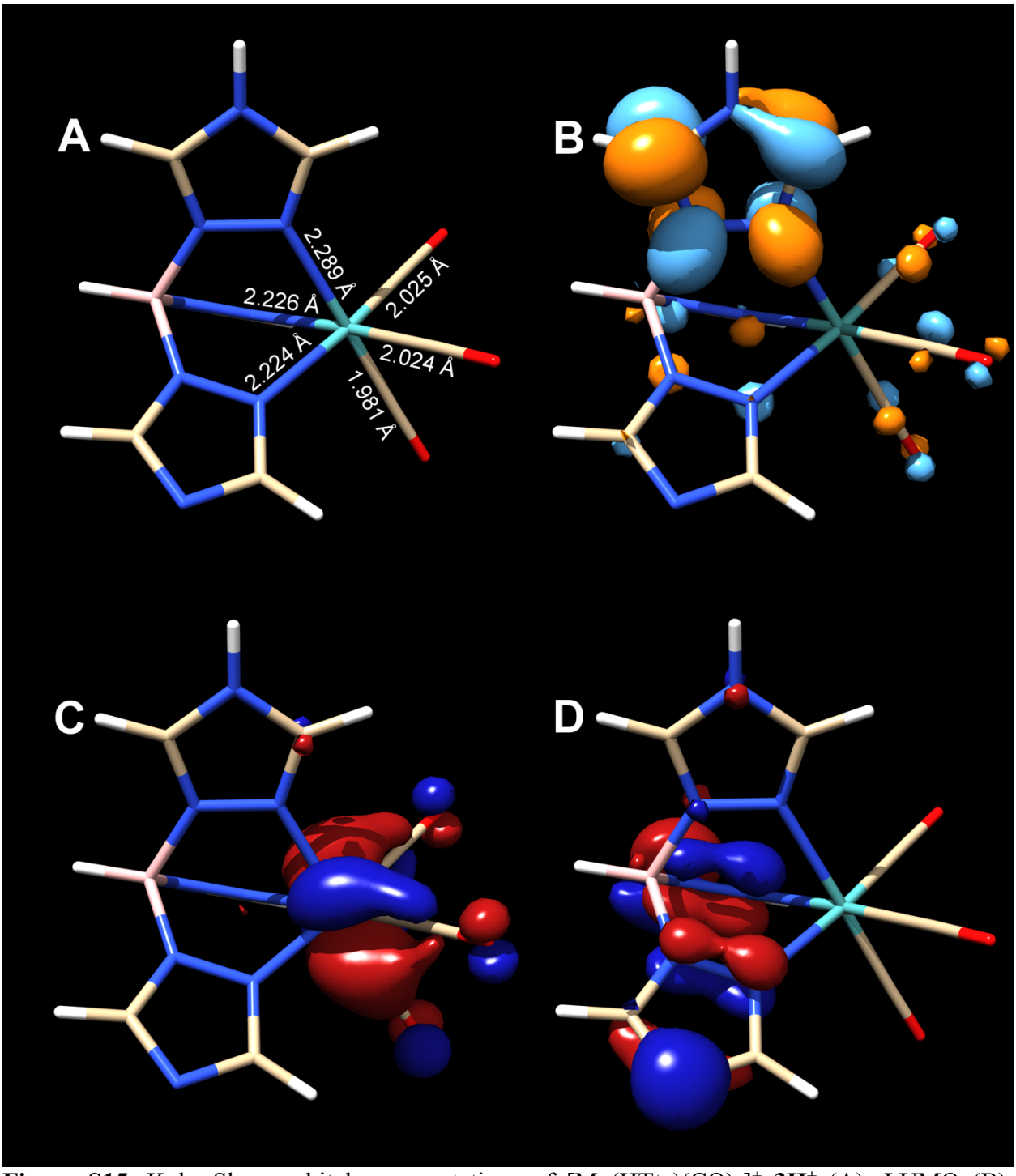



**Figure S15**. Kohn-Sham orbital representations of $[Mo(HTtz)(CO)_3]^+$ **3H**$^+$ (A); LUMO (B); SOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

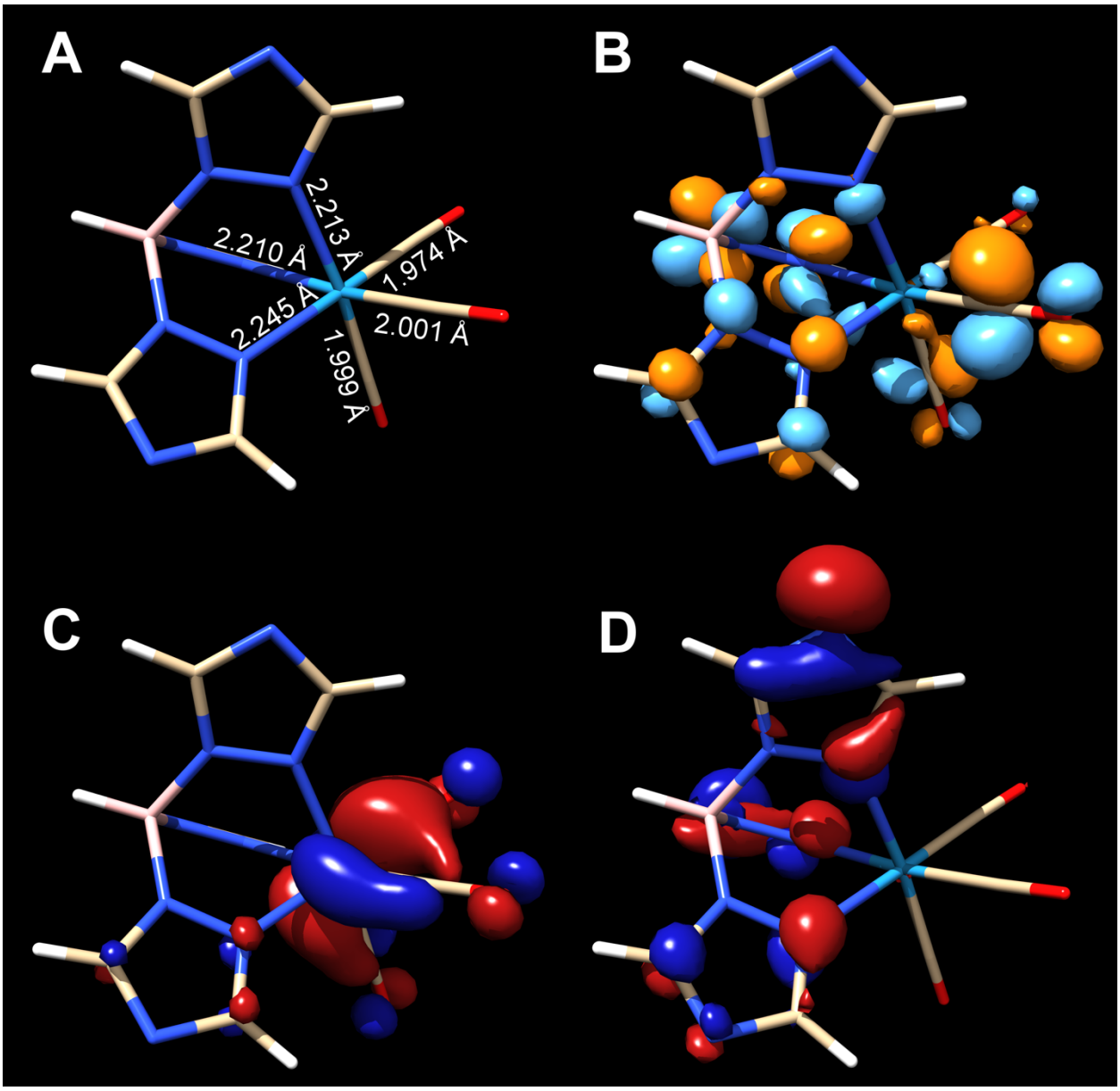



**Figure S16.** Kohn-Sham orbital representations of [W(Ttz)CO$_3$] **5** (A); LUMO (B); SOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

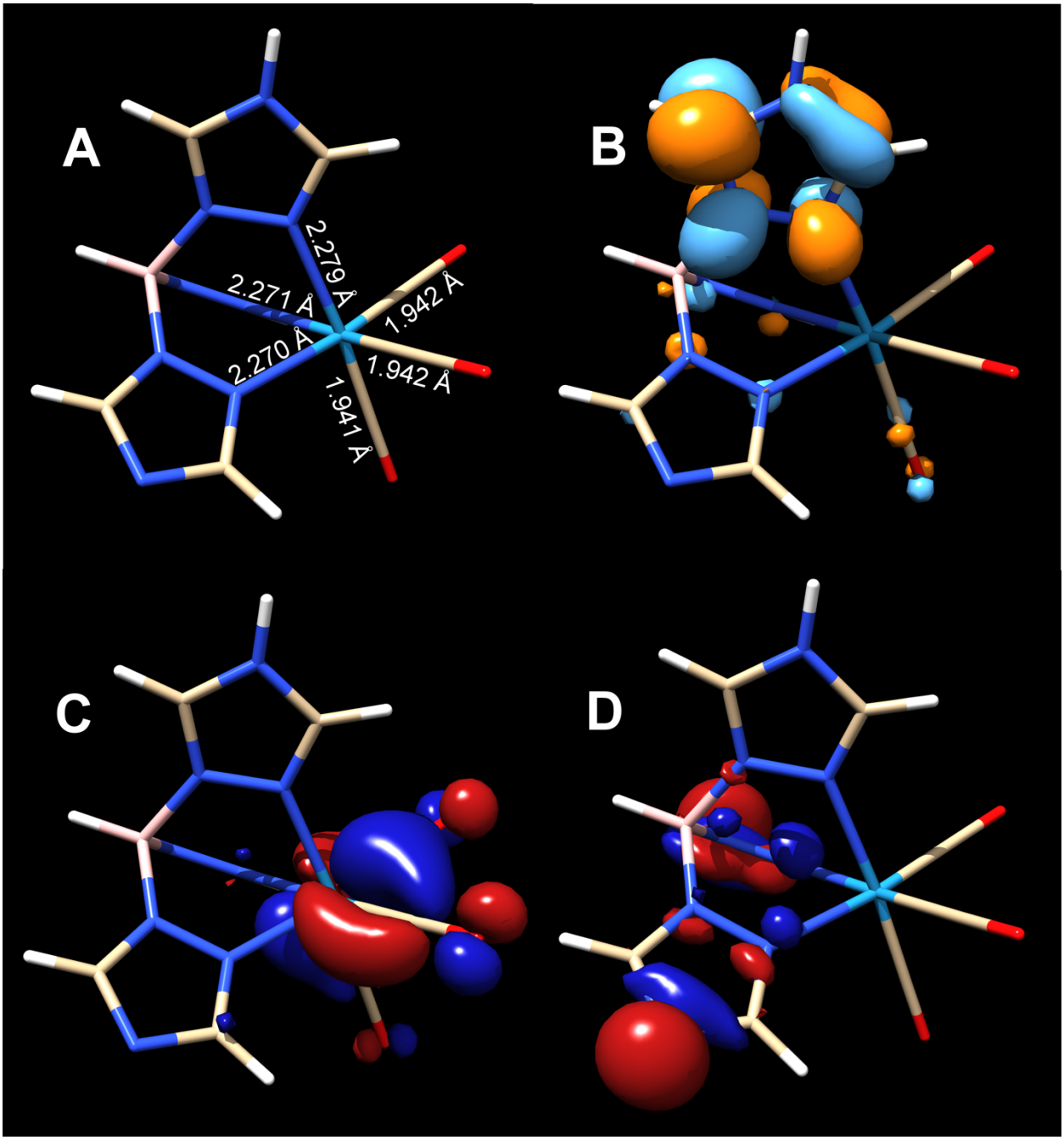



**Figure S17.** Kohn-Sham orbital representations of [W(HTtz)$(CO)_3$] **5H** (A); LUMO (B); HOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

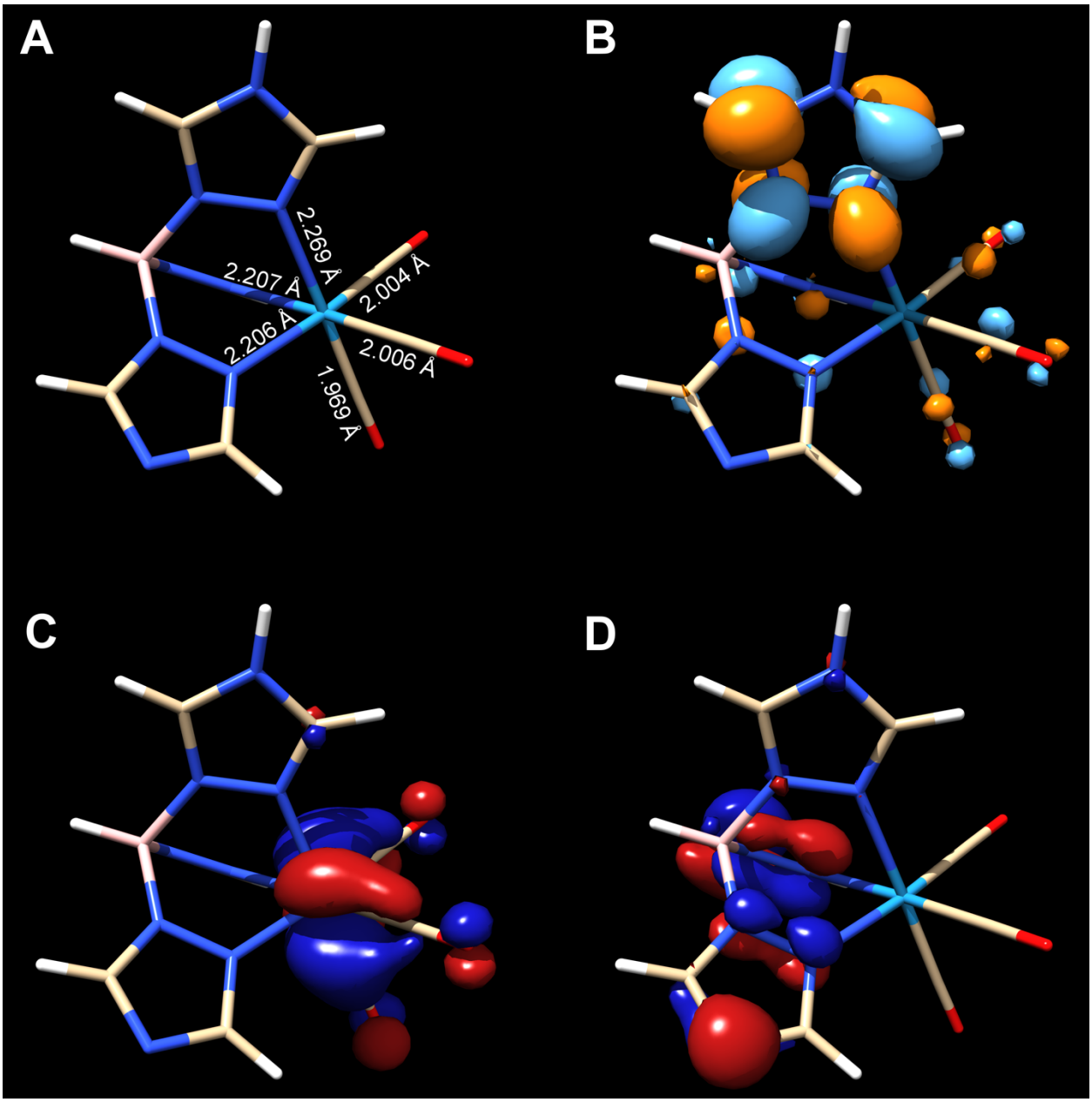



**Figure S18.** Kohn-Sham orbital representations of $[W(HTtz)(CO)_3]^+$ **5H**$^+$ (A); LUMO (B); SOMO (C); and (D) HOMO-7. ORCA 4.0.0; B3LYP/G; ZORA; def2-TZVP; CPCM(Acetonitrile).

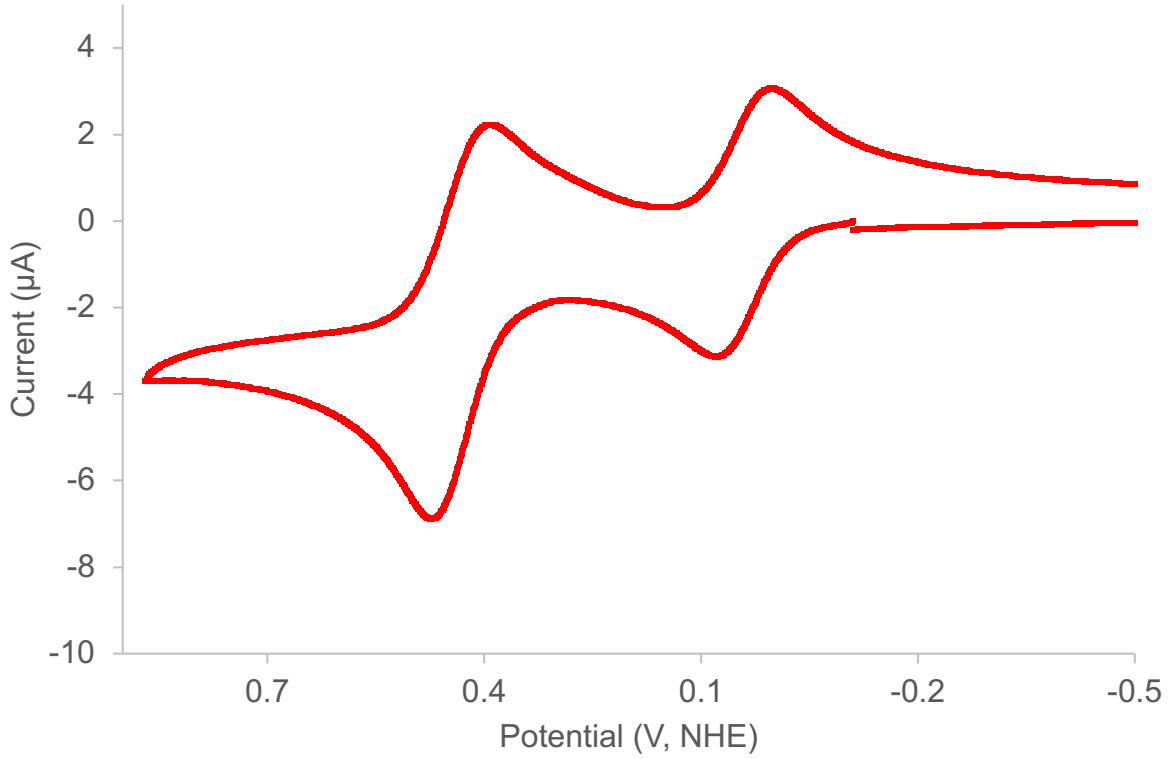



**Figure S19.** Cyclic Voltammogram of 0.002 M **3**$^{-}$ and 0.01 M $BF_3$-etherate with decamethylferrocene and tetrabutylammonium hexafluorophosphate in acetonitrile.

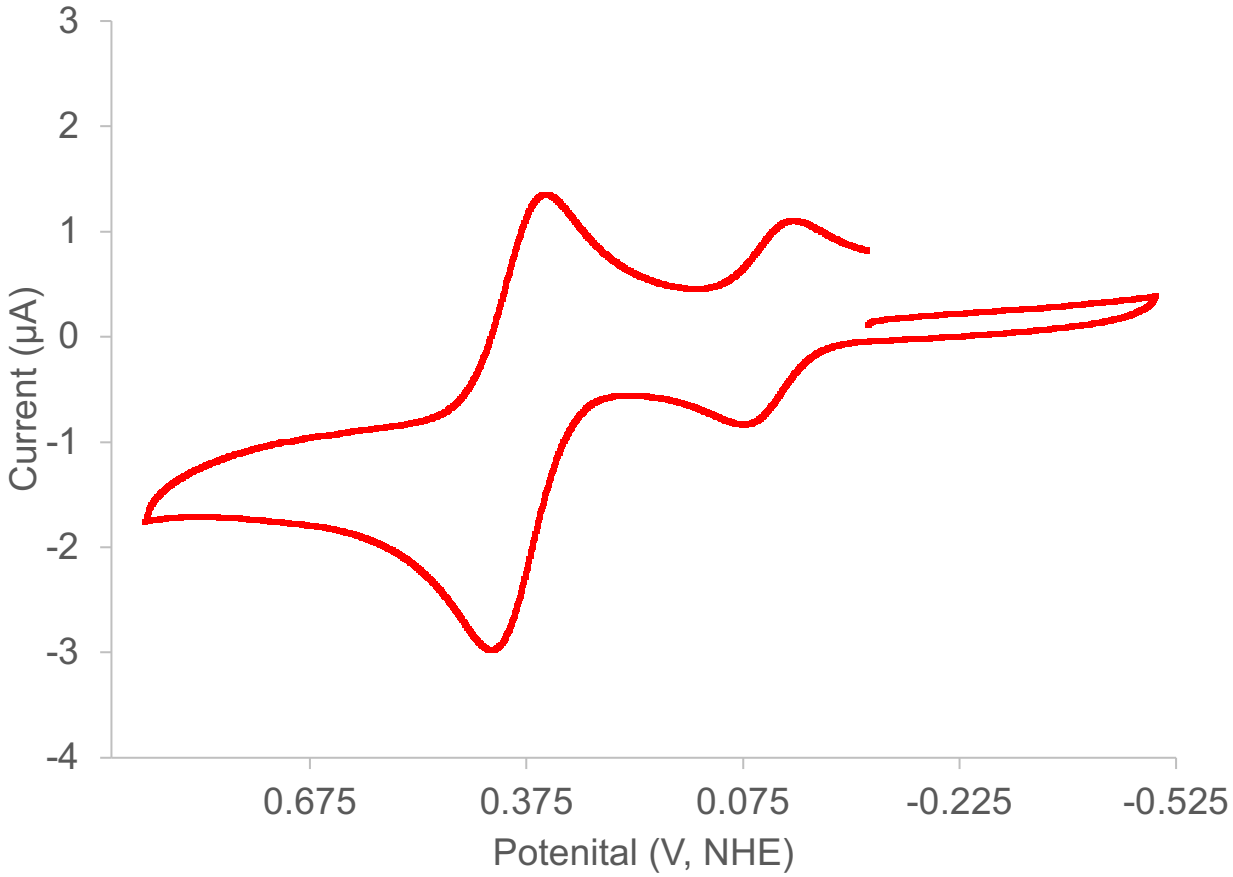
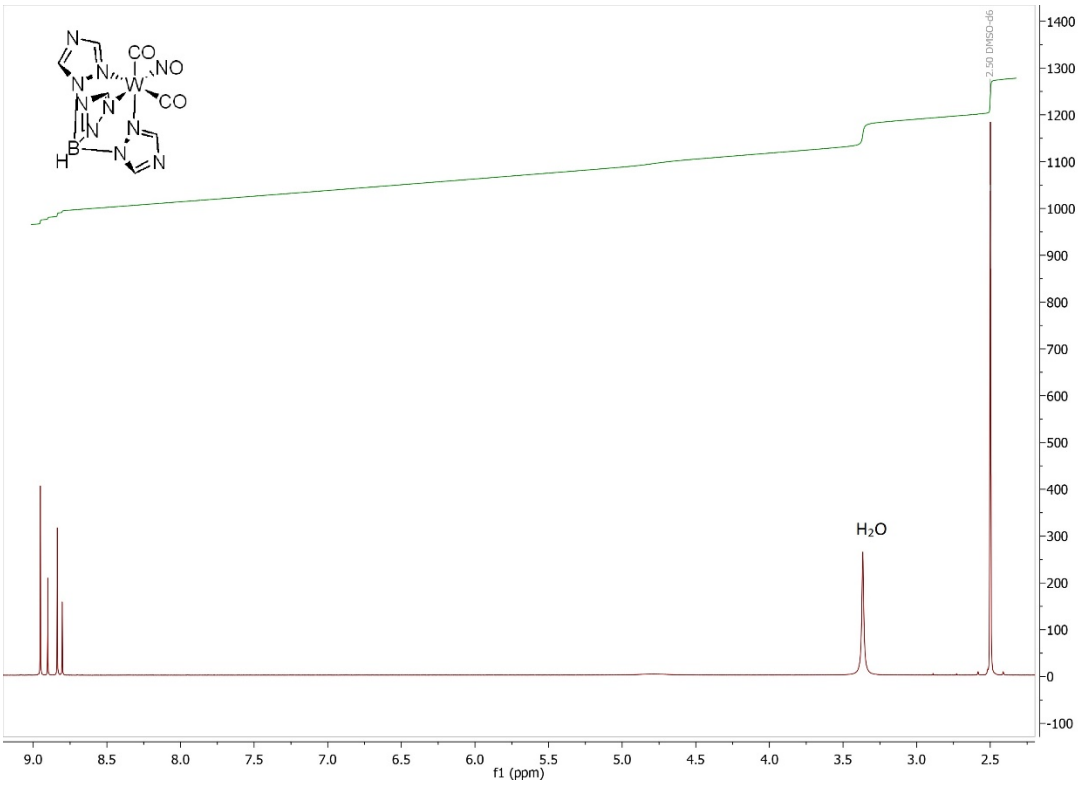
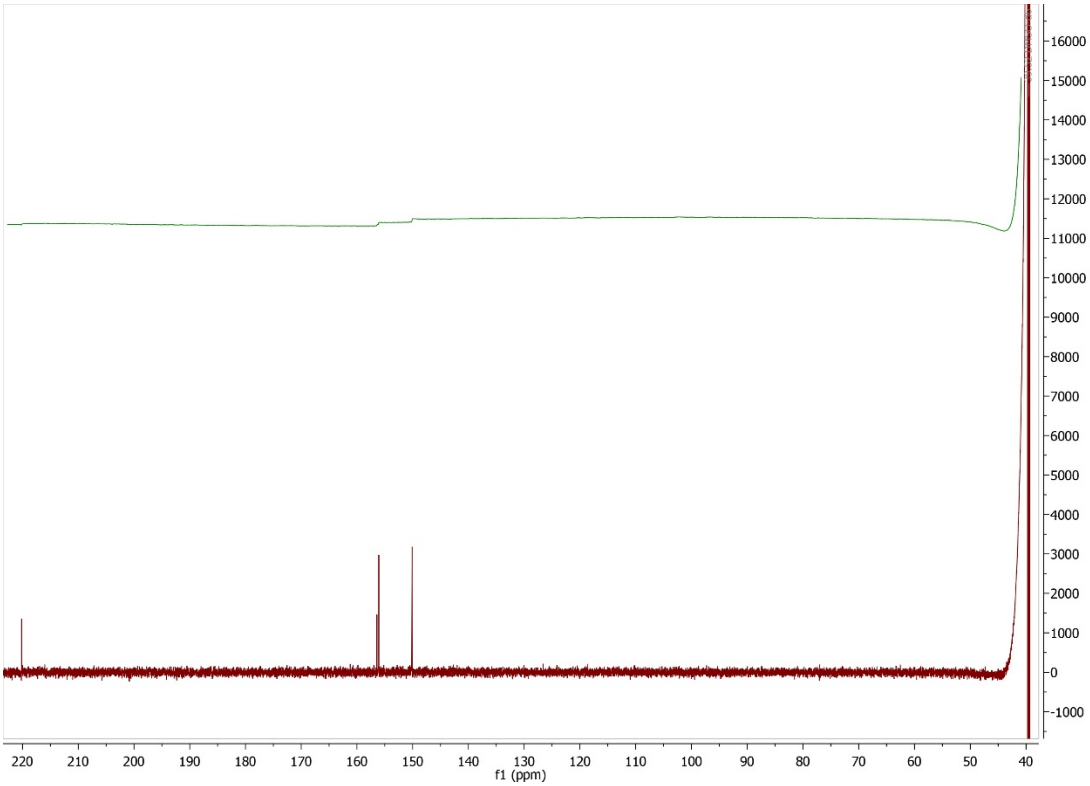



**Figure S20.** Cyclic Voltammogram of 0.002 M **5**$^{-}$ and 0.01 M $BF_3$-etherate with decamethylferrocene and tetrabutylammonium hexafluorophosphate in acetonitrile.

**$^{1}$H-NMR ($d_6$-DMSO) and $^{13}$C{$^{1}$H}-NMR ($d_6$-DMSO) of Compound 9:**



**$^{1}$H-NMR ($d_6$-MeCN) of $BF_3$•$Et_2O$ added to Compound 3:**

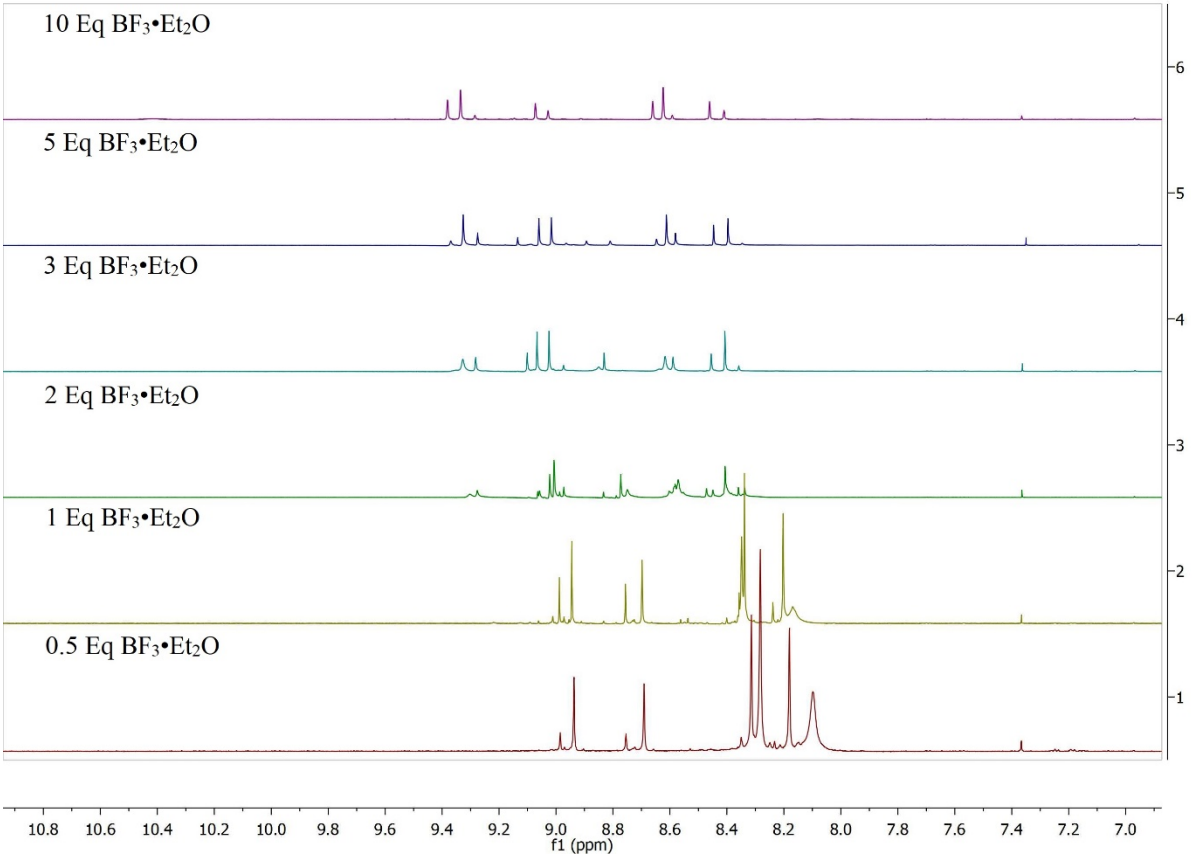


**Table S1**. Mulliken Charges

$[Mo(Ttz)(CO)_3]^-$ **3**$^-$

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | |
|---|---|---|
| 0 | Mo: | 1.022843 0.000000 |
| 1 | O : | -0.286466 0.000000 |
| 2 | C : | 0.002725 0.000000 |
| 3 | O : | -0.285554 0.000000 |
| 4 | N : | 0.072683 0.000000 |
| 5 | C : | 0.014449 0.000000 |
| 6 | N : | 0.052979 0.000000 |
| 7 | N : | 0.069447 0.000000 |
| 8 | C : | 0.010613 0.000000 |
| 9 | N : | -0.251737 0.000000 |
| 10 | C : | -0.010354 0.000000 |
| 11 | H : | 0.195144 0.000000 |
| 12 | Nexo: | -0.364909 0.000000 |
| 13 | B : | 0.096203 0.000000 |
| 14 | Nexo: | -0.363860 0.000000 |
| 15 | N : | -0.233705 0.000000 |
| 16 | C : | -0.005014 0.000000 |
| 17 | H : | 0.194208 0.000000 |
| 18 | C : | 0.002419 0.000000 |
| 19 | H : | 0.190573 0.000000 |
| 20 | N : | -0.251427 0.000000 |
| 21 | C : | -0.223501 0.000000 |
| 22 | Nexo: | -0.369147 0.000000 |
| 23 | C : | -0.231423 0.000000 |
| 24 | C : | -0.234940 0.000000 |
| 25 | H : | -0.057191 0.000000 |
| 26 | H : | 0.174151 0.000000 |
| 27 | O : | -0.288332 0.000000 |
| 28 | H : | 0.186068 0.000000 |
| 29 | H : | 0.173051 0.000000 |

Sum of atomic charges : -1.0000000

Sum of atomic spin populations: 0.0000000

[Mo(HTtz)(CO)$_3$] **3H**

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | | |
|---|---|---|---|
| 0 | Mo: | 0.993914 | 0.000000 |
| 1 | O : | -0.272912 | 0.000000 |
| 2 | C : | 0.008431 | 0.000000 |
| 3 | O : | -0.267500 | 0.000000 |
| 4 | N : | 0.076131 | 0.000000 |
| 5 | C : | 0.019779 | 0.000000 |
| 6 | N : | 0.074542 | 0.000000 |
| 7 | N : | 0.073832 | 0.000000 |
| 8 | C : | 0.092396 | 0.000000 |
| 9 | N : | -0.252274 | 0.000000 |
| 10 | C : | -0.006440 | 0.000000 |
| 11 | H : | 0.199758 | 0.000000 |
| 12 | Nexo: | -0.356498 | 0.000000 |
| 13 | B : | 0.089929 | 0.000000 |
| 14 | Nexo: | -0.355152 | 0.000000 |
| 15 | N : | -0.193300 | 0.000000 |
| 16 | C : | -0.001000 | 0.000000 |
| 17 | C : | 0.095662 | 0.000000 |
| 18 | H : | 0.249963 | 0.000000 |
| 19 | N : | -0.252836 | 0.000000 |
| 20 | C : | -0.211896 | 0.000000 |
| 21 | NexoH: | -0.174340 | 0.000000 |
| 22 | C : | -0.219620 | 0.000000 |
| 23 | C : | -0.223459 | 0.000000 |
| 24 | H : | -0.032532 | 0.000000 |
| 25 | H : | 0.178595 | 0.000000 |
| 26 | O : | -0.274933 | 0.000000 |
| 27 | H : | 0.189903 | 0.000000 |
| 28 | H : | 0.229887 | 0.000000 |
| 29 | H : | 0.323655 | 0.000000 |
| 30 | H : | 0.198317 | 0.000000 |

Sum of atomic charges : -0.0000000

Sum of atomic spin populations: 0.0000000

[Mo(Ttz)(CO)$_3$] **3**

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | | |
|---|---|---|---|
| 0 | Mo: | 0.915345 | 0.879662 |
| 1 | O : | -0.113064 | 0.055888 |
| 2 | C : | 0.013397 | 0.019202 |
| 3 | O : | -0.160774 | 0.021889 |
| 4 | N : | 0.064072 | -0.001595 |
| 5 | C : | 0.024814 | 0.020811 |
| 6 | N : | 0.055046 | 0.002034 |
| 7 | N : | 0.059136 | -0.002070 |
| 8 | C : | 0.022862 | 0.006873 |
| 9 | N : | -0.232456 | -0.021423 |
| 10 | C : | 0.014224 | 0.015370 |
| 11 | H : | 0.203686 | -0.000706 |
| 12 | Nexo: | -0.348578 | -0.001538 |
| 13 | B : | 0.097084 | -0.002329 |
| 14 | Nexo: | -0.346022 | -0.001773 |
| 15 | N : | -0.223744 | -0.024687 |
| 16 | C : | 0.018771 | 0.016901 |
| 17 | H : | 0.203521 | -0.000768 |
| 18 | C : | 0.015301 | -0.000265 |
| 19 | H : | 0.197698 | 0.000399 |
| 20 | N : | -0.230958 | -0.020628 |
| 21 | C : | -0.097666 | 0.000258 |
| 22 | Nexo: | -0.357256 | -0.000050 |
| 23 | C : | -0.101036 | 0.000883 |
| 24 | C : | -0.114942 | -0.015700 |
| 25 | H : | -0.039503 | 0.000028 |
| 26 | H : | 0.190442 | -0.000935 |
| 27 | O : | -0.116812 | 0.055038 |
| 28 | H : | 0.201418 | -0.000915 |
| 29 | H : | 0.185993 | 0.000144 |

Sum of atomic charges : -0.0000000

Sum of atomic spin populations: 1.0000000

$[Mo(HTtz)(CO)_3]^+$ **3H**$^+$

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | |
|---|---|---|
| 0 Mo: | 0.893124 | 0.884880 |
| 1 O : | -0.099176 | 0.057446 |
| 2 C : | 0.020379 | 0.020323 |
| 3 O : | -0.151743 | 0.016391 |
| 4 N : | 0.068164 | -0.001820 |
| 5 C : | 0.030694 | 0.021653 |
| 6 N : | 0.081223 | 0.001570 |
| 7 N : | 0.064991 | -0.002249 |
| 8 C : | 0.106532 | 0.006151 |
| 9 N : | -0.234347 | -0.021994 |
| 10 C : | 0.018359 | 0.016335 |
| 11 H : | 0.208494 | -0.000726 |
| 12 Nexo: | -0.339734 | -0.001669 |
| 13 B : | 0.089722 | -0.002225 |
| 14 Nexo: | -0.337326 | -0.001883 |
| 15 N : | -0.186716 | -0.020541 |
| 16 C : | 0.023312 | 0.017552 |
| 17 C : | 0.105682 | -0.000379 |
| 18 H : | 0.256250 | 0.000301 |
| 19 N : | -0.232698 | -0.021321 |
| 20 C : | -0.086653 | -0.000226 |
| 21 NexoH: | -0.166120 | 0.000051 |
| 22 C : | -0.091644 | -0.001911 |
| 23 C : | -0.104424 | -0.022648 |
| 24 H : | -0.016139 | 0.000014 |
| 25 H : | 0.194844 | -0.000958 |
| 26 O : | -0.099772 | 0.059564 |
| 27 H : | 0.205589 | -0.000976 |
| 28 H : | 0.242337 | 0.000117 |
| 29 H : | 0.328938 | -0.000046 |
| 30 H : | 0.207860 | -0.000774 |

Sum of atomic charges : 1.0000000

Sum of atomic spin populations: 1.0000000

$[W(Ttz)(CO)_3]^-$ **5**$^-$

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | |
|---|---|---|
| 0 | W : | 0.643111 0.000000 |
| 1 | O : | -0.314275 0.000000 |
| 2 | C : | 0.003133 0.000000 |
| 3 | O : | -0.313353 0.000000 |
| 4 | N : | 0.049875 0.000000 |
| 5 | C : | 0.017998 0.000000 |
| 6 | N : | 0.030681 0.000000 |
| 7 | N : | 0.046528 0.000000 |
| 8 | C : | 0.013006 0.000000 |
| 9 | N : | -0.210485 0.000000 |
| 10 | C : | -0.002776 0.000000 |
| 11 | H : | 0.197754 0.000000 |
| 12 | Nexo: | -0.355885 0.000000 |
| 13 | B : | 0.083659 0.000000 |
| 14 | Nexo: | -0.353495 0.000000 |
| 15 | N : | -0.192242 0.000000 |
| 16 | C : | 0.002091 0.000000 |
| 17 | H : | 0.197576 0.000000 |
| 18 | C : | 0.009693 0.000000 |
| 19 | H : | 0.193782 0.000000 |
| 20 | N : | -0.208779 0.000000 |
| 21 | C : | -0.113866 0.000000 |
| 22 | Nexo: | -0.359152 0.000000 |
| 23 | C : | -0.120093 0.000000 |
| 24 | C : | -0.131071 0.000000 |
| 25 | H : | -0.047177 0.000000 |
| 26 | H : | 0.179877 0.000000 |
| 27 | O : | -0.315233 0.000000 |
| 28 | H : | 0.190803 0.000000 |
| 29 | H : | 0.178315 0.000000 |

Sum of atomic charges : -1.0000000

Sum of atomic spin populations: 0.0000000

[W(HTtz)(CO)$_3$] **5H**

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | |
|---|---|---|
| 0 W : | 0.642378 | 0.000000 |
| 1 O : | -0.299064 | 0.000000 |
| 2 C : | 0.008934 | 0.000000 |
| 3 O : | -0.292848 | 0.000000 |
| 4 N : | 0.054240 | 0.000000 |
| 5 C : | 0.022671 | 0.000000 |
| 6 N : | 0.054558 | 0.000000 |
| 7 N : | 0.051412 | 0.000000 |
| 8 C : | 0.099970 | 0.000000 |
| 9 N : | -0.212949 | 0.000000 |
| 10 C : | 0.000968 | 0.000000 |
| 11 H : | 0.202401 | 0.000000 |
| 12 Nexo: | -0.347445 | 0.000000 |
| 13 B : | 0.071356 | 0.000000 |
| 14 Nexo: | -0.345191 | 0.000000 |
| 15 N : | -0.156620 | 0.000000 |
| 16 C : | 0.006543 | 0.000000 |
| 17 C : | 0.102200 | 0.000000 |
| 18 H : | 0.252338 | 0.000000 |
| 19 N : | -0.211543 | 0.000000 |
| 20 C : | -0.111336 | 0.000000 |
| 21 NexoH: | -0.170323 | 0.000000 |
| 22 C : | -0.115037 | 0.000000 |
| 23 C : | -0.125248 | 0.000000 |
| 24 H : | -0.023247 | 0.000000 |
| 25 H : | 0.184467 | 0.000000 |
| 26 O : | -0.300064 | 0.000000 |
| 27 H : | 0.195020 | 0.000000 |
| 28 H : | 0.235416 | 0.000000 |
| 29 H : | 0.324338 | 0.000000 |
| 30 H : | 0.201705 | 0.000000 |

Sum of atomic charges : -0.0000000

Sum of atomic spin populations: 0.0000000

[W(Ttz)(CO)$_3$] **5**

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | | |
|---|---|---|---|
| 0 | W : | 0.761113 | 0.785616 |
| 1 | O : | -0.141088 | 0.072163 |
| 2 | C : | 0.010430 | 0.020994 |
| 3 | O : | -0.190274 | 0.026798 |
| 4 | N : | 0.042280 | -0.002411 |
| 5 | C : | 0.027175 | 0.022481 |
| 6 | N : | 0.032584 | 0.001166 |
| 7 | N : | 0.039051 | -0.002817 |
| 8 | C : | 0.026167 | 0.002277 |
| 9 | N : | -0.196863 | -0.015593 |
| 10 | C : | 0.021897 | 0.017318 |
| 11 | H : | 0.207403 | -0.000775 |
| 12 | Nexo: | -0.337695 | -0.002054 |
| 13 | B : | 0.074477 | -0.001868 |
| 14 | Nexo: | -0.334053 | -0.002281 |
| 15 | N : | -0.182303 | -0.009518 |
| 16 | C : | 0.024786 | 0.018825 |
| 17 | H : | 0.208296 | -0.000833 |
| 18 | C : | 0.023444 | -0.000339 |
| 19 | H : | 0.201309 | 0.000407 |
| 20 | N : | -0.192795 | -0.014863 |
| 21 | C : | -0.069717 | 0.013013 |
| 22 | Nexo: | -0.347918 | 0.000142 |
| 23 | C : | -0.075962 | 0.013030 |
| 24 | C : | -0.052981 | -0.008492 |
| 25 | H : | -0.028396 | 0.000005 |
| 26 | H : | 0.196130 | -0.001108 |
| 27 | O : | -0.143641 | 0.071471 |
| 28 | H : | 0.206036 | -0.001140 |
| 29 | H : | 0.191110 | -0.001614 |

Sum of atomic charges : -0.0000000

Sum of atomic spin populations: 1.0000000

$[W(HTtz)(CO)_3]^+$ **5H**$^+$

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MULLIKEN ATOMIC CHARGES AND SPIN POPULATIONS

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| | | |
|---|---|---|
| 0 W : | 0.774498 | 0.778915 |
| 1 O : | -0.130326 | 0.074428 |
| 2 C : | 0.015835 | 0.022273 |
| 3 O : | -0.182330 | 0.021825 |
| 4 N : | 0.044556 | -0.002776 |
| 5 C : | 0.030404 | 0.023668 |
| 6 N : | 0.060330 | 0.000978 |
| 7 N : | 0.042587 | -0.003206 |
| 8 C : | 0.113059 | 0.001796 |
| 9 N : | -0.196571 | -0.015696 |
| 10 C : | 0.027514 | 0.018731 |
| 11 H : | 0.212440 | -0.000807 |
| 12 Nexo: | -0.328409 | -0.002150 |
| 13 B : | 0.061833 | -0.001806 |
| 14 Nexo: | -0.325101 | -0.002425 |
| 15 N : | -0.146643 | -0.007047 |
| 16 C : | 0.031969 | 0.019970 |
| 17 C : | 0.112604 | -0.000484 |
| 18 H : | 0.259547 | 0.000361 |
| 19 N : | -0.193291 | -0.015219 |
| 20 C : | -0.069815 | 0.013074 |
| 21 NexoH: | -0.161830 | 0.000166 |
| 22 C : | -0.073552 | 0.010484 |
| 23 C : | -0.049005 | -0.011135 |
| 24 H : | -0.004471 | -0.000004 |
| 25 H : | 0.201346 | -0.001253 |
| 26 O : | -0.126885 | 0.081090 |
| 27 H : | 0.210531 | -0.001340 |
| 28 H : | 0.246633 | -0.001513 |
| 29 H : | 0.330213 | -0.000045 |
| 30 H : | 0.212329 | -0.000854 |

Sum of atomic charges : 1.0000000

Sum of atomic spin populations: 1.0000000

**Table S2.** Bond lengths of the primary coordination sphere for computed structures.

| Complex | M–N1 | M–N2 | M–N3 | M–C1 | M–C2 | M–C3 |
|---|---|---|---|---|---|---|
| **3**$^{-}$ | 2.298 | 2.302 | 2.303 | 1.942 | 1.943 | 1.944 |
| **3** | 2.229 | 2.232 | 2.265 | 1.988 | 2.016 | 2.020 |
| **3H** | 2.296 | 2.297 | 2.305* | 1.944$^{\dagger}$ | 1.945 | 1.946 |
| **3H**$^{+}$ | 2.224 | 2.226 | 2.289* | 1.981$^{\dagger}$ | 2.024 | 2.025 |
| **5**$^{-}$ | 2.272 | 2.276 | 2.277 | 1.939 | 1.939 | 1.940 |
| **5** | 2.210 | 2.213 | 2.245 | 1.974 | 1.999 | 2.001 |
| **5H** | 2.270 | 2.271 | 2.279* | 1.941$^{\dagger}$ | 1.942 | 1.942 |
| **5H**$^{+}$ | 2.206 | 2.207 | 2.269* | 1.969$^{\dagger}$ | 2.004 | 2.006 |

All distances in Angstroms.

* - denotes protonated triazole; $^{\dagger}$ - denotes CO *trans* to protonated triazole.

***DFT Coordinates***

[Mo(Ttz)(CO)$_3$] **3**$^-$

| | | | |
|---|---|---|---|
| Mo | 2.94053312599688 | 3.18705611242101 | 1.18288972308944 |
| O | 3.60256869086909 | 0.17111569118379 | 1.59755270084902 |
| C | 6.11670203255854 | 3.71748108822551 | 2.15396839446395 |
| O | 4.14656418589984 | 2.89246855644533 | -1.67534515565584 |
| N | 4.75972248197280 | 5.07547375876729 | 3.06137519415467 |
| C | 2.00718469616080 | 6.23518404100160 | 0.12000144930377 |
| N | 2.46943367174854 | 4.69323344081944 | 3.99516154095068 |
| N | 2.79636642703574 | 6.28028439372096 | 2.09064104405124 |
| C | 1.31784672006476 | 2.91249610939942 | 4.10590385778166 |
| N | 2.51404526593553 | 5.44497857273495 | 1.05116536261387 |
| C | 5.99814767659202 | 5.33536012695533 | 3.48998414339332 |
| H | 6.21637374250865 | 6.12602533545816 | 4.18881489890518 |
| N | 6.88172038437140 | 4.50417612233311 | 2.94409870993163 |
| B | 3.41707136163032 | 5.75317455517388 | 3.39926863696688 |
| N | 1.94342835654231 | 7.53263551630874 | 0.49526140058066 |
| N | 2.13570603109389 | 3.56903474720462 | 3.30083736740675 |
| C | 2.44405378255408 | 7.51654014099768 | 1.72752448904063 |
| H | 2.56493695334742 | 8.36861541136962 | 2.37597000337323 |
| C | 1.83596766312187 | 4.64906076088199 | 5.17096483921664 |
| H | 1.93136959140903 | 5.42598522255481 | 5.91162872652436 |
| N | 4.83165934605281 | 4.02634912734640 | 2.19361051350874 |
| C | 1.24199674654645 | 2.60643418865510 | 0.44085321266339 |
| N | 1.10102940815714 | 3.54566457132295 | 5.28075128005196 |
| C | 3.36213747787799 | 1.31021429496619 | 1.45580342935933 |
| C | 3.69951625292853 | 3.01698276589910 | -0.59821684167689 |
| H | 3.58385750562170 | 6.64665483006443 | 4.17264946311480 |
| H | 1.68426848260489 | 5.85791524060293 | -0.83575072363788 |
| O | 0.22454971020014 | 2.23627876482005 | -0.00992521643871 |
| H | 6.49221168526404 | 2.91296906537051 | 1.54373556077476 |
| H | 0.88098054333284 | 1.96773744699510 | 3.82941199533876 |

[Mo(HTtz)(CO)$_3$] **3H**

| | | | |
|---|---|---|---|
| Mo | 2.93679797578977 | 3.17976942590953 | 1.17280029465206 |
| O | 3.63629974336095 | 0.17550040910978 | 1.61922649537977 |
| C | 6.08922809675283 | 3.73112720155813 | 2.18641477716172 |
| O | 4.15376265555864 | 2.89940155677636 | -1.67954231239017 |
| N | 4.71376481751842 | 5.08961915031585 | 3.06421512608165 |
| C | 1.93882890823557 | 6.19873046505546 | 0.10783582815679 |
| N | 2.42380213188530 | 4.69170852672495 | 3.98485617337274 |
| N | 2.73716634263816 | 6.26930647753234 | 2.07367074972017 |
| C | 1.30314736184892 | 2.87022936029467 | 4.06130735695494 |
| N | 2.47432892108096 | 5.42398883555548 | 1.03520989883268 |
| C | 5.94464045177123 | 5.35035035228590 | 3.51912629310962 |
| H | 6.14757380261382 | 6.14193510916180 | 4.22153592274043 |
| N | 6.83688867063729 | 4.52016828514443 | 2.99126658865512 |
| B | 3.37951689879262 | 5.77407169480719 | 3.37141956228469 |
| N | 1.83869683502382 | 7.49402861598519 | 0.48374361867875 |
| N | 2.10644284942543 | 3.55225762760328 | 3.29067407946196 |
| C | 2.34426803536322 | 7.49564349931723 | 1.71184542228402 |
| C | 1.81337982828259 | 4.68095425515493 | 5.14814492269049 |
| H | 1.87223463666574 | 5.44180746426560 | 5.90629686494104 |
| N | 4.80377644231638 | 4.03831751930215 | 2.19825864300702 |
| C | 1.24227936913962 | 2.58150385874198 | 0.42774780495702 |
| N | 1.10419123000610 | 3.54872740342981 | 5.21946410723134 |
| C | 3.38060751548696 | 1.30716591845183 | 1.46284052167710 |
| C | 3.70365537858794 | 3.01161160226207 | -0.60572288202766 |
| H | 3.51818993573275 | 6.66090299851839 | 4.15312029344334 |
| H | 1.62107413852450 | 5.81233191996597 | -0.84592209738615 |
| O | 0.22810935546341 | 2.20582203809962 | -0.02046024128093 |
| H | 6.47854729184155 | 2.92580658915132 | 1.58609283099270 |
| H | 0.86278219429173 | 1.91887287544180 | 3.82493954379837 |
| H | 0.52804664281470 | 3.25587179270757 | 5.99739390227309 |
| H | 2.44362154254907 | 8.35140717136939 | 2.35893991054627 |

[Mo(Ttz)(CO)$_3$] **3**

| | | | |
|---|---|---|---|
| Mo | 2.93844352795747 | 3.22980087492129 | 1.24285853244040 |
| O | 3.94931484451424 | 0.25628071039188 | 1.63912556635365 |
| C | 6.08495395804747 | 3.70202969844826 | 2.12644693671284 |
| O | 4.02866840012358 | 2.76466666881886 | -1.66468301827745 |
| N | 4.74144752299534 | 5.05864923819962 | 3.07323713055563 |
| C | 2.02215717855442 | 6.18971783410236 | 0.11384380722883 |
| N | 2.45644635805266 | 4.69281828896146 | 4.01910232816791 |
| N | 2.78592755259727 | 6.25979936676662 | 2.10248082232173 |
| C | 1.29729463854183 | 2.91175655655912 | 4.13022101956165 |
| N | 2.51571293232801 | 5.41133017657889 | 1.06850320849717 |
| C | 5.98581452374268 | 5.30591285202363 | 3.48092599348493 |
| H | 6.22125827716655 | 6.08946548059196 | 4.18198999234477 |
| N | 6.85794102832945 | 4.47450783258673 | 2.91103678392449 |
| B | 3.40529332360121 | 5.74810127606989 | 3.42032437086433 |
| N | 1.95530069621211 | 7.48421880286023 | 0.47249759640551 |
| N | 2.12105390243812 | 3.56729075517709 | 3.32796367604717 |
| C | 2.44054245013010 | 7.48639569773458 | 1.71401567554919 |
| H | 2.55511625496173 | 8.34944747208924 | 2.34873586770816 |
| C | 1.81783733726527 | 4.65080432473925 | 5.19088575987083 |
| H | 1.91187485971502 | 5.42912810177389 | 5.93013105767145 |
| N | 4.79808985815539 | 4.01737712439607 | 2.19303513232551 |
| C | 1.17789924060719 | 2.76337346499941 | 0.37806260572342 |
| N | 1.08033767746413 | 3.54878304797691 | 5.29912336261617 |
| C | 3.55709645929461 | 1.32636251278329 | 1.51390427294912 |
| C | 3.64645337661579 | 2.95974274114418 | -0.59453512946667 |
| H | 3.57856900664657 | 6.64572493368188 | 4.18286663575928 |
| H | 1.71475735493169 | 5.79927154289975 | -0.84185052681244 |
| O | 0.19123396738204 | 2.52302597275807 | -0.15490764071887 |
| H | 6.44740538538283 | 2.90446726904779 | 1.49930818735442 |
| H | 0.85770810624524 | 1.96732938091777 | 3.85593999283689 |

$[Mo(HTtz)(CO)_3]^+$ **3H$^+$**

| | | | |
|---|---|---|---|
| Mo | 2.93318657990802 | 3.22231436283638 | 1.22395407324680 |
| O | 3.96405415646527 | 0.25174540767824 | 1.61830311935622 |
| C | 6.05679729865814 | 3.71223619320201 | 2.15583623724696 |
| O | 4.06497920950428 | 2.80877972660893 | -1.66664777671747 |
| N | 4.69362159662878 | 5.06793187882601 | 3.07518518918857 |
| C | 1.95867193230610 | 6.15744945062051 | 0.09910355589363 |
| N | 2.40899866376963 | 4.69422079081993 | 4.01266099009466 |
| N | 2.72454296341143 | 6.24809094166106 | 2.08590102092241 |
| C | 1.28258046393747 | 2.87434698156006 | 4.09703030554470 |
| N | 2.47689174921123 | 5.39188331613476 | 1.05055060896335 |
| C | 5.93107462394700 | 5.31653230689035 | 3.50818924841467 |
| H | 6.15131586149316 | 6.10132921335637 | 4.21287839717715 |
| N | 6.81218750719945 | 4.48577103334007 | 2.95616765097086 |
| B | 3.36737474540225 | 5.76685129814577 | 3.39112331687106 |
| N | 1.85502182106067 | 7.44889226208628 | 0.46036118714376 |
| N | 2.08892518707522 | 3.55294617806505 | 3.32570731753230 |
| C | 2.34121916058624 | 7.46587654859708 | 1.69922329543535 |
| C | 1.79784112035205 | 4.68871400290186 | 5.17447843418345 |
| H | 1.85797881602009 | 5.45337868366808 | 5.92903322697135 |
| N | 4.76838539172520 | 4.02513272638431 | 2.19547581998119 |
| C | 1.17325804475271 | 2.71583575646128 | 0.36208426681280 |
| N | 1.08568450020720 | 3.55825487750239 | 5.24860669632048 |
| C | 3.56801781195768 | 1.31855887962602 | 1.49490394016202 |
| C | 3.66268244419275 | 2.97801708138527 | -0.60117270541066 |
| H | 3.51622394430472 | 6.65933270743331 | 4.16057745841640 |
| H | 1.66092472354453 | 5.76023599366461 | -0.85687075939082 |
| O | 0.18927850154668 | 2.43783514067236 | -0.15202407798376 |
| H | 6.43394307686051 | 2.91483348633914 | 1.53725948560710 |
| H | 0.83906964215852 | 1.92240172674736 | 3.86679199519246 |
| H | 0.50909648700015 | 3.26744641254622 | 6.02774963627673 |
| H | 2.43182197481287 | 8.33176463423890 | 2.33431884557631 |

$[W(Ttz)(CO)_3]^-$ **5**$^-$

| | | | |
|---|---|---|---|
| W | 2.94222128814805 | 3.20125266796477 | 1.19276095026035 |
| O | 3.61366300878097 | 0.18806246416501 | 1.62817751256666 |
| C | 6.09374313748545 | 3.70770533493603 | 2.14576566621358 |
| O | 4.16011740203261 | 2.92184425113896 | -1.66426673428429 |
| N | 4.75646252254617 | 5.08102119108279 | 3.06559509203702 |
| C | 2.01445845313921 | 6.21293944104041 | 0.12277979687242 |
| N | 2.47263911728119 | 4.70059711988190 | 3.99631451460257 |
| N | 2.79935046393552 | 6.28356118091835 | 2.09728274190509 |
| C | 1.32717387148907 | 2.91126554796474 | 4.08144744103294 |
| N | 2.52361774934061 | 5.43486869796743 | 1.06557261422891 |
| C | 6.00023921339936 | 5.32538111708556 | 3.48516905027059 |
| H | 6.23253547144444 | 6.11234214038988 | 4.18356251996069 |
| N | 6.87012730111268 | 4.48446261868827 | 2.93132823946189 |
| B | 3.41938101624149 | 5.76564992820667 | 3.40935937689912 |
| N | 1.94375550104318 | 7.51172206071700 | 0.48501972881484 |
| N | 2.14697444845631 | 3.58209109506607 | 3.28702227873089 |
| C | 2.44159426647869 | 7.51279154710911 | 1.71891799456366 |
| H | 2.55630116605827 | 8.37279239196762 | 2.35782091525349 |
| C | 1.83352600882500 | 4.63925134033187 | 5.16732423984958 |
| H | 1.92131920544415 | 5.40791743652821 | 5.91743359315088 |
| N | 4.81075191533549 | 4.03171016156584 | 2.19516373902211 |
| C | 1.24387088965848 | 2.62426669444550 | 0.45606516128480 |
| N | 1.10322281858950 | 3.53074184054270 | 5.26006495916935 |
| C | 3.36481452211700 | 1.32886731513455 | 1.46960074430470 |
| C | 3.70211629217285 | 3.03403541749590 | -0.58421815020575 |
| H | 3.58627243127932 | 6.65817574632959 | 4.18205071396745 |
| H | 1.69618763082535 | 5.82283314548484 | -0.82916890245090 |
| O | 0.21376607763083 | 2.26153612657550 | 0.01360662357096 |
| H | 6.45513694259651 | 2.90004353999820 | 1.53154578981642 |
| H | 0.89660986711227 | 1.96785043927667 | 3.79149178913001 |

[W(HTtz)(CO)$_3$] **5H**

| | | | |
|---|---|---|---|
| W | 2.93994157112239 | 3.19738158290982 | 1.18176591611343 |
| O | 3.63777417751337 | 0.19664368705623 | 1.65940523090201 |
| C | 6.06810591411622 | 3.72357829620991 | 2.17860828138884 |
| O | 4.16409587687395 | 2.90476935234965 | -1.66869142918484 |
| N | 4.71181989675146 | 5.09881181807308 | 3.06693037986350 |
| C | 1.94596926692906 | 6.18038530151515 | 0.11065340293778 |
| N | 2.42900741572341 | 4.70048855690512 | 3.98590992739725 |
| N | 2.73979484224115 | 6.27493887389733 | 2.08036517219128 |
| C | 1.31452061080418 | 2.87099221859523 | 4.03453348349252 |
| N | 2.48614889784743 | 5.41767578512476 | 1.04805286032138 |
| C | 5.94788849392770 | 5.34371089197319 | 3.51367579503760 |
| H | 6.16474324661743 | 6.13194415457423 | 4.21557077144298 |
| N | 6.82675846741774 | 4.50297556945896 | 2.97883371738627 |
| B | 3.38216642250488 | 5.78810131074826 | 3.38083909155728 |
| N | 1.83554112189481 | 7.47574422833336 | 0.47594392959997 |
| N | 2.11909052513031 | 3.56739496636925 | 3.27483875223436 |
| C | 2.33766178065118 | 7.49350542371947 | 1.70569759007281 |
| C | 1.81331042769272 | 4.67121578518764 | 5.14563256298202 |
| H | 1.86452057289998 | 5.42262435934899 | 5.91377284188619 |
| N | 4.78448408616369 | 4.04651483625053 | 2.19881120770906 |
| C | 1.24429251736768 | 2.60059243108880 | 0.44811128412665 |
| N | 1.10879588899388 | 3.53474916177631 | 5.19809104596462 |
| C | 3.37951821596969 | 1.33010991406718 | 1.48244191564506 |
| C | 3.70524725723684 | 3.02125052233700 | -0.59332544863900 |
| H | 3.52074869757275 | 6.67436981385554 | 4.16184451311331 |
| H | 1.63377707651473 | 5.78192235151559 | -0.83979349520827 |
| O | 0.21731029695943 | 2.22852533747944 | 0.01242184267560 |
| H | 6.44364382075685 | 2.91419674953478 | 1.57524991217124 |
| H | 0.87964744554609 | 1.92079695977562 | 3.78406474626235 |
| H | 0.53254403303248 | 3.22753543180050 | 5.97043360758771 |
| H | 2.42678113522652 | 8.35549432816906 | 2.34605059096908 |

[W(Ttz)(CO)$_3$] **5**

| | | | |
|---|---|---|---|
| W | 2.94129777684286 | 3.24029646272874 | 1.24998517533587 |
| O | 3.90514919762895 | 0.26263012885781 | 1.63269617523584 |
| C | 6.06686143758835 | 3.70246209950942 | 2.11803418421808 |
| O | 4.03632409712687 | 2.77513972835362 | -1.64825269882300 |
| N | 4.73969400053794 | 5.06888604525202 | 3.08010565117832 |
| C | 2.03446913850848 | 6.17271987128753 | 0.11719309957383 |
| N | 2.46046619550889 | 4.70207231253800 | 4.02309932113992 |
| N | 2.78861020205269 | 6.26678084102357 | 2.11158489625916 |
| C | 1.30932526309913 | 2.91136496312759 | 4.10830558515015 |
| N | 2.52881206807304 | 5.40548510578948 | 1.08366109321358 |
| C | 5.98851510795902 | 5.30443872750805 | 3.47686760053773 |
| H | 6.23643200859959 | 6.08485584781168 | 4.17714698945072 |
| N | 6.84924995768658 | 4.46650166616065 | 2.89757851545928 |
| B | 3.40757611864613 | 5.76339909733050 | 3.43286814385582 |
| N | 1.95754731362463 | 7.46737631596262 | 0.46430594986464 |
| N | 2.13400239365817 | 3.58220951179516 | 3.31646555570135 |
| C | 2.43694856859912 | 7.48564147351054 | 1.70873465303306 |
| H | 2.54273747744295 | 8.35602691842521 | 2.33483432334218 |
| C | 1.81708224269654 | 4.64165559161219 | 5.19026669115729 |
| H | 1.90302107625724 | 5.41156321271719 | 5.93921335231610 |
| N | 4.78067786716062 | 4.02787474454786 | 2.19633100353780 |
| C | 1.19839775337848 | 2.76202046318558 | 0.39627932867512 |
| N | 1.08517549581354 | 3.53376851929665 | 5.28137379594477 |
| C | 3.53424846060889 | 1.34682263765674 | 1.50898536041109 |
| C | 3.64551723838876 | 2.96818871894980 | -0.57434948088258 |
| H | 3.58047010065432 | 6.66001649999998 | 4.19497357696958 |
| H | 1.73532731748923 | 5.77031249396690 | -0.83609603645748 |
| O | 0.20414390571185 | 2.50540883882007 | -0.12763195862495 |
| H | 6.41741773905857 | 2.90365928596934 | 1.48582866455454 |
| H | 0.87645247959851 | 1.96800187630555 | 3.82020148867218 |

$[W(HTtz)(CO)_3]^+$ **5H**$^+$

| | | | |
|---|---|---|---|
| W | 2.93790027043882 | 3.23616388564903 | 1.22749575131175 |
| O | 3.94760615005262 | 0.27184531789064 | 1.60484494640664 |
| C | 6.03755119041783 | 3.70693017505799 | 2.15621387777008 |
| O | 4.05292020195647 | 2.81021861034359 | -1.66156343472846 |
| N | 4.69127352030344 | 5.08161453673651 | 3.07956263813857 |
| C | 1.96980610936651 | 6.14522902326627 | 0.10125788170029 |
| N | 2.41353440437949 | 4.70583368606731 | 4.01362972166267 |
| N | 2.72696844692799 | 6.25837086941897 | 2.09313014076411 |
| C | 1.30176964887367 | 2.87297020308618 | 4.07265916628061 |
| N | 2.48688216395540 | 5.38967782002534 | 1.06482978703617 |
| C | 5.93123598004702 | 5.30975254025284 | 3.51265845660271 |
| H | 6.16320522188504 | 6.08915236768178 | 4.21956901896124 |
| N | 6.80082387739149 | 4.46765824241452 | 2.95750241942359 |
| B | 3.36872783959365 | 5.78578203194434 | 3.40168658289331 |
| N | 1.86007443490107 | 7.43706215190139 | 0.45034910634983 |
| N | 2.10773294373945 | 3.56753388601520 | 3.31267378134580 |
| C | 2.34093006958355 | 7.46921993649564 | 1.69177854173239 |
| C | 1.79292119957362 | 4.68303154102787 | 5.16960744857275 |
| H | 1.83985666977019 | 5.44068176635571 | 5.93228280275614 |
| N | 4.75145981563885 | 4.03894115936956 | 2.19604815649761 |
| C | 1.18893792740347 | 2.71021846488960 | 0.39888023041158 |
| N | 1.09111491550170 | 3.54492239859733 | 5.22729834677411 |
| C | 3.55961883474744 | 1.34833362744739 | 1.48338098567109 |
| C | 3.65019513786899 | 2.98535002285282 | -0.59118979792019 |
| H | 3.51730657347821 | 6.67721248569216 | 4.17079057483771 |
| H | 1.67849327571584 | 5.73661392553071 | -0.85180139337515 |
| O | 0.18905226924754 | 2.42107162059538 | -0.09055527192628 |
| H | 6.40150852884213 | 2.90401114406942 | 1.53691548583551 |
| H | 0.86851327826598 | 1.91956511159349 | 3.82913297844477 |
| H | 0.51097111792398 | 3.24220890559368 | 5.99964410845433 |
| H | 2.42675798220857 | 8.34176254213732 | 2.31802696131474 |