

Supporting Information for:

Electrochemical Behaviors of Pincer-Type NNN-Fe Complex and Catalytic H₂ Evolution Activity

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Materials and methods

All complexes were synthesized under inert atmosphere of N₂ or Ar using glovebox and Schlenk techniques. Solvents were purified through solvent purification system (Vigor) and stored over with 4 Å molecular sieves until use. NMR solvents were purchased from Cambridge Isotope Laboratory and stored over with 4 Å molecular sieves until use at a glove box. Iron(II) chloride (anhydrous, STREM chemicals, ≥ 99 %), silver perchlorate (STREM chemicals, 99 %), 1-methylpiperazine (Tokyo Chemical Industry, ≥ 98 %), 2,6-pyridinedimethanol (ACROS, ≥ 98%), phosphorous tribromide (ACROS, ≥ 99 %), potassium carbonate (anhydrous, Daejung, 98 %), sodium sulfate (anhydrous, Daejung, 99 %), *tert*-butyl isocyanide (Alfa Aesar, ≥ 98%), sodium amalgam (Alfa Aesar, min 20 wt%), 2,6-lutidine (Tokyo Chemical Industry, ≥ 98 %), triethylamine (Daejung, ≥ 98 %), tetrafluoroboric acid, 50 wt% aqueous solution (Alfa Aesar), and tetrabutylammonium hexafluorophosphate (Alfa Aesar, ≥ 98%) were used as received. The Fe(CO)₄I₂¹, NNN Ligand², triethylammonium tetrafluoroborate³, and 2,6-lutidinium tetrafluoroborate⁴ were synthesized following the known procedures.

Characterization methods

¹H-NMR (400 MHz) and ¹³C-NMR(101 MHz) spectra were recorded on JEOL NMR spectrometer (JNM-ECS400). All IR samples were mixed with mineral oil as powder on KBr windows. IR spectra were obtained using ATR-IR spectrometer (ALPHA II) with universal sampling module (A230/D, QuickSnap) as necessary.

Electrochemical details

Electrochemical data were collected by INTERFACE 1010 E potentiostat/Galvanostat/ZRA using a three electrodes system. The working electrode was a 3 mm-diameter glassy carbon. The platinum wire and Ag/AgNO₃ were used as a counter electrode and a reference electrode, respectively. 0.1 M NBu₄PF₆ was used as an electrolyte in dry CH₃CN. A 25 ml four-neck pear flask was used as an electrochemical cell. After CV curves were obtained versus Ag/AgNO₃, the potential values were converted to values against ferrocene/ferrocenium (Fc^{0/+}) redox potential. All the electrochemical reactions were conducted under Ar or N₂ atmosphere.

Chronoamperometry was conducted in a 25ml of four-neck pear flask. A custom-made rubber septum was used to hold a working electrode (3 mm diameter glassy carbon electrode), reference electrode (Ag/AgNO₃), and counter electrode (Pt wire). 10 ml of sample was prepared as 5 mM of catalyst, 0.1 M of tetrabutylammonium hexafluorophosphate, and 0.1 M of acids. Chronoamperometry was conducted for an hour. Applied potential was referenced relative to ferrocene with the Fc^{+/0} couple at 0.0 V using Fc. Gas analysis for chronoamperometry experiments was performed using 1 ml sample aliquots taken from the headspace of the electrochemical cell and injected on GC equipment. The faradaic yield of each experiment was determined by dividing the measured amount of H₂ by passed charge during chronoamperometry.

Calculation methods of rate constant (k), and half-life time ($t_{1/2}$) of disproportionation

The rate constant of disproportionation and half-life time ($t_{1/2}$) of Fe(I) complex was calculated from cyclic voltammograms at variable scan rate (5 mV/s to 5 V/s) using developed by P. Hickey et.al⁵. (Figure S4, a) Disproportionation reaction of Fe(I) complex is a second-order reaction occurred by a collision of two molecules of Fe(I) complex (Eqn. 1). To figure out t and $[Fe(I)]_t$, a few assumptions is adapted for convenience. Reaction time can be calculated by dividing voltage that $E_{pc}[Fe(II/I)]$ to E_R (Return potential point) and E_R to $E_{pa}[Fe(I/II)]$ by scan rate (V/s) (Eqn. 2). Concentration of Fe(I) complex at starting time ($t = 0$) assumed to same as concentration of Fe(II) complex that used in cyclic voltammograms. From the Randles-Sevcik equation, current (i_p) can be used as a term of concentration at same cyclic voltammograms and anodic current at E_{pa} is proportional to concentration of Fe(I) complex after reaction ($[Fe(I)]_t$) (Eqn. 3). The plot of t vs $1/[Fe(I)]_t$ results in a linear fit with a slope that is the same as rate constant (k) of disproportionation (Eqn. 4). Calculated rate constant of disproportionation for complex is $54.047 \text{ dm}^{-3} \text{ mol}^{-1} \text{ s}^{-1}$. (Figure S4, b) Additionally, the half-life time ($t_{1/2}$) of Fe(I) complex can be calculated through the equation of half-life time for second-order reaction (Eqn. 5). The calculated half-life time of complex is 9.25 s.

$$kt = \frac{1}{[Fe(I)]_t} - \frac{1}{[Fe(I)]_0} \quad (\text{Eqn. 1})$$

$$t \text{ (s)} = \frac{[E_{pc} - E_R + E_{pa} + E_R](V)}{\text{Scan rate } (V \text{ s}^{-1})} \quad (\text{Eqn. 2})$$

$$\frac{1}{[Fe(I)]_t} = \frac{i_{pc}}{i_{pa}} \times [Fe(I)]_0 \quad (\text{Eqn. 3})$$

$$kt = \frac{i_{pc}}{i_{pa}} \times [Fe(I)]_0 - \frac{1}{[Fe(I)]_0} \quad (\text{Eqn. 4})$$

$$t_{1/2} = \frac{1}{k[Fe(I)]_0} \text{ (Eqn. 5)}$$

Calculation methods of TOF, and TON from electrochemical data

TOF and TON were calculated by using cyclic voltammograms.⁶ In cyclic voltammograms at a certain concentration of acid, the catalytic current is proportional to the concentration of catalyst ([cat]), acid concentration ([Q]^y), diffusion coefficient (D), electrode surface area (A), and rate constant of catalytic reaction (k_{cat}) (Eqn. 6).⁷ If the concentration of catalyst is sufficiently smaller than acid, the catalytic reaction can be assumed as pseudo-first-reaction for acid ($y=1$). The rate of catalytic reaction can be obtained by squaring (i_{cat}/i_p) and arranging the equation for $k_{cat}[Q]$. i_p can be illustrated by the Randles-Sevcik equation (Eqn. 7) and dividing i_{cat} by i_p can cancel out electrode surface area (A) and diffusion coefficient (D) (Eqn. 8). Equation 8 can be described easier by calculating constant as shown in Eqn. 9.

$$i_{cat} = n_{cat}FA[cat]\sqrt{Dk_{cat}[Q]^y} \quad (\text{Eqn. 6})$$

$$i_p = 0.4463n_p^{3/2}FA[cat]\sqrt{\frac{FvD}{RT}} \quad (\text{Eqn. 7})$$

$$\text{Rate of catalytic reaction } (s^{-1}) = TOF(s^{-1}) = k_{cat}[Q] = \frac{Fvn_p^3}{RT} \left(\frac{0.4463}{n_{cat}}\right)^2 \left(\frac{i_{cat}}{i_p}\right)^2 \quad (\text{Eqn. 8})$$

$$TOF = k_{cat}[Q] = 1.94 \times v \times \left(\frac{i_{cat}}{i_p}\right)^2 \quad (\text{Eqn. 9})$$

Computational details

The geometries were optimized in Gaussian 09 software⁸ using the B3P86 functional.^{9,10} 6-311+G(d,p) basis set for C, H, and N, 6-311++G(d,p) basis set for acidic proton and hydride,^{11, 12} and Stuttgart basis set with effective core potential (ECP) was used for the Fe atom.¹³ Each structure was confirmed by a frequency calculation at the same level of theory to be a real local minimum on the potential energy surface without imaginary frequency. Solvation free energies in acetonitrile were calculated by using the polarizable continuum model (C-PCM) using Bondi atomic radii.¹⁴⁻¹⁶ The experimental value of proton solvation energy in CH₃CN (−255.2 kcal/mol)¹⁷ and experimental Gibbs free energy of proton (−6.28 kcal/mol)^{18,19} were used to calculate the values of Gibbs free energy of the proposed catalytic cycle. The reduction potentials of cobalt complexes were calculated by eqn.10 and 11.²⁰

$$E^o = -\frac{\Delta G_{solv}^{redox}}{F} \left(F = 23.06 \frac{kcal}{mol * V} \right) \quad (eqn. 10)$$

$$\Delta G_{solv}^{redox} = \Delta G_{solv}^{red} - \Delta G_{solv}^{ox} \quad (eqn. 11)$$

All reduction potentials were converted to values against ferrocene/ferrocenium (Fc/Fc⁺) redox couple that was optimized in the same level of theory.

Synthetic procedure for [NNN-Fe(CH₃CN)₃](ClO₄)₂. Solution of AgClO₄ (0.19 g, 0.92 mmol) in acetonitrile (4 ml) was added dropwise into a solution of NNN-FeCl₂ (0.20 g, 0.46 mmol) in acetonitrile (4 ml). Yellow color solution was changed to a beige solution with white precipitate. The reaction mixture was stirred for 12 h and filtered through a Celite pad, and acetonitrile in filtrate was removed under a reduced pressure. Resulted fine brown powder was washed with diethyl ether and dried under a reduced pressure to afford product (92 %). ¹H-NMR (400 MHz, Acetonitrile-d₃) δ 7.69 (t, 1H), 7.20 (d, 2H), 3.59 (s, 4H), 2.48 (bs, 16H), 2.27 (s, 6H), IR(v(C≡N)): 2305 (w), 2272 (m), 2251 (w) cm⁻¹.

Synthetic procedure for NNN-FeCl₂ complex. Anhydrous FeCl₂ (0.10 g, 0.79 mmol) was added to solution of NNN Ligand (0.3 g, 0.99 mmol) in acetonitrile (8 mL) with stirring. Reaction mixture was stirred for 14 h at room temperature. Acetonitrile was removed from mixture under a reduced pressure. Resulted solid was washed with Et₂O to give fine yellow powder as product. (92 %). IR: 2953, 2922, 2854, 2808, 1611, 1581, 1459, 1376, 1300, 1290, 1152, 1085, 1004, 824, 791, 732 cm⁻¹. Calcd for C₁₇H₂₉Cl₂Fe N₅: C, 47.46; H, 6.79; N, 16.28. Found: C, 46.89; H, 7.401; N, 16.21.

Synthetic procedure for [NNN-Fe(^tBuNC)₃](ClO₄)₂ complex ([1](ClO₄)₂) Solution of AgClO₄ (0.14 g, 0.67 mmol) in acetonitrile (3 ml) was added dropwise to solution of NNN-FeCl₂ (0.14 g, 0.33 mmol) in acetonitrile.(3 ml). Yellow color solution was changed to a beige solution with white precipitation. After stirring for 30 min at room temperature, *tert*-butyl isocyanide (0.09 g, 1.08 mmol) in acetonitrile (3 ml) was added into reaction solution and solution color was changed to purple. The reaction mixture was stirred for 12 h and filtered through Celite pad. Acetonitrile in filtrate was removed under a reduced pressure and the residual solid was with Et₂O to afford purple

colored solid as product. (94 %) X-ray quality single crystal was grown from diffusion method (CH₃CN/Et₂O) at room temperature. ¹H-NMR (400 MHz, Acetonitrile-d₃) δ 8.10 (t, 1H), 7.65 (d, 2H), 3.87 (s, 4H), 2.44 (s, 8H), 2.21 (s, 8H), 2.12 (s, 6H), 1.76 (s, 9H), 1.62 (s, 18H), IR(v(C≡N)): 2195 (w), 2160 (bs) cm⁻¹. E_{1/2}: -1.38 V vs. Fc⁺⁰. ΔE_p = 125 mV.

*KPF₆ could be used instead of AgClO₄ to obtain complex with a PF₆ counter anion. Elemental analysis data for [NNN-Fe(^tBuNC)₃](PF₆)₂ was acquired.

Calcd for C₃₂H₅₆N₈P₂F₁₂Fe: C, 42.77; H, 6.28; N, 12.47. Found: C, 42.55; H, 6.42; N, 12.35.

Chemical reduction of [1](ClO₄)₂.

Na(Hg) (20 wt% Na) was added to solution of [NNN-Fe(^tBuNC)₃](ClO₄)₂ (0.1 g, 0.12 mmol) in mixture of THF (5 ml) and acetonitrile (1 ml) at room temperature. The purple color solution was changed to a brown solution after 5 min. After stirring for 3 h at room temperature, the reaction solution was decanted and the supernatant was dried under a reduced pressure. The resulting solid was washed with Et₂O (2 times) to give brown powder.

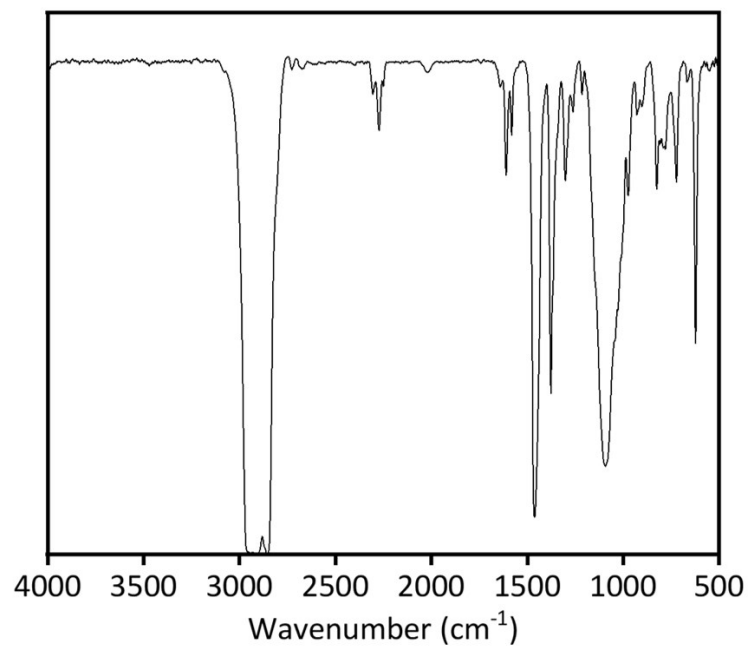


Figure S1. IR spectra of $[\text{NNN-Fe}(\text{CH}_3\text{CN})_3](\text{ClO}_4)_2$.

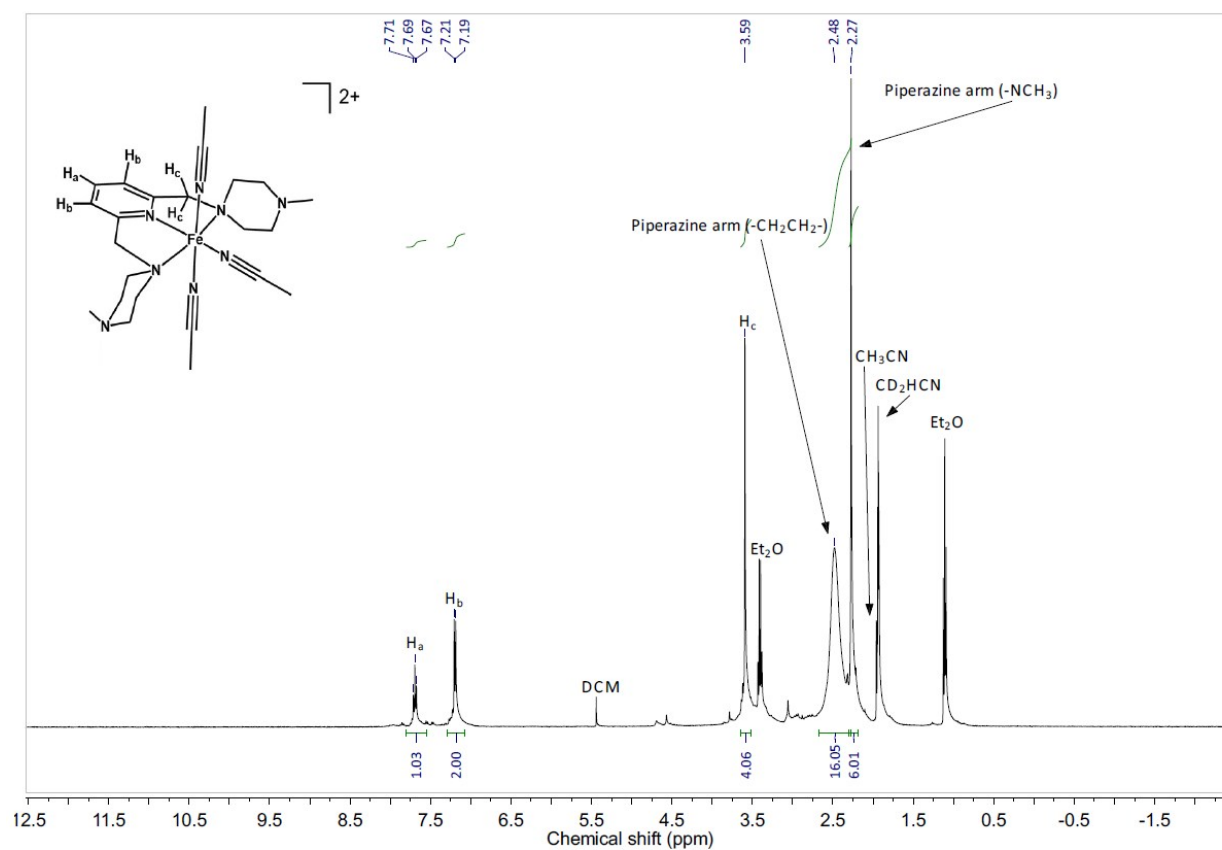


Figure S2. ^1H NMR spectrum of $[\text{NNN-Fe}(\text{CH}_3\text{CN})_3](\text{ClO}_4)_2$.

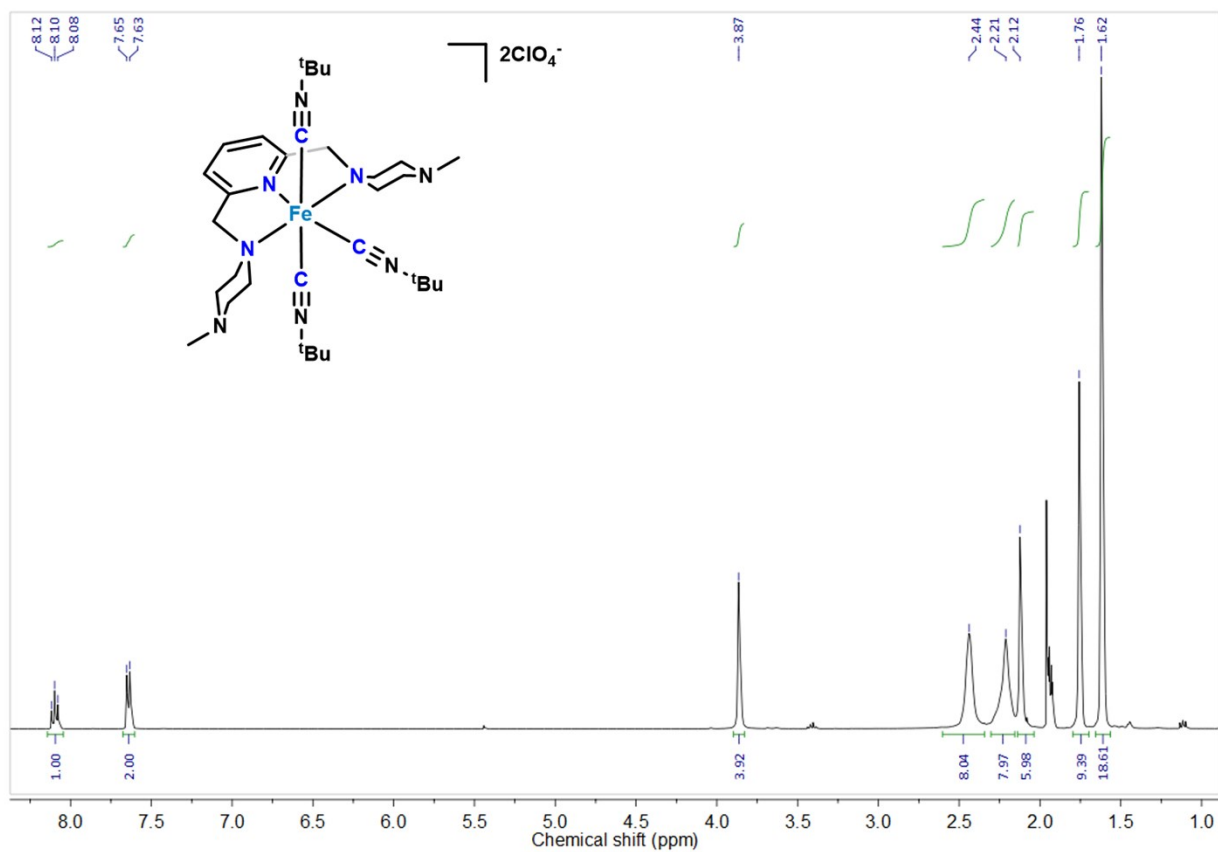


Figure S3. ^1H NMR spectrum of $[\text{NNN-Fe}(\text{tBuNC})_3](\text{ClO}_4)_2$ ([1](ClO_4) $_2$).

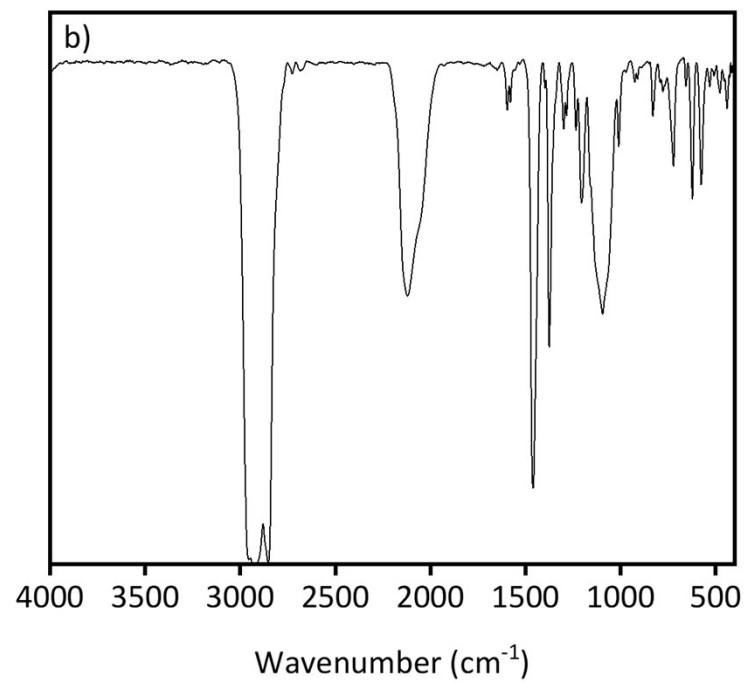
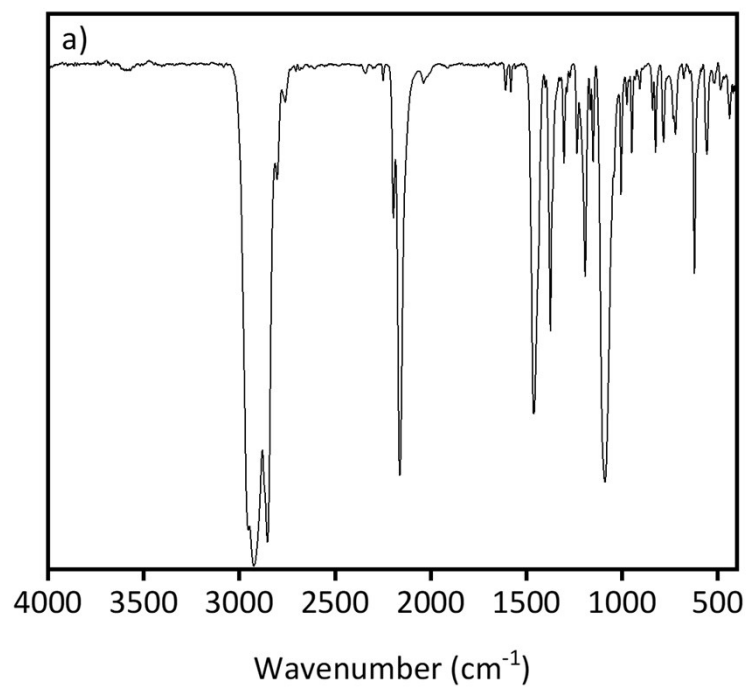


Figure S4. IR spectra of a) $[1](\text{ClO}_4)_2$ and b) $[[1](\text{ClO}_4)_2 + 2 \text{ equiv. of Na(Hg)}]$.

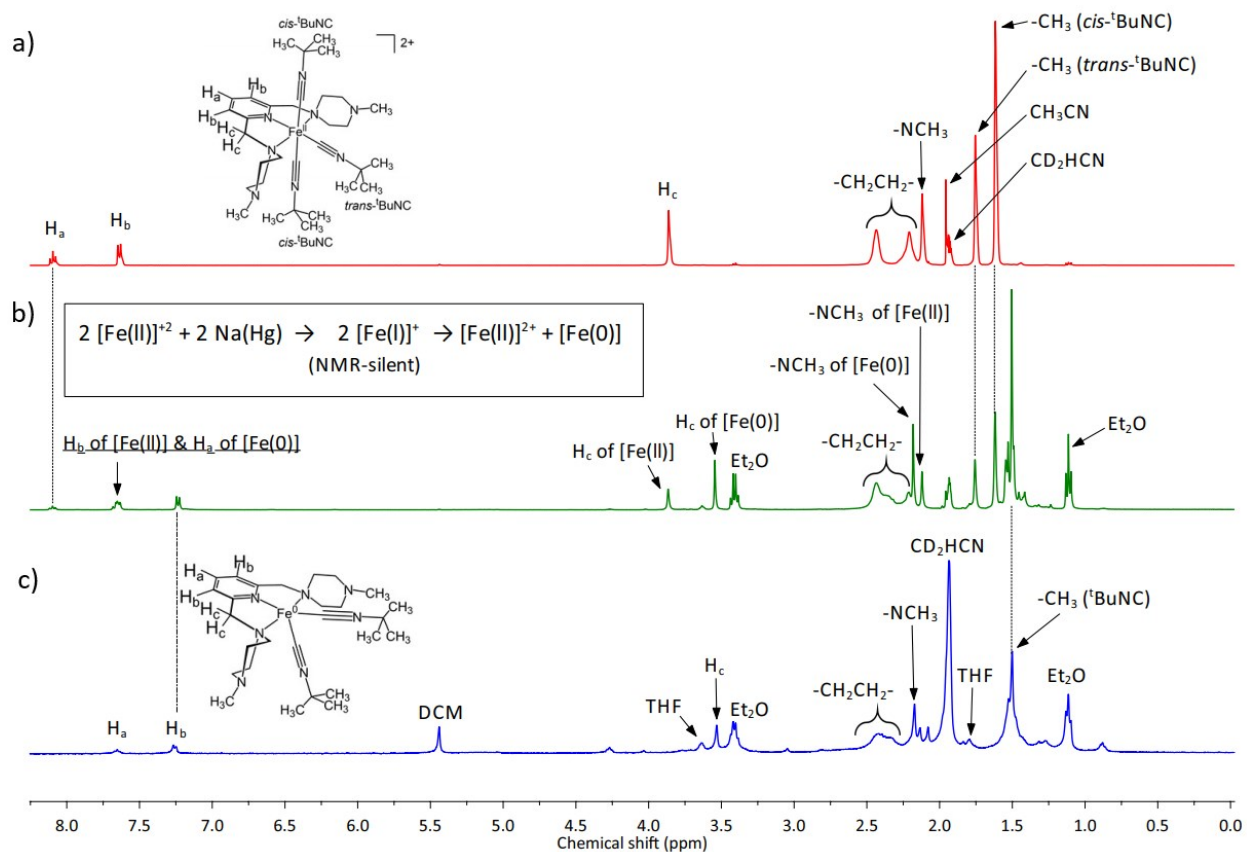


Figure S5. ^1H NMR spectrum of a) $[\mathbf{1}](\text{ClO}_4)_2$, b) mixture (~1:1 ratio) of $[\mathbf{1}](\text{ClO}_4)_2$ and $[\text{NNN-Fe}^0(^t\text{BuNC})_2]$ generated from reaction of $([\mathbf{1}](\text{ClO}_4)_2 + 1 \text{ equiv. of Na/Hg})$, and c) $[\text{NNN-Fe}^0(^t\text{BuNC})_2]$ species in situ generated from reaction of $([\mathbf{1}](\text{ClO}_4)_2 + 2 \text{ equiv. of Na/Hg})$.

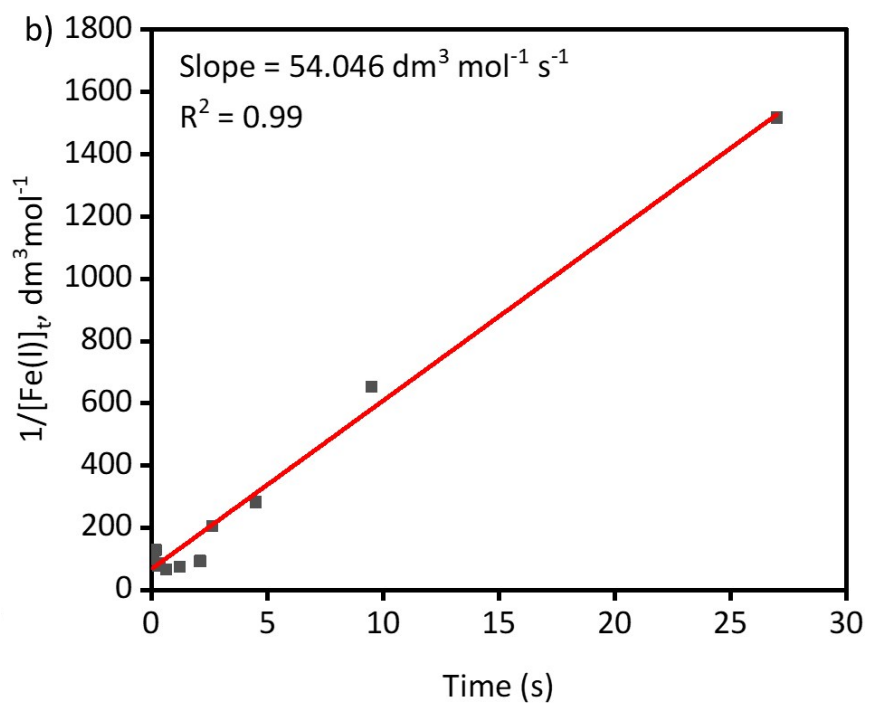
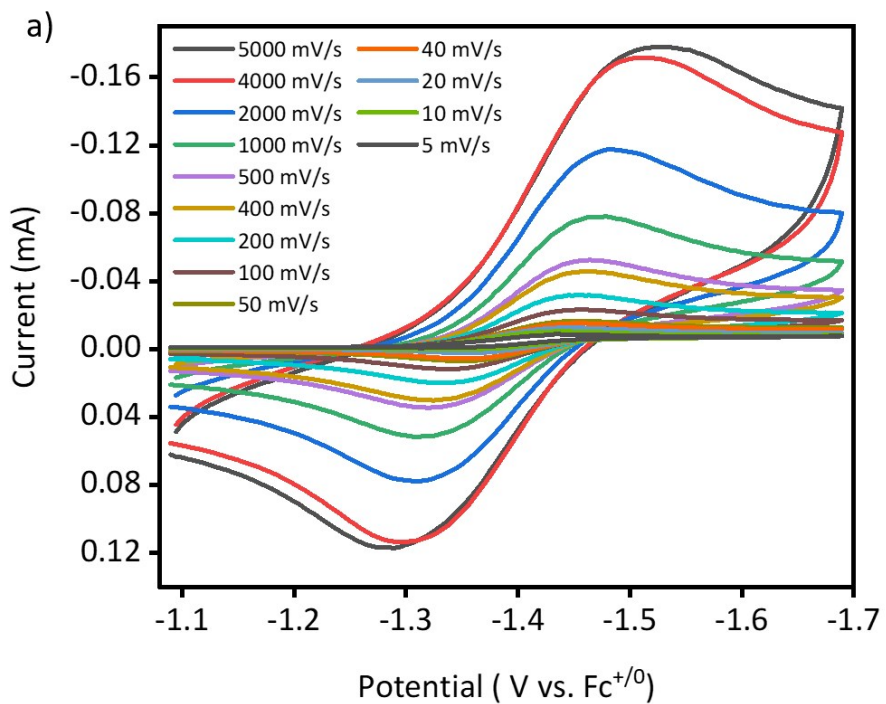


Figure S6. a) Cyclic voltammograms of $[\mathbf{1}](\text{ClO}_4)_2$ at various scan rates (5 mV/s to 5 V/s) b) corresponding plot of second-order-kinetics of disproportionation reaction.

X-Ray Crystallography

Reflection data for [1](ClO₄)₂ were collected using a Bruker APEX-II CCD-based diffractometer with graphite-monochromated MoK α radiation ($\lambda = 0.7107 \text{ \AA}$). The hemisphere of the reflection data was collected as multi-scan frames at 0.5°/frame and an exposure time of 10 s/frame. The cell parameters were determined and refined using the APEX2 program.²¹ The data were corrected for Lorentz and polarization effects and an empirical absorption correction was applied using the SADABS program.²² The compound structure was solved by direct methods and refined by full matrix least-squares using the SHELXTL program package²³ and Olex2²⁴ with anisotropic thermal parameters for all non-hydrogen atoms. The relevant data are summarized in Table S1. CCDC 2083139 contains the supplementary crystallographic data for this study. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data and parameters for [1](ClO₄)₂.

	[1](ClO ₄) ₂
formula	C ₃₄ H ₅₉ Cl ₂ FeN ₉ O ₈
formula weight	848.65
crystal system	Orthorhombic
space group	Pbca
<i>a</i> (Å)	13.5619(4)
<i>b</i> (Å)	16.3532(4)
<i>c</i> (Å)	39.3827(9)
α (°)	90
β (°)	90
γ (°)	90
<i>V</i> (Å ³)	8734.3(4)
<i>Z</i>	8
ρ_{calc} (g cm ⁻³)	1.291
μ (mm ⁻¹)	0.523
<i>F</i> (000)	3600.0
<i>T</i> (K)	100

2 Θ range for data collection/ $^{\circ}$	5.278 to 52.816
<i>hkl</i> range	-16 \leq h \leq 16, -20 \leq k \leq 20, -48 \leq l \leq 48
measd reflns	60727
unique reflns	8630
refined parameters	620
R ₁ ^a (I > 2 σ (I))	0.0387
wR ₂ ^b all data	0.0982
GOF on F ²	1.045
ρ_{fin} (max/min) (e \AA^{-3})	0.92/ -0.44

^a R₁ = $\sum||F_o| - |F_c||/\sum|F_o|$. ^b wR₂ = $\{[\sum w(F_o^2 - F_c^2)^2]/[\sum w(F_o^2)^2]\}^{1/2}$.

Cartesian coordinates of optimized structures

$\text{LFe}^{\text{II}}(\text{tBuNC})_3$

C	0.98115400	2.18787600	0.40562400
C	1.11935600	3.56708200	0.37365600
C	0.07180300	4.32548500	-0.13737500
C	-1.07522800	3.70052600	-0.61477300
C	-1.13539500	2.31586100	-0.57864700
N	-0.12339100	1.60686600	-0.07040100
H	0.14947100	5.40581600	-0.16377800
H	2.02096500	4.03515500	0.74768100
H	-1.90136700	4.27423600	-1.01514800
C	-2.23937000	1.47038700	-1.13580400
H	-3.18703300	2.01022200	-1.12083000
H	-2.01307100	1.25660200	-2.18464300
C	-3.11942000	0.33127600	0.83756000
C	-3.01379600	-0.85722800	-1.24093200
C	-4.59969200	0.59080300	0.60175500
H	-2.68657300	1.14518100	1.42045700
H	-3.01545400	-0.59471200	1.40380300
C	-4.48641500	-0.56542700	-1.47151000
H	-2.49306400	-0.94854800	-2.19310900
H	-2.92130200	-1.80545800	-0.70943000
H	-4.76608300	1.58552100	0.14959500
H	-5.08756800	0.61178800	1.58034900
H	-4.90639100	-1.39384500	-2.04846900
H	-4.61706700	0.34666800	-2.08290900
N	-2.31876500	0.16679100	-0.41179000

N	-5.18836500	-0.46478500	-0.20320500
C	-6.61328200	-0.26524200	-0.38975600
H	-7.02895600	-1.09507900	-0.96578600
H	-7.11212600	-0.23781000	0.58174800
H	-6.84315600	0.67421000	-0.92214800
C	-0.57095400	-4.78868400	0.08416900
C	0.27497600	-0.64775900	-4.49740000
C	-0.85897700	-0.34645100	4.45971700
C	1.95664000	1.22185900	1.00446800
H	2.97186600	1.61842200	0.95815500
H	1.71396700	1.09696000	2.06363300
N	1.84259300	-0.11387800	0.34851400
C	2.65074900	-0.12824000	-0.90745200
C	2.39001200	-1.18239000	1.23047100
C	4.15408600	-0.07078800	-0.68207900
H	2.33555500	0.70832600	-1.53262800
H	2.41248300	-1.05721500	-1.42614200
C	3.89097700	-1.09556400	1.44485300
H	1.87104800	-1.14400700	2.18737200
H	2.15590300	-2.13539500	0.75388900
H	4.46265200	0.91006800	-0.27530600
H	4.63584400	-0.16457000	-1.65941000
N	4.59180000	-1.15970100	0.17340000
H	4.19075300	-1.94637000	2.06289000
H	4.15620400	-0.18284400	2.01022800
C	6.03172700	-1.15278500	0.35209000
H	6.33152200	-2.00507500	0.96596200

H	6.52393100	-1.23872800	-0.61927900
H	6.39204900	-0.23091400	0.84124600
C	-0.52269800	-0.29880900	1.87245400
C	-0.39903200	-2.18707000	0.02504100
C	-0.01847000	-0.43228400	-1.91380000
N	-0.66258900	-0.32182900	3.02482100
N	-0.47986500	-3.34576400	0.05288200
N	0.10260000	-0.53617000	-3.06372900
C	-2.23687500	0.24899900	4.74964500
H	-2.29889700	1.28044300	4.39808000
H	-3.02512200	-0.33813900	4.27524100
H	-2.40253300	0.24082700	5.82855200
C	0.24781000	0.49451200	5.09605300
H	1.23219000	0.07382900	4.88287800
H	0.21307500	1.52372500	4.73411800
H	0.10436800	0.50310100	6.17812200
C	-0.77890700	-1.80347200	4.91438500
H	-0.92906900	-1.84429100	5.99484000
H	-1.55242700	-2.40439900	4.43316800
H	0.19869100	-2.23023700	4.68356300
C	-0.48712600	-5.22963400	1.54547000
H	0.46275700	-4.92600600	1.98902900
H	-1.30465900	-4.80120200	2.12800500
H	-0.55992900	-6.31787600	1.59247300
C	0.59757200	-5.34589000	-0.72947200
H	0.54917600	-5.00359000	-1.76473800
H	1.55279900	-5.04004300	-0.29890000

H	0.54653300	-6.43632900	-0.72123000
C	-1.91190100	-5.18417300	-0.53538000
H	-2.74343600	-4.76865000	0.03679000
H	-1.98222300	-4.83707500	-1.56779400
H	-1.99698500	-6.27250500	-0.52902300
C	-1.05782500	-1.10283600	-5.09219100
H	-1.35588500	-2.07188300	-4.68779900
H	-1.84515900	-0.37385000	-4.89116300
H	-0.94625300	-1.19924700	-6.17375600
C	1.37364500	-1.67940600	-4.75391500
H	2.31990000	-1.36176400	-4.31253900
H	1.09804600	-2.65226500	-4.34316500
H	1.51292300	-1.78423900	-5.83140500
C	0.67299700	0.73125700	-5.02409600
H	-0.10539600	1.46708900	-4.81457000
H	1.60877200	1.06592200	-4.57296000
H	0.81097100	0.66990900	-6.10518100
Fe	-0.26348900	-0.31221100	-0.02238300

LFe^I(^tBuNC)₃

C	0.93583700	2.13710400	0.40952200
C	1.06036000	3.52018100	0.36798600
C	0.01932500	4.27781000	-0.14895100
C	-1.11096400	3.62702000	-0.62243000
C	-1.16168000	2.23936700	-0.57842900
N	-0.15555400	1.51429200	-0.06341200
H	0.08778000	5.35893900	-0.18206300
H	1.96182300	3.98848200	0.74457600
H	-1.94799400	4.18106400	-1.03014700
C	-2.32171900	1.47483700	-1.15903600
H	-3.17548800	2.15508100	-1.26885300
H	-2.04263400	1.15702900	-2.16948700
C	-3.34058700	0.56913100	0.85826500
C	-3.37716700	-0.73004900	-1.14536600
C	-4.80245700	0.94056900	0.64185000
H	-2.82184100	1.37268800	1.38651600
H	-3.29183900	-0.32467400	1.48608200
C	-4.83664500	-0.35589600	-1.36519000
H	-2.87876200	-0.89756300	-2.10233700
H	-3.33104700	-1.66569000	-0.57938700
H	-4.88425300	1.90972900	0.11368800
H	-5.28320900	1.07142400	1.61594900
H	-5.34521500	-1.18069800	-1.87351900
H	-4.91169000	0.52698200	-2.02937200
N	-2.61937900	0.27128000	-0.38715900
N	-5.49681900	-0.11002300	-0.09013000

C	-6.89857900	0.21174300	-0.27276800
H	-7.40326200	-0.60822300	-0.78966000
H	-7.37715000	0.35150400	0.69972700
H	-7.04644900	1.13335100	-0.86428900
C	-0.61901200	-4.92673300	0.02539800
C	0.30656700	-0.93439000	-4.43561600
C	-0.84178800	-0.60192400	4.44200500
C	1.99144800	1.26989900	1.04153900
H	2.92303400	1.84471900	1.11854500
H	1.67350800	1.05231300	2.06709500
N	2.13720600	-0.00596300	0.34545600
C	2.88566800	0.12456600	-0.91247700
C	2.76732600	-1.04391300	1.16933000
C	4.38367100	0.31821400	-0.71402000
H	2.47002800	0.95554200	-1.48737200
H	2.71910900	-0.78973300	-1.48855100
C	4.26373500	-0.84425200	1.36783700
H	2.25775400	-1.08476500	2.13415900
H	2.60235300	-2.00137500	0.66593200
H	4.59153400	1.29799200	-0.24255600
H	4.87225900	0.32942100	-1.69294800
N	4.94018100	-0.76865800	0.07997600
H	4.66702600	-1.69152500	1.93055300
H	4.45568600	0.06452600	1.97050500
C	6.37404900	-0.62721900	0.24034800
H	6.76883200	-1.47358400	0.80790800
H	6.85792900	-0.61539800	-0.73954800

H	6.65167400	0.30145000	0.77102500
C	-0.51413700	-0.51143900	1.85233300
C	-0.41567100	-2.32143500	0.02711000
C	-0.04881000	-0.63870700	-1.86549100
N	-0.65839300	-0.55234400	3.01460100
N	-0.50829000	-3.49469300	0.04360500
N	0.10050200	-0.76838000	-3.02050800
C	-2.20896100	0.00207600	4.76938000
H	-2.26556500	1.03889200	4.43207400
H	-3.00916000	-0.56793700	4.29334300
H	-2.36340600	-0.02021900	5.85028500
C	0.27805500	0.21087900	5.09511000
H	1.25561000	-0.21198100	4.85481300
H	0.24994700	1.24935100	4.75885900
H	0.15109800	0.19396400	6.17965200
C	-0.77613700	-2.06616500	4.87983100
H	-0.91832500	-2.12714100	5.96091800
H	-1.55899400	-2.65091800	4.39292900
H	0.19439000	-2.50055000	4.63217700
C	-0.97165900	-5.40269300	1.43647800
H	-0.19223000	-5.11952100	2.14685800
H	-1.91970400	-4.97134600	1.76439600
H	-1.06566400	-6.49084800	1.44068900
C	0.72635800	-5.50804500	-0.41737300
H	0.98755400	-5.15713700	-1.41780000
H	1.51863100	-5.21654100	0.27516300
H	0.66532000	-6.59856000	-0.43663300

C	-1.72277200	-5.31197700	-0.96308700
H	-2.67990100	-4.88278100	-0.65964000
H	-1.48222100	-4.95830900	-1.96779100
H	-1.82357600	-6.39924600	-0.99241800
C	-1.06137100	-1.10458000	-5.09970000
H	-1.57643600	-1.98287300	-4.70563200
H	-1.68529100	-0.22449000	-4.93157900
H	-0.92746500	-1.23394700	-6.17582100
C	1.17117600	-2.17899500	-4.64705000
H	2.13979200	-2.06609300	-4.15606000
H	0.67565000	-3.06640500	-4.24844600
H	1.33921800	-2.32535100	-5.71616200
C	1.01363700	0.31552500	-4.96351500
H	0.40480300	1.20553300	-4.79217000
H	1.98005400	0.45003700	-4.47379500
H	1.18056200	0.21022400	-6.03763400
Fe	-0.28484000	-0.50986500	-0.00943100

(LH⁺)Fe^I(^tBuNC)₃

C	0.93945900	2.12870300	0.42782400
C	1.06672200	3.51214500	0.40772700
C	0.02720300	4.28023900	-0.09494200
C	-1.10493800	3.63924800	-0.57793100
C	-1.15691100	2.25189200	-0.55666600
N	-0.15346200	1.51446500	-0.05377700
H	0.09756800	5.36148200	-0.11082900

H	1.96974900	3.97230300	0.79024700
H	-1.94062900	4.20164600	-0.97657700
C	-2.31927500	1.50575200	-1.15806200
H	-3.15770600	2.20316500	-1.28606100
H	-2.02757000	1.18052700	-2.16173100
C	-3.36090700	0.58770400	0.85305400
C	-3.38289600	-0.70179200	-1.15322300
C	-4.82079200	0.97810700	0.65966500
H	-2.85902100	1.39530300	1.38875200
H	-3.30067600	-0.30098100	1.48798100
C	-4.83895200	-0.34459000	-1.41841700
H	-2.88647200	-0.87050500	-2.10935400
H	-3.33176200	-1.64439600	-0.59872400
H	-4.93470400	1.90681300	0.09877300
H	-5.32796900	1.08642400	1.61820600
H	-5.36092400	-1.16046800	-1.91798100
H	-4.94279500	0.55899700	-2.02122600
N	-2.65413300	0.30705700	-0.39370800
N	-5.54701900	-0.07876000	-0.12133200
C	-6.98032200	0.26479600	-0.32521900
H	-7.45952800	-0.54804200	-0.86663200
H	-7.44928100	0.39913800	0.64743600
H	-7.03726000	1.18639400	-0.90091000
C	-0.55304800	-4.93211800	0.04219900
C	0.28866100	-0.93831800	-4.44101800
C	-0.84642300	-0.60207100	4.44224400
C	1.99314600	1.25009700	1.04547700

H	2.93098100	1.81450200	1.11491800
H	1.68379000	1.03140800	2.07331800
N	2.12057400	-0.02555400	0.34136300
C	2.87006600	0.10758200	-0.91817600
C	2.75268900	-1.06958400	1.15980700
C	4.36841800	0.29692200	-0.72081600
H	2.45573200	0.94136200	-1.48976500
H	2.70041200	-0.80486300	-1.49569500
C	4.24916300	-0.87188800	1.35663700
H	2.24417500	-1.11505700	2.12487700
H	2.58600500	-2.02334600	0.65072600
H	4.58024500	1.27491600	-0.24769000
H	4.85401000	0.30991500	-1.70113000
N	4.92366500	-0.79378400	0.06819800
H	4.65085700	-1.72192900	1.91614300
H	4.44365000	0.03402700	1.96261200
C	6.35839800	-0.65694800	0.22615900
H	6.75170300	-1.50634500	0.79010100
H	6.84015400	-0.64353200	-0.75470900
H	6.63974500	0.26913700	0.75916800
C	-0.50413900	-0.51398400	1.85385800
C	-0.37275300	-2.32538200	0.02955100
C	-0.04083700	-0.63537800	-1.86804100
N	-0.66846800	-0.55331600	3.01305700
N	-0.45804100	-3.49809400	0.04803000
N	0.08844000	-0.76571900	-3.02489200
C	-2.21357500	-0.00099000	4.77434900

H	-2.27555400	1.03448800	4.43386700
H	-3.01521900	-0.57608400	4.30678700
H	-2.36126000	-0.01947400	5.85617800
C	0.27425100	0.21482300	5.08870000
H	1.25183600	-0.20606700	4.84536400
H	0.24192700	1.25274400	4.75125200
H	0.15154100	0.19901700	6.17369300
C	-0.77510800	-2.06582900	4.88019800
H	-0.91323000	-2.12597600	5.96179700
H	-1.55815600	-2.65317000	4.39678800
H	0.19576900	-2.49757200	4.62963000
C	-0.89807500	-5.39866600	1.45816600
H	-0.12063200	-5.10084500	2.16465200
H	-1.85041200	-4.97519700	1.78390800
H	-0.97988900	-6.48766500	1.47186900
C	0.79809600	-5.50124300	-0.39819800
H	1.05358500	-5.15588800	-1.40197600
H	1.58816600	-5.19552100	0.29063100
H	0.74866000	-6.59239800	-0.40822200
C	-1.65434100	-5.33658800	-0.94110800
H	-2.61559900	-4.91546300	-0.63935900
H	-1.41925800	-4.98906400	-1.94921100
H	-1.74332700	-6.42503100	-0.96083600
C	-1.08224700	-1.10999900	-5.09826600
H	-1.59666700	-1.98600700	-4.69823900
H	-1.70430900	-0.22803800	-4.93294700
H	-0.95242400	-1.24505800	-6.17410300

C	1.15071000	-2.18524200	-4.64871400
H	2.12157600	-2.07106600	-4.16261500
H	0.65559300	-3.06991700	-4.24368500
H	1.31391000	-2.33705500	-5.71776100
C	0.99519700	0.30857900	-4.97628700
H	0.38813300	1.20010100	-4.80672500
H	1.96366400	0.44380700	-4.49094000
H	1.15780700	0.19811500	-6.05049100
Fe	-0.24824300	-0.51060400	-0.00661400
H	-5.51518900	-0.94360500	0.42617700

(LH⁺)Fe⁰(^tBuNC)₂ [Chair conformation]

C	0.83812300	1.74332500	1.01222800
C	0.89315100	3.01167300	1.55906400
C	-0.16415300	3.89538300	1.32848200
C	-1.23800400	3.48197600	0.53683800
C	-1.21461500	2.21152700	-0.00762200
N	-0.19861900	1.35695100	0.23801500
H	-0.15024600	4.89038200	1.75622700
H	1.74058200	3.30316300	2.16887900
H	-2.07048400	4.14600200	0.33444700
C	-2.18934900	1.61794000	-0.97146200
H	-3.15351700	2.13479700	-0.94425200
H	-1.77647000	1.71379000	-1.98323500
C	-3.03963100	-0.12277200	0.52808100
C	-2.96052500	-0.55311200	-1.81954600
C	-4.52477600	0.19637600	0.45399200
H	-2.60003400	0.45281200	1.34338300
H	-2.89768600	-1.17873400	0.76271900
C	-4.44302800	-0.24695300	-1.95513200
H	-2.46099400	-0.30042400	-2.75423600
H	-2.81125000	-1.62300300	-1.65609700
H	-4.72903500	1.25332700	0.28011700
H	-5.02284700	-0.10322300	1.37558700
H	-4.88745900	-0.85747700	-2.74052200
H	-4.63939800	0.80247900	-2.17866000
N	-2.29240900	0.15356300	-0.71546000
N	-5.16365300	-0.55244400	-0.67624000

C	-6.62384000	-0.28516600	-0.77525200
H	-7.03392500	-0.88867700	-1.58221600
H	-7.09140300	-0.55039000	0.17050400
H	-6.76811500	0.77304700	-0.98373400
C	-0.91952400	-3.50455100	2.29333200
C	0.34911500	-2.25709700	-4.17684000
C	1.79583500	0.61718300	1.22516500
H	2.77946200	0.97504000	1.54054700
H	1.39286300	-0.03138700	2.01402500
N	1.84144500	-0.21609700	-0.00648400
C	2.57599000	0.49238800	-1.08623700
C	2.52621700	-1.50404700	0.23758900
C	4.07335700	0.60902600	-0.84187000
H	2.13137300	1.48181700	-1.21026400
H	2.40319700	-0.06824400	-2.00473500
C	4.02223800	-1.37383500	0.47628500
H	2.04235200	-1.99214700	1.08405500
H	2.35304700	-2.12124700	-0.64638500
H	4.28795700	1.27680300	0.01378000
H	4.52617200	1.07476200	-1.72231300
N	4.66716000	-0.70434400	-0.64302400
H	4.44291500	-2.37840500	0.58023500
H	4.22328600	-0.84529900	1.42749300
C	6.10251200	-0.61806400	-0.45756800
H	6.52289400	-1.62085400	-0.34890400
H	6.56112700	-0.14597700	-1.32983900
H	6.37970900	-0.03086700	0.43648700

C	-0.51262800	-1.85879800	0.49149400
C	0.03473700	-0.75813800	-2.21401600
N	-0.70827100	-2.98077100	0.93594300
N	0.22843300	-1.02326600	-3.38800800
C	-0.88547500	-2.39453000	3.34345600
H	0.07940100	-1.88145700	3.33461800
H	-1.66671200	-1.65398300	3.15595700
H	-1.04190500	-2.81481000	4.34076900
C	0.18825000	-4.52241200	2.56892600
H	0.18071100	-5.31127300	1.81280700
H	1.16929900	-4.04081200	2.55468300
H	0.04536800	-4.98134500	3.55104500
C	-2.27813600	-4.20681200	2.31075900
H	-3.08572400	-3.49850700	2.10796700
H	-2.31275100	-4.99406800	1.55360400
H	-2.45775600	-4.65961500	3.28967400
C	-0.69118000	-2.19168600	-5.29547500
H	-1.70283700	-2.16541400	-4.88247000
H	-0.54360000	-1.29693800	-5.90519800
H	-0.60745600	-3.06921500	-5.94239800
C	0.12271700	-3.49979300	-3.31795000
H	0.85628600	-3.55377900	-2.51006100
H	-0.87560200	-3.48877900	-2.87392100
H	0.21699500	-4.40086300	-3.93037000
C	1.75571400	-2.27865200	-4.77697400
H	1.92798800	-1.38640700	-5.38394400
H	2.51143400	-2.31049200	-3.98798100

H	1.88318300	-3.15971900	-5.41186800
H	-5.04585600	-1.55163900	-0.48791100
Fe	-0.22523600	-0.40019600	-0.48950300

(LH⁺)Fe⁰(^tBuNC)₂ (Twisted boat conformation)

C	1.17242100	1.08467200	1.05812200
C	1.42596400	2.12051200	1.94088000
C	0.43216000	3.07275700	2.16311700
C	-0.77985000	2.96976500	1.48174400
C	-0.95064900	1.92894900	0.58595400
N	0.00713900	1.00617900	0.39081500
H	0.59986600	3.88547700	2.85942600
H	2.37675600	2.17423400	2.45777700
H	-1.57020400	3.69528000	1.63298400
C	-2.10612700	1.72219300	-0.33578500
H	-3.01592200	2.22673800	0.00805200
H	-1.82772400	2.14222800	-1.30939800
C	-3.10137300	-0.28853900	0.58221700
C	-3.22853900	0.16249900	-1.75619700
H	-2.43354000	-0.30126500	1.44180000
H	-2.73749500	0.66727700	-2.58579500
N	-2.35427800	0.27334500	-0.56672700
C	-0.45479000	-3.45707900	2.36759800
C	-0.22654400	-0.32762200	-4.91960400
C	2.05315400	-0.09396400	0.79021500
H	3.10555600	0.14510900	0.96202500
H	1.77398900	-0.89534500	1.48450400

N	1.78620900	-0.60707900	-0.57967400
C	2.39657200	0.29684200	-1.59061100
C	2.36486700	-1.95519500	-0.77898700
C	3.91699100	0.26557700	-1.60945100
H	2.03648500	1.31087000	-1.40911500
H	2.02247100	-0.02345700	-2.56216700
C	3.88502000	-1.97640900	-0.80111500
H	1.98370400	-2.61220600	0.00259600
H	1.98277400	-2.31705300	-1.73602800
H	4.33860800	0.69412600	-0.68094300
H	4.25753400	0.90487100	-2.42931400
N	4.40078700	-1.08835200	-1.83167000
H	4.21026300	-2.99825900	-1.01712100
H	4.29435900	-1.71653700	0.19353600
C	5.84870600	-1.13210900	-1.89730400
H	6.17970700	-2.15244700	-2.10539000
H	6.20278600	-0.48506200	-2.70346300
H	6.32492100	-0.80139900	-0.95689800
C	-0.51135800	-1.95409300	0.38568000
C	-0.38102700	-0.68720000	-2.47378600
N	-0.60373900	-3.02115000	0.96931600
N	-0.42136400	-1.03611500	-3.64362600
C	-1.48731500	-4.55281100	2.62757100
H	-2.50498500	-4.16956000	2.51670800
H	-1.35278200	-5.38186600	1.92893000
H	-1.38043500	-4.93622900	3.64541100
C	-0.66593000	-2.28944200	3.33178000

H	0.04578700	-1.48435500	3.13443500
H	-1.67703300	-1.88455100	3.24067100
H	-0.52855700	-2.62497300	4.36312900
C	0.95357500	-4.03201800	2.52817600
H	1.12604000	-4.83744500	1.81047100
H	1.71263200	-3.26112700	2.37376000
H	1.07874900	-4.43486400	3.53665300
C	-1.43199200	-0.64034800	-5.80642000
H	-1.53784300	-1.71912300	-5.94457600
H	-2.35419600	-0.25662100	-5.36227700
H	-1.30860300	-0.17577600	-6.78829900
C	1.04357500	-0.88887000	-5.56079500
H	1.91779100	-0.68476600	-4.93740100
H	0.96065700	-1.97032000	-5.69318000
H	1.20563700	-0.43093800	-6.54026900
C	-0.09697200	1.18177800	-4.71846300
H	-0.99814700	1.59432000	-4.25779600
H	0.75327600	1.42066700	-4.07560400
H	0.04988200	1.67636400	-5.68236800
Fe	-0.34058800	-0.53914100	-0.69194300
C	-3.49010400	-1.29781400	-2.13421600
H	-2.91056800	-1.58868800	-3.00873600
H	-4.54874200	-1.47778000	-2.32263800
C	-3.61584200	-1.70442500	0.26883100
H	-4.70283000	-1.72755100	0.18100300
H	-3.31307900	-2.41267400	1.03633800
N	-3.06482500	-2.18917000	-1.02509900

H	-2.00980900	-2.07332800	-0.96413100
C	-3.38242400	-3.61035700	-1.28204100
H	-4.46401600	-3.74095000	-1.29887700
H	-2.95771700	-3.89430700	-2.24320600
H	-2.93921100	-4.21075100	-0.48986100
H	-3.95751500	0.35569700	0.81631700
H	-4.17468300	0.67870800	-1.55323700

LFe^{II}(H)(^tBuNC)₂

C	1.64566800	1.59127800	1.39995800
C	1.91680800	2.63846200	2.26877900
C	0.94419800	3.61660400	2.45208000
C	-0.25941100	3.53749400	1.75747200
C	-0.44965900	2.47479700	0.88728400
N	0.48694000	1.53296100	0.73696900
H	1.12491800	4.44057100	3.13229000
H	2.86311100	2.68422000	2.79355000
H	-1.02888900	4.28942600	1.88188800
C	-1.61871100	2.26097000	-0.02363500
H	-2.51175300	2.79224500	0.32340700
H	-1.35258800	2.66589900	-1.00543000
C	-2.60009600	0.31801100	1.03418700
C	-2.79471300	0.63846600	-1.34567800
H	-1.86077100	-0.10220900	1.71201200
H	-2.32734600	1.07210100	-2.22919900
N	-1.88544400	0.80961500	-0.19362500
C	-0.22173300	-3.36985100	2.38640800
C	0.26393600	1.86243800	-4.54101500
C	2.53244000	0.41350700	1.12990400
H	3.57787700	0.66036400	1.32731900
H	2.25470700	-0.39393500	1.81468000
N	2.30870300	-0.08374300	-0.25621800
C	3.01969300	0.78801200	-1.23005700
C	2.84361500	-1.45738600	-0.42426600
C	4.53615300	0.69111300	-1.16287600

H	2.69525000	1.81846400	-1.07467200
H	2.69708000	0.47846800	-2.22386000
C	4.35979300	-1.54235200	-0.35548400
H	2.39589400	-2.09853200	0.33430500
H	2.50270500	-1.80528400	-1.40117700
H	4.92481100	1.10591100	-0.21424200
H	4.94718100	1.31271000	-1.96374600
N	4.97155400	-0.68259600	-1.35641300
H	4.65254600	-2.57824200	-0.54985700
H	4.72055200	-1.29645000	0.66134700
C	6.41756300	-0.79143100	-1.34309900
H	6.71218400	-1.82681300	-1.53001100
H	6.84330600	-0.16559200	-2.13104700
H	6.85679500	-0.47757900	-0.37939200
C	-0.01497300	-1.31155800	0.79375300
C	0.24093500	0.90935100	-2.10938300
N	-0.10125200	-2.22075000	1.52665500
N	0.24748000	1.35305500	-3.19375500
C	-1.58327000	-3.30292300	3.07999600
H	-1.67266300	-2.39078100	3.67338900
H	-2.39085000	-3.32810900	2.34620500
H	-1.69215900	-4.16204700	3.74517200
C	0.91043100	-3.31615000	3.41411700
H	1.88475500	-3.34463800	2.92201300
H	0.84552500	-2.40685800	4.01509100
H	0.83524400	-4.17857700	4.07984500
C	-0.11403000	-4.62819700	1.52288200

H	-0.90795900	-4.65192200	0.77396900
H	0.85155000	-4.66879700	1.01484200
H	-0.20882400	-5.51179100	2.15774800
C	-0.57515800	0.92870500	-5.41580500
H	-0.16675400	-0.08375200	-5.40356100
H	-1.60955500	0.89524200	-5.06797400
H	-0.56803400	1.29361800	-6.44512300
C	1.71781700	1.88909300	-5.01739500
H	2.32402900	2.53481800	-4.37899400
H	2.14680600	0.88503100	-5.01380200
H	1.75459800	2.27704900	-6.03745200
C	-0.32638000	3.27356400	-4.52577800
H	-1.35616800	3.25996600	-4.16309400
H	0.26361900	3.93296100	-3.88607700
H	-0.32178400	3.67856700	-5.53996300
Fe	0.16777400	0.04323600	-0.46727100
C	-3.11522900	-0.82572300	-1.60712500
H	-2.31579400	-1.28602000	-2.19456700
H	-4.03806900	-0.85150000	-2.21231200
C	-3.69017100	-0.70550200	0.71803200
H	-4.64699900	-0.19576800	0.49888700
H	-3.86221800	-1.30791100	1.61360200
N	-3.27781300	-1.57306700	-0.36330800
C	-4.14229100	-2.72021400	-0.53645900
H	-5.17781000	-2.43877000	-0.80279100
H	-3.75302300	-3.35746800	-1.33484400
H	-4.17459800	-3.31047700	0.38276400

H	-3.06916300	1.16935200	1.53960100
H	-3.71799900	1.20251600	-1.15647300
H	-0.05809800	-1.14084500	-1.41014100

(LH⁺)Fe^{II}(H)(^tBuNC)₂

C	1.59835200	1.48283400	1.35654300
C	1.91200900	2.47957400	2.26934700
C	0.95164600	3.44461300	2.55301500
C	-0.28543700	3.40426500	1.91729400
C	-0.51576200	2.39817000	0.99190800
N	0.41458800	1.47501000	0.73710600
H	1.16523500	4.22672200	3.27175700
H	2.87886800	2.49100800	2.75687600
H	-1.04893800	4.14239000	2.12834300
C	-1.73191400	2.26506000	0.12776800
H	-2.61506200	2.71632000	0.59101600
H	-1.53533700	2.80938500	-0.80071400
C	-2.77009700	0.19078800	0.83541400
C	-2.88794500	0.85608800	-1.43335300
H	-2.13533700	0.10163600	1.71447800
H	-2.44453700	1.47545200	-2.20948600
N	-1.99619600	0.84584600	-0.24720400
C	-0.17996000	-3.04001300	2.82758500
C	0.22003700	2.09577000	-4.43369600
C	2.45671100	0.29740700	1.02603800
H	3.51484600	0.54093700	1.13748700
H	2.23649000	-0.49453200	1.74810300
N	2.13099100	-0.22414400	-0.33125000
C	2.86230700	0.56855100	-1.36043800
C	2.56015900	-1.63823700	-0.48650200
C	4.36917600	0.35894300	-1.35608800

H	2.62408000	1.62422600	-1.21910800
H	2.47707400	0.25675400	-2.33080500
C	4.06765800	-1.83182400	-0.48044900
H	2.10466200	-2.23000400	0.30626400
H	2.15150200	-1.98134500	-1.43846500
H	4.83214500	0.76688800	-0.43856100
H	4.78480300	0.92997200	-2.19129800
N	4.69190300	-1.04666500	-1.53269700
H	4.27372400	-2.89153800	-0.65547000
H	4.48981900	-1.58569500	0.51201000
C	6.12562300	-1.26226200	-1.58413400
H	6.33417400	-2.32125500	-1.75282100
H	6.55570900	-0.69150800	-2.41049900
H	6.63255800	-0.95461100	-0.65252800
C	-0.15375900	-1.22878200	0.94256800
C	0.11727000	0.94861300	-2.09043600
N	-0.20908500	-2.03683600	1.78408800
N	0.14262500	1.47002600	-3.13417200
C	-1.57882700	-3.14078800	3.43601200
H	-1.90262300	-2.17880500	3.83767700
H	-2.30516200	-3.48593800	2.69750100
H	-1.55740000	-3.86574800	4.25182100
C	0.83454100	-2.58876300	3.87964700
H	1.83553100	-2.50848300	3.45139700
H	0.55076100	-1.62439900	4.30484900
H	0.86444900	-3.32737300	4.68305700
C	0.23661600	-4.36710600	2.19239100

H	-0.47031700	-4.66585700	1.41623700
H	1.23415900	-4.29525700	1.75476200
H	0.25356100	-5.14041100	2.96292500
C	-0.81032200	1.42609000	-5.34392400
H	-0.60739300	0.35780400	-5.43962900
H	-1.82179100	1.56098900	-4.95585900
H	-0.75921200	1.87959800	-6.33583500
C	1.63750700	1.88518000	-4.96846600
H	2.37615400	2.34154000	-4.30681300
H	1.86079400	0.82153800	-5.07154300
H	1.71934800	2.35241900	-5.95179400
C	-0.08282000	3.58456000	-4.25975700
H	-1.08523900	3.73423100	-3.85406400
H	0.64216600	4.05218500	-3.59089400
H	-0.02656600	4.07757300	-5.23237000
Fe	0.00445700	0.01445700	-0.46637800
C	-3.10849700	-0.55454000	-1.97860900
H	-2.46124000	-0.75606000	-2.83137800
H	-4.14649300	-0.70514500	-2.27468800
C	-3.29696900	-1.18427800	0.38982600
H	-4.38430500	-1.18370700	0.30746600
H	-3.00948800	-1.96434900	1.09134400
N	-2.76085200	-1.56682000	-0.94478100
H	-1.70009700	-1.51783200	-0.91198900
C	-3.15989800	-2.93604200	-1.34408500
H	-4.24603400	-2.99031800	-1.39783600
H	-2.72592900	-3.15370100	-2.31836700

H	-2.78493900	-3.64072600	-0.60464900
H	-3.62337000	0.82505000	1.09980300
H	-3.84300600	1.31218900	-1.14895000
H	-0.28477300	-1.19590400	-1.39889300

LFe^I(^tBuNC)₂

C	0.88140300	2.22994600	0.41275800
C	0.94043500	3.60271800	0.59825500
C	-0.12499000	4.38161900	0.15639600
C	-1.22706500	3.77161100	-0.43793500
C	-1.20554900	2.39863200	-0.61704200
N	-0.15278700	1.66424100	-0.22493400
H	-0.10781400	5.45596800	0.29615100
H	1.79148500	4.04997700	1.09704400
H	-2.08612600	4.35079900	-0.75360500
C	-2.28117500	1.56408100	-1.23819600
H	-3.25216500	2.06055600	-1.16675400
H	-2.05779100	1.42562500	-2.30110100
C	-2.84188900	0.23417300	0.75415700
C	-3.05773600	-0.74508900	-1.42701700
C	-4.34611400	0.46405400	0.78978500
H	-2.32858700	1.00411300	1.33363700
H	-2.61301200	-0.73367500	1.20524200
C	-4.55559000	-0.48939300	-1.38559400
H	-2.68717600	-0.71201800	-2.45255400
H	-2.85684900	-1.74081000	-1.02797100
H	-4.59446100	1.49035900	0.46064200
H	-4.67962500	0.37999900	1.82807400
H	-5.05454700	-1.27353000	-1.96231000
H	-4.80522500	0.47177300	-1.87318400
N	-2.26748300	0.21020600	-0.61774800
N	-5.04157800	-0.52891200	-0.01419200

C	-6.47939500	-0.34953700	0.04697800
H	-6.97466100	-1.13319500	-0.53131800
H	-6.81757300	-0.42158200	1.08341100
H	-6.80045400	0.62871500	-0.35307300
C	-0.75189400	-4.58135900	0.38509400
C	0.43588400	-0.78233300	-4.91836300
C	1.84147300	1.23046600	0.98091300
H	2.83955300	1.66102200	1.09180700
H	1.49211900	0.97464100	1.98740400
N	1.83583100	-0.02022400	0.17931200
C	2.72575100	0.12314800	-1.00354100
C	2.33802600	-1.15926000	0.98492700
C	4.20750800	0.18871800	-0.66248400
H	2.42215400	1.01269600	-1.55834100
H	2.54490400	-0.74333600	-1.64020000
C	3.81665900	-1.06504900	1.32722200
H	1.73431900	-1.23226700	1.89121900
H	2.16939100	-2.06176600	0.39539400
H	4.45771000	1.12763200	-0.13443800
H	4.76826200	0.20405900	-1.60168200
N	4.61309700	-0.97329200	0.11250600
H	4.10179700	-1.96951500	1.87224100
H	4.01210100	-0.21098200	2.00284700
C	6.03337400	-0.94681700	0.40482000
H	6.31690400	-1.85085500	0.94899900
H	6.60178200	-0.91460600	-0.52776800
H	6.32359500	-0.07256900	1.01451300

C	-0.41389100	-2.04134900	-0.13208200
C	0.06107900	-0.41829100	-2.35633300
N	-0.56977800	-3.18389500	0.10317900
N	0.21368500	-0.57118600	-3.51357400
C	-1.00797100	-4.74132200	1.88582900
H	-0.16105200	-4.36644800	2.46417800
H	-1.90601400	-4.19695600	2.18509600
H	-1.14868300	-5.79861400	2.12105500
C	0.52185400	-5.32369000	-0.02663300
H	0.71451200	-5.19914000	-1.09411300
H	1.38365000	-4.95323700	0.53220900
H	0.40501400	-6.38918500	0.18345200
C	-1.95148400	-5.08045000	-0.42369400
H	-2.85815900	-4.53958400	-0.14472300
H	-1.77776600	-4.94879800	-1.49362600
H	-2.10754900	-6.14305600	-0.22495200
C	-0.92401300	-0.95876500	-5.59757800
H	-1.45396700	-1.81898300	-5.18349400
H	-1.54083100	-0.06779500	-5.46330100
H	-0.77861600	-1.12239000	-6.66767400
C	1.29012300	-2.04167900	-5.08367700
H	2.25316600	-1.92396600	-4.58255600
H	0.78023900	-2.91155800	-4.66465200
H	1.47156300	-2.22309700	-6.14539200
C	1.16386500	0.44208100	-5.47829200
H	0.56251700	1.34355400	-5.34350700
H	2.12441300	0.58277700	-4.97840400

H	1.34572000	0.30211700	-6.54621000
Fe	-0.20617100	-0.24024700	-0.47968100

LF⁰(^tBuNC)₃

C	0.91867500	2.09781100	0.48230100
C	1.01865400	3.48326500	0.49063700
C	0.00902900	4.24463900	-0.07810300
C	-1.06644200	3.57800000	-0.64610200
C	-1.09348000	2.18964500	-0.62933900
N	-0.11935100	1.44296000	-0.07141800
H	0.05772100	5.32745300	-0.07734700
H	1.88880100	3.94757100	0.94077800
H	-1.88803500	4.11876300	-1.10160000
C	-2.22624200	1.42688200	-1.24521500
H	-3.05749600	2.11542200	-1.45019800
H	-1.89781500	1.02100300	-2.20873400
C	-3.23809300	0.71140100	0.84418400
C	-3.40810200	-0.68808800	-1.07261800
C	-4.67634400	1.17271800	0.64093300
H	-2.65503700	1.50367800	1.32035600
H	-3.23334100	-0.14892200	1.51985500
C	-4.84307600	-0.22477200	-1.29091900
H	-2.94031100	-0.95060100	-2.02390400
H	-3.42446100	-1.58933400	-0.45160300
H	-4.70510300	2.11787700	0.06445900
H	-5.12461000	1.38515300	1.61673900
H	-5.41866100	-1.03952500	-1.74157100
H	-4.87405800	0.62254700	-2.00325000
N	-2.56371800	0.29647600	-0.39176700
N	-5.45931000	0.13781900	-0.02112300

C	-6.83758900	0.54883700	-0.19840000
H	-7.41004600	-0.25934800	-0.66082900
H	-7.28584100	0.77541600	0.77240100
H	-6.93319400	1.44572100	-0.83742100
C	-0.33660100	-4.63887100	0.13728300
C	0.21384900	-1.16378500	-4.39123500
C	-0.94167200	-0.94438300	4.36450200
C	1.97704000	1.23976400	1.10639900
H	2.89198800	1.83770800	1.23792500
H	1.63841100	0.95208700	2.10856300
N	2.13569700	0.02657700	0.33635000
C	2.81827500	0.23995900	-0.93778200
C	2.82195800	-1.03056600	1.07001000
C	4.32118600	0.46291600	-0.80827400
H	2.35869600	1.08759200	-1.45371500
H	2.63989000	-0.64909700	-1.55205600
C	4.32288800	-0.80818400	1.21500100
H	2.35824400	-1.12936900	2.05495800
H	2.64141900	-1.96791500	0.53573500
H	4.52754200	1.42412700	-0.29710200
H	4.76601800	0.53385600	-1.80641400
N	4.94365400	-0.64415400	-0.09392100
H	4.77327100	-1.67492100	1.71027700
H	4.52557300	0.07136100	1.85777300
C	6.37648600	-0.46132400	0.01766900
H	6.82263100	-1.32031100	0.52568400
H	6.82080600	-0.38182900	-0.97802700

H	6.64457600	0.44902100	0.58530400
C	-0.51909700	-0.66640100	1.80037400
C	0.12100700	-2.25565600	0.07735100
C	-0.11303800	-0.78508000	-1.82463900
N	-0.65548700	-0.75104200	2.97288100
N	0.51722800	-3.42842400	0.16182700
N	-0.01207300	-0.95654400	-2.99099500
C	-2.34529400	-1.54160800	4.50361700
H	-3.09426100	-0.86767000	4.08235900
H	-2.40752000	-2.50149500	3.98679300
H	-2.57609500	-1.69933200	5.56005900
C	-0.86841700	0.41407600	5.06750700
H	0.12786400	0.84912000	4.96230600
H	-1.59899300	1.10682400	4.64414900
H	-1.08234200	0.29124900	6.13186700
C	0.10385200	-1.90023000	4.94611200
H	-0.09171800	-2.05755800	6.00948600
H	0.06664600	-2.86692700	4.43941500
H	1.10830900	-1.48603000	4.83524100
C	-1.27326400	-4.63583200	1.34690800
H	-0.69749700	-4.58856900	2.27560000
H	-1.93743500	-3.76849600	1.31261300
H	-1.88481800	-5.54357400	1.36821700
C	0.58780300	-5.85276200	0.20820100
H	1.27636000	-5.86056700	-0.64156000
H	1.18135700	-5.83062500	1.12652800
H	0.01150400	-6.78275300	0.19291800

C	-1.15376100	-4.69168400	-1.15446700
H	-1.81423100	-3.82414000	-1.22332500
H	-0.49376300	-4.69093700	-2.02651800
H	-1.76509900	-5.59909200	-1.18945900
C	-1.13887500	-1.36528900	-5.08060300
H	-1.65555100	-2.23426900	-4.66761600
H	-1.77255800	-0.48569600	-4.94769400
H	-0.98858600	-1.52629000	-6.15083800
C	1.09069100	-2.40731300	-4.56330300
H	2.04894900	-2.27622200	-4.05609800
H	0.59458600	-3.28845800	-4.15097300
H	1.28023600	-2.58108500	-5.62523200
C	0.92062400	0.07094100	-4.95872400
H	0.30667500	0.96347700	-4.81933100
H	1.88124700	0.22663200	-4.46323100
H	1.09881500	-0.06424300	-6.02828300
Fe	-0.26302900	-0.58018600	-0.01596100

TS_H₂ evolution

C	2.00594700	1.17913600	1.13897500
C	2.57976200	2.11309100	1.98833400
C	1.80195200	3.18199300	2.41946500
C	0.48369200	3.30326200	1.99363800
C	-0.01570900	2.35233900	1.11720600
N	0.74816200	1.33336500	0.71447900
H	2.22169900	3.91897300	3.09365800
H	3.60485300	1.99690600	2.31657200
H	-0.14052200	4.12235300	2.32757800
C	-1.36836200	2.39008400	0.47285600
H	-2.11313300	2.85886200	1.12286500
H	-1.28681500	3.01428200	-0.42200500
C	-2.60970200	0.39395000	1.11695100
C	-2.79256500	1.23033600	-1.08175400
H	-1.96506300	0.24218100	1.98049700
H	-2.32163100	1.82268800	-1.86187000
N	-1.82543000	1.03927000	0.03413800
C	-0.17646900	-2.79740200	3.16578100
C	0.16383500	2.37608000	-4.22572600
C	2.64520200	-0.10427300	0.69727300
H	3.72715700	0.01002300	0.61632600
H	2.46654500	-0.85406000	1.47292600
N	2.03189100	-0.59832300	-0.56931900
C	2.72241200	0.03055800	-1.73389100
C	2.19372300	-2.07199600	-0.71196000
C	4.15331600	-0.44093900	-1.93998500

H	2.69779300	1.11370500	-1.60615500
H	2.14518700	-0.22676500	-2.62165200
C	3.63081300	-2.52030000	-0.91574800
H	1.77171700	-2.55619600	0.16748200
H	1.59874200	-2.36625900	-1.57865700
H	4.81450100	-0.09717600	-1.12312100
H	4.52465600	0.02865400	-2.85527400
N	4.20227300	-1.88453600	-2.09050600
H	3.62725900	-3.60416700	-1.06051100
H	4.23621200	-2.32218500	-0.01115700
C	5.55166500	-2.34970400	-2.35147700
H	5.54675900	-3.43214500	-2.49822700
H	5.93369400	-1.88143300	-3.26149400
H	6.24606400	-2.11629600	-1.52546700
C	-0.14010400	-1.19209600	1.10456300
C	0.07281600	1.02233900	-1.99647600
N	-0.16659600	-1.91387900	2.01581900
N	0.09572500	1.63677300	-2.98315800
C	-1.60069600	-3.32274800	3.34498500
H	-2.29991300	-2.50693800	3.53781100
H	-1.92781400	-3.87825800	2.46402400
H	-1.61928400	-3.99775800	4.20250000
C	0.26546800	-1.98043100	4.38011800
H	1.27779700	-1.59589100	4.24507400
H	-0.41308100	-1.14332900	4.55327600
H	0.25394800	-2.62496500	5.26103500
C	0.79563100	-3.94354600	2.88502600

H	0.49855700	-4.50038600	1.99437000
H	1.81416600	-3.57389300	2.75378700
H	0.78724300	-4.62591200	3.73705700
C	1.30925000	3.38197600	-4.10721200
H	1.13308700	4.07685000	-3.28417000
H	2.26123400	2.87343000	-3.94532400
H	1.37530100	3.95260100	-5.03549300
C	-1.17440900	3.08887700	-4.42116200
H	-1.99483100	2.37127900	-4.48260200
H	-1.36911800	3.78721400	-3.60494500
H	-1.14049000	3.65283300	-5.35514000
C	0.42090300	1.37193300	-5.35000300
H	1.36705900	0.84921900	-5.19880800
H	-0.38492700	0.63807600	-5.40800200
H	0.47068200	1.90897200	-6.29912800
Fe	-0.02073400	-0.01562900	-0.40615100
C	-3.26925200	-0.11318100	-1.64943400
H	-2.82138400	-0.29789700	-2.62841300
H	-4.35786800	-0.10635500	-1.77536100
C	-3.22254000	-0.93308000	0.62700800
H	-4.31458800	-0.89865000	0.72130300
H	-2.87089700	-1.76791600	1.23126800
N	-2.85758900	-1.20571300	-0.76736100
H	-1.39830300	-1.15329000	-0.97640100
C	-3.34174900	-2.50436600	-1.22749900
H	-4.43687300	-2.54878300	-1.21856000
H	-2.98851000	-2.67790400	-2.24531300

H	-2.94715600	-3.28748900	-0.57889000
H	-3.40884300	1.08017900	1.41852800
H	-3.64029200	1.80723900	-0.69611600
H	-0.54275500	-1.20341800	-1.36133300

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