Supporting Information:

Nitrogen Oxide Atom-Transfer Redox Chemistry; Mechanism of $NO_{(g)}$ to Nitrite Conversion Utilizing μ-oxo Heme-Fe^{III}–O–Cu^{II}(L) Constructs

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3. $[(TMPP)Fe^{III}(THF)_2](SbF_6)$.

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- **Table S2**. Absolute energies of studied compounds at the OLYP/6-311+G(d,p) level
- **Table S3**. Absolute energies and zero-point correction energy of studied compounds at the BP86/6-31G(d) level
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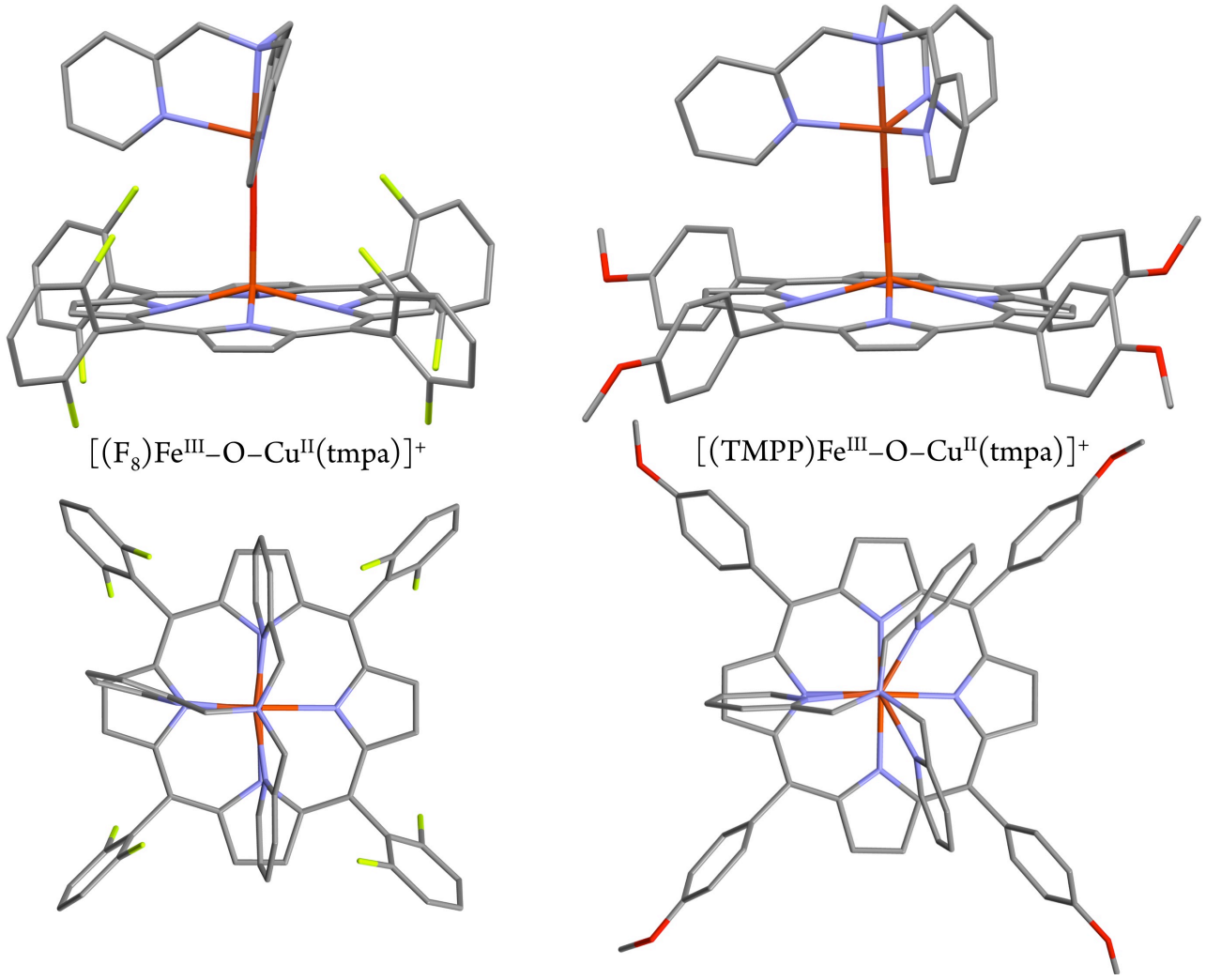

Figure S1. Molecular structures (side and top views) of the oxo-bridged heteronuclear cations $[(F_8)Fe^{III}–O–Cu^{II}(tmpa)]^+$ (adapted from text reference #14) and $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)]^+$ showing that the cupric center adapted different geometries; in the former compound Cu(II) adjusts to a distorted square pyramidal geometry ($\tau = 0.3$) while in the latter it is present in a trigonal bipyramidal arrangement ($\tau = 0.9$). All the hydrogen atoms are omitted for clarity.

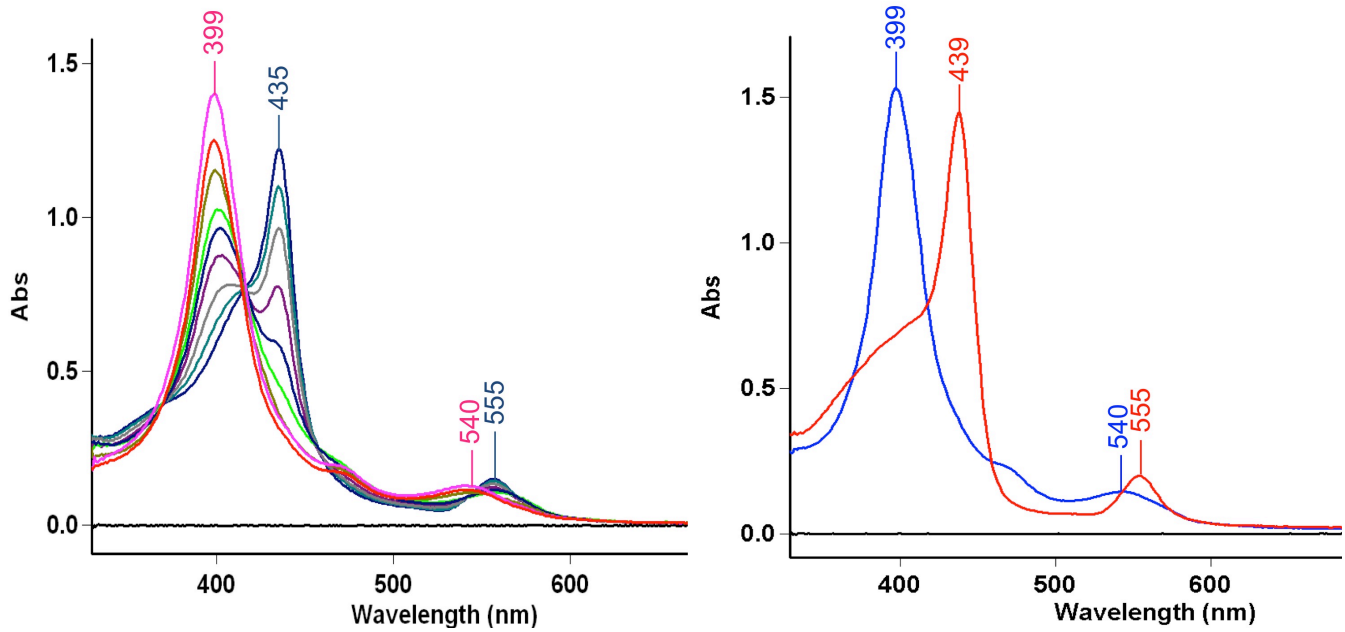

Figure S2. UV–vis spectra of: *Left*) (adapted from text reference # 11) $[(F_8)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$ (blue), $(F_8)Fe^{II}(NO)$ (red) generated from addition of 1 mL of $NO_{(g)}$. Addition of second mL of $NO_{(g)}$ to the solution resulted in completion of the reaction (purple) 10 μM in acetone at RT. *Right*)$[(F_8)Fe^{III}–O–Cu^{II}(AN)][B(C_6F_5)_4]$ (red) and $(F_8)Fe^{II}(NO)$ (blue) immediately generated after addition of 1 mL $NO_{(g)}$ into the μ-oxo complex solution 10 μM in acetone at RT.

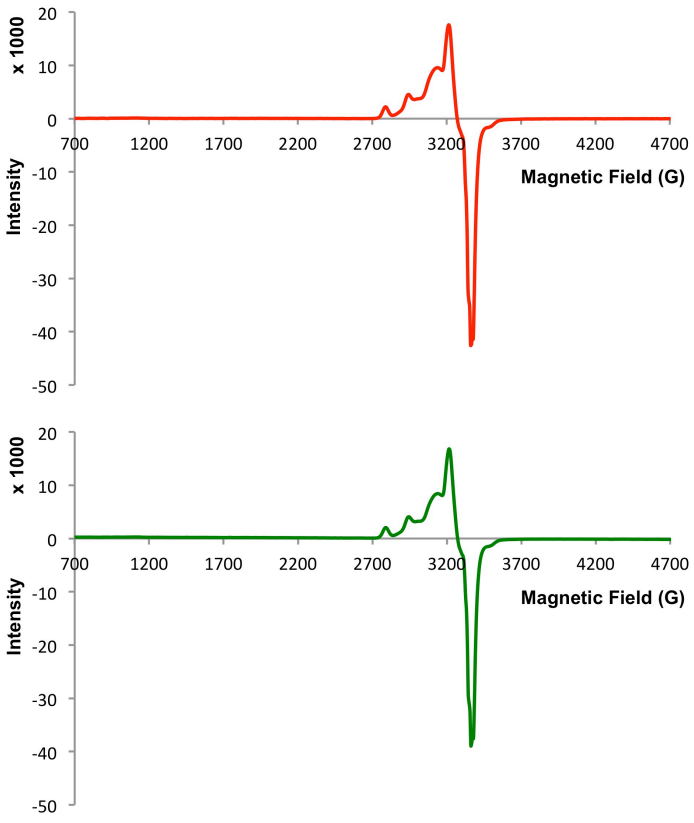

Figure S3. EPR spectrum comparison between the reaction mixture and an authentic sample: the products of the reaction of $NO_{(g)}$ and $[(F_8)Fe^{III}–O–Cu^{II}(AN)][B(C_6F_5)_4]$, giving signals of $(F_8)Fe^{II}(NO)$ and Cu(II) (red); an authentic sample of a 1:1 mixture of $(F_8)Fe^{II}(NO)$ and $[(AN)Cu^{II}(NO_2)](CF_3SO_3)$ (green) 1 mM in MeCN/toluene (1:1) at 20 K.

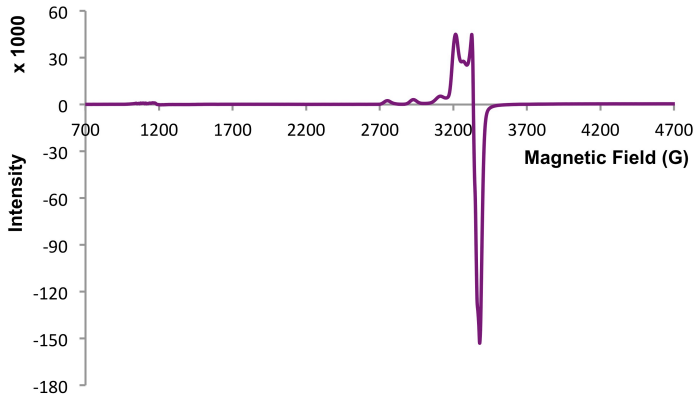

Figure S4. EPR spectrum of the products of the reaction of $NO_{(g)}$ and $[(F_8)Fe^{III}–O–Cu^{II}(MePY2)][B(C_6F_5)_4]$ (purple), giving signals of $(F_8)Fe^{II}(NO)$ and Cu(II) in acetone 2 mM at 12 K.

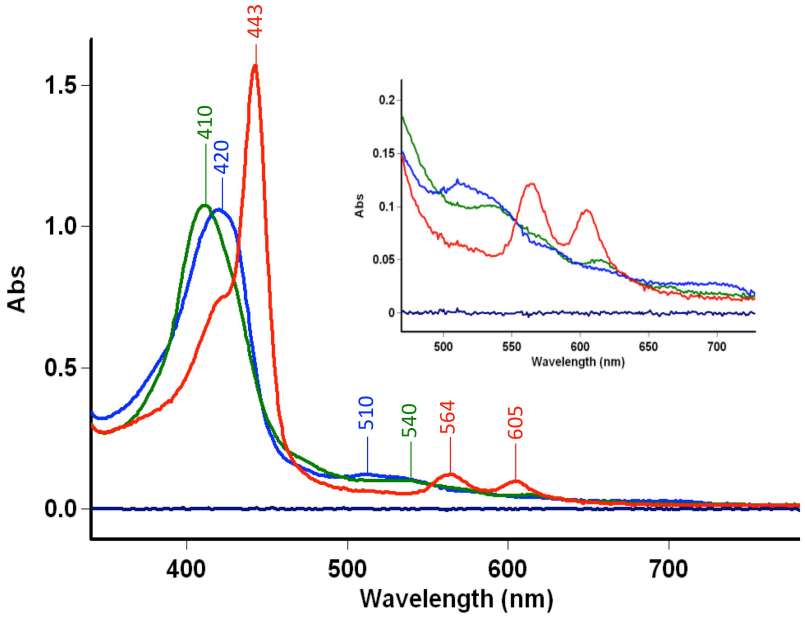

Figure S5. UV–vis spectra of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$ (red) 35 μM in acetone in a 2-mm cuvette at RT, right after addition of 1 mL of $NO_{(g)}$ into the solution (blue), after stirring for 4 min forming $(TMPP)Fe^{II}(NO)$ (green).

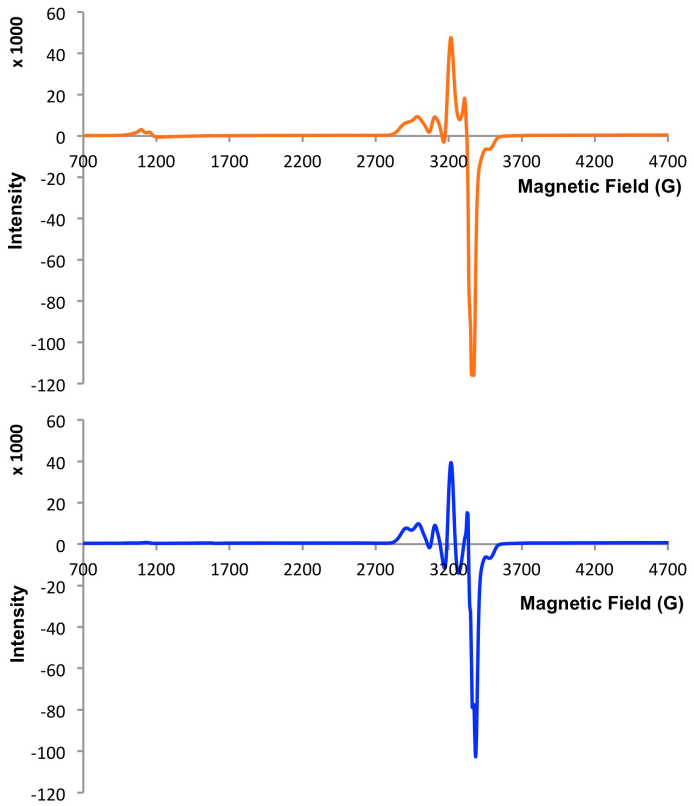

Figure S6. EPR spectra of the products of the reaction of $NO_{(g)}$ and $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$, giving signals of $(TMPP)Fe^{II}(NO)$ and Cu(II) in acetone (orange) and in MeTHF (blue) 2 mM at 12 K.

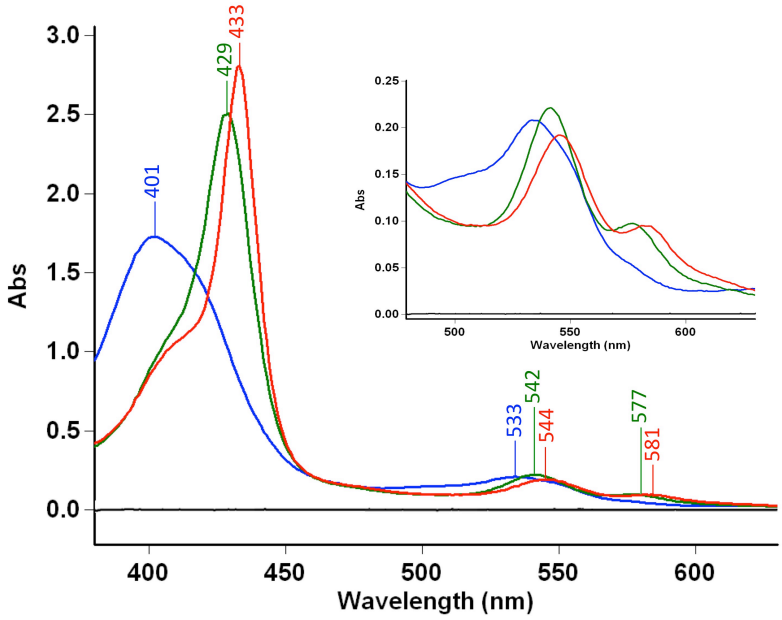

Figure S7. UV–vis spectra of $[(TMPP)Fe^{III}(THF)_2]SbF_6$ (blue) 50 μM in acetone in a 2-mm cuvette at –20 °C, right after addition of 1 mL of $NO_{(g)}$ into the solution generating $(TMPP)Fe^{III}(NO)$ (green), after addition of 10 equiv $(n\text{Bu})_4N(NO_2)$ forming $(TMPP)Fe^{III}(NO)(NO_2)$ (red).

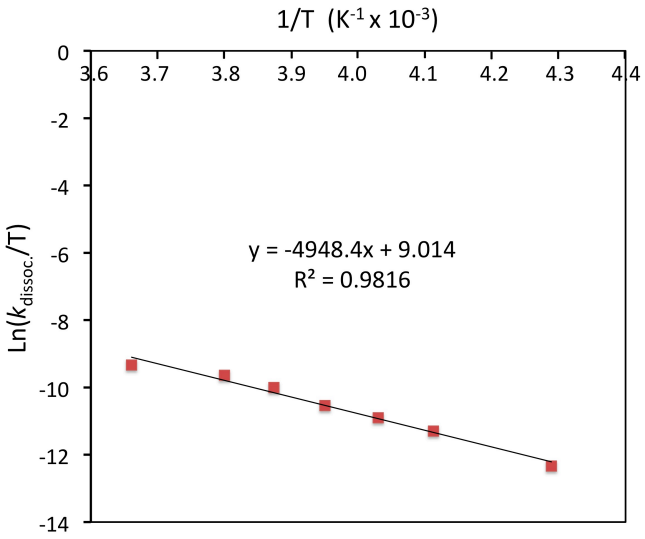

Figure S8. Eyring plot, $\ln(k_{obs}/T)$ vs 1/T, for the final step, slow dissociation of the "intermediate", [(NO)(TMPP)Fe^{II}–(NO_2)–Cu^{II}(tmpa)][$B(C_6F_5)_4$], generated from reaction of [(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][$B(C_6F_5)_4$] with $NO_{(g)}$ to the two final Cu-nitrite and heme-Fe^{II}(NO) products. The rate constants ($k_{dissoc.}$) were obtained from monitoring of the decay of the 433 nm intermediate in acetone at 0, –10, –15, –20, –25, –30, –40 °C. From the plot, activation parameters for the final step were obtained, $\Delta S^{\ddagger}_{dissoc.} = R(\text{intercept} - \ln k_B/h) = -123 \pm 2$ J $mole^{-1}$ K^{-1} and $\Delta H^{\ddagger}_{dissoc.} = -R(\text{slope}) = +41{,}141 \pm 100$ J mol^{-1}.

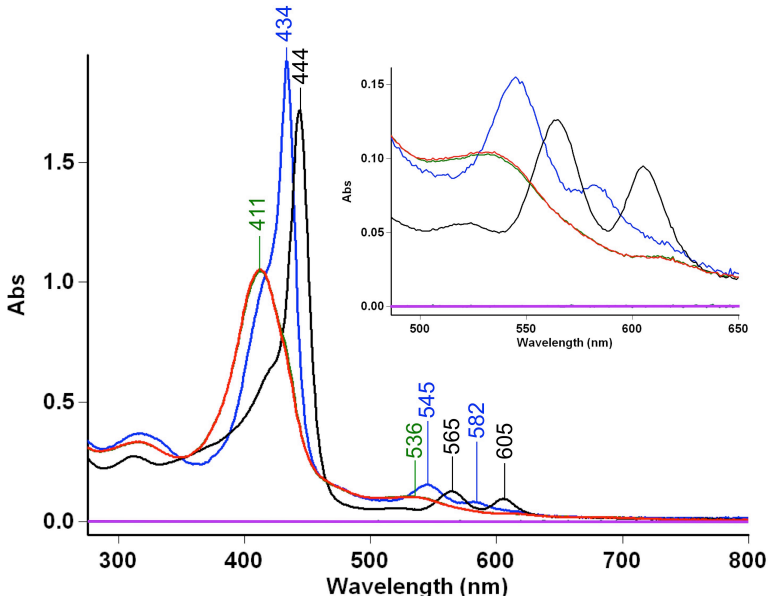

Figure S9. UV–vis spectra of [(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][$B(C_6F_5)_4$] (black) 35 μM in MeTHF in a 2-mm cuvette at RT, after addition of 1 mL of $NO_{(g)}$ into the solution forming final products, (TMPP)Fe^{II}(NO) and [(tmpa)Cu^{II}(NO_2)][$B(C_6F_5)_4$] (green). The excess $NO_{(g)}$ was then removed and the sample was cooled to –125 °C generating a new species formulated as [(NO)(TMPP)Fe^{II}–(NO_2)–Cu^{II}(tmpa)][$B(C_6F_5)_4$] (blue). Warming up to RT resulted the reformation of initial spectrum of the final products (red).

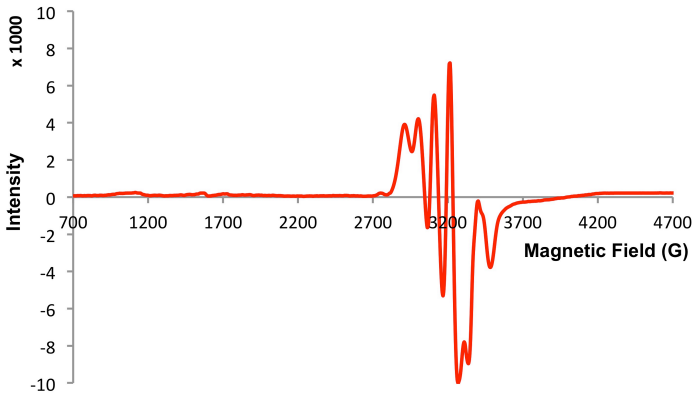

Figure S10. EPR spectrum of the "intermediate" for the reaction of $NO_{(g)}$ and $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$ at 12 K giving signals of Cu(II) and ferrous heme nitrosyl species, but with a different hyperfine coupling observed in the spectrum of products mixture (Figure S9). Sample was prepared by addition of 1 mL $NO_{(g)}$ into the 1 mM solution of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$ in MeTHF at –80 °C (dry ice-acetone bath). Then excess $NO_{(g)}$ was removed via vacuum/Ar-purge cycles and the EPR sample was frozen in liquid nitrogen prior to measurement.

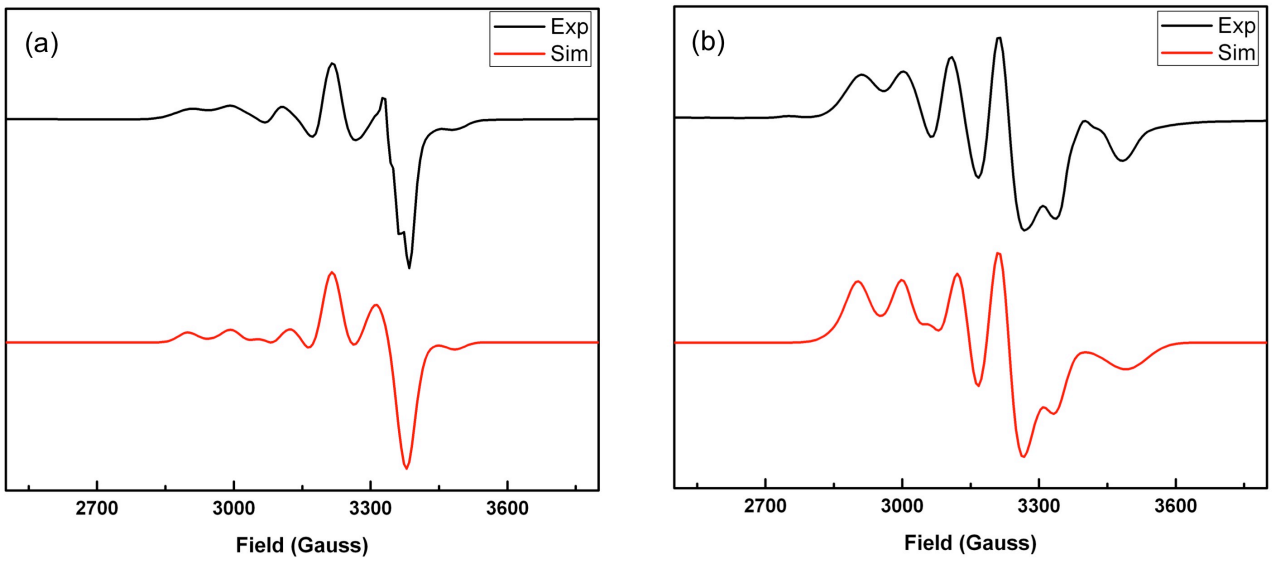

Figure S11. Experimental (black) and simulated (red) spectra (for the reaction of $NO_{(g)}$ with $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$) of the product species (**a**) $g_{1,Cu}$ = 2.153, $g_{2,Cu}$ = 2.195, $g_{3,Cu}$ = 1.987, $A_{1,Cu}$ = 82.1 G, $A_{2,Cu}$ = 115 G, $A_{3,Cu}$ = 69.2 G, $g_{1,FeNO}$ = 2.094, $g_{2,FeNO}$ = 2.009, $g_{3,FeNO}$ = 1.993, $A_{1,FeNO}$ = 10.3 G, $A_{2,FeNO}$ = 22.8 G, $A_{3,FeNO}$ = 7.1 G and the "intermediate" species (**b**) $g_{1,Cu}$ = 2.161, $g_{2,Cu}$ = 2.187 $g_{3,Cu}$ = 2.056, $A_{1,Cu}$ = 73.1 G, $A_{2,Cu}$ = 110 G, $A_{3,Cu}$ = 51.2 G, $g_{1,FeNO}$ = 2.340, $g_{2,FeNO}$ = 1.920, $g_{3,FeNO}$ = 2.066, $A_{2,NO}$ = 18.9 G, $A_{2,Nitrite}$ = 7.74 G. EPR conditions: microwave frequency, 9.41 GHz; microwave power, 0.2 mW; modulation frequency, 100 kHz; modulation amplitude, 10 G; temperature, 12 K. EPR simulations were performed using EasySpin v. 4.5.5 (Stoll, S.; Schweiger, A. *J. Magn. Reson.* **2006**, 178, 42; http://www.easyspin.org).

Table S1. Observed Rate Constants for the First Reaction Step ($k_{1(obs)}$, Binding of 1st NO) and Second Reaction Step ($k_{2(obs)}$, Binding of 2nd NO) as a Function of Temperature and Concentration.

[NO] mM	Temperature						
	−60 °C		−67 °C		−74 °C		−83 °C*
	$k_{1(obs)}$	$k_{2(obs)}$	$k_{1(obs)}$	$k_{2(obs)}$	$k_{1(obs)}$	$k_{2(obs)}$	$k_{1(obs)}$
0.281	4.35 ± 0.15	0.25 ± 0.02	3.11 ± 0.26	0.20 ± 0.04	1.81 ± 0.26	0.16 ± 0.03	0.92 ± 0.04
0.563	6.11 ± 0.66	0.45 ± 0.06	4.36 ± 0.23	0.37 ± 0.03	2.34 ± 0.03	0.23 ± 0.01	1.16 ± 0.03
0.750	6.72 ± 0.06	0.53 ± 0.04	4.64 ± 0.26	0.50 ± 0.04	2.90 ± 0.03	0.38 ± 0.02	1.38 ± 0.05
1.13	9.84 ± 0.86	0.82± 0.11	7.43 ± 0.18	0.72 ± 0.05	3.66 ± 0.06	0.46 ± 0.02	1.88 ± 0.10
1.69	12.76 ± 0.19	1.19 ± 0.03	10.33 ± 0.36	0.98 ± 0.08	4.91 ± 0.13	0.77 ± 0.06	2.52 ± 0.08
2.25	16.19 ± 0.37	1.65 ± 0.11	12.67 ± 1.47	1.51 ± 0.10	6.49 ± 0.09	1.16 ± 0.15	3.22 ± 0.11

* The second step at −83 °C was very slow and $k_{2(obs)}$ could not be accurately determined.

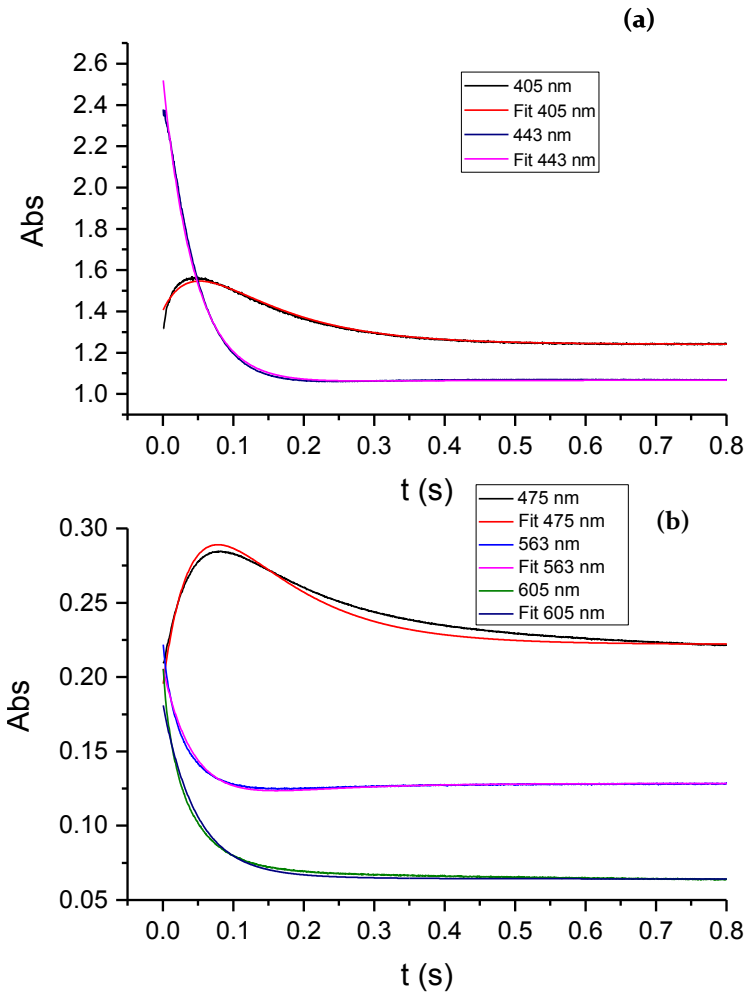

Figure S12. Kinetic traces with a two-exponential fit for the reaction of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)][B(C_6F_5)_4]$ with 2.3 mM NO at -60 °C in acetone monitored (**a**) at 405 and 443 nm, as well as (**b**) at 475, 563 and 605 nm.

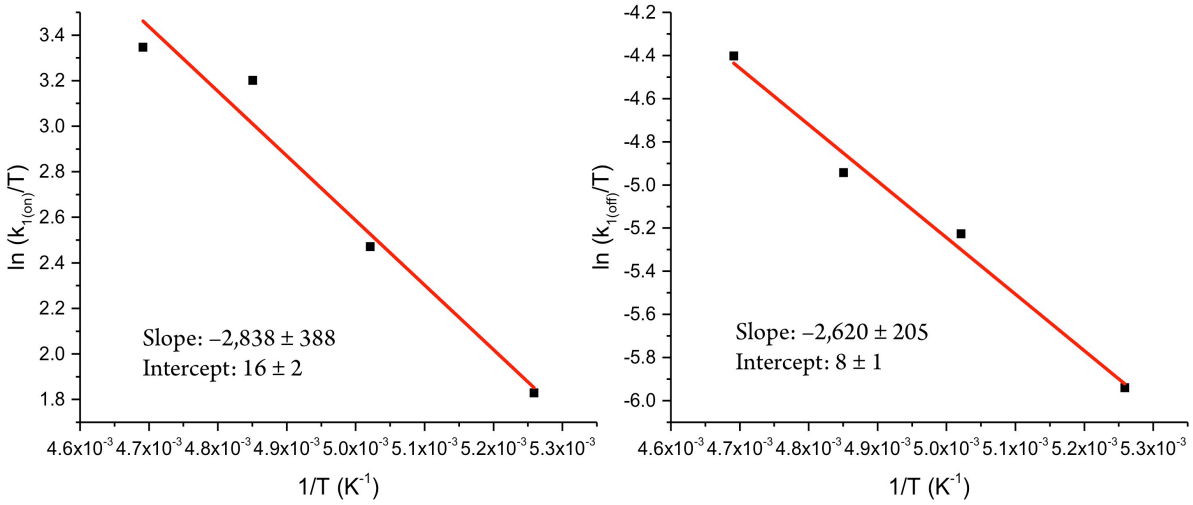

Figure S13. Eyring plots $(\ln(k/T) = -(\Delta H^{\ddagger}/R)(1/T) + \Delta S^{\ddagger}/R + \ln(k_b/h);\ k = k_{1(on)}$ or $k_{1(off)})$ for the forward and reverse reactions for the first reaction step, reaction of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)]^{+}$ with the first $NO_{(g)}$.

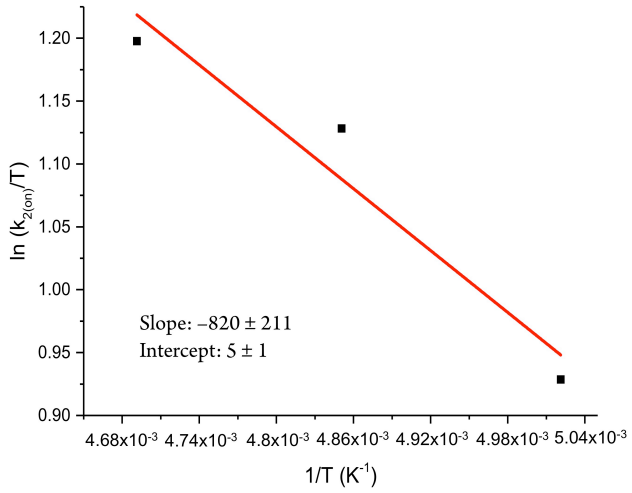

Figure S14. Eyring plot $(\ln(k/T) = -(\Delta H^{\ddagger}/R)(1/T) + \Delta S^{\ddagger}/R + \ln(k_b/h);\ k = k_{2(on)})$ for the forward reaction for the second reaction step, binding of the second $NO_{(g)}$.

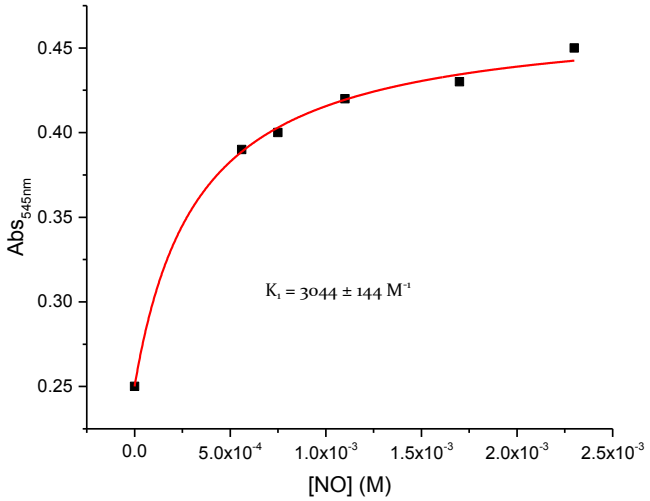

Figure S15. Absorbance at 545 nm (at the end of the first reaction step at –74 °C) as a function of $NO_{(g)}$ concentration (data fitted by Eq. 1 given in the main text).

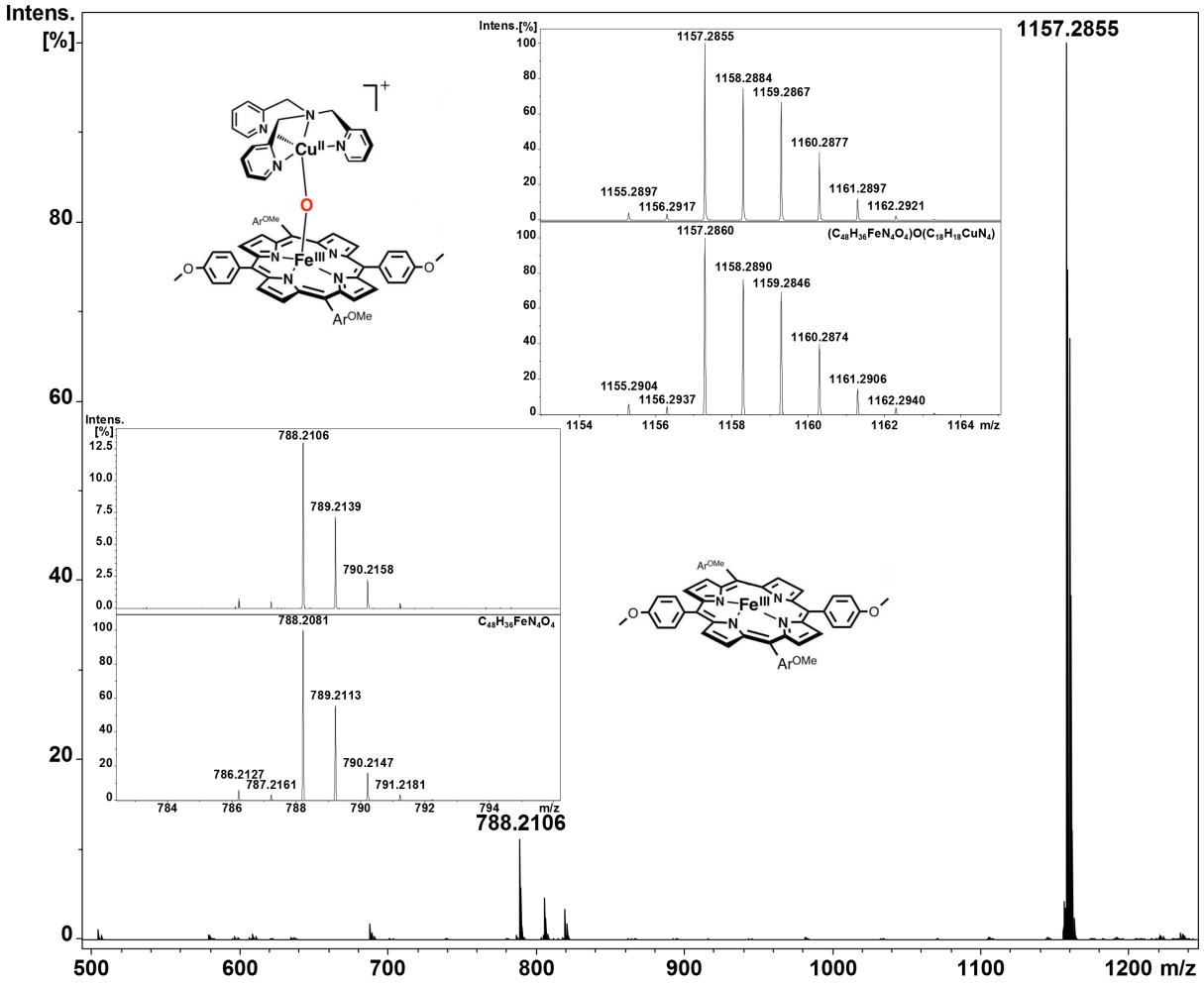

Figure S16. Mass spectrum of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)]^+$ in acetone before bubbling with $NO_{(g)}$, spray gas temperature –60 °C, dry gas temperature –55 °C; main species m/z = 1157.2855, which is assigned to the μ-oxo compound.

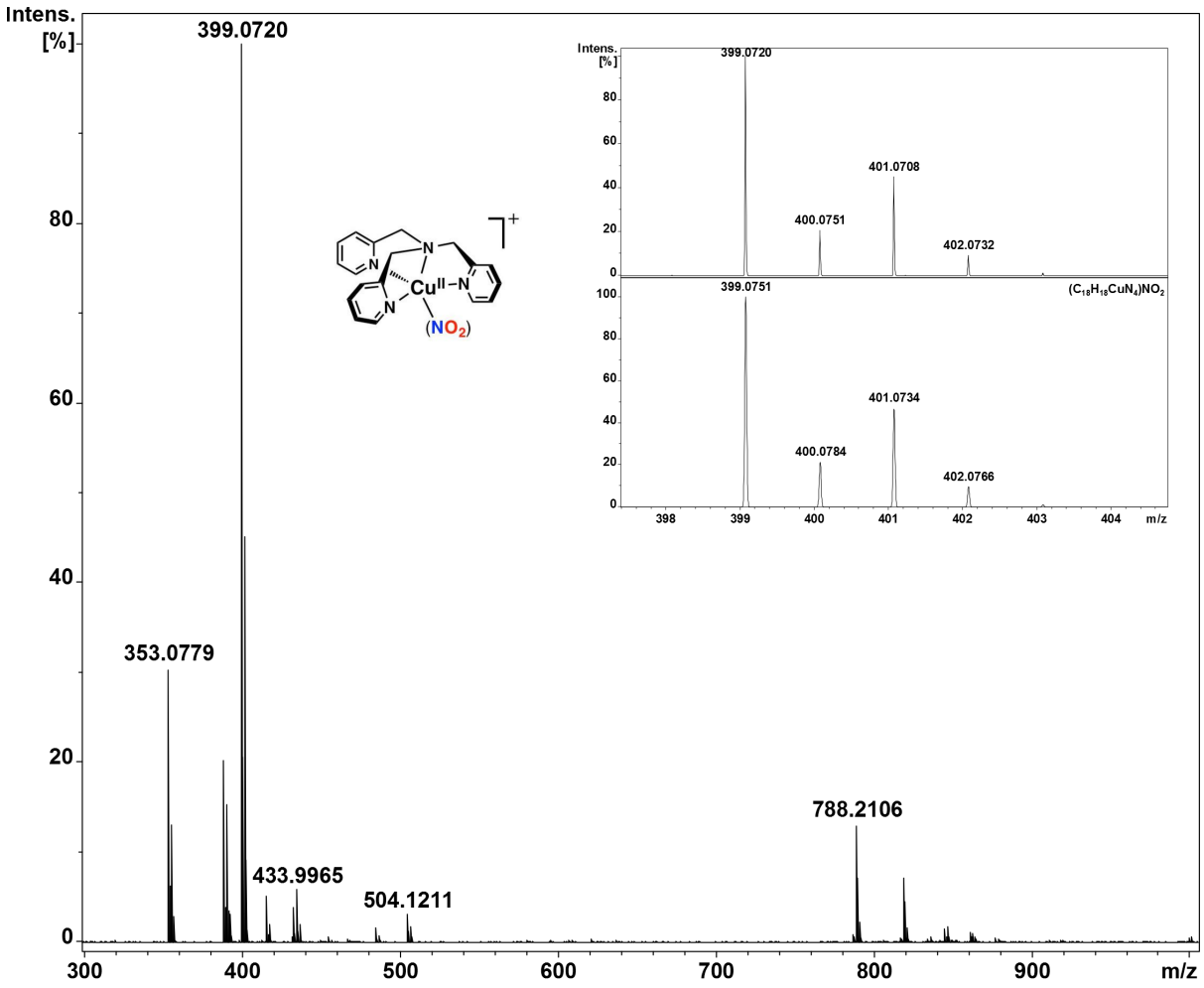

Figure S17. Mass spectrum of $[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)]^+$ in acetone 20 min after bubbling with $NO_{(g)}$. Experimental conditions: spray gas temperature –60 °C; dry gas temperature –55 °C. (Main species m/z = 399.0720, which can be assigned to the $[(tmpa)Cu^{II}(NO_2)]^+$ complex; the ferrous heme nitrosyl $(TMPP)Fe^{II}(NO)$ compound cannot be observed because it is not charged.)

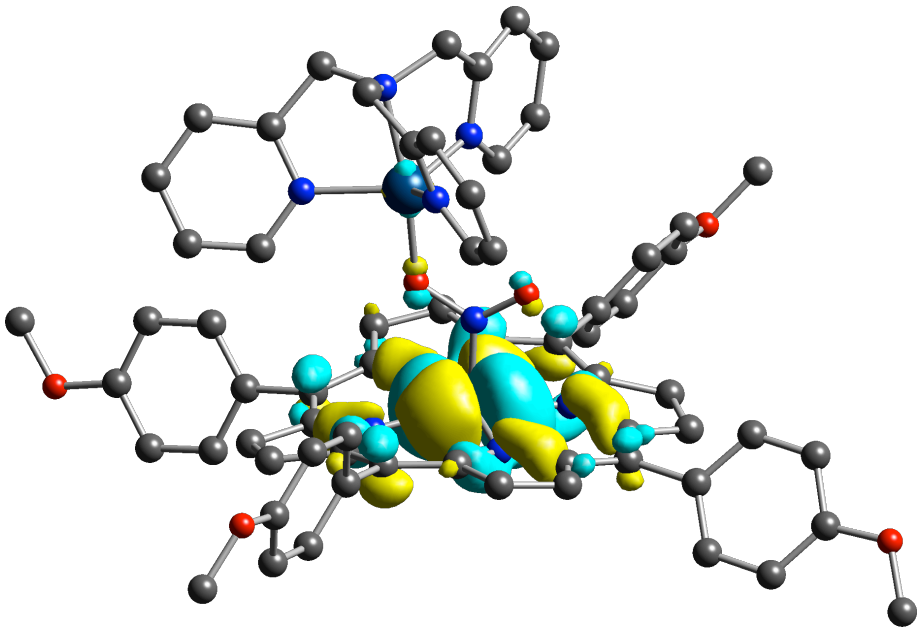

Figure S18. SOMO of the *mono*-NO adduct (BP86/6–31G(d)). Isodensity value α = 0.02.

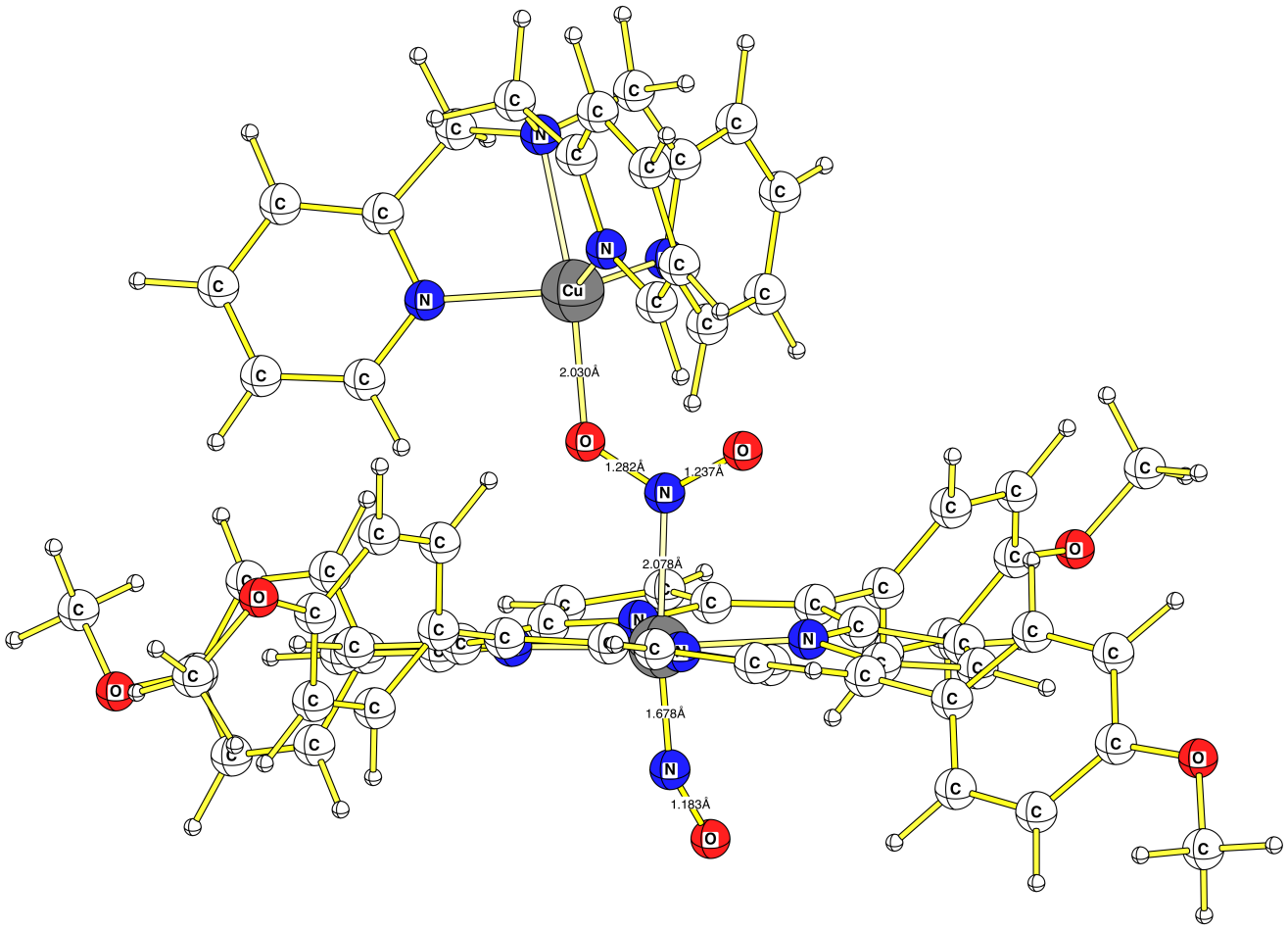

Figure S19. Optimized geometry of the *bis*-NO complex, BP86/6–31G(d).

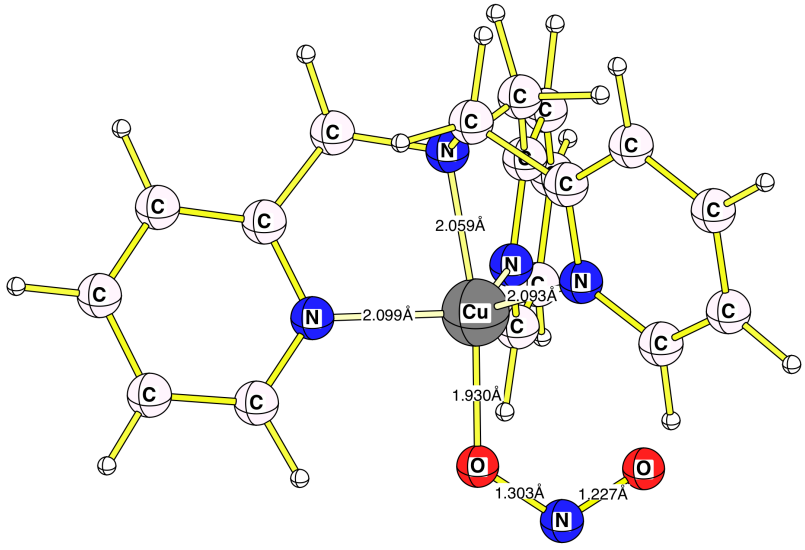

Figure S20. Optimized geometry of $[(tmpa)Cu^{II}(NO_2)]^+$ complex, BP86/6–31G(d).

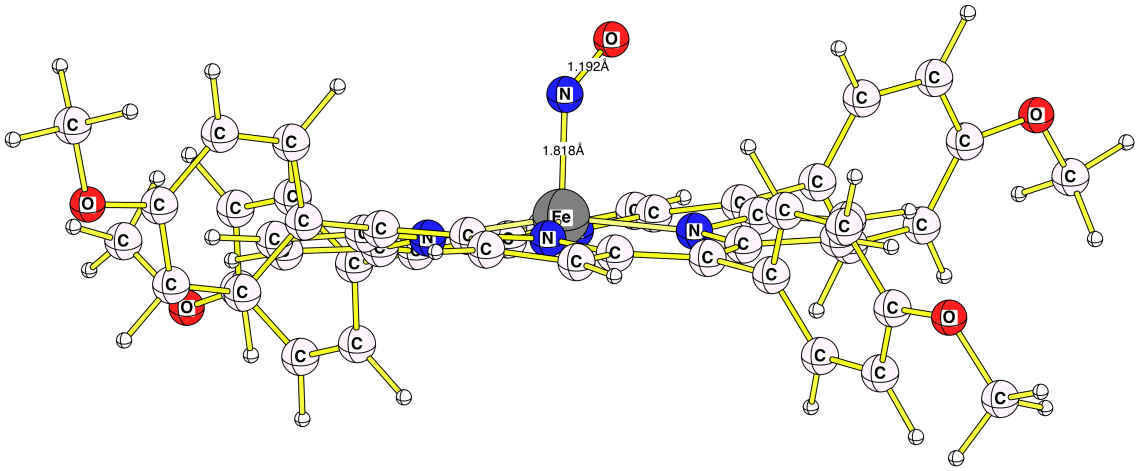

Figure S21. Optimized geometry of (TMPP)Fe^{II}(NO) complex, BP86/6–31G(d).

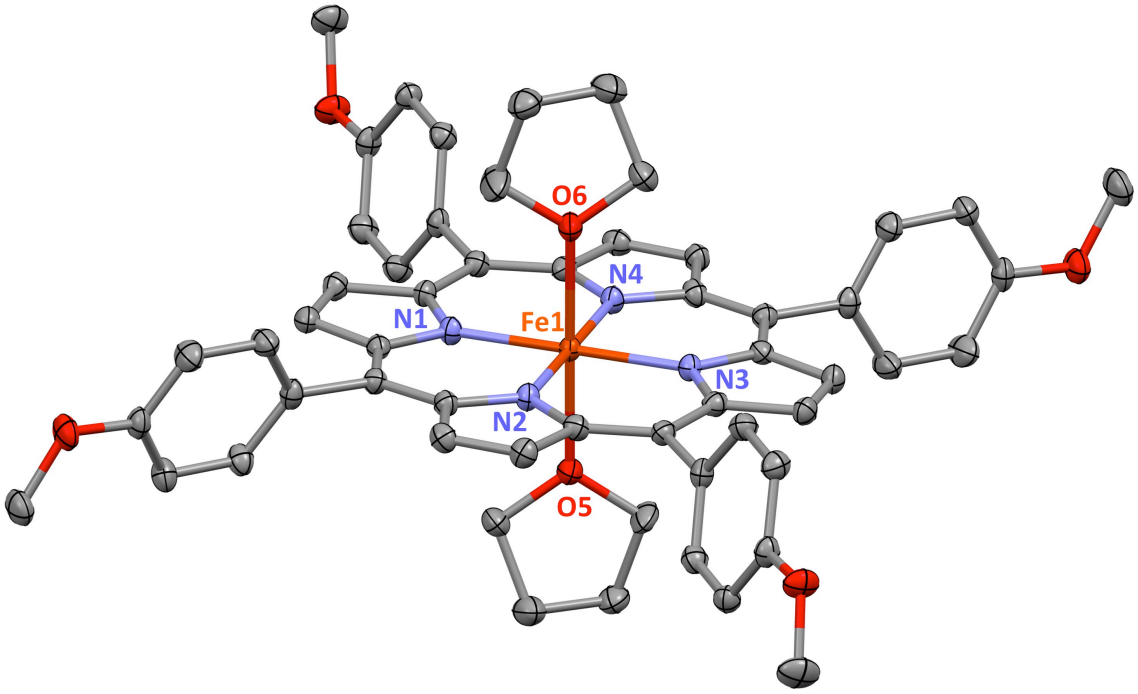

Figure S22. Displacement ellipsoid plot (50% probability level) of $[(TMPP)Fe^{III}(THF)_2]^+$, showing the atom-labeling scheme. Lattice solvent molecules and hydrogen atoms have been omitted for the sake of clarity. Selected bond lengths (Å) and angles (deg): Fe1–O6, 2.156(2); Fe1–O5, 2.154(2); Fe1–N1, 2.015(3); Fe1–N2, 2.025(3); Fe1–N3, 2.032(3); Fe1–N4, 2.014(3); O5–Fe1–O6, 179.68(10); N1–Fe1–N2, 89.40(10); N1–Fe1–N3, 179.70(11); N1–Fe1–N4, 90.98(10); N1–Fe1–O5, 90.58(9); N1–Fe1–O6, 89.67(9); N2–Fe1–N3, 90.30(10); N2–Fe1–N4, 179.26(10); N2–Fe1–O5, 90.68(9); N2–Fe1–O6, 89.13(9); N3–Fe1–N4, 89.32(10); N3–Fe1–O5, 89.38(9); N3–Fe1–O6, 90.37(9); N4–Fe1–O5, 89.96(9); N4–Fe1–O6, 90.24(9).

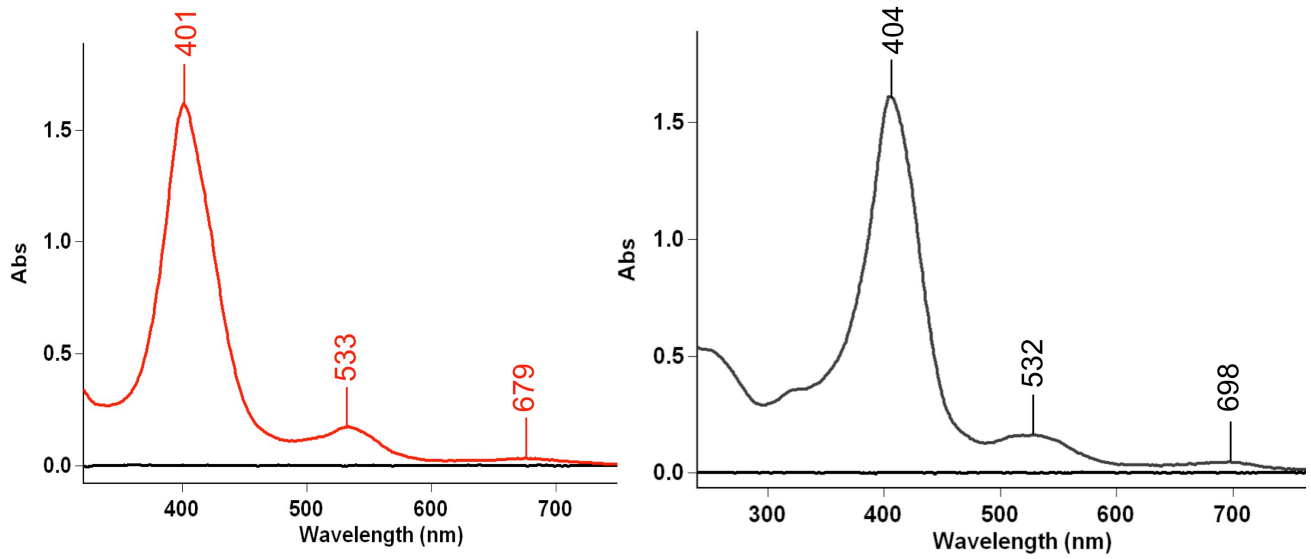

Figure S23. UV–vis spectra of $[(TMPP)Fe^{III}(THF)_2](SbF_6)$ in acetone (*left*, red) and MeCN (*right*, black) 50 μM in a 2-mm cuvette at RT.

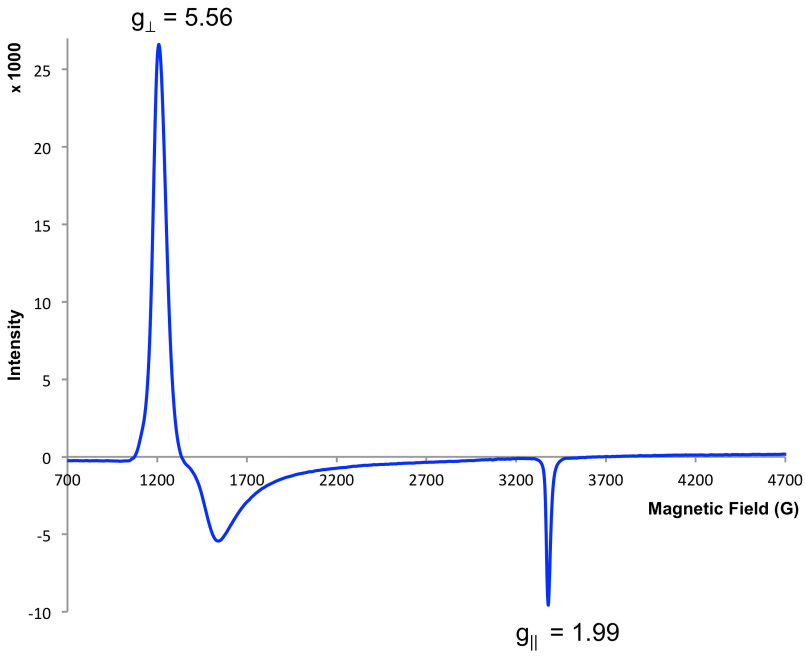

Figure S24. EPR spectrum of $[(TMPP)Fe^{III}(THF)_2](SbF_6)$ (1 mM) in THF/MeTHF (1:4) at 12 K.

Computational details

All structures were fully optimized in the presence of solvent (acetone, PCM model) within Gaussian 09 program.[1] The BP86[2,3] functional with the 6–31G(d)[4-18] basis sets for all the atoms were used. In all case the nature of stationary points were checked (full optimization, NIMag= 0 for minima and NIMag=1 – for transition state).

Various spin states of the complexes were considered in our calculations (high spin (HS), intermediate spin (IS) and low spin (LS)). Single-point energy evaluation was performed at the OLYP[19–22]/6–311+G(d,p) level of theory, including solvent correction via PCM model.

1. Gaussian 09 Revision A.2 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C. Iyengar, S. S. Tomasi, J. Cossi, M. Rega, Millam, N. J., Klene, M. Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, O., Foresman, J. B., Ortiz, J. V., Cioslowski, J., and Fox, D. J. Gaussian, Inc., Wallingford CT **2009.**
2. Becke, A. D. *Phys. Rev. A At. Mol. Opt. Phys.* **1988**, *38*, 3098.
3. Perdew, J. P. *Phys. Rev. B Condens. Matter Mater. Phys.* **1986**, *33*, 8822.
4. Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724.
5. Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213.
6. Hariharan, P. C.; Pople, J. A. *Mol. Phys.* **1974**, *27*, 209.
7. Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654.
8. Rassolov, V. A.; Pople, J. A.; Ratner, M. A.; Windus, T. L. *J. Chem. Phys.* **1998**, *109*, 1223.
9. Rassolov, V. A.; Ratner, M. A.; Pople, J. A.; Redfern, P. C.; Curtiss, L. A. *J. Comput. Chem.* **2001**, *22*, 976.
10. Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257.
11. Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257.
12. Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213.
13. Hariharan, P. C.; Pople, J. A. *Mol. Phys.* **1974**, *27*, 209.
14. Gordon, M. S. *Chem. Phys. Lett.* **1980**, *76*, 163.
15. Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; DeFrees, D. J.; Pople, J. A.; Gordon, M. S. *J. Chem. Phys.* **1982**, *77*, 3654.
16. Binning, R. C. J.; L. A. Curtiss *J. Comput. Chem.* **1990**, *11*, 1206.
17. Blaudeau, J.-P.; McGrath, M. P.; Curtiss, L. A.; Radom, L. *J. Chem. Phys.* **1997**, *107*, 5016.
18. Rassolov, V. A.; Ratner, M. A.; Pople, J. A.; Redfern, P. C.; Curtiss, L. A. *J. Comput. Chem.* **2001**, *22*, 976.
19. Handy, N.C.; Cohen, A.J. *Mol. Phys.*, **2001**, *99*, 403.
20. Hoe, W.-M.; Cohen, A.J.; Handy, N.C. *Chem. Phys. Lett.*, **2001**, *341*, 319.
21. Lee, C.; Yang, W.; Parr, R.G. *Phys. Rev. B*, **1988**, *37*, 785.
22. Miehlich, B.; Savin. A.; Stoll, H.; Preuss, H. *Chem. Phys. Lett.*, **1989**, *157*, 200.

Table S2. Absolute energies (E, Hartree) of studied compounds at the OLYP/6-311+G(d,p) level, for different (HS – high spin, IS – intermediate spin, LS – low spin) states in the presence of solvent (acetone).

Compounds	HS	IS	LS
	E	E	E
$[(\mathbf{TMPP})\mathbf{Fe^{III}}–\mathbf{O}–\mathbf{Cu^{II}}(\mathbf{tmpa})]^+$	-6266.15854	-6266.15260	–
INIT1	-6396.06924	-6396.07014	–
TS1	-6396.06936	-6396.06993	–
***mono*-NO**	-6396.08632	-6396.08955	-6396.08947
***bis*-NO**	-6525.96359	-6526.02858	-6526.03250
NO	–	–	-129.895151

Table S3. Absolute energies (E, Hartree) and zero-point correction energy (ZPE, kcal/mol) of studied compounds at the BP86/6-31G(d) level, for different (HS – high spin, IS – intermediate spin, LS – low spin) states in the presence of solvent (acetone).

Compounds	HS		IS		LS	
	E	ZPE	E	ZPE	E	ZPE
$[(\mathbf{TMPP})\mathbf{Fe^{III}}–\mathbf{O}–\mathbf{Cu^{II}}(\mathbf{tmpa})]^+$	-6266.00970	648.85	-6266.021454	649.37	–	–
INIT1	-6395.90702	652.47	-6395.925409	653.50	–	–
TS1	-6395.90517	652.52	*-6395.923805*	*653*	–	–
***mono*-NO**	-6395.92571	655.67	-6395.94428	654.00	-6395.96122	655.55
***bis*-NO**	-6525.85606	658.31	-6525.90377	659.56	-6525.90605	659.87
NO	–	–	–	–	-129.895151	2.70

XYZ Coordinates

NO

2

N	-0.62483	-0.00000	0.00000
O	0.54711	0.00000	0.00000

[(TMPP)Fe^{III}–O–Cu^{II}(tmpa)]$^{+}$

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Fe	-0.05373	-1.86193	0.08131
C	2.61924	-2.22350	-1.55535
C	4.04803	-2.39887	-1.38933
H	4.77127	-2.46632	-2.20086
C	4.28455	-2.51253	-0.04429
H	5.23772	-2.69142	0.45137
C	3.00175	-2.40947	0.62202
C	2.82882	-2.55675	2.02081
C	1.56911	-2.64379	2.66265
C	1.38831	-2.82795	4.08915
H	2.18986	-2.89372	4.82354
C	0.03886	-2.92076	4.31330
H	-0.46858	-3.09267	5.26165
C	-0.61637	-2.76179	3.03117
C	-2.01830	-2.81947	2.84496
C	-2.66140	-2.72701	1.58709
C	-4.09966	-2.73301	1.40812
H	-4.83292	-2.82589	2.20826
C	-4.33768	-2.58422	0.06521
H	-5.30241	-2.53262	-0.43774
C	-3.04741	-2.49163	-0.58701
C	-2.87259	-2.31388	-1.98098
C	-1.61301	-2.19795	-2.61638
C	-1.43287	-2.10925	-4.05086
H	-2.23537	-2.10702	-4.78725
C	-0.08275	-2.05000	-4.28383
H	0.42414	-1.97490	-5.24488
C	0.57355	-2.12880	-2.99450
C	1.97837	-2.13560	-2.81458
N	1.99153	-2.23690	-0.31583
N	0.33267	-2.59287	2.03064
N	-2.03011	-2.57881	0.35683
N	-0.37605	-2.20875	-1.98219
C	1.62965	1.00128	2.68957
H	1.62106	0.03262	2.18152
C	2.43973	1.25559	3.80188
H	3.09366	0.46864	4.18804
N	-0.43510	3.82910	0.68812
C	0.66336	4.38774	-0.14022
C	0.81960	3.57900	-1.41423
C	1.28110	4.12826	-2.61678
H	1.49448	5.19964	-2.68137
C	1.46509	3.28350	-3.72224
H	1.82509	3.68896	-4.67302
C	1.17504	1.91760	-3.58900
H	1.30448	1.22152	-4.42225
C	0.70354	1.44568	-2.35870
H	0.45308	0.39396	-2.19248
N	0.52584	2.25627	-1.29098
O	-0.20015	-0.14262	0.28478
Cu	-0.31088	1.71869	0.47822
N	0.80028	1.93255	2.16715
C	2.39907	2.52877	4.38921
H	3.02718	2.76630	5.25353
C	1.54345	3.50000	3.84746
H	1.48601	4.50539	4.27597
C	0.75119	3.16441	2.74228
C	-0.26241	4.11597	2.13440
C	-1.77903	4.21294	0.18707
C	-2.80515	3.17404	0.59865
C	-4.15202	3.48038	0.82859
H	-4.49584	4.51734	0.76334
C	-4.55160	1.12769	1.21246
H	-5.20504	0.28370	1.44911
C	-3.18962	0.90271	0.98231
H	-2.74535	-0.09527	1.03358
N	-2.32958	1.90200	0.68167
C	-5.04156	2.43964	1.13735
H	-6.09916	2.65355	1.32089
H	0.51098	5.46249	-0.35695
H	1.59497	4.30344	0.44995
H	-2.06911	5.22724	0.52238
H	-1.72207	4.23881	-0.91726
H	0.01385	5.17276	2.31368
H	-1.24114	3.94997	2.62196
C	-4.09755	-2.26097	-2.84040
C	4.06345	-2.66088	2.86087
C	4.34691	-3.81502	3.62137
H	3.65253	-4.66192	3.59171
C	5.51019	-3.91852	4.40115
H	5.69481	-4.83573	4.96662
C	6.42580	-2.84642	4.43403
C	6.16136	-1.68396	3.67561
H	6.87836	-0.85718	3.70938
C	5.00199	-1.59966	2.90144
H	4.81138	-0.69205	2.31825
C	7.89699	-3.99533	5.94114
H	7.12141	-4.18138	6.70708
H	8.85446	-3.77373	6.43411
H	8.00862	-4.89238	5.30425
C	-4.42162	-1.10380	-3.57930
H	-3.76962	-0.22545	-3.51455
C	-5.56952	-1.03993	-4.38588
H	-5.78761	-0.11977	-4.93446
C	-6.42515	-2.15763	-4.46923
C	-6.11376	-3.32714	-3.73998
H	-6.78010	-4.19221	-3.82057
C	-4.96983	-3.37265	-2.94003
H	-4.73642	-4.29046	-2.38927
C	-7.91981	-1.04510	-5.97978
H	-8.08954	-0.17202	-5.32243
H	-8.85446	-1.30020	-6.49967
H	-7.13880	-0.79959	-6.72321
O	7.58867	-2.83206	5.15677
O	-7.56979	-2.21221	-5.21975
C	-2.87794	-2.99311	4.05924
C	-3.66324	-4.15095	4.23870
H	-3.63432	-4.94204	3.48110
C	-4.47113	-4.32632	5.37409
H	-5.05654	-5.24352	5.47835
C	-4.50893	-3.32261	6.36363

C	-3.73015	-2.15507	6.19947
H	-3.77291	-1.37976	6.97148
C	-2.92803	-1.99899	5.06678
H	-2.33539	-1.08488	4.94994
C	-6.06709	-4.54870	7.71505
H	-6.81833	-4.66564	6.91187
H	-6.57815	-4.38874	8.67537
H	-5.44705	-5.46249	7.77458
C	2.84484	-2.08464	-4.03427
C	2.79552	-3.10805	-5.01287
H	2.11767	-3.95668	-4.86999
C	3.60844	-3.06602	-6.14746
H	3.57335	-3.86450	-6.89581
C	4.50254	-1.98919	-6.34232
C	4.57031	-0.96122	-5.37956
H	5.24971	-0.11397	-5.50497
C	3.74862	-1.02115	-4.24209
H	3.80397	-0.21276	-3.50462
C	6.17917	-0.96714	-7.71968
H	5.65841	0.00513	-7.80115
H	6.66937	-1.20219	-8.67537
H	6.93919	-0.91167	-6.91836
O	-5.25810	-3.37998	7.50903
O	5.25216	-2.03916	-7.48739

INIT1_IS

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Initial complex in acetone

Fe	0.22176	-1.83067	-0.27991
C	2.67357	-1.84956	-2.06462
C	4.05870	-2.25149	-2.07368
H	4.70494	-2.23912	-2.95031
C	4.36444	-2.66594	-0.80356
H	5.31202	-3.05397	-0.43283
C	3.17451	-2.48862	-0.00788
C	3.13883	-2.65632	1.38732
C	1.96248	-2.45224	2.12964
C	1.90603	-2.48718	3.57092
H	2.76494	-2.62844	4.22527
C	0.59044	-2.32964	3.92257
H	0.15650	-2.33268	4.92171
C	-0.16162	-2.19868	2.69760
C	-1.56546	-2.21970	2.64349
C	-2.26302	-2.25610	1.42284
C	-3.68714	-2.45676	1.31837
H	-4.35952	-2.59497	2.16395
C	-4.00160	-2.43476	-0.01636
H	-4.98102	-2.54574	-0.47949
C	-2.77626	-2.17596	-0.73161
C	-2.73412	-1.87679	-2.10353
C	-1.54313	-1.49902	-2.74723
C	-1.47186	-1.06769	-4.12052
H	-2.32775	-0.94958	-4.78318
C	-0.14767	-0.85098	-4.40242
H	0.29027	-0.51387	-5.34084
C	0.59977	-1.21251	-3.22273
C	1.99941	-1.35909	-3.19745
N	2.11446	-2.04277	-0.80089
N	0.69369	-2.22941	1.59298
N	-1.69609	-2.09045	0.15521
N	-0.26660	-1.54937	-2.17920
C	0.25199	1.56896	3.22825
H	0.45143	0.59479	2.77320
C	0.54026	1.81449	4.57418
H	0.97396	1.02021	5.18794
N	-1.03590	4.39381	0.58581
C	0.16418	5.09025	0.07001
C	0.65182	4.39552	-1.18562
C	1.29839	5.07160	-2.22723
H	1.44267	6.15472	-2.16601
C	1.75046	4.34037	-3.33565
H	2.25978	4.84589	-4.16201
C	1.52858	2.95603	-3.36808
H	1.85832	2.34337	-4.21173
C	0.86910	2.35293	-2.29160
H	0.67736	1.27680	-2.26793
N	0.44045	3.05076	-1.21390
O	0.45322	0.48554	0.24469
Cu	-0.50620	2.31943	0.40437
N	-0.28702	2.50309	2.40819
C	0.27463	3.08782	5.09949
H	0.50439	3.32378	6.14323
C	-0.29341	4.05635	4.26085
H	-0.52361	5.05994	4.63227
C	-0.57773	3.72583	2.92845
C	-1.31315	4.68535	2.01010
C	-2.22645	4.57470	-0.27816
C	-3.17935	3.40888	-0.09230
C	-4.57037	3.56371	-0.14764
H	-5.00135	4.55717	-0.30652
C	-4.78330	1.18911	0.22113
H	-5.37399	0.27951	0.35784
C	-3.38500	1.11907	0.26856
H	-2.87194	0.16944	0.44185
N	-2.58600	2.20046	0.11426
C	-5.38853	2.43454	0.00645
H	-6.47827	2.53046	-0.03021
H	-0.02484	6.16634	-0.11424
H	0.94403	5.02026	0.85190
H	-2.73306	5.54081	-0.08899
H	-1.87686	4.59087	-1.32661
H	-1.08478	5.73805	2.26511
H	-2.39808	4.54861	2.17452
N	1.77261	0.60500	0.51265
O	2.13738	1.74441	0.79433
C	-4.00195	-1.95298	-2.89830
C	4.38951	-3.04248	2.10992
C	4.46364	-4.25300	2.83076
H	3.59502	-4.92068	2.84965
C	5.62954	-4.63631	3.51261
H	5.64621	-5.58797	4.05019
C	6.75976	-3.79348	3.48769
C	6.70150	-2.57368	2.77661
H	7.58169	-1.92237	2.77345
C	5.53552	-2.20993	2.09921
H	5.50237	-1.25637	1.56098
C	8.04773	-5.28880	4.85188
H	7.31270	-5.32379	5.67741
H	9.06608	-5.30263	5.26631
H	7.90500	-6.16634	4.19425
C	-4.62231	-0.79822	-3.41582
H	-4.17779	0.18421	-3.22201
C	-5.80651	-0.87219	-4.16854
H	-6.25754	0.04833	-4.54831
C	-6.39727	-2.12823	-4.41584
C	-5.79180	-3.29500	-3.89807
H	-6.25823	-4.26505	-4.09896
C	-4.61384	-3.20397	-3.15262
H	-4.15012	-4.11842	-2.76621

C	-8.18489	-1.16669	-5.69487
H	-8.50913	-0.46458	-4.90421
H	-9.06608	-1.54552	-6.23247
H	-7.51818	-0.64044	-6.40326
O	7.94810	-4.06040	4.11422
O	-7.54544	-2.32510	-5.13732
C	-2.33459	-2.29485	3.92775
C	-3.00611	-3.47425	4.30979
H	-2.96200	-4.35328	3.65703
C	-3.72165	-3.55801	5.51578
H	-4.22348	-4.49357	5.77638
C	-3.77345	-2.44017	6.37356
C	-3.10325	-1.25177	6.00717
H	-3.15293	-0.38945	6.68018
C	-2.39617	-1.18544	4.80385
H	-1.88498	-0.25507	4.53288
C	-5.12647	-3.59277	7.98515
H	-5.92065	-3.86837	7.26648
H	-5.57949	-3.34947	8.95705
H	-4.42848	-4.44212	8.10544
C	2.79442	-1.06268	-4.42853
C	2.57756	-1.76846	-5.63811
H	1.81558	-2.55450	-5.67364
C	3.33301	-1.49732	-6.78047
H	3.16908	-2.05325	-7.70939
C	4.33544	-0.50158	-6.75135
C	4.57167	0.21005	-5.55705
H	5.34018	0.98570	-5.50523
C	3.80756	-0.08002	-4.41478
H	3.99764	0.47970	-3.49236
C	6.05009	0.68623	-7.93697
H	5.64462	1.69092	-7.71509
H	6.46010	0.67286	-8.95705
H	6.85081	0.44419	-7.21369
O	-4.43658	-2.40295	7.57204
O	5.01510	-0.30974	-7.92416

TS1_IS

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Fe	-0.645382	0.077981	-1.339409
C	-3.525808	-0.912272	-1.482112
C	-4.878476	-0.413685	-1.510218
H	-5.761994	-1.019227	-1.705228
C	-4.811111	0.926968	-1.232023
H	-5.627915	1.643666	-1.158440
C	-3.415492	1.257223	-1.086668
C	-2.953549	2.551626	-0.781396
C	-1.600979	2.902717	-0.925737
C	-1.104081	4.253361	-0.829248
H	-1.689236	5.107905	-0.492259
C	0.180868	4.242118	-1.309906
H	0.856763	5.085240	-1.447024
C	0.499602	2.873207	-1.630180
C	1.723568	2.456912	-2.179837
C	2.037349	1.095527	-2.346226
C	3.329625	0.627061	-2.776588
H	4.133152	1.269699	-3.134568
C	3.341880	-0.735299	-2.604409
H	4.158842	-1.430252	-2.794031
C	2.045856	-1.110701	-2.103094
C	1.684123	-2.426101	-1.762245
C	0.357776	-2.767544	-1.441250
C	-0.096436	-4.126019	-1.278357
H	0.554352	-4.998740	-1.247452
C	-1.467993	-4.088885	-1.246679
H	-2.163222	-4.923735	-1.169163
C	-1.855962	-2.708007	-1.383272
C	-3.191201	-2.277090	-1.493901
N	-2.622456	0.135855	-1.298356
N	-0.588142	2.042669	-1.357083
N	1.232381	0.018847	-1.960741
N	-0.727490	-1.887795	-1.444225
C	0.351262	2.798922	2.741260
H	-0.063161	2.571103	1.755343
C	0.164438	4.051543	3.334128
H	-0.402079	4.821280	2.802394
N	2.135594	-0.386491	4.600700
C	1.068796	-1.055127	5.364262
C	0.395058	-2.117859	4.512876
C	-0.130347	-3.297713	5.052887
H	-0.029348	-3.499554	6.124801
C	-0.786552	-4.203265	4.204713
H	-1.207356	-5.131956	4.603647
C	-0.885426	-3.894884	2.840787
H	-1.380355	-4.566500	2.133414
C	-0.329274	-2.697948	2.375893
H	-0.389424	-2.409701	1.322445
N	0.302076	-1.817525	3.188794
O	-0.106554	0.130104	1.002243
Cu	1.164187	-0.094768	2.606744
N	1.044312	1.796817	3.334981
C	0.698366	4.282273	4.609530
H	0.553783	5.242331	5.115622
C	1.425651	3.254728	5.226826
H	1.866962	3.394522	6.219889
C	1.596132	2.037673	4.553916
C	2.496239	0.943812	5.114721
C	3.296711	-1.240568	4.294700
C	3.967223	-0.774860	3.010864
C	5.355160	-0.813376	2.834264
H	5.998601	-1.161951	3.649453
C	5.031990	0.037447	0.601112
H	5.400279	0.367731	-0.373727
C	3.654711	0.052581	0.856268
H	2.941497	0.389824	0.098490
N	3.118464	-0.338835	2.036634
C	5.900891	-0.402441	1.607517
H	6.983768	-0.421820	1.447046
H	1.431622	-1.487938	6.321585
H	0.321583	-0.278028	5.617235
H	4.029821	-1.284350	5.127729
H	2.917248	-2.269026	4.146084
H	2.508070	0.977732	6.224450
H	3.531256	1.156180	4.785493
N	-1.385153	0.359075	1.408083
O	-1.535664	0.408816	2.623738
C	2.708560	-3.514474	-1.837697
C	-3.950081	3.574188	-0.343221
C	-4.225615	4.731302	-1.100311
H	-3.707484	4.886135	-2.053303
C	-5.173530	5.676719	-0.677549
H	-5.369516	6.553376	-1.300899
C	-5.868281	5.475201	0.532984
C	-5.604828	4.319541	1.302151
H	-6.151820	4.179741	2.239930
C	-4.666185	3.384752	0.865106
H	-4.463056	2.494981	1.471220
C	-7.124529	7.500993	0.294378

H -6.240616 8.157278 0.179031
H -7.895892 8.025666 0.876644
H -7.526753 7.247153 -0.704935
C 3.122574 -4.202635 -0.679976
H 2.697763 -3.920296 0.290340
C 4.070381 -5.237841 -0.736659
H 4.368445 -5.744656 0.185341
C 4.625923 -5.606427 -1.978746
C 4.218821 -4.929156 -3.149597
H 4.648678 -5.236776 -4.108039
C 3.274728 -3.904102 -3.076186
H 2.951964 -3.402807 -3.995353
C 5.978611 -7.328937 -1.008976
H 6.473414 -6.670419 -0.268923
H 6.702348 -8.069149 -1.379945
H 5.131483 -7.852786 -0.525779
O -6.809309 6.323826 1.046277
O 5.552524 -6.595810 -2.161299
C 2.739899 3.483894 -2.572404
C 3.052827 3.703679 -3.928790
H 2.531355 3.124702 -4.699342
C 4.007042 4.657260 -4.318633
H 4.214459 4.803303 -5.382080
C 4.674569 5.417592 -3.336910
C 4.373887 5.207469 -1.972621
H 4.906100 5.801870 -1.223097
C 3.422368 4.255495 -1.601705
H 3.205701 4.096138 -0.539128
C 5.954108 6.626880 -4.961505
H 6.371232 5.726465 -5.451857
H 6.718727 7.416854 -4.936757
H 5.075488 6.982932 -5.532544
C -4.271381 -3.303081 -1.596477
C -4.296963 -4.212762 -2.683280
H -3.524380 -4.145367 -3.457045
C -5.300416 -5.174448 -2.798585
H -5.328844 -5.866636 -3.645906
C -6.315343 -5.263292 -1.819498
C -6.304855 -4.372151 -0.726530
H -7.072102 -4.424751 0.050750
C -5.291654 -3.405785 -0.627901
H -5.284710 -2.726023 0.231459
C -8.310489 -6.357416 -1.071147
H -7.924123 -6.602606 -0.063161
H -8.941132 -7.183043 -1.431486
H -8.912138 -5.429942 -1.018889
O 5.620455 6.371536 -3.592291
O -7.249091 -6.239771 -2.024829

NORMALMODES 405
Fe -0.04 0.00 -0.09
C -0.05 0.00 -0.09
C -0.07 0.00 -0.06
H -0.07 0.00 -0.05
C -0.06 0.00 -0.06
H -0.05 0.00 -0.05
C -0.04 -0.01 -0.07
C -0.03 -0.02 -0.05
C -0.03 -0.02 -0.02
C -0.02 -0.03 0.02
H -0.02 -0.04 0.06
C -0.01 -0.01 0.03
H -0.01 -0.01 0.07
C -0.02 0.00 -0.03
C -0.02 0.00 -0.02
C -0.02 0.01 -0.01
C -0.02 0.00 -0.02
H -0.03 -0.01 -0.04
C -0.03 0.00 0.00
H -0.04 0.00 0.00
C -0.03 0.01 0.02
C -0.04 0.02 0.02
C -0.05 0.02 0.00
C -0.05 0.02 0.01
H -0.05 0.03 0.04
C -0.06 0.01 -0.02
H -0.05 0.00 -0.03
C -0.06 0.00 -0.05
C -0.06 0.01 -0.07
N -0.05 0.00 -0.11
N -0.03 0.00 -0.07
N -0.03 0.01 0.01
N -0.06 0.01 -0.05
C -0.03 0.00 0.09
H -0.02 0.00 0.09
C -0.04 0.00 0.10
H -0.05 -0.01 0.10
N 0.04 0.02 0.04
C 0.05 0.01 0.05
C 0.05 0.01 0.05
C 0.05 0.00 0.04
H 0.05 -0.01 0.03
C 0.04 0.02 0.03
H 0.04 0.01 0.01
C 0.03 0.04 0.03
H 0.03 0.05 0.02
C 0.03 0.04 0.04
H 0.03 0.06 0.05
N 0.03 0.03 0.06
O 0.36 0.02 0.04
Cu 0.09 0.02 0.12
N 0.00 0.01 0.09
C -0.03 0.00 0.09
H -0.03 0.00 0.09
C 0.00 0.01 0.09
H 0.00 0.02 0.08
C 0.01 0.02 0.08
C 0.03 0.02 0.06
C 0.07 0.03 0.07
C 0.08 0.01 0.06
C 0.07 -0.01 0.05
H 0.08 -0.01 0.05
C 0.06 -0.05 0.03
H 0.05 -0.08 0.02
C 0.06 -0.02 0.05
H 0.05 -0.03 0.05
N 0.08 0.01 0.06
C 0.06 -0.04 0.03
H 0.06 -0.06 0.02
H 0.07 0.01 0.04
H 0.05 0.00 0.07
H 0.05 0.06 0.08
H 0.08 0.02 0.09
H 0.05 0.00 0.05
H 0.02 0.04 0.04
N 0.28 -0.15 -0.30
O -0.08 -0.04 -0.35
C -0.04 0.01 0.02
C -0.02 -0.02 -0.03
C -0.01 -0.01 -0.01

H -0.01 0.00 -0.01
C 0.00 0.00 0.00
H 0.01 0.01 0.01
C 0.00 -0.01 0.00
C -0.01 -0.02 -0.01
H -0.01 -0.03 -0.01
C -0.02 -0.03 -0.03
H -0.03 -0.04 -0.04
C 0.01 0.00 0.02
H 0.01 0.00 0.02
H 0.01 0.00 0.02
H 0.01 0.01 0.02
C -0.03 0.02 0.01
H -0.02 0.02 0.02
C -0.03 0.02 0.01
H -0.02 0.02 0.01
C -0.04 0.02 0.01
C -0.05 0.01 0.01
H -0.05 0.01 0.01
C -0.05 0.01 0.01
H -0.06 0.00 0.01
C -0.02 0.02 0.00
H -0.02 0.02 0.00
H -0.02 0.02 0.00
H -0.02 0.02 0.01
O 0.01 -0.01 0.01
O -0.03 0.02 0.00
C -0.01 0.00 -0.02
C -0.02 0.02 -0.02
H -0.03 0.04 -0.02
C -0.01 0.02 -0.01
H -0.02 0.03 -0.01
C 0.00 0.00 0.00
C 0.00 -0.02 0.00
H 0.01 -0.03 0.00
C 0.00 -0.01 -0.01
H 0.00 -0.03 -0.01
C 0.00 0.01 0.00
H -0.01 0.01 -0.01
H 0.01 0.00 0.01
H 0.00 0.02 0.01
C -0.05 0.00 -0.05
C -0.06 -0.01 -0.04
H -0.06 -0.01 -0.05
C -0.05 -0.02 -0.02
H -0.05 -0.03 -0.02
C -0.04 -0.02 -0.01
C -0.03 -0.01 -0.02
H -0.03 -0.01 -0.01
C -0.04 0.00 -0.04
H -0.04 0.01 -0.05
C -0.02 -0.02 0.01
H -0.02 -0.01 0.01
H -0.02 -0.03 0.03
H -0.03 -0.03 0.01
O 0.00 0.00 0.00
O -0.03 -0.03 0.01
-49.5795

TS1_HS

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Fe -0.638549 0.168130 -1.105222
C -3.018175 -1.870703 -1.436591
C -4.463211 -1.941471 -1.354220
H -5.060000 -2.838697 -1.513321
C -4.909277 -0.677823 -1.059778
H -5.939785 -0.345385 -0.940141
C -3.741475 0.176475 -0.983571
C -3.800069 1.572643 -0.750197
C -2.705425 2.456584 -0.907148
C -2.793210 3.897209 -0.787399
H -3.682154 4.452621 -0.491308
C -1.569789 4.405457 -1.146927
H -1.276596 5.452928 -1.206764
C -0.710057 3.276918 -1.436975
C 0.646688 3.381360 -1.827301
C 1.492248 2.269223 -2.055297
C 2.899458 2.370698 -2.382272
H 3.446746 3.301643 -2.524957
C 3.390076 1.090354 -2.449150
H 4.413076 0.780350 -2.658666
C 2.284992 0.196040 -2.172637
C 2.394539 -1.215343 -2.141070
C 1.304552 -2.098010 -1.943430
C 1.392234 -3.535747 -2.074566
H 2.308188 -4.096518 -2.255960
C 0.115916 -4.029579 -1.959890
H -0.200332 -5.070615 -2.013274
C -0.762798 -2.895835 -1.769198
C -2.172452 -2.984212 -1.659497
N -2.595076 -0.563656 -1.237149
N -1.416101 2.091051 -1.280220
N 1.128936 0.932115 -1.928720
N -0.017269 -1.720094 -1.726541
C 0.064480 2.425563 3.565224
H -0.388749 2.401720 2.571856
C -0.198961 3.476885 4.448330
H -0.866207 4.287703 4.142905
N 2.261338 -0.890594 4.507090
C 1.323911 -1.840437 5.145027
C 0.682940 -2.722596 4.091600
C 0.286338 -4.040174 4.350347
H 0.466961 -4.477153 5.337317
C -0.337305 -4.777279 3.332825
H -0.657974 -5.808306 3.511409
C -0.526917 -4.171171 2.082444
H -0.996043 -4.705996 1.251796
C -0.094816 -2.853832 1.898509
H -0.209902 -2.346658 0.936390
N 0.492422 -2.128265 2.880759
O 0.071523 0.153899 1.053222
Cu 1.239332 -0.260897 2.727948
N 0.881775 1.387093 3.870289
C 0.396283 3.455756 5.717931
H 0.199549 4.250546 6.444162
C 1.255306 2.395964 6.038453
H 1.750766 2.345870 7.013221
C 1.491230 1.393100 5.088238
C 2.524682 0.306239 5.332636
C 3.497638 -1.527540 3.996778
C 4.087892 -0.677126 2.885622
C 5.467561 -0.522938 2.705107
H 6.164704 -1.015654 3.390053
C 4.997271 0.890389 0.805846
H 5.307172 1.524740 -0.028736
C 3.633489 0.688831 1.052102
H 2.870515 1.154888 0.421921
N 3.174586 -0.078339 2.068701

C 5.932829 0.271428 1.645722
H 7.006856 0.410592 1.487754
H 1.813713 -2.448390 5.931501
H 0.537784 -1.237990 5.638634
H 4.239025 -1.705636 4.799966
H 3.216439 -2.515891 3.588421
H 2.594902 0.057268 6.409116
H 3.512480 0.706451 5.037768
N -1.256870 0.279553 1.270520
O -1.636941 0.125159 2.421967
C 3.740154 -1.825504 -2.391135
C -5.122320 2.140686 -0.337028
C -5.829941 3.057481 -1.142000
H -5.410865 3.360975 -2.107822
C -7.073185 3.578250 -0.746792
H -7.594115 4.278102 -1.405401
C -7.634460 3.183914 0.485244
C -6.939779 2.265297 1.303885
H -7.383549 1.970163 2.260388
C -5.707895 1.751962 0.893013
H -5.174842 1.046359 1.539711
C -9.576103 4.558673 0.173355
H -9.006884 5.493104 0.012552
H -10.489475 4.778775 0.744573
H -9.848857 4.120837 -0.804859
C 4.399086 -2.562397 -1.385706
H 3.924648 -2.673233 -0.404235
C 5.656401 -3.149401 -1.604173
H 6.135401 -3.706177 -0.794563
C 6.282578 -3.006046 -2.859265
C 5.634559 -2.274771 -3.879895
H 6.125999 -2.179339 -4.853695
C 4.385043 -1.695979 -3.645302
H 3.889339 -1.143349 -4.451016
C 8.191701 -4.292432 -2.183925
H 8.413944 -3.676010 -1.292917
H 9.133443 -4.615421 -2.650607
H 7.606757 -5.180561 -1.880352
O -8.834877 3.625771 0.975234
O 7.504085 -3.531494 -3.188943
C 1.229346 4.750952 -1.997859
C 1.652936 5.205278 -3.264131
H 1.542126 4.548927 -4.134575
C 2.200869 6.486007 -3.443789
H 2.508594 6.801051 -4.444288
C 2.337602 7.346451 -2.335307
C 1.921788 6.906571 -1.058601
H 2.041007 7.580438 -0.203834
C 1.376656 5.630453 -0.897919
H 1.068949 5.300323 0.100423
C 3.293082 9.098243 -3.666931
H 4.107400 8.472770 -4.077610
H 3.667769 10.115872 -3.485235
H 2.457459 9.136114 -4.390326
C -2.804216 -4.334606 -1.791687
C -2.684794 -5.081053 -2.990040
H -2.132075 -4.655983 -3.834918
C -3.274249 -6.339980 -3.122103
H -3.188162 -6.907631 -4.054399
C -4.004291 -6.899803 -2.049382
C -4.135268 -6.175076 -0.847142
H -4.689025 -6.584925 0.001512
C -3.540937 -4.907509 -0.732931
H -3.645303 -4.356762 0.208572
C -5.300314 -8.740270 -1.218658
H -4.677340 -8.904798 -0.319811
H -5.640014 -9.709229 -1.611889
H -6.177344 -8.122209 -0.950938
O 2.855997 8.613578 -2.387569
O -4.540620 -8.138683 -2.278892

NORMALMODES 405
Fe 0.05 0.00 0.04
C 0.03 0.00 0.02
C 0.03 0.00 0.00
H 0.03 0.01 -0.02
C 0.03 0.00 0.00
H 0.03 0.01 -0.01
C 0.03 0.00 0.02
C 0.02 0.00 0.02
C 0.02 0.00 0.02
C 0.02 0.00 0.00
H 0.01 0.00 -0.02
C 0.02 0.00 0.00
H 0.01 0.00 -0.02
C 0.02 0.00 0.03
C 0.02 -0.01 0.02
C 0.02 -0.01 0.01
C 0.01 0.00 0.00
H 0.01 0.00 0.01
C 0.02 0.00 -0.01
H 0.02 0.00 -0.02
C 0.03 -0.01 -0.01
C 0.03 -0.01 -0.02
C 0.02 0.00 -0.03
C 0.02 -0.01 -0.02
H 0.02 -0.01 -0.01
C 0.02 0.00 -0.01
H 0.02 0.00 0.01
C 0.03 0.00 -0.02
C 0.03 0.00 0.00
N 0.04 0.00 0.04
N 0.03 -0.01 0.05
N 0.03 -0.01 0.01
N 0.03 0.00 -0.04
C 0.06 0.05 -0.08
H 0.11 0.08 -0.11
C 0.03 0.03 -0.07
H 0.05 0.04 -0.07
N -0.02 0.00 -0.04
C -0.02 0.00 -0.04
C -0.01 0.00 -0.04
C -0.01 0.00 -0.03
H -0.02 0.01 -0.02
C -0.01 0.00 -0.02
H -0.01 0.00 -0.02
C -0.01 -0.01 -0.03
H -0.02 -0.01 -0.02
C -0.01 -0.01 -0.03
H -0.03 0.00 -0.03
N 0.00 0.00 -0.04
O -0.40 -0.03 -0.06
Cu -0.05 0.00 -0.06
N 0.04 0.03 -0.08
C -0.02 0.00 -0.05
H -0.04 -0.02 -0.03
C -0.03 -0.01 -0.04
H -0.06 -0.03 -0.03
C 0.00 0.01 -0.06
C -0.02 0.00 -0.04

C -0.03 0.00 -0.05
C -0.04 0.00 -0.04
C -0.03 0.01 -0.03
H -0.04 0.01 -0.02
C -0.02 0.02 -0.02
H -0.02 0.03 -0.01
C -0.03 0.01 -0.04
H -0.02 0.01 -0.04
N -0.04 0.00 -0.05
C -0.03 0.02 -0.02
H -0.03 0.03 -0.01
H -0.02 0.01 -0.03
H -0.02 0.00 -0.04
H -0.03 -0.01 -0.05
H -0.04 0.00 -0.05
H -0.03 0.00 -0.04
H -0.01 -0.01 -0.03
N -0.36 0.05 0.42
O 0.11 -0.06 0.55
C 0.03 0.00 -0.01
C 0.02 0.00 0.00
C 0.02 0.00 0.00
H 0.02 0.00 0.00
C 0.02 0.00 -0.01
H 0.02 -0.01 -0.01
C 0.01 0.00 -0.01
C 0.01 0.00 -0.01
H 0.00 0.00 -0.01
C 0.01 0.00 0.00
H 0.00 0.00 0.00
C 0.01 0.00 -0.01
H 0.01 0.00 -0.01
H 0.01 0.00 -0.02
H 0.01 0.00 -0.02
C 0.02 0.00 -0.01
H 0.02 0.00 -0.01
C 0.02 0.00 0.00
H 0.02 0.00 0.00
C 0.02 -0.01 0.00
C 0.03 -0.01 -0.01
H 0.03 -0.01 -0.01
C 0.03 -0.01 -0.01
H 0.03 -0.01 -0.01
C 0.02 -0.01 0.00
H 0.02 -0.01 0.00
H 0.02 -0.01 0.01
H 0.02 -0.01 0.00
O 0.01 0.00 -0.01
O 0.02 -0.01 0.00
C 0.02 -0.01 0.01
C 0.01 -0.01 0.01
H 0.01 -0.01 0.01
C 0.00 -0.01 0.00
H 0.00 -0.01 0.00
C 0.00 0.00 0.00
C 0.00 0.00 0.00
H 0.00 0.01 0.00
C 0.01 0.00 0.00
H 0.01 0.00 0.01
C 0.00 0.00 -0.01
H 0.00 0.00 0.00
H 0.00 0.00 -0.01
H 0.00 -0.01 -0.01
C 0.02 0.00 0.00
C 0.02 0.00 0.00
H 0.02 0.00 0.00
C 0.01 0.00 0.00
H 0.01 0.00 0.00
C 0.01 0.01 0.00
C 0.01 0.01 0.00
H 0.01 0.01 0.00
C 0.01 0.01 0.00
H 0.01 0.01 0.00
C 0.00 0.01 0.00
H 0.00 0.01 0.00
H 0.00 0.01 0.00
H 0.00 0.01 0.00
O 0.00 0.00 -0.01
O 0.00 0.01 0.00
-82.9500

***mono*-NO LS**

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Final complex in acetone

Fe	0.17437	-2.30689	-0.21933
C	2.88849	-2.56758	-1.56501
C	4.25724	-2.93830	-1.29179
H	5.03843	-3.03346	-2.04460
C	4.34479	-3.17310	0.05316
H	5.21394	-3.49418	0.62548
C	3.03590	-2.91964	0.60960
C	2.76652	-2.92672	1.98733
C	1.48054	-2.68614	2.49927
C	1.18997	-2.56587	3.90991
H	1.93044	-2.63087	4.70585
C	-0.16067	-2.37693	4.02346
H	-0.75290	-2.26940	4.93130
C	-0.69902	-2.38249	2.68315
C	-2.07371	-2.35242	2.40126
C	-2.56802	-2.51084	1.09582
C	-3.97200	-2.63400	0.78075
H	-4.77887	-2.61551	1.51194
C	-4.06422	-2.77446	-0.57758
H	-4.96167	-2.88840	-1.18415
C	-2.71916	-2.69141	-1.10051
C	-2.44171	-2.59321	-2.47346
C	-1.14917	-2.34297	-2.96325
C	-0.85016	-2.11607	-4.35822
H	-1.58762	-2.09388	-5.15908
C	0.50417	-1.94373	-4.45309
H	1.09402	-1.74732	-5.34718
C	1.04365	-2.13000	-3.12577
C	2.41670	-2.24768	-2.84950
N	2.12022	-2.60856	-0.39968
N	0.31823	-2.55767	1.74100
N	-1.79113	-2.55967	-0.06433
N	0.01722	-2.33001	-2.19805
C	-0.19153	1.87645	2.55991
H	0.17758	0.88728	2.27834
C	-0.09602	2.35012	3.87352
H	0.33174	1.70914	4.64930
N	-1.22906	4.17273	-0.61523
C	0.08890	4.79135	-0.91087
C	0.86880	3.91134	-1.86834
C	1.80015	4.41857	-2.78232
H	1.96198	5.49840	-2.85416
C	2.51190	3.52230	-3.59356
H	3.24630	3.89366	-4.31502
C	2.25727	2.14846	-3.47260

H	2.78165	1.41321	-4.08929
C	1.30424	1.71839	-2.54299
H	1.05710	0.65969	-2.42269
N	0.62415	2.57742	-1.74896
O	-0.73744	0.15962	-0.56917
Cu	-0.86199	2.12168	-0.45373
N	-0.71012	2.61611	1.54845
C	-0.53935	3.64924	4.15903
H	-0.46756	4.05702	5.17214
C	-1.06970	4.42399	3.11803
H	-1.42193	5.44484	3.29518
C	-1.15168	3.87240	1.83297
C	-1.79840	4.61628	0.68105
C	-2.19809	4.31302	-1.73340
C	-3.24134	3.21569	-1.64742
C	-4.55992	3.37960	-2.08836
H	-4.88902	4.34712	-2.47961
C	-4.96850	1.06975	-1.50496
H	-5.61729	0.19308	-1.42942
C	-3.63890	0.98680	-1.07425
H	-3.21905	0.06202	-0.66760
N	-2.78831	2.03678	-1.14067
C	-5.43813	2.28721	-2.01879
H	-6.47441	2.38947	-2.35568
H	-0.02113	5.82053	-1.30288
H	0.63944	4.86070	0.04576
H	-2.66386	5.31645	-1.74502
H	-1.63243	4.20255	-2.67706
H	-1.71552	5.71239	0.80836
H	-2.87680	4.37217	0.66553
N	0.26653	-0.53899	-0.06805
O	1.19959	0.08585	0.48105
C	-3.57190	-2.74760	-3.44541
C	3.89035	-3.16622	2.94510
C	3.88569	-4.27940	3.81144
H	3.05012	-4.98710	3.77131
C	4.93373	-4.51525	4.71617
H	4.89480	-5.39580	5.36288
C	6.02022	-3.61812	4.77198
C	6.04002	-2.49562	3.91403
H	6.88498	-1.80173	3.97300
C	4.99230	-2.27916	3.01638
H	5.01671	-1.39941	2.36409
C	7.10975	-4.86274	6.50977
H	6.24503	-4.83908	7.19874
H	8.04132	-4.76792	7.08614
H	7.11379	-5.82053	5.95697
C	-4.03321	-1.66891	-4.22665
H	-3.56459	-0.68492	-4.11553
C	-5.08980	-1.81883	-5.14073
H	-5.41988	-0.95489	-5.72368
C	-5.71154	-3.07572	-5.28682
C	-5.26406	-4.16680	-4.50894
H	-5.75169	-5.13920	-4.63391
C	-4.21241	-4.00018	-3.60445
H	-3.87116	-4.85719	-3.01312
C	-7.22872	-2.26020	-6.95640
H	-7.62468	-1.43543	-6.33492
H	-8.04132	-2.68497	-7.56327
H	-6.43565	-1.87095	-7.62175
O	7.09450	-3.74097	5.61333
O	-6.74654	-3.34206	-6.14477
C	-3.03802	-2.19526	3.53670
C	-3.88977	-3.24636	3.93330
H	-3.83876	-4.20697	3.40854
C	-4.79831	-3.09918	4.99476
H	-5.43699	-3.94150	5.27328
C	-4.86642	-1.87353	5.68828
C	-4.01491	-0.81213	5.30847
H	-4.07817	0.13555	5.85341
C	-3.11682	-0.97563	4.25089
H	-2.46701	-0.14146	3.96364
C	-6.60189	-2.65981	7.14688
H	-7.28456	-2.95479	6.32826
H	-7.18609	-2.24138	7.97918
H	-6.04362	-3.54762	7.49801
C	3.41062	-2.10694	-3.95797
C	3.40201	-2.97633	-5.07666
H	2.65314	-3.77368	-5.13291
C	4.34479	-2.85127	-6.09924
H	4.34039	-3.53309	-6.95596
C	5.33382	-1.84394	-6.03675
C	5.36492	-0.97089	-4.92992
H	6.11919	-0.18346	-4.85261
C	4.41248	-1.11426	-3.90738
H	4.44813	-0.43315	-3.04977
C	7.24298	-0.80952	-7.05770
H	6.81942	0.21198	-7.04905
H	7.82417	-0.95784	-7.97918
H	7.90211	-0.94284	-6.17985
O	-5.71246	-1.61085	6.73388
O	6.20814	-1.80489	-7.09000

***bis*-NO LS**

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Final complex 2 in acetone

Fe	0.23083	-2.49634	-0.24598
C	2.99168	-2.33999	-1.53369
C	4.38497	-2.59362	-1.23598
H	5.18831	-2.59304	-1.97097
C	4.46585	-2.86182	0.10358
H	5.35019	-3.11801	0.68493
C	3.12818	-2.74321	0.64039
C	2.81765	-2.85645	2.00843
C	1.51551	-2.66053	2.50955
C	1.20424	-2.57313	3.91889
H	1.93326	-2.66029	4.72303
C	-0.14392	-2.35609	4.01907
H	-0.74274	-2.24632	4.92202
C	-0.66775	-2.31843	2.67185
C	-2.04113	-2.23340	2.37272
C	-2.53883	-2.34938	1.06136
C	-3.94811	-2.37667	0.73127
H	-4.75903	-2.29350	1.45344
C	-4.03710	-2.52027	-0.62748
H	-4.93488	-2.57083	-1.24209
C	-2.68264	-2.53546	-1.13971
C	-2.37791	-2.48664	-2.51337
C	-1.07212	-2.27333	-2.99719
C	-0.74984	-2.08605	-4.39377
H	-1.47496	-2.08747	-5.20600
C	0.60477	-1.90298	-4.47383
H	1.20478	-1.71990	-5.36374
C	1.13036	-2.03886	-3.13330
C	2.50601	-2.08349	-2.83089
N	2.23144	-2.44468	-0.37841
N	0.36228	-2.48990	1.75607
N	-1.77561	-2.44471	-0.09425
N	0.08635	-2.21633	-2.23149

C	0.08313	2.23358	2.40363
H	0.40464	1.21882	2.15654
C	0.30682	2.77904	3.67250
H	0.79258	2.17512	4.44410
N	-1.21229	4.38481	-0.79483
C	0.08554	4.92928	-1.24725
C	0.75916	3.95618	-2.19830
C	1.59578	4.37830	-3.23813
H	1.75191	5.44815	-3.40814
C	2.22068	3.41787	-4.04723
H	2.87962	3.72591	-4.86492
C	1.97357	2.06095	-3.79509
H	2.43137	1.27295	-4.39954
C	1.11711	1.71540	-2.74468
H	0.88495	0.66976	-2.52518
N	0.51851	2.63602	-1.95010
O	-0.71696	0.27277	-0.34538
Cu	-0.83739	2.29081	-0.52436
N	-0.51325	2.92147	1.39736
C	-0.08744	4.10200	3.91863
H	0.08270	4.56687	4.89475
C	-0.69777	4.82423	2.88373
H	-1.01593	5.86130	3.03035
C	-0.90696	4.20235	1.64601
C	-1.64470	4.90327	0.51780
C	-2.27293	4.43903	-1.82405
C	-3.29319	3.34014	-1.57953
C	-4.64777	3.48381	-1.90275
H	-5.01217	4.43184	-2.31065
C	-5.00036	1.21296	-1.16294
H	-5.63748	0.34387	-0.97795
C	-3.63651	1.14842	-0.85523
H	-3.18678	0.24488	-0.43366
N	-2.78992	2.18657	-1.05626
C	-5.51751	2.40213	-1.69611
H	-6.58056	2.49175	-1.94075
H	-0.01585	5.93170	-1.70817
H	0.72063	5.04733	-0.34903
H	-2.75992	5.43262	-1.87393
H	-1.78981	4.26599	-2.80409
H	-1.53062	6.00279	0.59160
H	-2.72484	4.68612	0.61809
N	0.34845	-4.15589	-0.46592
O	0.90478	-5.11455	-0.87900
N	0.31777	-0.42834	-0.06165
O	1.34846	0.13213	0.33192
C	-3.50175	-2.62941	-3.49262
C	3.91352	-3.15018	2.98321
C	3.88535	-4.32561	3.76309
H	3.05881	-5.03373	3.63645
C	4.89761	-4.62157	4.68984
H	4.84091	-5.54861	5.26628
C	5.97180	-3.72363	4.85775
C	6.01392	-2.53877	4.08881
H	6.84748	-1.84414	4.23563
C	5.00107	-2.26169	3.16782
H	5.04115	-1.33170	2.59018
C	7.00290	-5.09117	6.53772
H	6.10994	-5.12915	7.18896
H	7.90830	-5.03300	7.15884
H	7.04196	-6.00279	5.91291
C	-3.90331	-1.56325	-4.32337
H	-3.39073	-0.59818	-4.24574
C	-4.95798	-1.70008	-5.24101
H	-5.24159	-0.84624	-5.86190
C	-5.63928	-2.93048	-5.34110
C	-5.25432	-4.00737	-4.51151
H	-5.78894	-4.95883	-4.59976
C	-4.20453	-3.85386	-3.60291
H	-3.91217	-4.70008	-2.97128
C	-7.09711	-2.11599	-7.06370
H	-7.45664	-1.24472	-6.48512
H	-7.92451	-2.52701	-7.65989
H	-6.27900	-1.79863	-7.73685
O	7.01157	-3.90278	5.73093
O	-6.67814	-3.18234	-6.19794
C	-3.00535	-2.05673	3.50470
C	-3.91240	-3.07367	3.86641
H	-3.90977	-4.01888	3.31216
C	-4.81130	-2.91425	4.93410
H	-5.49271	-3.73100	5.18611
C	-4.81397	-1.71081	5.66875
C	-3.91065	-0.68180	5.32036
H	-3.92487	0.24984	5.89552
C	-3.02183	-0.85731	4.25693
H	-2.32967	-0.04901	3.99573
C	-6.57195	-2.46442	7.11677
H	-7.27732	-2.70059	6.29847
H	-7.12619	-2.04948	7.97098
H	-6.04853	-3.38709	7.42915
C	3.50069	-1.92493	-3.93778
C	3.56181	-2.84437	-5.01395
H	2.86861	-3.69222	-5.03822
C	4.50475	-2.70386	-6.03433
H	4.55469	-3.42362	-6.85791
C	5.42374	-1.63056	-6.01173
C	5.38300	-0.70553	-4.94836
H	6.08008	0.13538	-4.90479
C	4.43125	-0.86420	-3.92740
H	4.40944	-0.14016	-3.10532
C	7.26983	-0.51692	-7.06375
H	6.77698	0.47198	-7.10935
H	7.87205	-0.66898	-7.97098
H	7.92451	-0.56160	-6.17369
O	-5.64169	-1.44203	6.72691
O	6.30606	-1.58195	-7.05754

(TMPP)Fe^{II}(NO)

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Fe	-0.022283	0.025569	0.170534
C	2.995722	-0.038785	0.094107
C	4.142632	0.829757	0.064419
H	5.163409	0.515156	0.221960
C	3.687326	2.082146	-0.205030
H	4.262170	2.990937	-0.303561
C	2.253922	1.999327	-0.299248
C	1.427030	3.116177	-0.455927
C	0.033865	3.044867	-0.348610
C	-0.830984	4.195243	-0.380686
H	-0.506726	5.211519	-0.547044
C	-2.092786	3.749602	-0.142160
H	-2.999521	4.331962	-0.075407
C	-2.018383	2.316232	-0.026264
C	-3.138420	1.488286	0.109393
C	-3.059510	0.092813	0.029877
C	-4.214098	-0.757617	-0.102481

H	-5.238331	-0.415439	-0.096427
C	-3.755862	-2.024533	-0.282929
H	-4.332372	-2.922812	-0.445822
C	-2.318941	-1.964133	-0.221489
C	-1.487914	-3.086705	-0.303176
C	-0.098347	-3.005424	-0.170247
C	0.764612	-4.154326	-0.097851
H	0.438167	-5.179735	-0.186672
C	2.026276	-3.692991	0.112717
H	2.935255	-4.267088	0.214602
C	1.949474	-2.256846	0.151978
C	3.068973	-1.424712	0.268635
N	1.840072	0.690782	-0.118801
N	-0.706702	1.895852	-0.143664
N	-1.902712	-0.657316	-0.047188
N	0.642335	-1.844744	-0.024577
N	0.120438	0.029165	1.983374
O	0.932479	-0.343465	2.772123
C	-2.107803	-4.433722	-0.502276
C	2.070607	4.444801	-0.701925
C	2.068414	5.452728	0.270259
H	1.589259	5.270134	1.228136
C	2.678708	6.689655	0.045655
H	2.659275	7.440146	0.827244
C	3.310696	6.937276	-1.179528
C	3.322940	5.936945	-2.164433
H	3.813347	6.141827	-3.111273
C	2.713425	4.711836	-1.924468
H	2.729362	3.948593	-2.697586
C	3.958389	9.153240	-0.545012
H	2.944124	9.482817	-0.289544
H	4.499653	9.976123	-1.013953
H	4.481946	8.846415	0.368444
C	-1.916301	-5.140883	-1.695834
H	-1.317714	-4.699107	-2.487757
C	-2.483331	-6.401432	-1.901009
H	-2.315069	-6.911304	-2.842355
C	-3.261553	-6.982489	-0.891958
C	-3.461288	-6.288002	0.311818
H	-4.061138	-6.751485	1.089189
C	-2.892458	-5.034427	0.499139
H	-3.050302	-4.513780	1.439515
C	-3.685598	-8.957802	-2.177275
H	-4.093982	-8.428280	-3.046436
H	-4.237119	-9.886930	-2.027144
H	-2.627826	-9.186342	-2.354661
O	3.936262	8.102809	-1.508829
O	-3.860511	-8.203869	-0.979765
C	-4.490104	2.109596	0.271650
C	-5.193031	1.974755	1.475343
H	-4.742344	1.425541	2.297432
C	-6.460347	2.536194	1.652353
H	-6.966410	2.413579	2.602752
C	-7.053672	3.249040	0.603076
C	-6.364955	3.388740	-0.612441
H	-6.838760	3.936358	-1.421504
C	-5.104369	2.826684	-0.771406
H	-4.589752	2.935685	-1.721962
C	-9.031946	3.718583	1.867752
H	-9.247738	2.669466	2.103057
H	-9.967723	4.250352	1.690161
H	-8.505430	4.179777	2.711967
C	4.398088	-2.058828	0.531317
C	4.666174	-2.661369	1.774220
H	3.903581	-2.650370	2.547945
C	5.891331	-3.262689	2.032934
H	6.097065	-3.721305	2.995387
C	6.890827	-3.283069	1.047237
C	6.642051	-2.692152	-0.198036
H	7.391685	-2.698986	-0.980712
C	5.404935	-2.089412	-0.441568
H	5.221341	-1.643337	-1.415111
C	9.107000	-3.949720	0.433597
H	8.800431	-4.501999	-0.462872
H	9.930065	-4.475573	0.919447
H	9.436181	-2.943904	0.146190
O	-8.282432	3.836491	0.660511
O	8.056548	-3.897510	1.396113

$[(tmpa)Cu^{II}(NO_2)]^+$

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C	1.777276	-2.540808	0.888299
H	1.333709	-2.579644	1.875153
C	2.683553	-3.505088	0.459913
H	2.974788	-4.306497	1.129695
N	0.101618	0.239174	-1.516887
C	-0.990768	-0.576704	-2.106883
C	-2.240151	-0.466233	-1.260553
C	-3.521996	-0.596580	-1.788363
H	-3.658709	-0.746635	-2.853979
C	-4.614058	-0.529037	-0.923620
H	-5.623588	-0.628450	-1.309663
C	-4.391421	-0.321865	0.437471
H	-5.213140	-0.254650	1.141621
C	-3.081101	-0.192714	0.885714
H	-2.853789	-0.023382	1.931905
N	-2.027778	-0.268710	0.056418
O	-0.079340	0.029224	2.449548
Cu	-0.018795	-0.024587	0.521278
N	1.381551	-1.523116	0.103030
C	3.187801	-3.421385	-0.837232
H	3.887881	-4.163190	-1.208443
C	2.772579	-2.373682	-1.657741
H	3.137550	-2.279493	-2.675074
C	1.876263	-1.436836	-1.149299
C	1.445124	-0.225284	-1.944066
C	-0.081321	1.690722	-1.779428
C	0.640898	2.510106	-0.732658
C	1.151440	3.780455	-0.985954
H	1.085956	4.205757	-1.981856
C	1.808452	3.899208	1.326200
H	2.260975	4.414755	2.165918
C	1.285313	2.620686	1.495254
H	1.308522	2.110021	2.451821
N	0.715327	1.941776	0.486908
C	1.741797	4.486127	0.062749
H	2.147452	5.478495	-0.107176
H	-1.183741	-0.287299	-3.146440
H	-0.654436	-1.619518	-2.115078
H	0.247926	1.949760	-2.792225
H	-1.153556	1.906524	-1.720725
H	1.469164	-0.423841	-3.021680
H	2.150725	0.589924	-1.750019
N	-0.506911	-0.954104	3.190115
O	-0.853581	-1.964382	2.587114