Supporting information for Geometric control of Fe(I) intermediates in CO_2 photoreduction by tetrahedral tripodal phosphine complexes

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1. Experimental section

1.1. General remarks

All reagents were used without further purification. The reagents used were purchased from different companies such as Sigma Aldrich, Acros Organics, Fluorochem and/or TCI. Solvent purifications were performed according to the book "Purification of Laboratory Chemicals" by Armarego and Perrin.[1] All reactions were done using standard Schlenk techniques and freshly distilled solvents. NMR spectra were recorded on a Bruker Advance 400 spectrometer using deuterated solvents ($CDCl_3$ and CD_2Cl_2). Infrared spectroelectrochemistry experiments were performed with CO_2 or N_2 saturated solutions of acetonitrile (MeCN) and dichloroethane (DCE) without further purification with a purity of 99%. 2,4,5,6-Tetra(9H-carbazol-9-yl)isophthalonitrile (4CzIPN) was synthesized through a reported procedure.[2] FTIR spectra were obtained on a Bruker INVENIO S FTIR spectrometer in the 400-4000 cm^{-1} range with 4 cm^{-1} resolution using KBr pellets. Elemental analysis (EA) for C, H and N were performed in monoplicate with a Truspec Micro CHNS 630 200 200 elemental analyzer at the Department of Chemistry, University of Aveiro.Analysis parameters: sample amount 1.3 - 2.0 mg; combustion furnace temperature 1075 ºC; afterburner temperature 850 ºC. Detection method: C, H and S through infrared absorption; N by thermal conductivity. Gases required: combustion - oxygen; carrier helium; pneumatic - compressed air.

1.2. Synthesis

Tris(2-bromo-*p*-tolyl)amine

Tris(2-bromo-*p*-tolyl)amine was synthesized according to the literature.[3,4] Tri-*p*-tolylamine (2.50 g, 8.6 mmol) was dissolved in $CHCl_3$ (25 mL) and a solution of bromine (1.34 mL) in $CHCl_3$ (5 mL) was added dropwise at ambient temperature resulting in a deep blue colour. The reaction mixture was stirred at room temperature for 24 h, and the reaction was stopped by the addition of a saturated, aqueous Na_2SO_3 solution (60 mL). The aqueous layer was extracted with $CHCl_3$ (3×15 mL). The combined organic layers were washed with saturated, aqueous $NaHCO_3$ solution (2×20 mL), brine (1×20 mL) and dried over $MgSO_4$. After evaporation of the solvent under reduced pressure the compound was obtained as a white solid (2.27 g, 4.3 mmol, η = 50 %) .^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm): δ = 2.30 (s, 9H, CH_3), 6.69 (d, J = 8.1 Hz, 3H), 7.00 (dd, 3H), 7.40 (d, 3H).

Tris(2-diisopropylphosphine-*p*-tolyl)amine (**NP^{iso}**)

Tris(2-diisopropylphosphine-*p*-tolyl)amine was synthesised according to the literature procedure.[3] In a degassed Schlenk flask, tris(2-bromo-*p*-tolyl)amine (1 g, 1.89 mmol) was dissolved in dry Et_2O (20 mL) and cooled down to -78 °C. A solution of *tert*-BuLi (1.70 M in heptane, 7 mL) was added portionwise over 15 min. The resulting mixture was warmed up to room temperature after 30 min. After 3 h of stirring, the reaction mixture showed a yellow colour and a white precipitate (LiBr). The Schlenk flask was cooled down again to –78 °C and chlorodiisopropylphosphine (1 mL, 6.24 mmol) was added over 5 min. The mixture was stirred at room temperature for 18 h an then it was filtered through a silica plug and the solvent removed under vacuum. The resulting tacky solid was dissolved in CH_2Cl_2 (30 mL), filtered through Celite®, and dried to a solid. Trituration of the filtrate in cold MeOH (150 mL) afforded an analytically pure fine white solid, which was collected on a fritted glass funnel and dried under vacuum (0.94 g, 1.50 mmol, η = 78 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm): δ = 7.23 (s), 7.07 (br s), 6.93 (s), 6.91 (s), 6.85 (m), 6.63 (m), 6.57 (br s), 6.45 (m), 2.54 (m), 2.30 (s), 2.28 (s), 1.51 (m), 1.21 (m), 1.10 (m), 1.00 (br s), 0.91 (m), 0.80 (br s), 0.41 (m); ^{31}P NMR (400 MHz, $CDCl_3$, 298 K, ppm): δ = -11.73.

^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$)

The ligand tris(2-diisopropylphosphine-*p*-tolyl)amine (**NP^{iso}**) and corresponding Fe(II) complex, abbreviated as ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$), were prepared following modifications of previously reported procedures for the tripodal **NP^{iso}** ligand and its metal complexes.[3] The ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) was obtained with a yield of 52% by stirring the ligand **NP^{iso}** with the $FeCl_2$ precursor and $NaBPh_4$ in dry tetrahydrofuran at 65 ºC for 12 h under N_2 atmosphere. Single

crystals of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) were obtained as yellow blocks by slow diffusion of diethyl ether into a saturated dichloromethane solution under N_2 atmosphere.

The ^{1}H NMR spectrum of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) was obtained in deuterated dichloromethane (CD_2Cl_2) and matched the data previously reported by Peters and co-workers (Figures S1 to S5).[3] FTIR confirmed the presence of the characteristic vibrational modes of the $B^{Ph}_{4}^{-}$ anion $\tilde{\nu}(B^{Ph}_{4}^{-})$ at 731, 704 cm^{-1}, as well as the bands attributed to aromatic and aliphatic groups $\tilde{\nu}$(C–H) at ~3047, 2971 and 2916 cm^{-1}, $\tilde{\nu}$(C═C) and $\tilde{\nu}$(C-P) ~1630, 1471 and 645 cm^{-1}, respectively (Figure S6).

In a degassed J Young glass reactor, to a solution of **NP^{iso}** (0.55 g, 0.90 mmol) in dry THF (20 mL) was added $FeCl_2$ (0.110 g, 0.84 mmol) and sodium tetraphenylborate (0.297 g, 0.84 mmol). The mixture was heated up to 70 °C for 12 h. After this time the reaction mixture was cooled down to room temperature and the solvent was removed under vacuum. The resulting yellow crude product was washed with petroleum ether (2 × 20 mL) and dried under reduced pressure. The product was extracted with CH_2Cl_2 and filtered through Celite®. The remaining CH_2Cl_2 solution was layered with Et_2O affording pure yellow single crystals suitable for X-ray diffraction (0.495 g, 0.470 mmol, η = 52%). ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, ppm): δ = 141.9 (br s), 30.6 (br s), 19.6 (br s), 15.4 (s), 7.8 (s), 7.2 (s), 5.5 (m), 3.1 (s), 2.6 (m), 1.66 (s), 1.1 (s) –2.8 (br s), –16.0 (br s), –20.6 (br s); UV-Vis bands (nm) were as follows: 198 (ε = 400000 M^{-1} cm^{-1}), 297 (ε = 23000 M^{-1} cm^{-1}); FTIR vibration modes ($\tilde{\nu}$/cm^{-1}) were as follows: 3047, 2971, 2916 (C-H aromatic, stretching); 1471 (C=C, stretching); 731, 704 ($B^{Ph}_{4}^{-}$, stretching); 645 (P-C, stretching); Elemental Analysis (**1** • 0.2 CH_2Cl_2) **exp. C** 71.32, **H** 6.83, **N** 1.40 **calc. C** 71.39, **H** 7.62, **N** 1.32.

2. ^{1}H and ^{13}C NMR spectra of the precursors and $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$

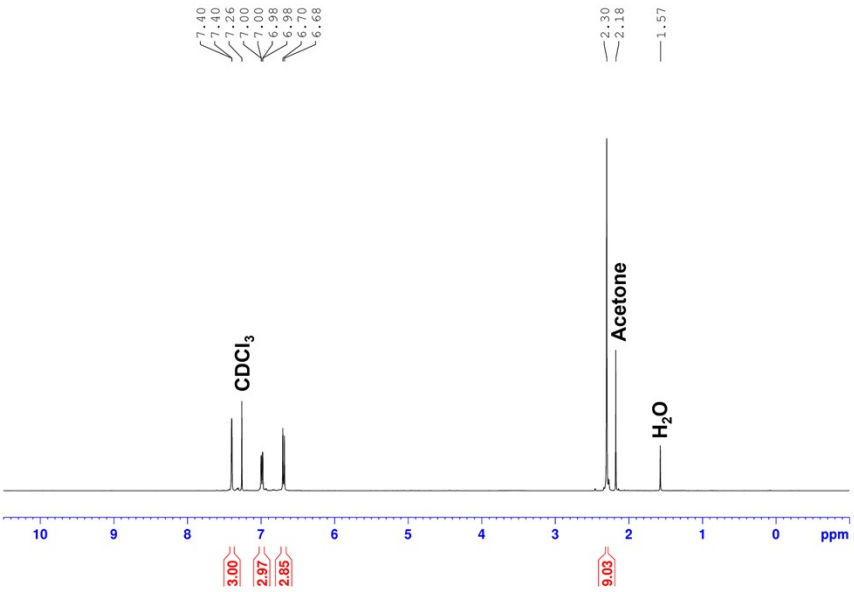


Figure S1: ^{1}H NMR spectrum of tris(2-bromo-*p*-tolyl)amine, in $CDCl_3$.

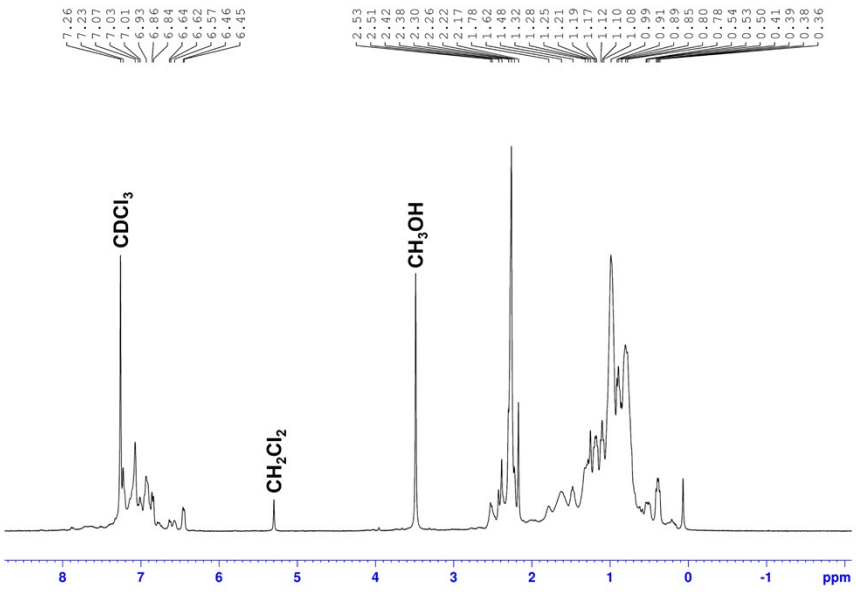


Figure S2: ^{1}H NMR spectrum of $\mathbf{NP^{iso}}$, in $CDCl_3$.

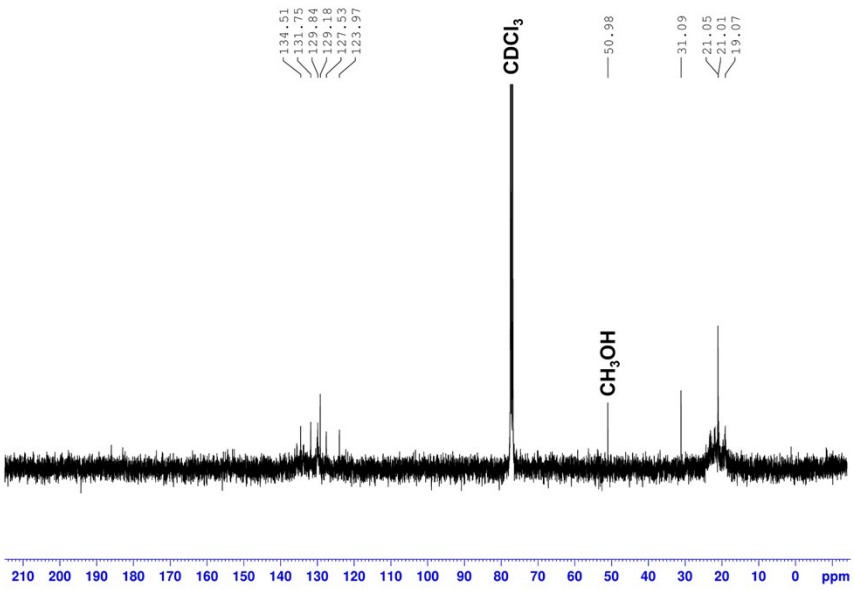


Figure S3: ^{13}C NMR spectrum of **NP^{iso}**, in $CDCl_3$.

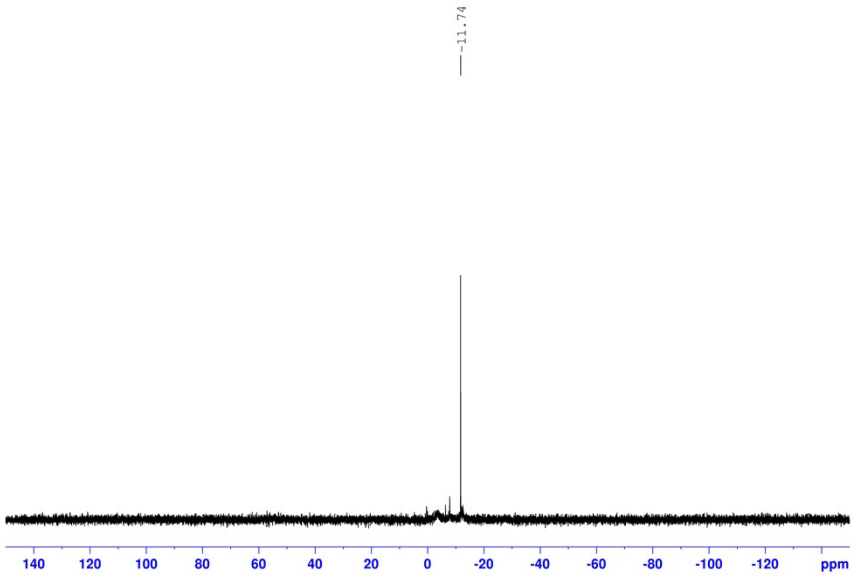


Figure S4: ^{31}P NMR spectrum of **NP^{iso}**, in $CDCl_3$.

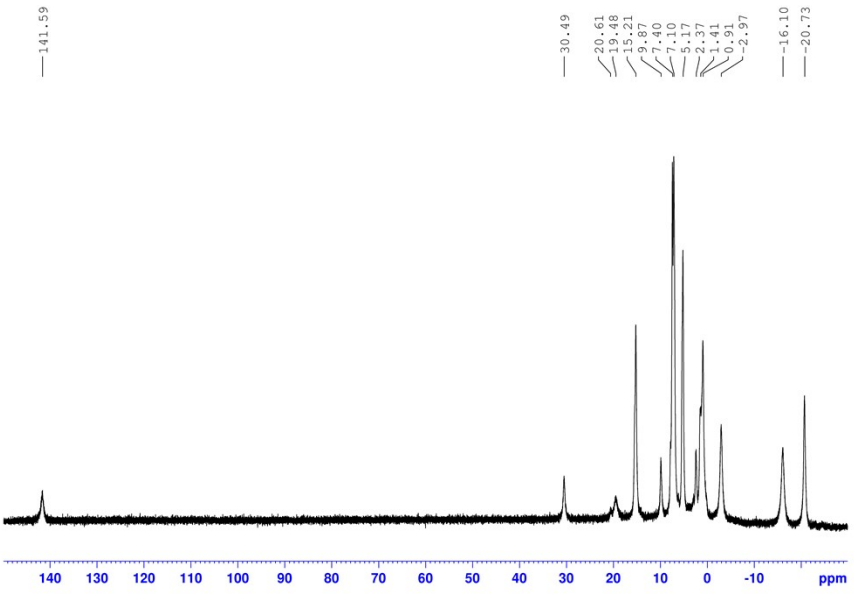


Figure S5: ^{1}H NMR spectrum of **NP^{iso}**, in CD_2Cl_2.

3. FTIR characterisation of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$)

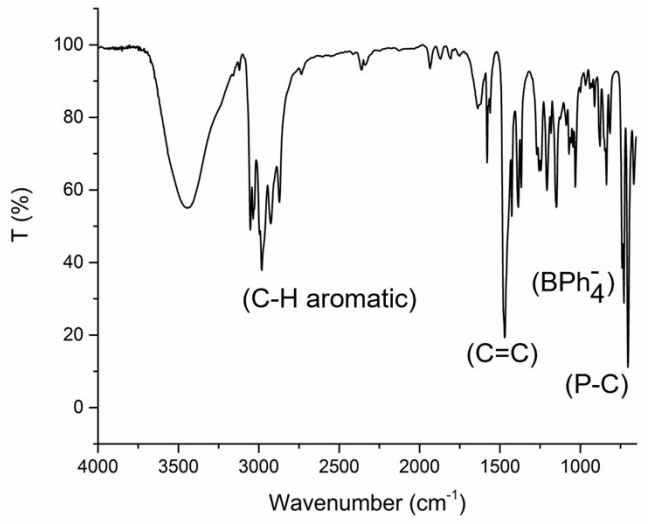


Figure S6:FTIR spectrum of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) in KBr pellet.

4. Single crystal and powder X-ray diffraction data of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$

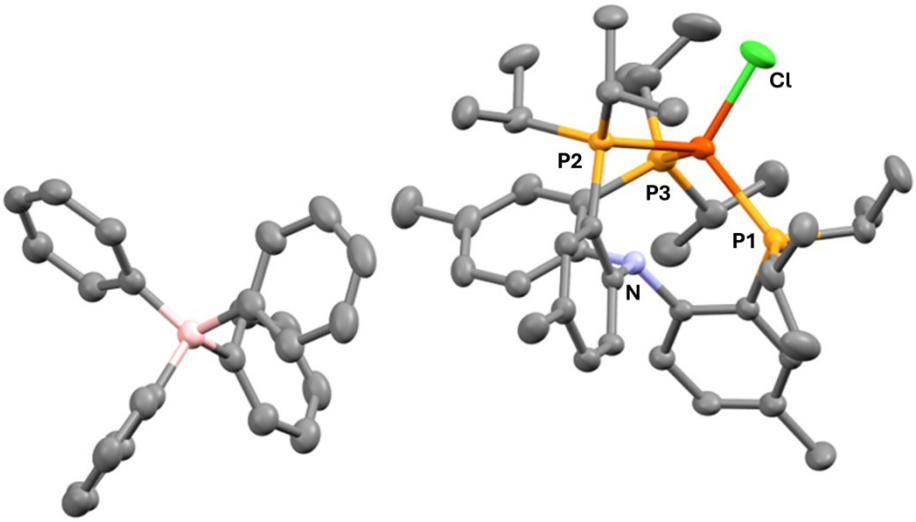


Figure S7: X-ray crystal structure of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$. Fe (dark orange); Cl (green); P (light orange); N (blue); C (grey); B (pink). Hydrogens were omitted for clarity.

Table S1:Crystal data and structure refinement for $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ at 150 K (CCDC #261769).

Compound	**$^{5}[Fe^{II}(NP^{iso})(Cl)](BPh_4)$**
Empirical formula	$C_{63}H_{80}BClFeNP_3$
Formula weight	1046.346
Temperature (K)	150
Wavelength ($\dot{A}$)	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions:	
a ($\dot{A}$)	10.9752(9)
b ($\dot{A}$)	15.0135(11)
c ($\dot{A}$)	17.9619(14)
α (º)	84.014(3)
β (º)	79.191(3)
λ (º)	89.227(3)
Volume ($\dot{A}$)³	2891.27
Z	2

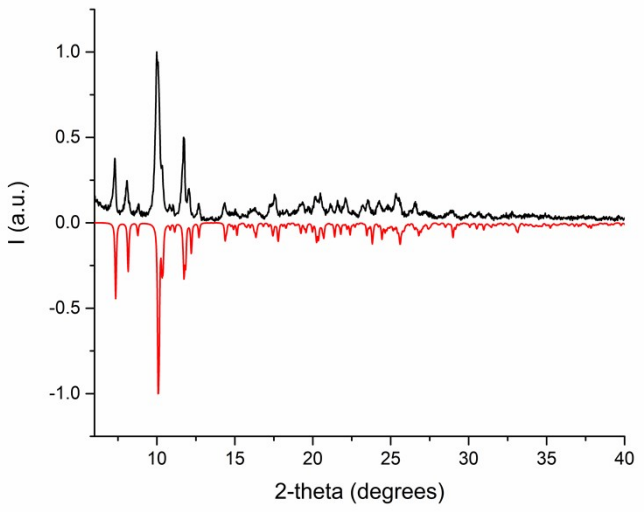


Figure S8: Powder X-ray diffraction patterns for ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) experimental data (black) and simulated data obtained from the SC-XRD structure (red).

5. UV-vis spectroscopy studies of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$

UV-vis studies

UV-vis spectra were recorded on a Shimadzu 50/60 Hz spectrometer using a 3 mL solution of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ in acetonitrile (1×10^{-5} M).

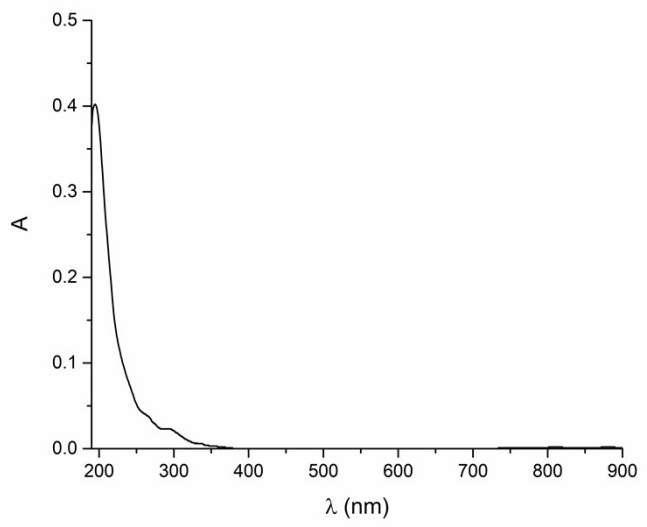


Figure S9:UV-vis spectrum of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ (1×10^{-6} M) in MeCN.

6. Electrochemical characterization of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$

Electrochemical procedures

Cyclic voltammetry experiments were performed using 1 mM MeCN or DCE solutions of the complex, under N_2 (obtained by direct evaporation of liquid N_2) or CO_2 (99.995%) saturated atmosphere in a three-electrode one compartment electrochemical cell at 0.1 mV s^{-1}. The solvents used in these studies had a purity of 99% and were bubbled for 30 min prior to the addition of the complex. Glassy carbon (CHI Instruments, 3 mm diameter) and platinum wire were used as working and counter electrodes, respectively. Ag wire was used as the pseudo-reference electrode and tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (0.1 M) as the supporting electrolyte (recrystallized from hot ethanol). Ferrocene was used as an internal standard, and all potentials are referenced to ferrocene/ferrocenium couple. The working electrode was polished with alumina paste of 1 and 0.05 μm diameter sizes and washed thoroughly with Milli-Q water and dried with nitrogen.

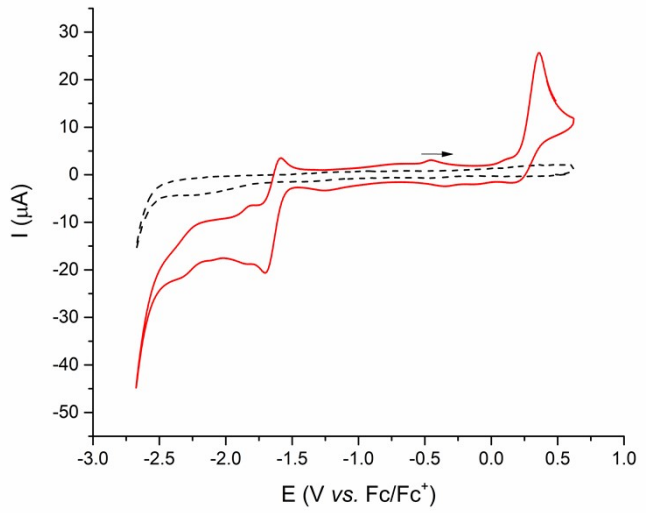


Figure S10: Cyclic voltammogram of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere in DCE.

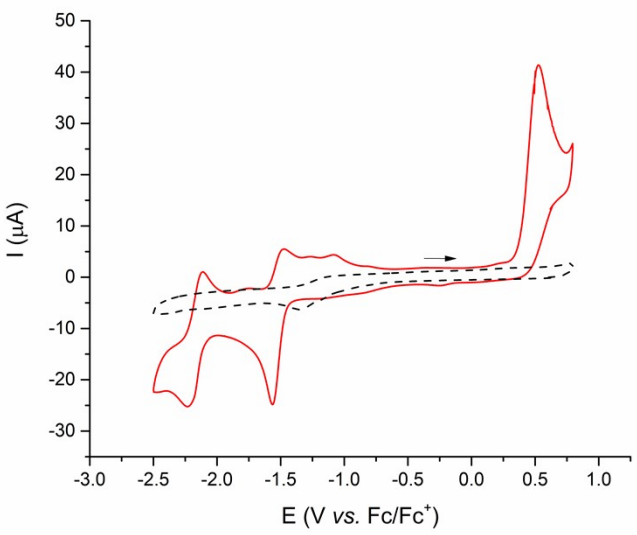


Figure S11: Cyclic voltammogram of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere in MeCN.

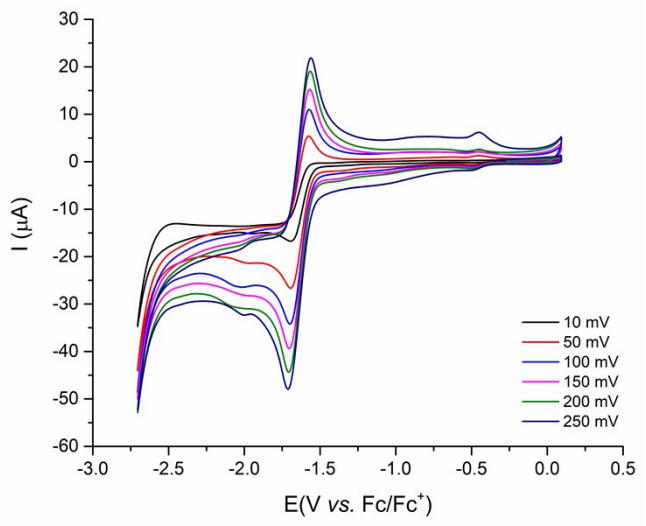


Figure S12: Cyclic voltammogram of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere in DCE at different scan rates.

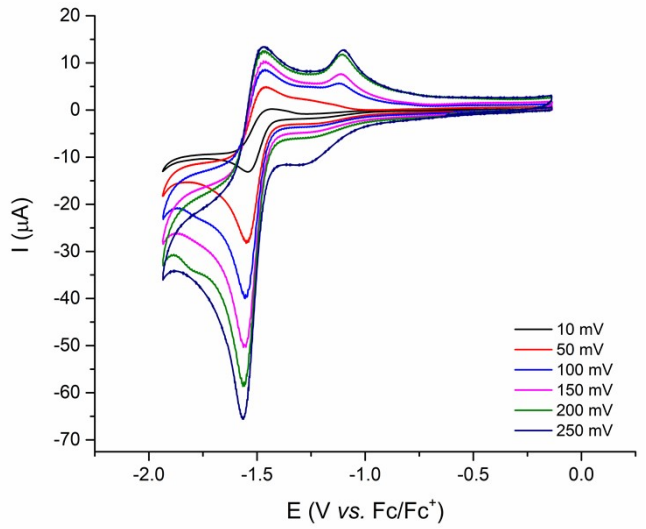


Figure S13: Cyclic voltammogram of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere in MeCN at different scan rates.

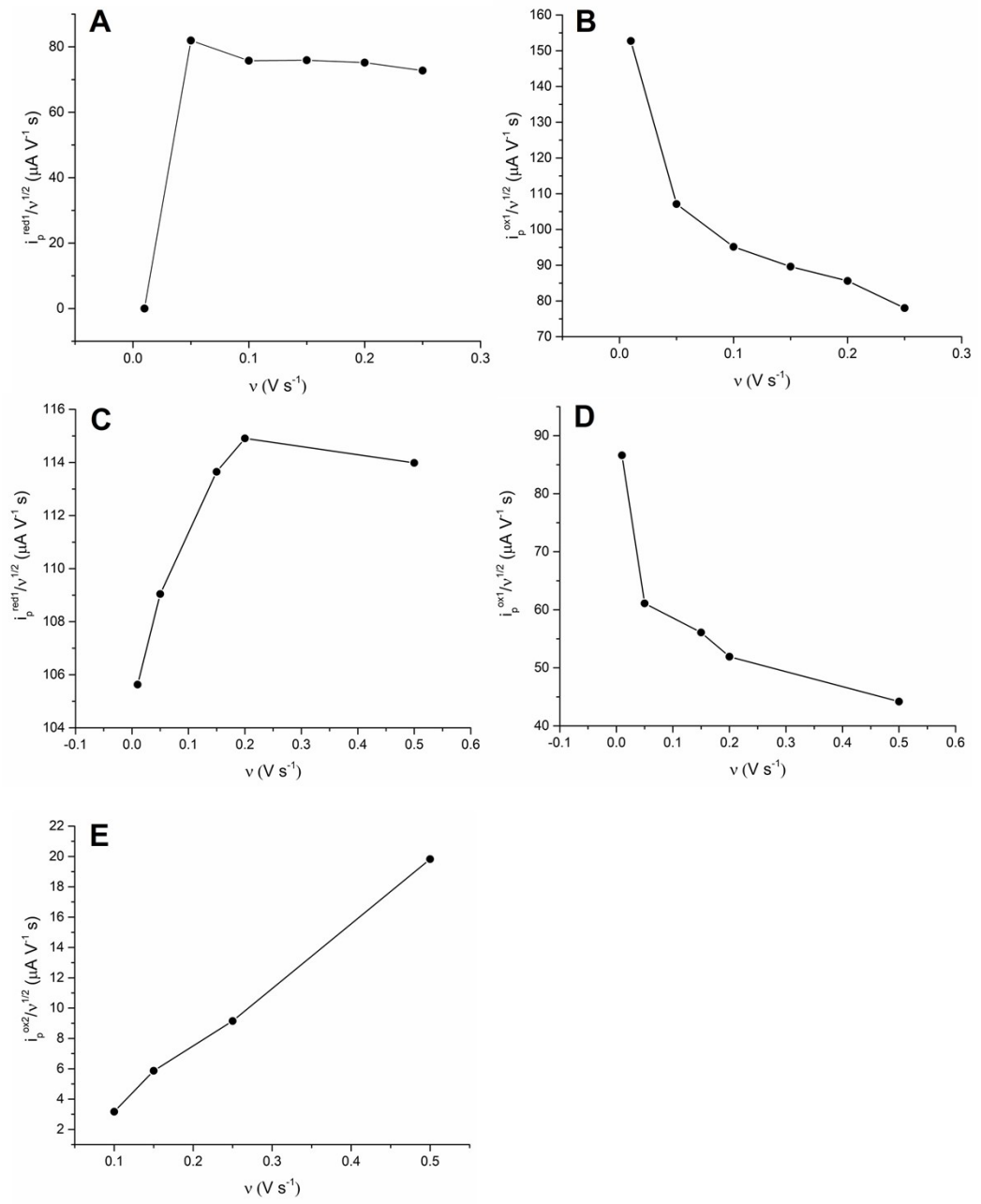


Figure S14: Diagnostic criteria showing the variation of the parameter $i_p/\nu^{1/2}$ as a function of the scan rate (ν) in DCE (Panel A and B) and in MeCN (Panel C, D and E) under N_2 atmospheres. Panel A refers to the reduction wave and Panel B to the oxidation wave in DCE (Figure S12). Panel C refers to the reduction wave, Panel D refers to the 1st oxidation wave and Panel E to the 2nd oxidation wave in MeCN (Figure S13). $TBAPF_6$ was used as supporting electrolyte (0.1 M). Glassy carbon (3 mm diameter) was used as working, platinum wire as counter and Ag/Ag^+ as reference electrodes. Fc was used as internal standard.

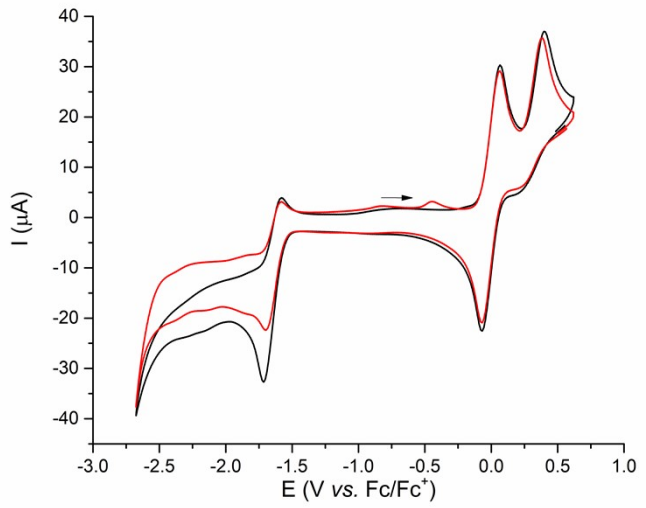


Figure S15: Cyclic voltammogram overlay of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere (red) and under CO_2 atmosphere (black) in DCE.

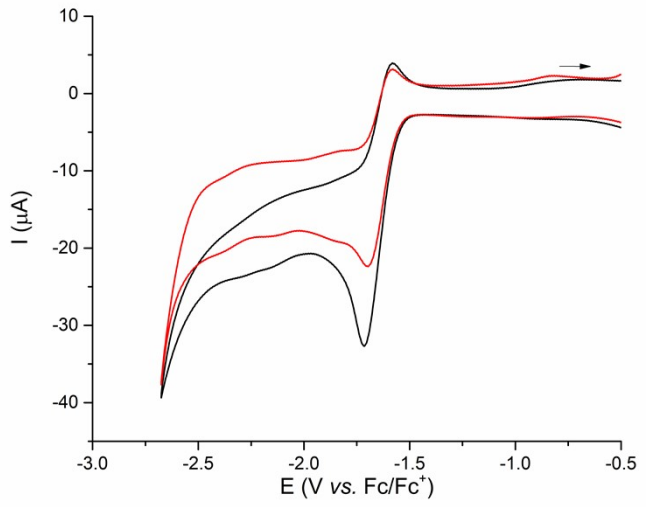
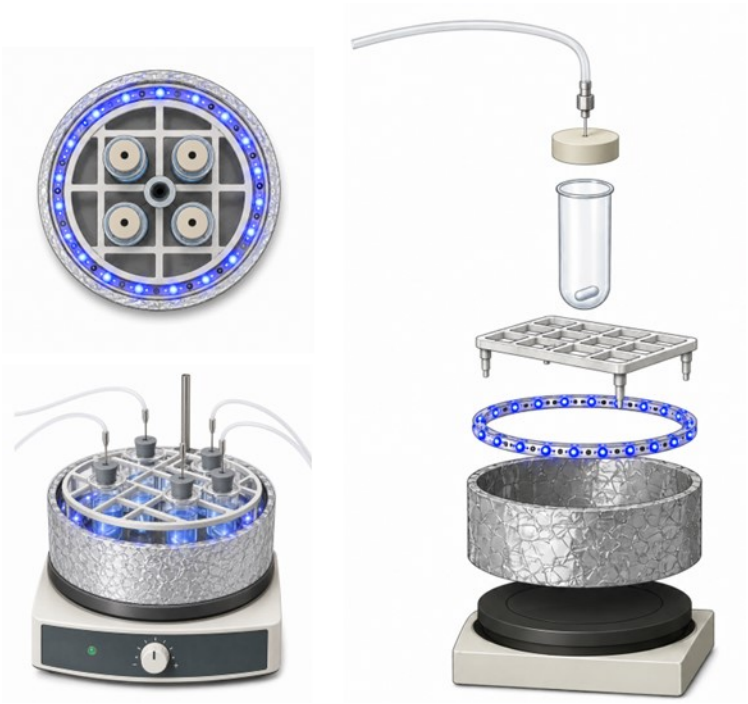


Figure S16: Cyclic voltammogram overlay ampliation of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ under N_2 atmosphere (red) and under CO_2 atmosphere (black) in DCE.

7. Photocatalytic reactions

Photoreduction experiments

CO_2 photoreduction experiments were performed in a 16 mL quartz reactor, directly exposed to 30 W blue LED light (300 LEDs strip RGB+W SMD5050 IP20 12VDC 18 W/m (90 W) 6000 K (cold white) 1250 lm/m – strip length: 5.0 m.). The experiments were carried out under a saturated CO_2 atmosphere using 5 mL solutions of different concentrations of the catalyst (0.5 μM, 5 μM and 50 μM), BIH (0.1 M), $[Ir(dtbbpy)(ppy)_2](PF_6)$ (0.2 mM) and phenol (1 M) in MeCN. These solutions were stirred with a magnetic bar and irradiated for several periods of time. The gases produced were analyzed by gas chromatography equipment fitted with a thermal conductivity detector (GC-TCD) using gas-tight syringes (500 μL) previously purged with CO_2 and the liquid products were not analyzed. Following each injection, the temperature of the quartz reactor was measured using a thermometer.



Scheme S1: Schematic representation of the photoreactor setup used for the CO_2 photoreduction experiments. Left: top view showing the circular arrangement of the LEDs surrounding the sample holder, which accommodates multiple sealed quartz tubes. Right: exploded side view illustrating the assembly of the photoreactor components. From bottom to top: fan-cooled base unit, LED strip mounted inside the reactor chamber, sample holder rack, and sealed quartz tube fitted with a septum cap.

For gaseous products quantification, GC-TCD was used from Agilent Technology (GC-TCD 7820A) controlled by OpenLAB ChemStation edition software. A HP-MOLESIEVE capillary GC Column (L×I.D. 30 m×0.32 mm, average thickness 12 μm) was used for H_2, CO, CH_4, and CO_2 detection. The temperature was held at 200 ºC and 220 ºC both for the injector and the detector (respectively). The carrier gas was Ar flowing at 1.7 mL min-1 and injections were performed with gas-tight syringes (250 or 500 μL) previously purged with CO_2. The method was based on a temperature ramp in the oven starting at 40 ºC for 8 min and gradually increased to 200 ºC for 12 min (retention times (min): H_2 1.91, O_2 2.02, N_2 2.20, CO 3.18, CO_2 10.18). Calibration curves were obtained for H_2, CO and CH_4 separately by injecting known volumes of the pure gas.

7.1. Details on the TON, TOF, selectivity and quantum yield calculations

The control experiments without $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ (Table S2, Entry 4), reveal that $[Ir(dtbbpy)(ppy)_2](PF_6)$ can be active for the CO_2 photoreduction reaction producing 1.35 μmol of CO, however the use of $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ as a catalyst is crucial to improve the amount of CO produced in this system. In table S3, the results of the photoreduction reactions shown are relative to the modification of the PS component, demonstrating that $[Ir(dtbbpy)(ppy)_2](PF_6)$ is the

best PS used in this system. The variation of the SED was also tested by changing BIH for triethanolamine (0.3 M), unfortunately, no CO was detected in the same conditions described in table S3.

The photoreduction experiments under a N_2 atmosphere reveal that the CO produced by $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ comes from the CO_2 reduction reaction and not from degradation of any other compounds present in the system (Table S2, Entry 5). A series of control experiments without the PS, SED and proton source component were conducted (Table S2, Entry 6-8). The results obtained demonstrate that $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ did not produce CO when the PS or the SED were not used, demonstrating that without a light absorber or a molecule able to promote the electron transfer in the system the production of active species able to reduce CO_2 is not achieved. When the proton source was not used, it was possible to detect CO in only trace amounts, suggesting that the residual amount of H_2O present in MeCN was sufficient to act as a proton source.

Upon using simple iron salts such as anhydrous $FeCl_2$ (Table S2, Entry 9), the results show that the molecular structure of $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ is important to enhance both the amount of CO produced and the selectivity of the system. To understand the effect of the proton source in the system, phenol was substituted by H_2O and isopropanol (*i*PrOH) (Table S2, Entry 10-13, Figure S17).

Table S2: Optimization of the catalyst concentration and control experiments for CO_2 reduction reaction.

Entry	[Cat] [µM]	n_{H_2} [µmol]	n_{CO} [µmol]	Selectivity$_{CO}$ [%]	TON$_{CO}$	TOF$_{CO}$ [h^{-1}]	Φ_{CO} [%]
1	50	74.47	15.61	17	62	21	3.01
2	5	13.72	5.94	30	238	79	1.15

3	0.5	5.11	2.96	37	1183	394	0.57
4	0	3.47	1.35	-	-	-	-
5[a]	0.5	1.38	0	-	-	-	-
6[b]	0.5	0	0	-	-	-	-
7[c]	0.5	0	0	-	-	-	-
8[d]	0.5	0.02	0.33	94	132	44	0.06
9[e]	0.5	3.74	1.38	27	551	183	0.27
10[f]	0	2.19	1.07	-	-	-	-
11[f]	0.5	0.53	3.34	86	1335	445	0.64
12[g]	0	0.70	tr.	-	-	-	-
13[g]	0.5	0.37	tr.	-	-	-	-

In a typical run, a CO_2-saturated acetonitrile (MeCN) solution containing $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$, $[Ir(dtbbpy)(ppy)_2](PF_6)$ (0.2 mM), BIH (0.1 M) and phenol (1 M) was irradiated using blue LED strip lights (30 W) for 3 h under a CO_2 atmosphere. [a]Under an N_2 atmosphere. [b]Without $[Ir(dtbbpy)(ppy)_2](PF_6)$. [c]Without BIH. [d]Without Phenol. [e]Using anhydrous $FeCl_2$ as catalyst. [f]Using H_2O as a proton source in a ratio of 4.5:0.5 (MeCN:H_2O). [g]Using isopropanol (*i*PrOH) as a proton source in a ratio of 4.5:0.5 (MeCN:*i*PrOH). For the quantum yield calculation to the CO formation, the number of photons was calculated using $K_3[Fe(C_2O_4)_3]$ actinometer method (2.63×10^{17} photons per second).

All the equations used to calculate all the parameters discussed in this paper are summarized below, and were used according to the literature.[5-8]

$$TON = \frac{n_{CO}}{n_{catalyst}} \quad (1)$$

$$TOF = \frac{TON}{time\ (h)} \quad (2)$$

$$Selectivity\ (\%) = \frac{n_{CO}}{n_{all\ products}} \quad (3)$$

$$\phi_{CO} = \frac{n_{CO} \times n_{e^-}}{n_{incident\ photons}} \times 100\% \quad (4)$$

7.2. Photocatalytic experiments

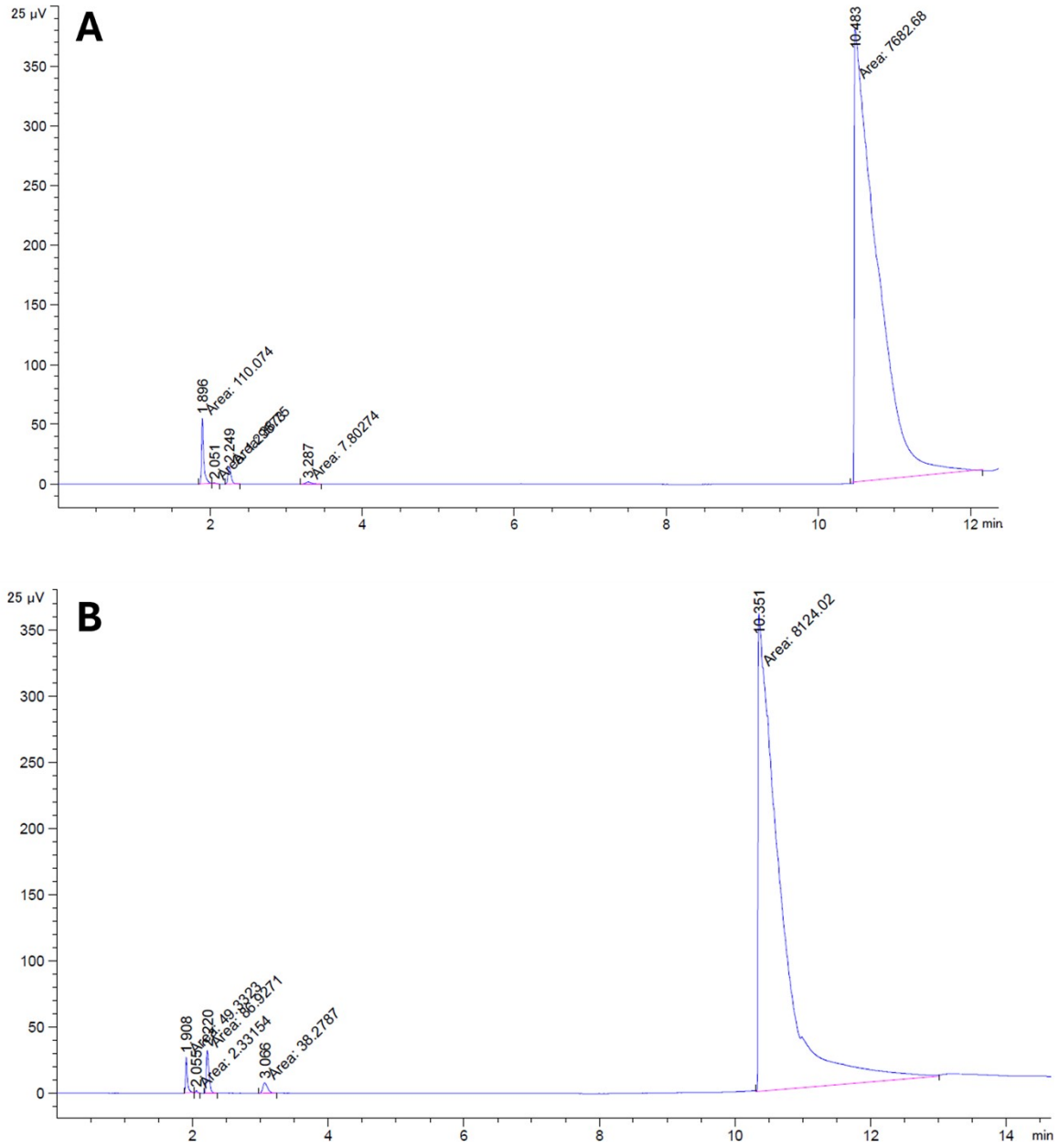


Figure S17: GC-TCD chromatograms of CO_2 photoreduction experiment using a mixture of MeCN:H_2O (4.5:0.5), BIH (0.1 M), [Ir(dtbbpy)(ppy)$_2$](PF$_6$)(0.2 mM) 30 W blue LED light (300 LEDs strip RGB+W SMD5050 IP20 12VDC 18 W/m (90 W) 6000 K (cold white) 1250 lm/m – strip length: 5.0 m.) without ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) for 3 h using a) 0 µM and b) 0.5 µM of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$).

7.3. Control experiments of the photosensitizer

Table S3: Control experiments of the photosensitizer for CO_2 reduction reaction.

PS	n_{H_2} [µmol]	n_{CO} [µmol]	Selectivity$_{CO}$ [%]	TON$_{CO}$	TOF$_{CO}$ [h^{-1}]	Φ_{CO} [%]
[Ru(bpy)$_3$](PF$_6$)$_2$[a]	0.39	0	-	-	-	-
[Ru(bpy)$_3$](PF$_6$)$_2$	5.84	1.43	20	6	2	0.28
[Ru(phen)$_3$](PF$_6$)$_2$[a]	0.10	0	-	-	-	-
[Ru(phen)$_3$](PF$_6$)$_2$	7.46	1.63	18	7	2	0.31
4CzIPN [a]	0	0	-	-	-	-
4CzIPN	0	0	-	-	-	-
[Ir(dtbbpy)(ppy)$_2$](PF$_6$) [a]	3.47	1.35	-	-	-	-
[Ir(dtbbpy)(ppy)$_2$](PF$_6$)	74.47	15.61	17	62	21	3.01

In a typical run, a CO_2-saturated MeCN solution containing [5][Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) (50 µM), [Ir(dtbbpy)(ppy)$_2$](PF$_6$) (0.2 mM), BIH (0.1 M) and phenol (1 M) was irradiated using blue LED strip lights (30 W) for 3 h under a CO_2 atmosphere. [a]Without catalyst. For the quantum yield calculation to the CO formation, the number of photons was calculated using $K_3[Fe(C_2O_4)_3]$ actinometer method (2.63×10^{17} photons per second).[6]

8. Mechanistic studies

8.1. Quenching mechanism studies

Fluorescence studies

UV-vis spectra were recorded on a Shimadzu 50/60 Hz spectrometer using a 3 mL solution of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ in acetonitrile (1×10^{-5} M). Emission spectra were recorded on a Fluorolog 3.22 spectrofluorometer from Horiba-Jobin-Yvon (Model FL-1065). Excited-state quenching experiments were carried out by adding either BIH or $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ in 100 µM increments to a CO_2-saturated solution of $[Ir(dtbbpy)(ppy)_2](PF_6)$ (1.25×10^{-5} M). The relative emission lifetime of the photosensitizer in the presence of quencher was used to calculate the Stern-Volmer quenching constant (k_q) using the following equation:

$$I_0/I_Q = 1+ \tau_f k_q [Q]$$

where I_0/I_Q is the emission intensity in the absence (I_0) or presence (I_Q) of quencher, τ_f is the [9]

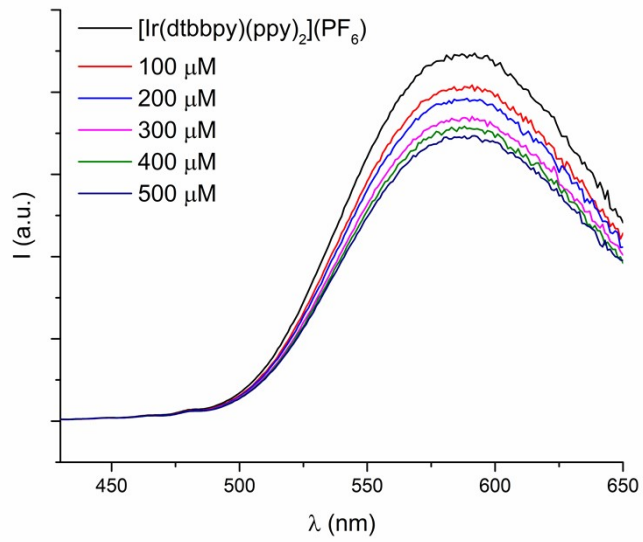


Figure S18: Normalized emission spectra of $[Ir(dtbbpy)(ppy)_2](PF_6)$ (2.5×10^{-5} M) in MeCN (λ_{exc} = 420 nm, T = 298 K) at various concentrations of BIH (indicated in the figure).

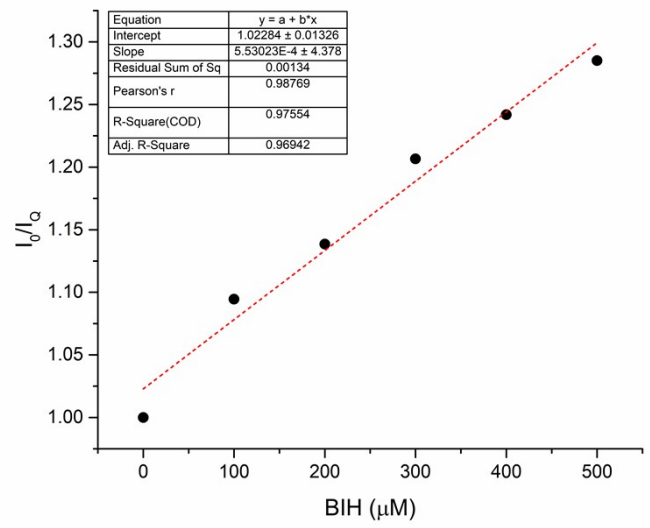


Figure S19: Stern-Volmer plots for $[Ir(dtbbpy)(ppy)_2](PF_6)$ quenching with BIH.

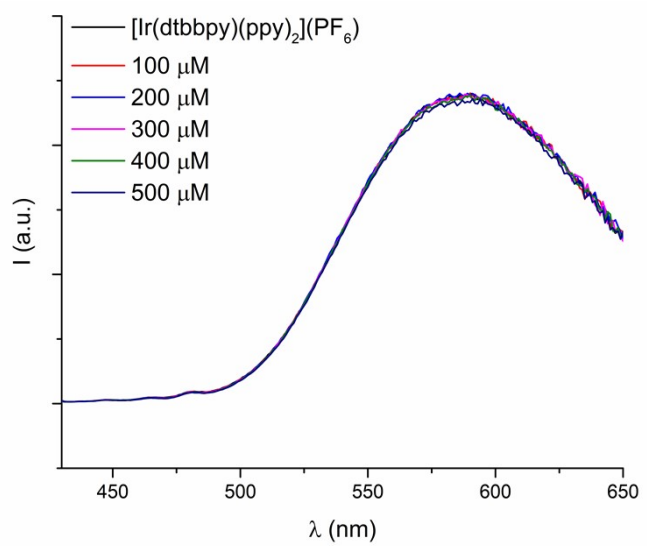


Figure S20: Normalized emission spectra of $[Ir(dtbbpy)(ppy)_2](PF_6)$ (2.5×10^{-5} M) in MeCN (λ_{exc} = 420 nm, T = 298 K) at various concentrations of $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ (indicated in the figure).

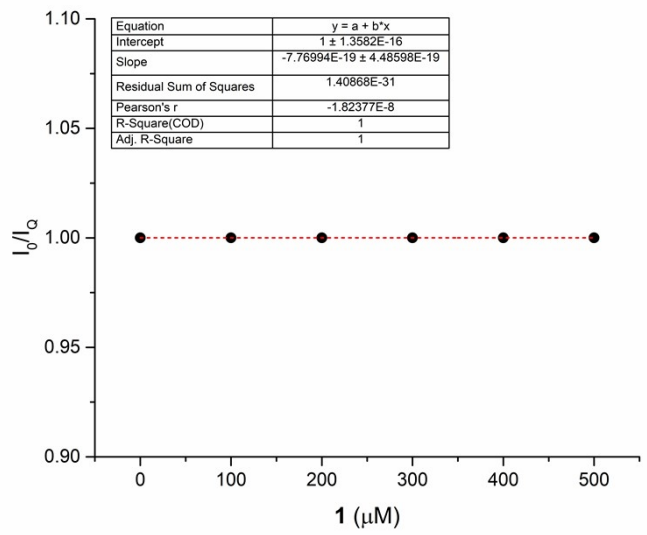


Figure S21: Stern-Volmer plots for $[Ir(dtbbpy)(ppy)_2](PF_6)$ quenching with $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$.

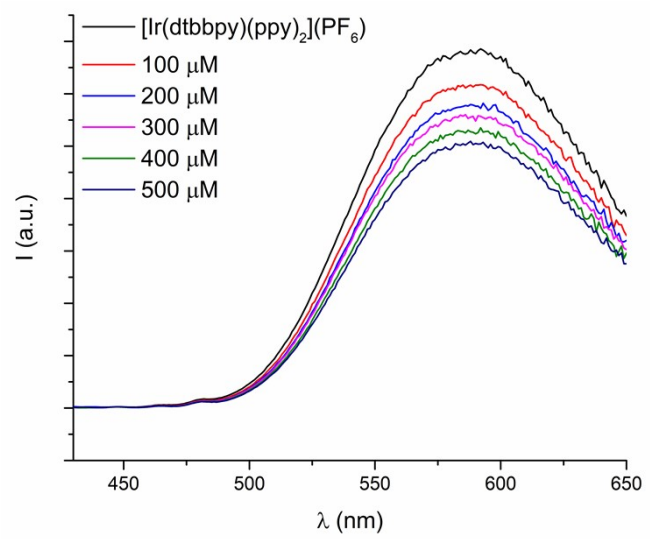


Figure S22: Normalized emission spectra of $[Ir(dtbbpy)(ppy)_2](PF_6)$ (2.5×10^{-5} M) in MeCN (λ_{exc} = 420 nm, T = 298 K) at various concentrations of **TTA** (indicated in the figure).

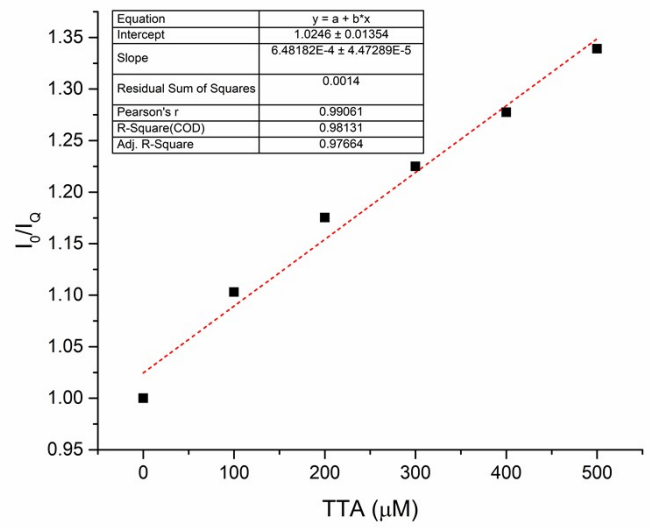


Figure S23: Stern-Volmer plots for $[Ir(dtbbpy)(ppy)_2](PF_6)$ quenching with **TTA**.

8.2. FTIR spectroelectrochemical studies

Electrochemical procedures

SEC-IR experiments were performed using a cell acquired from OTTLE. This cell has two platinum grids as working and counter electrodes and an Ag wire as the pseudo-reference electrode. A CO_2 or N_2 saturated MeCN or DCE/MeCN solution with 5 mM ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) and 0.1 M TBAPF$_6$ was injected in the SEC-IR cell. The studies performed using DCE/MeCN solutions were performed adding 5 µL of MeCN in a 5 mM solution of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) in 5 mL of DCE. A linear voltammogram was performed using a scan rate of 10 mV s^{-1} to reach the suitable potential. The IR spectra were obtained using a Bruker INVENIO S FTIR spectrometer with a resolution of 4 cm^{-1} after 32 scans between 2200–1600 cm^{-1}. The background spectrum was performed with the sample at the open circuit potential.

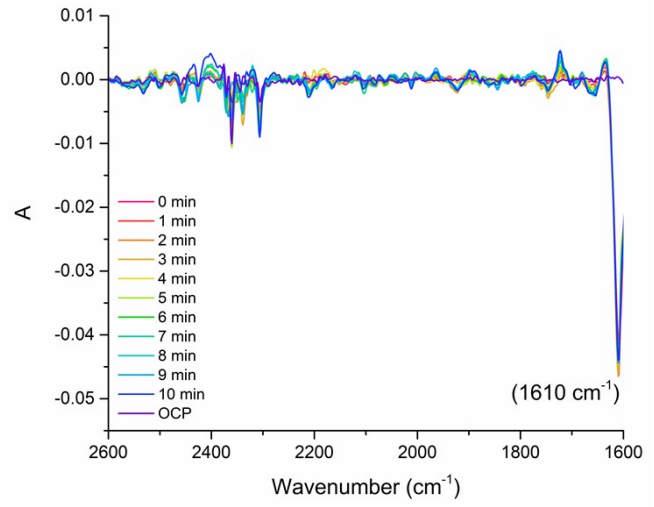


Figure S24: SEC-IR experiment at -1.65 V *vs.* Ag pseudo-reference under a N_2 atmosphere using 5 mM of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh$_4$) and 0.1 M TBAPF$_6$ in a N_2 saturated DCE/MeCN solution, Pt grids as working and counter electrodes and Ag wire as a pseudo-reference electrode.

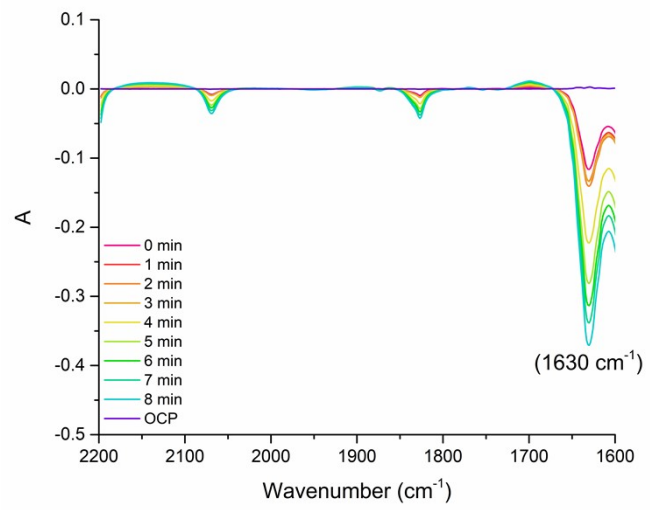


Figure S25: SEC-IR experiment at -1.45 V *vs.* Ag pseudo-reference under a CO_2 atmosphere using 5 mM of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ and 0.1 M $TBAPF_6$ in a CO_2 saturated MeCN solution, Pt grids as working and counter electrodes and Ag wire as a pseudo-reference electrode.

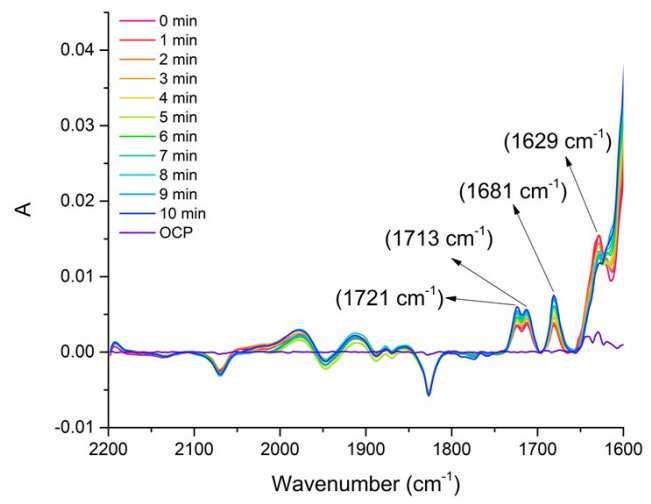


Figure S26: SEC-IR experiment at -1.85 V *vs.* Ag pseudo-reference under a N_2 atmosphere using 5 mM of $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ and 0.1 M $TBAPF_6$ in a N_2 saturated MeCN solution, Pt grids as working and counter electrodes and Ag wire as a pseudo-reference electrode.

8.3. Electrospray Ionization Mass spectrometry (ESI-MS) solution studies

All MS data were collected using a Q-trap, time-of-flight MS (Maxis Impact MS) instrument supplied by Bruker Daltonics Ltd. The detector was a time-of-flight, micro-channel plate detector and all data was processed using the Bruker Daltonics Data Analysis 4.1 software, whilst simulated isotope patterns were investigated using Bruker Isotope Pattern software and Molecular Weight Calculator 6.45. The calibration solution used was Agilent ES tuning mix solution, Recorder No. G2421A, enabling calibration between approximately 100 *m/z* and 2000 *m/z*. This solution was diluted 60:1 with MeCN. The reaction mixture was introduced into the MS *via* direct injection at 180 μL h^{-1}. The ion polarity for all MS scans recorded was positive, at 180 °C, with the voltage of the capillary tip set at 4000 V, endplate offset at –500 V, funnel 1 RF at 300 Vpp and funnel 2 RF at 400 Vpp.

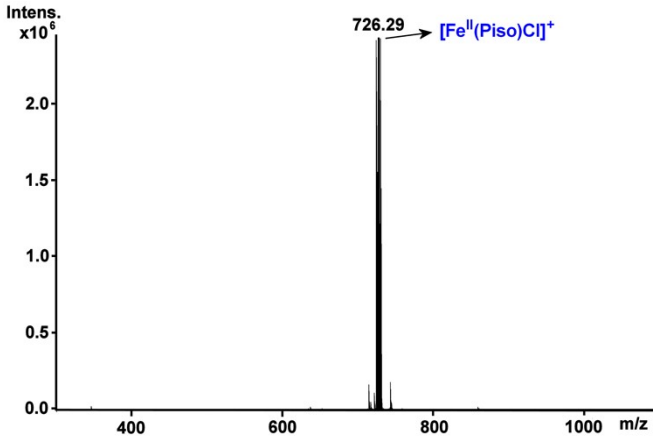


Figure S27: Positive ion mass spectrum of ^{5}[Fe^{II}(**NP^{iso}**)(Cl)](BPh_4) in MeCN. The isotopic distribution envelope correspond to singly charged species centred at 726.29 m/z and can be attributed to the {FeN($C_{13}H_{20}P)_3$Cl}$^+$ iron species.

Table S4: Representation of the experimentally identified and simulated m/z values of distribution envelopes of catalytic mixture after 4 h of irradiation, using a MeCN:H_2O (4.5:0.5) solvent mixture as eluent.

Exp.	Theor.	+ν	Formula
690.40	690.38	+1	$\{Fe^{I}(P^{iso})\}^{+}$
773.30	773.15	+1	$\{[Fe^{I}(P^{iso})CH_3CN]\bullet CH_3CN\}^{+}$
817.30	817.14	+1	$\{[Fe^{I}(P^{iso})CO_2](CH_3CN)_2\}^{+}$
879.30	879.20	+1	$\{[Fe^{I}(P^{iso})CO_2](H_2O)_4(HCl)_2\}^{+}$
923.30	923.32	+1	$\{Ir(C_{40}H_{40}N_4)(CH_3CN)_2(H_2O)_2(HCl)\}^{+}$
995.40	995.32	+1	$\{Ir(C_{40}H_{39}N_4)(CH_3CN)_2)PF_6\}^{+}$
1039.40	1040.15	+1	$\{[Fe^{III}(P^{iso})COCl_2](CH_3CN)_3(H_2O)_5(HCl)\}^{+}$

9. Additional Computational Data

9.1 Electronic structure of initial species

Initially, the 3d orbital splitting was examined in both the $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^{+}$ and $\mathbf{[Fe^{II}(NP^{iso})(NCMe)]^{2+}}$ complexes in order to compare them. These are displayed in Figure S31. Both complexes were optimized in the quintet state since the ligands are either weak- or mid-field and the similarity to the tetrahedral steric arrangement both point to a high spin solution.[10-33]

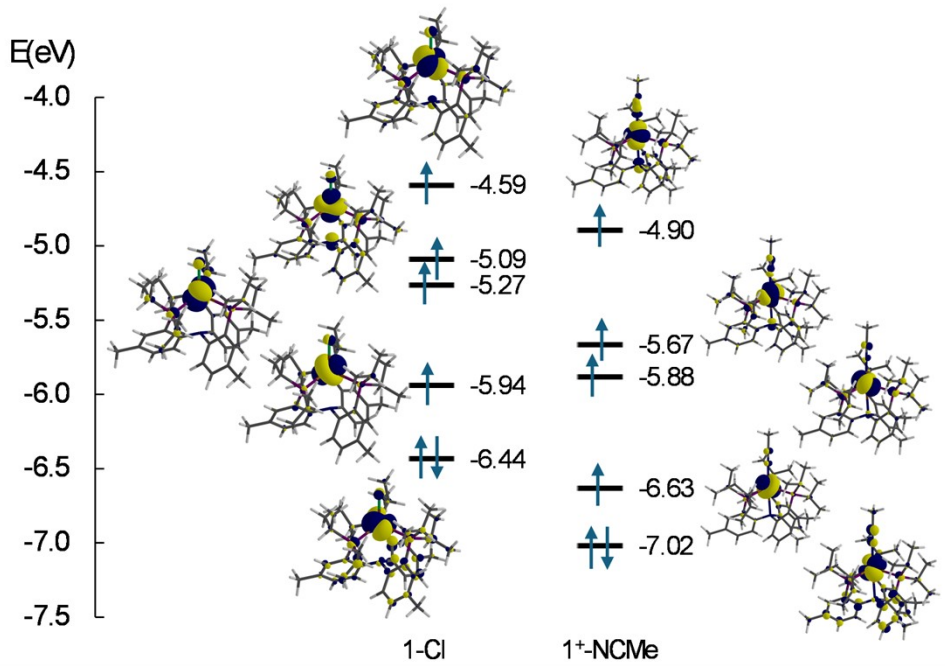


Figure S28: Kohn-Sham quasi-restricted molecular orbital comparison between complexes $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^{+}$ (left) and $[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+}$ (right).

The most noticeable difference between $^{5}[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^{+}$ and $[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+}$ lies is the clustering of the 3d levels in accordance to a pseudo-tetrahedral ligand field $e^{3}\ t_{2}^{3}$ (T_d point group) in

the case of the former but the latter is more in the pattern of a pseudo-trigonal bipyramid $(e'')^3$ $(e')^2$ $(a_1')^1$ (D_{5h} point group).

Since $[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+}$ is more cationic, the metal center will draw the axial nitrogen nearer. This difference is seen in the optimized distances where the Fe-N distance is close to 2.6 Å whereas in the neutral $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^+$ complex it is close to 0.2 Å longer (Figure S32).

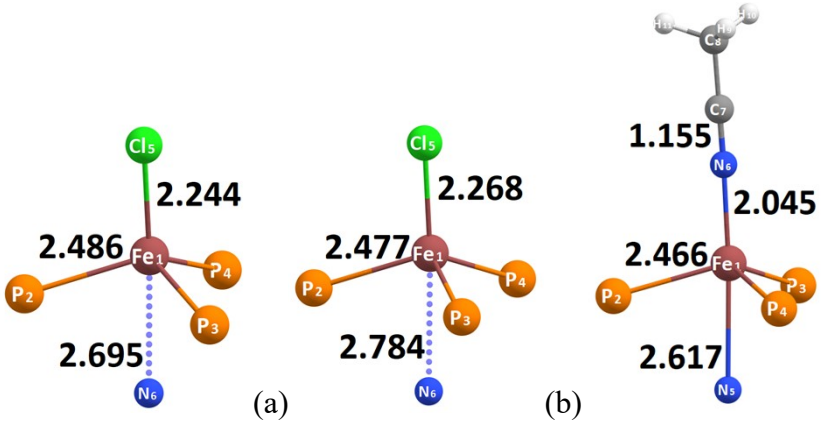


Figure S29: Essential bond lengths of the crystal structure of $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)](BPh_4)$ (a) and optimized structures of $^5[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^+$ (b) and $^5[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+}$ (c) highlighting the Fe-N internuclear distances in Å. Atoms in the second coordination sphere are omitted for clarity.

9.2 Reduction potential calculations

While the presence in solution of the $[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+}$ species in the Fe(II) oxidation state should only be residual given that its formation is endergonic the reduction wave shows up above the detection limit of the cyclic voltametric experiment. The remainder Fe(I)/Fe(0) pairs are estimated to be beyond -3.4 V.

Table S5: Calculated half pair reduction potentials and their assignment to the experimental values.

Redox pair	**Calc. E^0 (vs Fc^+/Fc)/V**	**Exp. E^0 (vs Fc^+/Fc)/V**
$[Fe^{II}(\mathbf{NP^{iso}})(Cl)]^+ + e^- \rightarrow [Fe^{I}(\mathbf{NP^{iso}})(Cl)]^0$	-2.19	-2.17
$[Fe^{II}(\mathbf{NP^{iso}})(NCMe)]^{2+} + e^- \rightarrow [Fe^{I}(\mathbf{NP^{iso}})(NCMe)]^+$	-1.54	-1.53
$[Fe^{I}(\mathbf{NP^{iso}})(Cl)]^0 + e^- \rightarrow [Fe^{0}(\mathbf{NP^{iso}})(Cl)]^-$	-3.67	—
$[Fe^{I}(\mathbf{NP^{iso}})(NCMe)]^+ + e^- \rightarrow [Fe^{0}(\mathbf{NP^{iso}})(NCMe)]^0$	-3.49	—

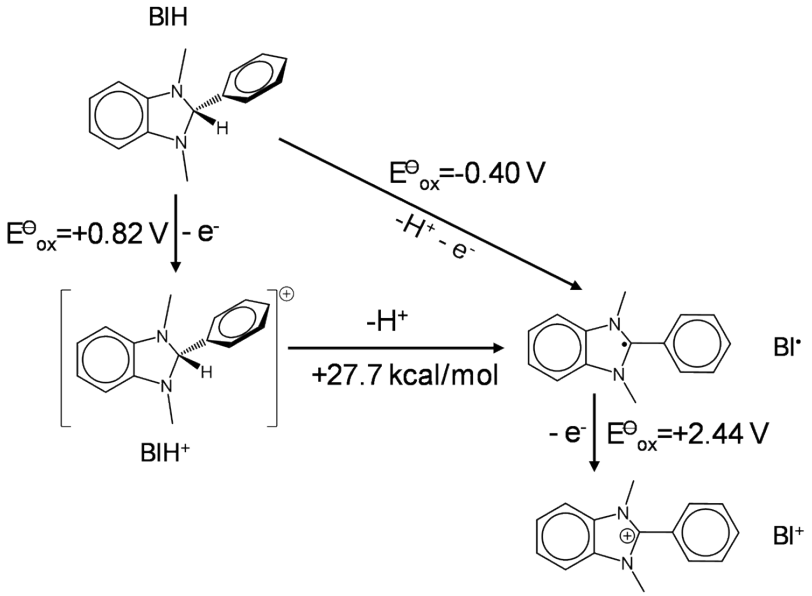


Figure S30: Oxidation potentials of the sacrificial reagent BIH with and without proton coupled steps.

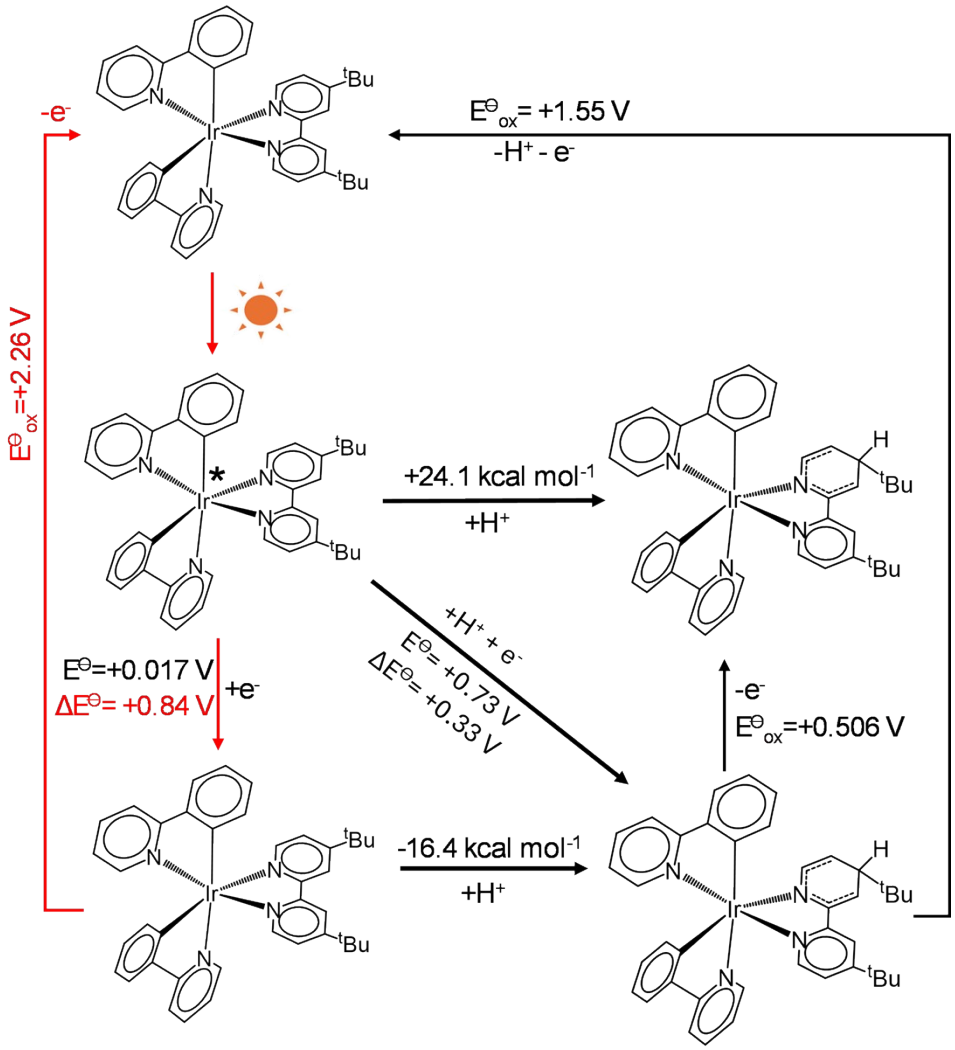


Figure S31: Calculated redox potentials (*vs.* Fc/Fc^+) for the $[Ir(ppy)_2(dtb\text{-}bpy)]^+$ complex. Difference in reduction potentials are calculated with respect to the proton coupled step of BIH (E^{e}_{ox} = -0.40 V) and single electron transfer (E^{e}_{ox} = +0.82 V) at the appropriate steps. Most favorable pathway using BIH as an electron donor is signaled in red.

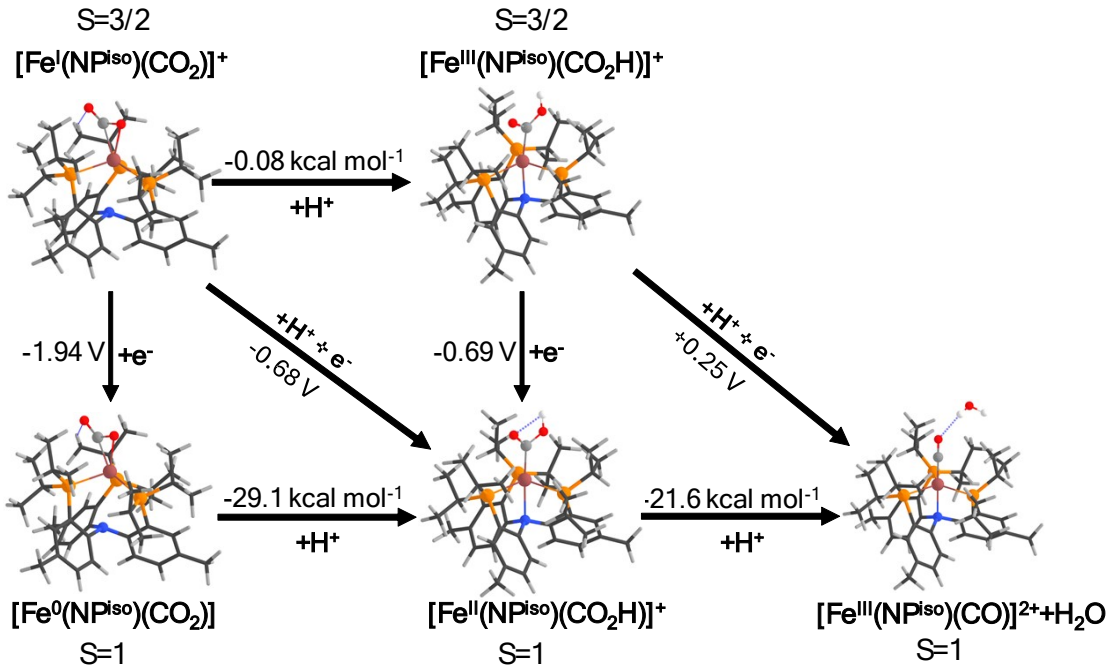


Figure S32: Calculated molecular Pourbaix diagram of the several stages of reduction of the CO_2 adduct complex and the respective oxidation states of the iron center.

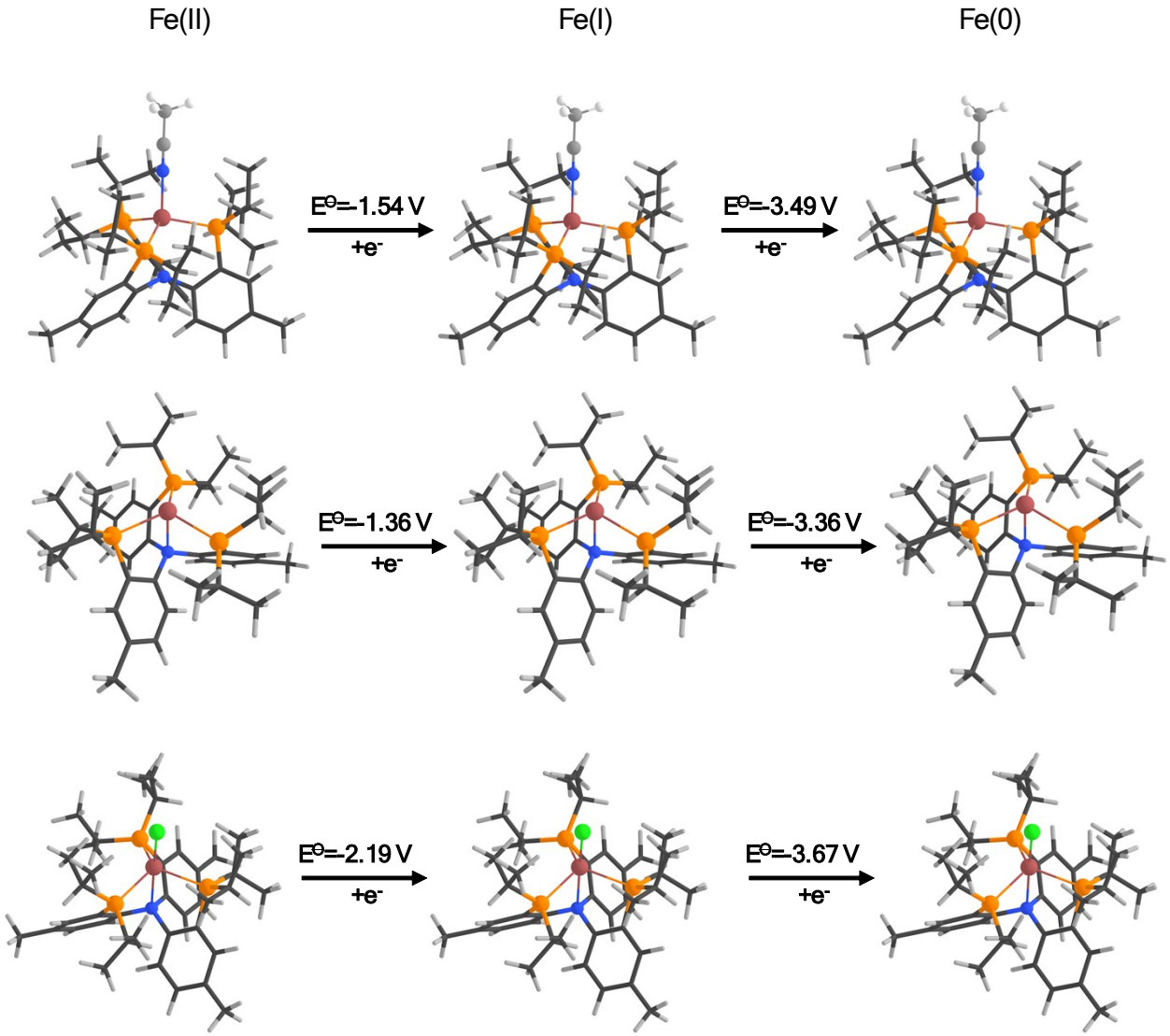


Figure S33: Calculated redox potentials for the non-coordinate, chloro and acetonitrile complexes.

9.3 Electronic structure of intermediates

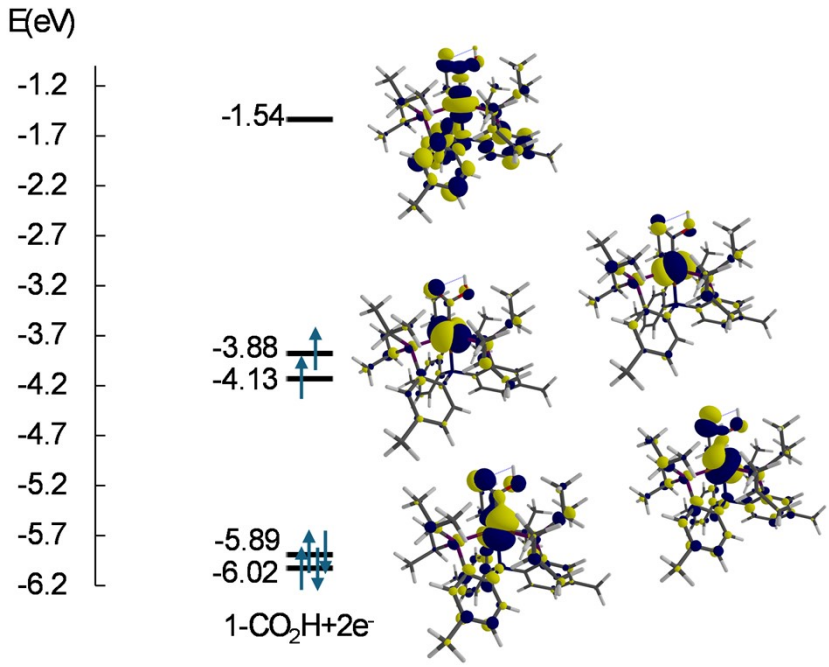


Figure S34: Ligand field splitting (quasi-restricted molecular orbitals) in the doubly reduced species $^{3}[Fe^{II}(\mathbf{NP^{iso}})(CO_2H)]^{+}$. Note that the complex is still $3d^6$ i.e. Fe(II). As the total charge of the complex is +1 it may be concluded that the ligand bears a $[:CO_2H]^-$ formal charge.

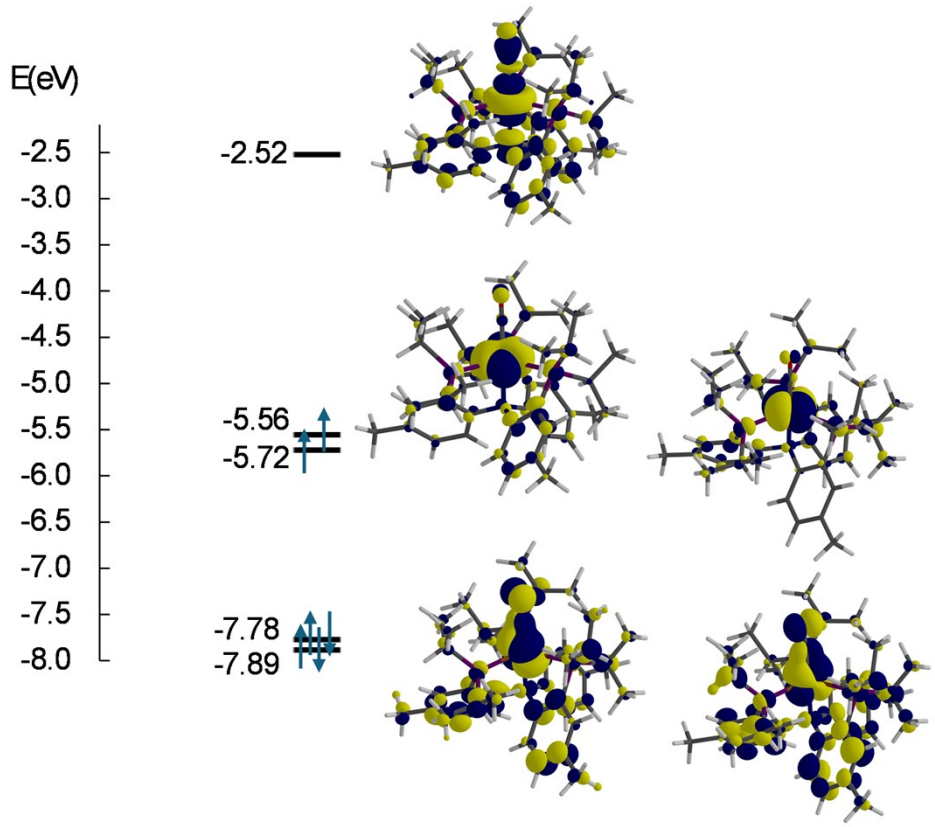
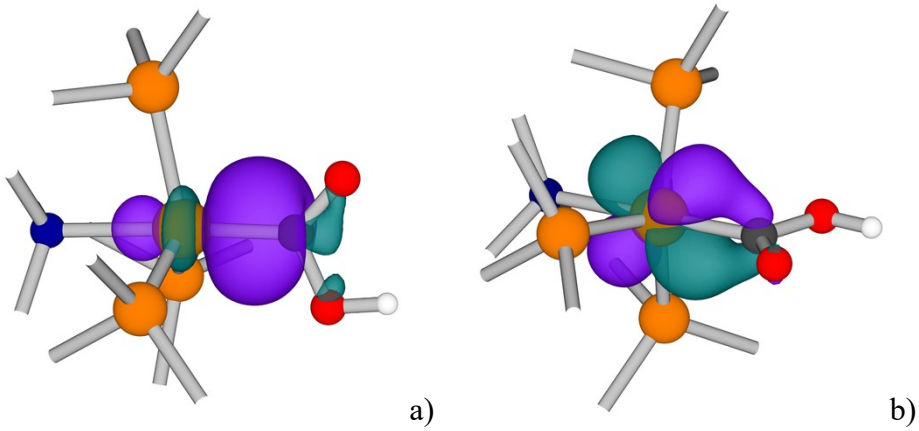


Figure S35: Ligand field splitting (quasi-restricted molecular orbitals) in the doubly reduced species $^{3}[Fe^{II}(\mathbf{NP^{iso}})(CO)]^{2+}$.

A natural bond orbital analysis[34-36] was carried out on the $[Fe^{II}(\mathbf{NP^{iso}})(CO_2H)]^{+}$ and $[Fe^{II}(\mathbf{NP^{iso}})(CO)]^{2+}$ species, in particular the composition of the natural localized molecular orbitals to assess the amount of σ M←L bonding donation and π M→L backbonding between the iron center and the carbonite and carbonyl ligands. The carbonite complex may only exhibit backbonding through the plane that is perpendicular to the ligand (see NLMOs below in Figure S40). As such the electron donation will be less. The overall results are displayed below (Table S7).

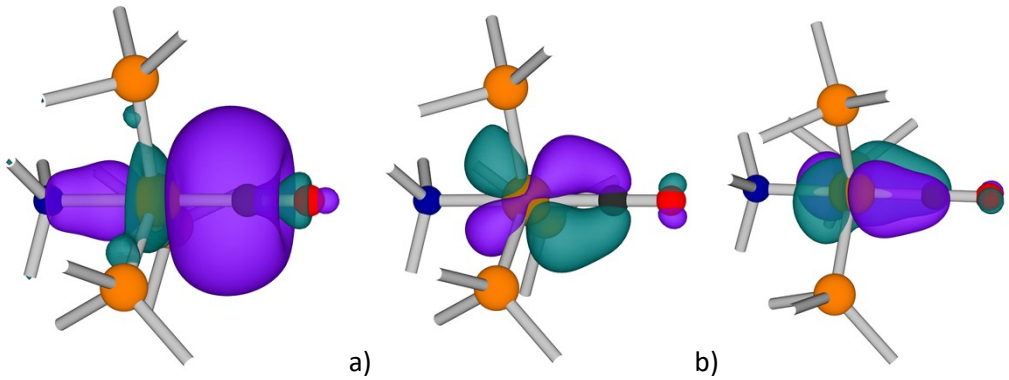
Table S6: Electron donation and backdonation from the population analysis of NLMOs. The electronic donor acceptor values are normalised to two electrons per bond.

Donor-acceptor NLMOs	**M←L σ NLMOs (α+β)**	**M→L π NLMOs (α+β)**
$[Fe^{II}(NP^{iso})(CO_2H)]^+$	0.68e$^-$	0.084e$^-$
$[Fe^{II}(NP^{iso})(CO)]^{2+}$	0.62e$^-$	0.11e$^-$
		0.11e$^-$



a) b)

Figure S36: NLMOs of the $^3[Fe^{II}(\mathbf{NP^{iso}})(CO_2H)]^+$ + 2e- intermediate showing the detail of the a) σ iron-carbanionic bond and b) the π backbonding component of the CO_2H^- ligand.



a) b) c)

Figure S37: NLMOs of the $^3[Fe^{II}(\mathbf{NP^{iso}})(CO)]^{2+}$ intermediate.

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11. Optimized coordinates

/db/nbandeira/Fe(NPiso)/L=Cl/2e-/1-NCMe+Cl
Energy (POTENTIAL) = -4466.93296750 Eh

	Atom	X	Y	Z
1	Fe	-0.3129	1.4417	2.7669
2	P	-0.9836	-0.6993	1.9499
3	P	-1.9045	3.0661	2.1084
4	P	1.7728	2.0894	1.8001
5	N	-0.5241	1.5020	-0.1113
6	C	0.0754	0.2688	-0.4646
7	C	0.8542	0.1820	-1.6243
8	H	0.9914	1.0710	-2.2378
9	C	1.4531	-1.0244	-1.9962
10	H	2.0655	-1.0651	-2.8985
11	C	1.2627	-2.1774	-1.2363
12	C	0.4698	-2.0789	-0.0797
13	H	0.3331	-2.9798	0.5178
14	C	-0.1129	-0.8775	0.3354
15	C	1.8743	-3.4941	-1.6267
16	H	2.5406	-3.3845	-2.4921
17	H	1.1010	-4.2317	-1.8906
18	H	2.4585	-3.9257	-0.8007
19	C	-1.9396	1.5903	-0.2751
20	C	-2.5759	0.8821	-1.2805
21	H	-1.9778	0.2325	-1.9219
22	C	-3.9701	0.9855	-1.4854
23	H	-4.4598	0.4044	-2.2679
24	C	-4.7125	1.9177	-0.7020
25	C	-4.0667	2.6455	0.2804
26	H	-4.6599	3.3523	0.8641
27	C	-2.6691	2.4836	0.5866
28	C	-6.1831	2.1005	-0.9613
29	H	-6.3756	2.4463	-1.9905
30	H	-6.6288	2.8315	-0.2726
31	H	-6.7318	1.1512	-0.8469
32	C	0.2022	2.6773	-0.4463
33	C	-0.2612	3.5064	-1.4756
34	H	-1.1615	3.2096	-2.0126

35	C	0.3980	4.6863	-1.7969
36	H	0.0112	5.3197	-2.5971
37	C	1.5518	5.0685	-1.1008
38	C	2.0048	4.2299	-0.0784
39	H	2.8876	4.5462	0.4702
40	C	1.3492	3.0430	0.2805
41	C	2.2771	6.3412	-1.4392
42	H	3.0949	6.5337	-0.7330
43	H	1.5990	7.2065	-1.4184
44	H	2.7099	6.2969	-2.4500
45	C	-0.3534	-2.1789	2.9147
46	H	-0.5184	-3.0860	2.3144
47	C	1.1414	-2.0000	3.1622
48	H	1.3154	-1.1189	3.7959
49	H	1.7125	-1.8677	2.2359
50	H	1.5464	-2.8780	3.6882
51	C	-1.0686	-2.3568	4.2544
52	H	-0.4886	-3.0494	4.8837
53	H	-2.0715	-2.7801	4.1473
54	H	-1.1735	-1.4151	4.8099
55	C	-2.7609	-1.1067	1.4823
56	H	-3.0725	-0.1700	1.0009
57	C	-2.8868	-2.2291	0.4593
58	H	-2.5142	-3.1852	0.8581
59	H	-2.3409	-2.0069	-0.4654
60	H	-3.9470	-2.3710	0.1962
61	C	-3.6914	-1.3660	2.6677
62	H	-4.7271	-1.1467	2.3672
63	H	-3.4692	-0.7610	3.5542
64	H	-3.6630	-2.4211	2.9710
65	C	-3.3557	3.3588	3.2602
66	H	-4.0505	4.0344	2.7388
67	C	-4.0779	2.0484	3.5504
68	H	-3.4766	1.4014	4.2041
69	H	-4.3152	1.4957	2.6330
70	H	-5.0221	2.2462	4.0829
71	C	-2.9380	4.0242	4.5704
72	H	-3.7829	4.0189	5.2770
73	H	-2.6334	5.0682	4.4359
74	H	-2.1062	3.4850	5.0466
75	C	-1.2905	4.8182	1.7439

76	H	-0.6474	4.6263	0.8752
77	C	-2.3844	5.7813	1.3035
78	H	-3.0579	6.0439	2.1329
79	H	-2.9920	5.3492	0.4954
80	H	-1.9469	6.7206	0.9280
81	C	-0.4048	5.3969	2.8448
82	H	0.2898	6.1443	2.4311
83	H	0.1961	4.6151	3.3317
84	H	-0.9894	5.8971	3.6276
85	C	2.7963	3.3341	2.7854
86	H	2.2426	4.2689	2.6107
87	C	4.2588	3.5810	2.4102
88	H	4.6275	4.4516	2.9743
89	H	4.4201	3.7893	1.3471
90	H	4.8976	2.7312	2.6786
91	C	2.6922	3.0223	4.2784
92	H	3.1656	2.0619	4.5277
93	H	1.6485	2.9735	4.6086
94	H	3.2031	3.8051	4.8600
95	C	2.9624	0.7582	1.1985
96	H	2.2670	-0.0089	0.8313
97	C	3.8660	1.1451	0.0336
98	H	4.6180	1.8910	0.3193
99	H	3.2888	1.5464	-0.8090
100	H	4.4032	0.2531	-0.3255
101	C	3.7502	0.1446	2.3553
102	H	4.1749	-0.8214	2.0433
103	H	3.1229	-0.0397	3.2358
104	H	4.5861	0.7816	2.6693
105	C	-0.2581	1.2466	5.9035
106	N	-0.2402	1.3286	4.7458
107	C	-0.3427	1.1161	7.3404
108	H	0.4674	0.4762	7.7152
109	H	-1.3224	0.6519	7.5602
110	H	-0.2735	2.1014	7.8209
111	Cl	-3.3929	-0.3240	6.6589

/db/nbandeira/Fe(NPiso)/_Ir(ppy)2(dtb-bpy)_+/0e-/Ground_state

Energy (POTENTIAL) = -19596.30441929004155 Eh

	Atom	X	Y	Z
1	Ir	0.0208	0.1044	0.0859
2	C	-1.5530	2.7564	-0.1515
3	H	-0.5436	3.1746	-0.1608
4	C	-2.6691	3.5690	-0.2570
5	C	-3.9533	3.0060	-0.2396
6	C	-4.0201	1.6172	-0.1178
7	H	-4.9862	1.1163	-0.1045
8	C	-2.8586	0.8520	-0.0145
9	C	-2.8678	-0.6176	0.1198
10	C	-4.0327	-1.3722	0.2013
11	H	-4.9981	-0.8668	0.1655
12	C	-3.9814	-2.7654	0.3327
13	C	-2.7077	-3.3387	0.3797
14	C	-1.5805	-2.5316	0.2916
15	H	-0.5759	-2.9605	0.3228
16	C	1.4624	1.4818	-0.0738
17	C	2.1457	2.1486	0.9548
18	H	1.9230	1.9129	1.9999
19	C	3.1112	3.1161	0.6737
20	H	3.6279	3.6215	1.4965
21	C	3.4262	3.4455	-0.6492
22	H	4.1833	4.2048	-0.8655
23	C	2.7690	2.7988	-1.6904
24	H	3.0160	3.0570	-2.7243
25	C	1.7988	1.8267	-1.4073
26	C	1.0578	1.0984	-2.4333
27	C	1.2170	1.2456	-3.8153
28	H	1.9457	1.9601	-4.2010
29	C	0.4527	0.4828	-4.6870
30	H	0.5759	0.5934	-5.7678
31	C	-0.4701	-0.4243	-4.1647
32	H	-1.0932	-1.0479	-4.8090
33	C	-0.5879	-0.5275	-2.7878
34	H	-1.2911	-1.2254	-2.3305
35	C	1.4464	-1.2851	0.2819
36	C	2.1510	-1.9566	-0.7292
37	H	1.9579	-1.7182	-1.7795

38	C	3.1007	-2.9324	-0.4237
39	H	3.6346	-3.4414	-1.2332
40	C	3.3779	-3.2657	0.9066
41	H	4.1226	-4.0315	1.1419
42	C	2.6990	-2.6144	1.9309
43	H	2.9166	-2.8757	2.9706
44	C	1.7447	-1.6339	1.6235
45	C	0.9827	-0.9006	2.6304
46	C	1.1033	-1.0515	4.0158
47	H	1.8151	-1.7732	4.4195
48	C	0.3226	-0.2836	4.8682
49	H	0.4157	-0.3974	5.9518
50	C	-0.5779	0.6324	4.3231
51	H	-1.2128	1.2602	4.9516
52	C	-0.6579	0.7387	2.9437
53	H	-1.3431	1.4430	2.4694
54	N	-1.6393	1.4272	-0.0270
55	N	-1.6510	-1.2060	0.1600
56	N	0.1510	0.2089	-1.9458
57	N	0.0971	-0.0025	2.1204
58	H	-2.5194	4.6467	-0.3511
59	H	-2.5650	-4.4144	0.4841
60	C	-5.1906	3.8887	-0.3432
61	C	-5.2702	-3.5739	0.4139
62	C	-4.9963	-5.0704	0.5699
63	H	-5.9553	-5.6132	0.6235
64	H	-4.4298	-5.4743	-0.2869
65	H	-4.4344	-5.2896	1.4944
66	C	-6.0733	-3.3486	-0.8776
67	H	-5.5021	-3.6855	-1.7604
68	H	-7.0147	-3.9244	-0.8359
69	H	-6.3333	-2.2858	-1.0201
70	C	-5.1222	4.6901	-1.6532
71	H	-4.2298	5.3374	-1.6942
72	H	-5.1009	4.0156	-2.5272
73	H	-6.0129	5.3370	-1.7388
74	C	-6.4834	3.0716	-0.3325
75	H	-7.3468	3.7538	-0.4110
76	H	-6.5317	2.3711	-1.1842
77	H	-6.5967	2.4948	0.6016
78	C	-5.2022	4.8523	0.8547

79	H	-6.0901	5.5063	0.7982
80	H	-5.2440	4.2957	1.8075
81	H	-4.3074	5.4978	0.8705
82	C	-6.0860	-3.0901	1.6236
83	H	-6.3519	-2.0225	1.5408
84	H	-7.0247	-3.6673	1.6921
85	H	-5.5226	-3.2342	2.5622

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/0e-/1-NCMe+Cl-
Energy (POTENTIAL) = -4456.34027303 Eh

	Atom	X	Y	Z
1	Fe	-0.2984	1.4266	2.6661
2	P	-1.0737	-0.7925	1.9417
3	P	-1.9415	3.1656	2.1502
4	P	1.8928	2.1387	1.8075
5	N	-0.4968	1.5303	0.0354
6	C	0.0823	0.2844	-0.3848
7	C	0.8733	0.2247	-1.5343
8	H	1.0608	1.1312	-2.1067
9	C	1.4226	-0.9819	-1.9549
10	H	2.0416	-1.0013	-2.8525
11	C	1.1773	-2.1675	-1.2546
12	C	0.3736	-2.0949	-0.1126
13	H	0.1807	-3.0167	0.4346
14	C	-0.1647	-0.8899	0.3509
15	C	1.7771	-3.4734	-1.6892
16	H	1.9686	-3.4852	-2.7697
17	H	1.1202	-4.3172	-1.4415
18	H	2.7389	-3.6474	-1.1826
19	C	-1.9126	1.6393	-0.1944
20	C	-2.5073	0.9721	-1.2676
21	H	-1.8976	0.3462	-1.9169
22	C	-3.8706	1.0969	-1.5079
23	H	-4.3159	0.5567	-2.3441
24	C	-4.6729	1.9137	-0.7019
25	C	-4.0617	2.5846	0.3618
26	H	-4.6861	3.2100	0.9988
27	C	-2.6972	2.4507	0.6443
28	C	-6.1437	2.0544	-0.9683
29	H	-6.3252	2.4530	-1.9768
30	H	-6.6191	2.7281	-0.2449
31	H	-6.6493	1.0798	-0.9109
32	C	0.2371	2.6993	-0.3713
33	C	-0.2152	3.4769	-1.4414
34	H	-1.1167	3.1840	-1.9762
35	C	0.4602	4.6330	-1.8135
36	H	0.0792	5.2288	-2.6436
37	C	1.6152	5.0403	-1.1354
38	C	2.0664	4.2428	-0.0805

39	H	2.9552	4.5670	0.4544
40	C	1.4003	3.0780	0.3196
41	C	2.3486	6.2885	-1.5328
42	H	3.1212	6.5491	-0.7989
43	H	1.6608	7.1400	-1.6276
44	H	2.8402	6.1593	-2.5086
45	C	-0.4071	-2.2322	2.9197
46	H	-0.5531	-3.1361	2.3107
47	C	1.0850	-2.0099	3.1530
48	H	1.2482	-1.1262	3.7863
49	H	1.6509	-1.8797	2.2231
50	H	1.5071	-2.8765	3.6819
51	C	-1.1200	-2.4344	4.2567
52	H	-0.5158	-3.1141	4.8752
53	H	-2.1067	-2.8916	4.1422
54	H	-1.2561	-1.5033	4.8228
55	C	-2.8636	-1.1142	1.4948
56	H	-3.1798	-0.1463	1.0841
57	C	-3.0092	-2.1747	0.4089
58	H	-2.6182	-3.1478	0.7405
59	H	-2.4964	-1.8955	-0.5197
60	H	-4.0765	-2.3065	0.1763
61	C	-3.7587	-1.4325	2.6933
62	H	-4.7995	-1.2070	2.4199
63	H	-3.5217	-0.8662	3.6026
64	H	-3.7139	-2.5002	2.9424
65	C	-3.3571	3.3804	3.3320
66	H	-4.1053	4.0038	2.8211
67	C	-3.9719	2.0260	3.6691
68	H	-3.3091	1.4280	4.3098
69	H	-4.2243	1.4389	2.7779
70	H	-4.8998	2.1811	4.2390
71	C	-2.9179	4.1068	4.6036
72	H	-3.7275	4.0472	5.3453
73	H	-2.7119	5.1685	4.4294
74	H	-2.0247	3.6489	5.0515
75	C	-1.3550	4.8630	1.6483
76	H	-0.7170	4.6421	0.7837
77	C	-2.4876	5.7682	1.1790
78	H	-3.1669	6.0343	2.0009
79	H	-3.0773	5.3044	0.3766

80	H	-2.0644	6.7033	0.7833
81	C	-0.4780	5.5215	2.7117
82	H	0.1151	6.3215	2.2463
83	H	0.2201	4.8132	3.1760
84	H	-1.0733	5.9753	3.5126
85	C	2.8446	3.3644	2.8530
86	H	2.2943	4.2991	2.6673
87	C	4.3130	3.5995	2.4987
88	H	4.6764	4.4562	3.0848
89	H	4.4850	3.8295	1.4418
90	H	4.9394	2.7387	2.7596
91	C	2.6935	3.0281	4.3367
92	H	3.1118	2.0422	4.5807
93	H	1.6438	3.0432	4.6509
94	H	3.2336	3.7767	4.9343
95	C	3.0244	0.7667	1.2269
96	H	2.3109	0.0207	0.8502
97	C	3.9448	1.1471	0.0734
98	H	4.7072	1.8766	0.3724
99	H	3.3857	1.5611	-0.7753
100	H	4.4655	0.2444	-0.2793
101	C	3.7752	0.1352	2.3985
102	H	4.1925	-0.8303	2.0789
103	H	3.1252	-0.0541	3.2616
104	H	4.6113	0.7589	2.7361
105	C	-0.2570	1.1948	5.8444
106	N	-0.2555	1.3198	4.6953
107	C	-0.2874	1.0189	7.2709
108	H	-0.1761	1.9891	7.7725
109	H	0.5235	0.3461	7.5798
110	H	-1.2739	0.5668	7.4978
111	Cl	-3.3017	-0.3107	6.5957

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/1e-/1-NCMe+Cl-
Energy (POTENTIAL) = -4456.33882696966066 Eh

	Atom	X	Y	Z
1	Fe	-0.3091	1.4462	2.7758
2	P	-1.0323	-0.6841	1.9364
3	P	-1.8704	3.0830	2.1366
4	P	1.7833	2.1159	1.8220
5	N	-0.5123	1.5344	-0.1086
6	C	0.0706	0.2864	-0.4675
7	C	0.8639	0.1906	-1.6159
8	H	1.0268	1.0787	-2.2246
9	C	1.4404	-1.0191	-1.9864
10	H	2.0601	-1.0660	-2.8830
11	C	1.2166	-2.1765	-1.2327
12	C	0.4096	-2.0686	-0.0955
13	H	0.2370	-2.9715	0.4888
14	C	-0.1514	-0.8564	0.3242
15	C	1.8458	-3.4871	-1.6125
16	H	1.8551	-3.6265	-2.7021
17	H	1.3129	-4.3334	-1.1601
18	H	2.8912	-3.5348	-1.2707
19	C	-1.9228	1.6510	-0.2796
20	C	-2.5555	1.0005	-1.3419
21	H	-1.9619	0.3934	-2.0242
22	C	-3.9289	1.1206	-1.5327
23	H	-4.4033	0.5963	-2.3634
24	C	-4.7009	1.9203	-0.6840
25	C	-4.0502	2.5779	0.3675
26	H	-4.6554	3.1931	1.0329
27	C	-2.6788	2.4427	0.6090
28	C	-6.1877	2.0432	-0.8621
29	H	-6.4821	1.8739	-1.9061
30	H	-6.5479	3.0343	-0.5561
31	H	-6.7180	1.2996	-0.2473
32	C	0.2335	2.6999	-0.4505
33	C	-0.1891	3.5063	-1.5133
34	H	-1.0726	3.2174	-2.0806
35	C	0.4863	4.6778	-1.8346
36	H	0.1276	5.2961	-2.6585
37	C	1.6184	5.0667	-1.1099
38	C	2.0375	4.2425	-0.0607

39	H	2.9057	4.5635	0.5083
40	C	1.3681	3.0654	0.2979
41	C	2.3703	6.3207	-1.4553
42	H	3.0200	6.6382	-0.6298
43	H	1.6850	7.1455	-1.6930
44	H	3.0084	6.1654	-2.3388
45	C	-0.4040	-2.1647	2.8973
46	H	-0.5739	-3.0696	2.2954
47	C	1.0925	-1.9850	3.1362
48	H	1.2701	-1.1099	3.7765
49	H	1.6619	-1.8482	2.2094
50	H	1.4985	-2.8671	3.6538
51	C	-1.1120	-2.3453	4.2410
52	H	-0.5170	-3.0249	4.8697
53	H	-2.1075	-2.7867	4.1402
54	H	-1.2300	-1.4037	4.7930
55	C	-2.8128	-1.0799	1.4571
56	H	-3.1487	-0.1272	1.0266
57	C	-2.9327	-2.1568	0.3843
58	H	-2.5115	-3.1149	0.7241
59	H	-2.4278	-1.8745	-0.5476
60	H	-3.9954	-2.3270	0.1517
61	C	-3.7317	-1.4047	2.6361
62	H	-4.7723	-1.2013	2.3425
63	H	-3.5251	-0.8268	3.5444
64	H	-3.6742	-2.4692	2.8978
65	C	-3.3042	3.3307	3.3061
66	H	-4.0522	3.9699	2.8150
67	C	-3.9338	1.9838	3.6410
68	H	-3.2428	1.3583	4.2218
69	H	-4.2383	1.4254	2.7474
70	H	-4.8276	2.1320	4.2662
71	C	-2.8435	4.0289	4.5860
72	H	-3.6391	3.9669	5.3434
73	H	-2.6237	5.0910	4.4290
74	H	-1.9473	3.5502	5.0068
75	C	-1.3480	4.8138	1.6339
76	H	-0.7246	4.6150	0.7530
77	C	-2.4992	5.7124	1.2004
78	H	-3.1591	5.9674	2.0420
79	H	-3.1093	5.2444	0.4157

80	H	-2.1038	6.6567	0.7956
81	C	-0.4549	5.4809	2.6781
82	H	0.1270	6.2883	2.2095
83	H	0.2536	4.7716	3.1252
84	H	-1.0369	5.9270	3.4938
85	C	2.7809	3.3601	2.8268
86	H	2.2406	4.2983	2.6314
87	C	4.2530	3.5920	2.4824
88	H	4.6150	4.4616	3.0517
89	H	4.4368	3.7969	1.4222
90	H	4.8790	2.7381	2.7666
91	C	2.6319	3.0569	4.3178
92	H	3.0711	2.0850	4.5829
93	H	1.5797	3.0437	4.6247
94	H	3.1505	3.8287	4.9065
95	C	2.9636	0.7754	1.2342
96	H	2.2649	0.0144	0.8596
97	C	3.8861	1.1534	0.0812
98	H	4.6362	1.8979	0.3751
99	H	3.3254	1.5525	-0.7737
100	H	4.4244	0.2571	-0.2640
101	C	3.7267	0.1576	2.4052
102	H	4.1417	-0.8151	2.1024
103	H	3.0854	-0.0143	3.2783
104	H	4.5669	0.7850	2.7264
105	C	-0.2390	1.1585	5.9132
106	N	-0.2294	1.2742	4.7600
107	C	-0.3121	0.9931	7.3456
108	H	0.4835	0.3215	7.6941
109	H	-1.3045	0.5503	7.5587
110	H	-0.2124	1.9646	7.8478
111	Cl	-3.3896	-0.3621	6.7240

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/2e-/1-Cl+NCMe
Energy (POTENTIAL) = -4456.33553582472450 Eh

	Atom	X	Y	Z
1	Fe	-0.0297	-0.1152	0.0353
2	P	-0.7673	-2.2263	-0.7603
3	P	-1.6281	1.4896	-0.5325
4	P	2.0227	0.5765	-1.0248
5	Cl	0.1428	-0.3075	2.4323
6	N	-0.3465	-0.0256	-2.8216
7	C	0.2502	-1.2615	-3.1891
8	C	1.0525	-1.3371	-4.3336
9	H	1.2162	-0.4308	-4.9151
10	C	1.6115	-2.5476	-4.7334
11	H	2.2400	-2.5828	-5.6252
12	C	1.3605	-3.7228	-4.0126
13	C	0.5627	-3.6306	-2.8686
14	H	0.3698	-4.5445	-2.3069
15	C	0.0298	-2.4139	-2.4140
16	C	1.9566	-5.0358	-4.4398
17	H	1.8841	-5.1754	-5.5277
18	H	1.4536	-5.8811	-3.9521
19	H	3.0249	-5.0923	-4.1791
20	C	-1.7573	0.0604	-2.9375
21	C	-2.4137	-0.6150	-3.9709
22	H	-1.8294	-1.2082	-4.6727
23	C	-3.8059	-0.5387	-4.0993
24	H	-4.3039	-1.0884	-4.9000
25	C	-4.5592	0.2415	-3.2249
26	C	-3.8813	0.9356	-2.2040
27	H	-4.4757	1.5378	-1.5171
28	C	-2.4966	0.8436	-2.0252
29	C	-6.0552	0.3394	-3.3401
30	H	-6.3814	1.3831	-3.4626
31	H	-6.5522	-0.0453	-2.4366
32	H	-6.4288	-0.2339	-4.1985
33	C	0.3587	1.1523	-3.2053
34	C	-0.1564	1.9811	-4.1899
35	H	-1.1000	1.7070	-4.6627
36	C	0.5112	3.1689	-4.5755
37	H	0.0839	3.8245	-5.3351
38	C	1.7668	3.4673	-3.9812

39	C	2.2898	2.6140	-3.0246
40	H	3.2527	2.8778	-2.5926
41	C	1.6041	1.4335	-2.5602
42	C	2.5171	4.7024	-4.4018
43	H	3.4503	4.8229	-3.8345
44	H	1.9112	5.6106	-4.2513
45	H	2.7744	4.6762	-5.4734
46	C	-0.1396	-3.7396	0.1621
47	H	-0.4529	-4.6384	-0.3915
48	C	1.3832	-3.7019	0.2631
49	H	1.6916	-2.8621	0.8992
50	H	1.8849	-3.5890	-0.7053
51	H	1.7503	-4.6287	0.7305
52	C	-0.7058	-3.8120	1.5830
53	H	-0.1910	-4.6132	2.1361
54	H	-1.7761	-4.0314	1.6151
55	H	-0.5313	-2.8667	2.1165
56	C	-2.5666	-2.6533	-1.1717
57	H	-2.9220	-1.7124	-1.6119
58	C	-2.7242	-3.7522	-2.2164
59	H	-2.2995	-4.7067	-1.8697
60	H	-2.2419	-3.4907	-3.1660
61	H	-3.7939	-3.9226	-2.4182
62	C	-3.4445	-2.9552	0.0416
63	H	-4.5006	-2.7983	-0.2265
64	H	-3.2259	-2.3210	0.9077
65	H	-3.3459	-4.0032	0.3553
66	C	-3.0292	1.7585	0.6806
67	H	-3.8149	2.3571	0.1960
68	C	-3.6037	0.4078	1.0914
69	H	-2.8265	-0.2031	1.5701
70	H	-3.9942	-0.1545	0.2341
71	H	-4.4256	0.5418	1.8124
72	C	-2.5412	2.5202	1.9130
73	H	-3.3128	2.4866	2.6977
74	H	-2.3394	3.5758	1.6986
75	H	-1.6272	2.0679	2.3240
76	C	-1.1292	3.2175	-1.0683
77	H	-0.5314	2.9879	-1.9604
78	C	-2.2857	4.1127	-1.4936
79	H	-2.9193	4.4006	-0.6414

80	H	-2.9237	3.6208	-2.2412
81	H	-1.9004	5.0410	-1.9450
82	C	-0.2002	3.9020	-0.0677
83	H	0.3857	4.6837	-0.5753
84	H	0.5091	3.1904	0.3762
85	H	-0.7484	4.3851	0.7512
86	C	3.0568	1.8597	-0.0939
87	H	2.5263	2.7903	-0.3486
88	C	4.5244	2.0500	-0.4818
89	H	4.9152	2.9542	0.0124
90	H	4.6864	2.1685	-1.5585
91	H	5.1448	1.2091	-0.1473
92	C	2.9543	1.6659	1.4178
93	H	3.4971	0.7662	1.7426
94	H	1.9162	1.5472	1.7519
95	H	3.4007	2.5273	1.9411
96	C	3.2175	-0.8233	-1.4747
97	H	2.5054	-1.5893	-1.8153
98	C	4.1673	-0.5544	-2.6344
99	H	4.9832	0.1256	-2.3576
100	H	3.6274	-0.1141	-3.4837
101	H	4.6246	-1.4968	-2.9775
102	C	3.9339	-1.3797	-0.2474
103	H	4.3292	-2.3864	-0.4545
104	H	3.2619	-1.4614	0.6174
105	H	4.7831	-0.7520	0.0528
106	C	-3.1757	-1.4339	4.2608
107	N	-3.6651	-2.3865	3.8181
108	C	-2.5477	-0.2404	4.7931
109	H	-1.6016	-0.0703	4.2552
110	H	-2.3480	-0.3613	5.8656
111	H	-3.2035	0.6273	4.6450

/db/nbandeira/Fe(NPiso)/1_with_vacancy_+_1e-
Energy (POTENTIAL) = -3872.82755323 Eh

	Atom	X	Y	Z
1	Fe	-0.0515	-0.0185	0.1333
2	P	2.2444	-0.0801	0.6709
3	P	-1.1496	-1.9970	0.6737
4	P	-1.2452	1.8963	0.7775
5	N	-0.0012	-0.0773	2.6961
6	C	2.1967	0.9126	2.2163
7	C	1.0413	0.8543	3.0187
8	C	0.9267	1.6975	4.1246
9	H	0.0334	1.6534	4.7456
10	C	1.9407	2.6014	4.4347
11	H	1.8236	3.2596	5.2964
12	C	3.1080	2.6637	3.6686
13	C	3.2171	1.7971	2.5736
14	H	4.1254	1.8377	1.9720
15	C	4.2048	3.6414	3.9811
16	H	4.2108	4.4695	3.2561
17	H	5.1927	3.1631	3.9330
18	H	4.0803	4.0756	4.9811
19	C	3.1959	-1.6166	1.2056
20	H	2.4087	-2.2342	1.6606
21	C	3.8033	-2.4056	0.0485
22	H	3.1082	-2.5555	-0.7851
23	H	4.1027	-3.3988	0.4147
24	H	4.7074	-1.9153	-0.3374
25	C	4.2586	-1.3312	2.2616
26	H	5.0207	-0.6305	1.8895
27	H	4.7703	-2.2694	2.5248
28	H	3.8312	-0.9140	3.1810
29	C	3.3626	0.8827	-0.4738
30	H	4.3818	0.8889	-0.0575
31	C	2.8437	2.3108	-0.6214
32	H	1.8503	2.2979	-1.0908
33	H	3.5143	2.8826	-1.2799
34	H	2.7593	2.8522	0.3276
35	C	3.3810	0.2392	-1.8638
36	H	3.8544	-0.7458	-1.8874
37	H	3.9358	0.8897	-2.5559
38	H	2.3578	0.1341	-2.2569

39	C	-0.2393	-2.4755	2.1972
40	C	0.3030	-1.4501	2.9940
41	C	1.1199	-1.7746	4.0793
42	H	1.5351	-0.9780	4.6946
43	C	1.4090	-3.1032	4.3754
44	H	2.0563	-3.3332	5.2227
45	C	0.8704	-4.1438	3.6104
46	C	0.0430	-3.8035	2.5337
47	H	-0.3680	-4.6112	1.9284
48	C	1.1908	-5.5787	3.9189
49	H	2.2268	-5.8195	3.6366
50	H	0.5290	-6.2628	3.3731
51	H	1.0923	-5.7874	4.9931
52	C	-0.9246	-3.4515	-0.4669
53	H	-1.2696	-4.3611	0.0462
54	C	-1.7569	-3.2618	-1.7344
55	H	-2.8340	-3.3387	-1.5462
56	H	-1.4944	-4.0399	-2.4662
57	H	-1.5596	-2.2849	-2.2023
58	C	0.5520	-3.5978	-0.8161
59	H	0.9168	-2.7027	-1.3415
60	H	0.6985	-4.4615	-1.4818
61	H	1.1782	-3.7475	0.0721
62	C	-2.9375	-2.0469	1.2326
63	H	-2.9056	-1.4283	2.1402
64	C	-3.8802	-1.3602	0.2484
65	H	-3.4666	-0.4092	-0.1077
66	H	-4.8390	-1.1443	0.7423
67	H	-4.0943	-1.9839	-0.6287
68	C	-3.4244	-3.4370	1.6242
69	H	-3.4973	-4.1033	0.7530
70	H	-4.4289	-3.3660	2.0682
71	H	-2.7669	-3.9113	2.3655
72	C	-2.0231	1.2790	2.3214
73	C	-1.3241	0.3270	3.0850
74	C	-1.9363	-0.2473	4.2023
75	H	-1.3955	-0.9869	4.7904
76	C	-3.2391	0.0929	4.5522
77	H	-3.7008	-0.3821	5.4189
78	C	-3.9614	1.0293	3.8041
79	C	-3.3271	1.6134	2.7027

80	H	-3.8916	2.3334	2.1139
81	C	0.0308	4.3333	0.0982
82	H	0.3887	3.7552	-0.7617
83	H	0.8335	5.0272	0.3873
84	H	-0.8196	4.9392	-0.2358
85	C	-2.6882	2.3577	-0.3248
86	H	-3.4227	1.5759	-0.0810
87	C	-3.3738	3.7098	-0.1359
88	H	-3.6831	3.9035	0.8975
89	H	-4.2798	3.7379	-0.7596
90	H	-2.7362	4.5423	-0.4548
91	C	-2.2694	2.1556	-1.7826
92	H	-1.4845	2.8642	-2.0820
93	H	-3.1321	2.3132	-2.4469
94	H	-1.8909	1.1375	-1.9578
95	C	-0.3294	3.4523	1.2939
96	H	0.6073	3.0349	1.6896
97	C	-0.9920	4.2492	2.4118
98	H	-1.9489	4.6854	2.0975
99	H	-0.3313	5.0771	2.7116
100	H	-1.1743	3.6308	3.2998
101	C	-5.3666	1.4048	4.1794
102	H	-5.3789	2.0187	5.0927
103	H	-5.9771	0.5140	4.3814
104	H	-5.8531	1.9817	3.3829

/db/nbandeira/Fe(NPiso)/L=Cl/2e-/1-Cl
Energy (POTENTIAL) = -4334.38680599 Eh

	Atom	X	Y	Z
1	Fe	0.0111	-0.0046	-0.0045
2	P	-0.6976	-2.1779	-0.6659
3	P	-1.6131	1.5882	-0.6589
4	P	2.0199	0.5563	-1.1172
5	Cl	0.1200	-0.0473	2.3881
6	N	-0.3846	-0.1083	-2.8599
7	C	0.1865	-1.3589	-3.1971
8	C	0.8827	-1.5067	-4.4004
9	H	0.9861	-0.6478	-5.0617
10	C	1.4371	-2.7420	-4.7554
11	H	1.9866	-2.8368	-5.6936
12	C	1.2758	-3.8562	-3.9333
13	C	0.5586	-3.6960	-2.7346
14	H	0.4362	-4.5683	-2.0927
15	C	0.0321	-2.4616	-2.3334
16	C	1.8660	-5.1924	-4.2912
17	H	2.2139	-5.2106	-5.3324
18	H	1.1339	-6.0026	-4.1617
19	H	2.7273	-5.4338	-3.6491
20	C	-1.8074	-0.0249	-2.9408
21	C	-2.5088	-0.8023	-3.8473
22	H	-1.9564	-1.5005	-4.4783
23	C	-3.9152	-0.7027	-3.9669
24	H	-4.4580	-1.3422	-4.6644
25	C	-4.6014	0.2896	-3.2098
26	C	-3.8885	1.0873	-2.3320
27	H	-4.4392	1.8416	-1.7664
28	C	-2.4737	0.9408	-2.1120
29	C	-6.0873	0.4578	-3.3769
30	H	-6.3559	0.6995	-4.4186
31	H	-6.4799	1.2585	-2.7348
32	H	-6.6274	-0.4699	-3.1256
33	C	0.3170	1.0511	-3.2903
34	C	-0.2222	1.8381	-4.3153
35	H	-1.1507	1.5133	-4.7833
36	C	0.3986	3.0174	-4.7156
37	H	-0.0499	3.6240	-5.5043
38	C	1.5860	3.4351	-4.1042

39	C	2.1181	2.6332	-3.0885
40	H	3.0278	2.9799	-2.6065
41	C	1.5050	1.4487	-2.6508
42	C	2.2755	4.7026	-4.5281
43	H	2.9861	5.0464	-3.7650
44	H	1.5536	5.5102	-4.7121
45	H	2.8401	4.5560	-5.4621
46	C	-0.0136	-3.6203	0.3253
47	H	-0.3060	-4.5563	-0.1754
48	C	1.5082	-3.5295	0.3916
49	H	1.8035	-2.6415	0.9671
50	H	1.9826	-3.4641	-0.5949
51	H	1.9159	-4.4132	0.9067
52	C	-0.5567	-3.6402	1.7567
53	H	0.0079	-4.3786	2.3474
54	H	-1.6123	-3.9198	1.8124
55	H	-0.4322	-2.6577	2.2346
56	C	-2.5082	-2.6254	-0.9715
57	H	-2.8623	-1.7162	-1.4761
58	C	-2.7140	-3.7977	-1.9224
59	H	-2.3070	-4.7342	-1.5109
60	H	-2.2436	-3.6176	-2.8964
61	H	-3.7915	-3.9524	-2.0942
62	C	-3.3409	-2.8165	0.2951
63	H	-4.4027	-2.6423	0.0632
64	H	-3.0620	-2.1291	1.1022
65	H	-3.2597	-3.8426	0.6784
66	C	-2.9993	1.9225	0.5620
67	H	-3.7532	2.5405	0.0512
68	C	-3.6432	0.6050	0.9741
69	H	-2.9139	-0.0185	1.5092
70	H	-4.0087	0.0404	0.1067
71	H	-4.4955	0.7857	1.6488
72	C	-2.5190	2.6797	1.7986
73	H	-3.3301	2.7290	2.5427
74	H	-2.2239	3.7104	1.5717
75	H	-1.6651	2.1675	2.2654
76	C	-1.0526	3.3233	-1.1551
77	H	-0.4646	3.0913	-2.0525
78	C	-2.1845	4.2516	-1.5753
79	H	-2.8006	4.5619	-0.7180

80	H	-2.8429	3.7643	-2.3086
81	H	-1.7855	5.1682	-2.0400
82	C	-0.1001	3.9733	-0.1535
83	H	0.5385	4.7160	-0.6567
84	H	0.5595	3.2291	0.3158
85	H	-0.6319	4.4979	0.6509
86	C	3.1218	1.8308	-0.2635
87	H	2.5461	2.7567	-0.4150
88	C	4.5432	2.0715	-0.7759
89	H	4.9524	2.9713	-0.2903
90	H	4.6119	2.2240	-1.8584
91	H	5.2105	1.2393	-0.5208
92	C	3.1591	1.5643	1.2418
93	H	3.7342	0.6562	1.4744
94	H	2.1545	1.4274	1.6627
95	H	3.6495	2.4048	1.7579
96	C	3.1674	-0.8031	-1.7488
97	H	2.4437	-1.5835	-2.0219
98	C	3.9834	-0.4825	-2.9956
99	H	4.7668	0.2613	-2.8020
100	H	3.3485	-0.1075	-3.8083
101	H	4.4799	-1.3974	-3.3565
102	C	4.0399	-1.3640	-0.6269
103	H	4.4387	-2.3474	-0.9192
104	H	3.4789	-1.5001	0.3058
105	H	4.8977	-0.7156	-0.4098

/db/nbandeira/Fe(NPiso)/BIH/1e-/BI
Energy (POTENTIAL) = -688.91773017287005 Eh

	Atom	X	Y	Z
1	C	1.4482	-2.6896	-2.1851
2	C	2.8064	-2.9580	-2.4288
3	C	1.1335	-1.9572	-1.0439
4	H	3.0829	-3.5290	-3.3152
5	C	3.8018	-2.5030	-1.5623
6	C	2.1380	-1.5061	-0.1639
7	H	4.8472	-2.7234	-1.7787
8	C	3.4833	-1.7675	-0.4074
9	H	4.2605	-1.4274	0.2752
10	H	0.6755	-3.0315	-2.8718
11	N	-0.0768	-1.5473	-0.5280
12	N	1.5134	-0.8142	0.8506
13	C	2.2244	0.0513	1.7594
14	H	2.5017	-0.4625	2.6905
15	H	3.1399	0.4064	1.2704
16	H	1.6045	0.9198	2.0047
17	C	-1.3409	-2.0759	-0.9790
18	H	-2.0252	-2.1716	-0.1296
19	H	-1.8083	-1.4393	-1.7432
20	H	-1.1781	-3.0726	-1.4070
21	C	0.1375	-0.8324	0.6460
22	C	-0.8504	-0.2408	1.4715
23	C	-2.0865	0.2480	0.9371
24	C	-0.6650	-0.0987	2.8849
25	C	-3.0458	0.8250	1.7541
26	C	-1.6353	0.4859	3.6831
27	C	-2.8415	0.9578	3.1381
28	H	-2.2625	0.2115	-0.1365
29	H	0.2328	-0.4978	3.3540
30	H	-3.9671	1.1979	1.3032
31	H	-1.4592	0.5610	4.7576
32	H	-3.6001	1.4144	3.7730

/db/nbandeira/Fe(NPiso)/L=CO2/0e-/1-CO2
Energy (POTENTIAL) = -4061.04119678 Eh

	Atom	X	Y	Z
1	Fe	-0.0487	0.0030	-0.3122
2	P	-0.8412	-2.2651	-0.6985
3	P	-1.7185	1.7476	-0.6822
4	P	2.1597	0.6740	-1.0950
5	N	-0.3201	-0.0194	-2.7062
6	C	0.2441	-1.2908	-3.1004
7	C	0.9889	-1.3992	-4.2763
8	H	1.1552	-0.5194	-4.8946
9	C	1.5196	-2.6241	-4.6647
10	H	2.1017	-2.6832	-5.5848
11	C	1.3042	-3.7788	-3.9035
12	C	0.5478	-3.6568	-2.7348
13	H	0.3752	-4.5527	-2.1396
14	C	0.0257	-2.4312	-2.3061
15	C	1.8859	-5.1002	-4.3136
16	H	1.8373	-5.2360	-5.4021
17	H	1.3601	-5.9351	-3.8337
18	H	2.9458	-5.1640	-4.0240
19	C	-1.7470	0.0810	-2.9238
20	C	-2.3613	-0.6424	-3.9453
21	H	-1.7693	-1.3104	-4.5684
22	C	-3.7305	-0.5260	-4.1641
23	H	-4.1934	-1.1131	-4.9577
24	C	-4.5165	0.3330	-3.3881
25	C	-3.8845	1.0580	-2.3716
26	H	-4.4948	1.7139	-1.7514
27	C	-2.5148	0.9398	-2.1163
28	C	-5.9870	0.4865	-3.6464
29	H	-6.1635	1.2101	-4.4569
30	H	-6.5146	0.8519	-2.7565
31	H	-6.4391	-0.4650	-3.9548
32	C	0.4016	1.1274	-3.2167
33	C	-0.0922	1.8350	-4.3150
34	H	-1.0115	1.5113	-4.7988
35	C	0.5689	2.9640	-4.7842
36	H	0.1586	3.5046	-5.6375
37	C	1.7465	3.4141	-4.1759
38	C	2.2422	2.6806	-3.0944

39	H	3.1551	3.0302	-2.6180
40	C	1.5935	1.5429	-2.5998
41	C	2.4397	4.6568	-4.6532
42	H	3.4547	4.7329	-4.2441
43	H	1.8846	5.5543	-4.3417
44	H	2.5034	4.6796	-5.7494
45	C	-0.1359	-3.6344	0.3454
46	H	-0.3158	-4.5766	-0.1928
47	C	1.3665	-3.4125	0.5023
48	H	1.5645	-2.5044	1.0898
49	H	1.8924	-3.3257	-0.4557
50	H	1.8055	-4.2593	1.0490
51	C	-0.7922	-3.7330	1.7231
52	H	-0.2038	-4.4245	2.3426
53	H	-1.8144	-4.1176	1.6833
54	H	-0.8124	-2.7652	2.2411
55	C	-2.6383	-2.6194	-1.0857
56	H	-2.9681	-1.6830	-1.5547
57	C	-2.8026	-3.7545	-2.0901
58	H	-2.4139	-4.7036	-1.6934
59	H	-2.3006	-3.5464	-3.0428
60	H	-3.8736	-3.8946	-2.2984
61	C	-3.5030	-2.8489	0.1535
62	H	-4.5528	-2.6636	-0.1141
63	H	-3.2489	-2.1867	0.9893
64	H	-3.4338	-3.8870	0.5006
65	C	-3.0666	1.9669	0.5719
66	H	-3.8708	2.5355	0.0823
67	C	-3.5987	0.6008	0.9924
68	H	-2.8234	0.0120	1.5023
69	H	-3.9706	0.0164	0.1422
70	H	-4.4320	0.7335	1.6973
71	C	-2.5768	2.7661	1.7794
72	H	-3.3449	2.7289	2.5649
73	H	-2.4060	3.8211	1.5394
74	H	-1.6498	2.3515	2.1996
75	C	-1.1658	3.4213	-1.2818
76	H	-0.5702	3.1649	-2.1674
77	C	-2.3308	4.2957	-1.7302
78	H	-2.9686	4.5916	-0.8855
79	H	-2.9563	3.7927	-2.4799

80	H	-1.9372	5.2152	-2.1877
81	C	-0.2414	4.1273	-0.2911
82	H	0.3200	4.9106	-0.8197
83	H	0.4868	3.4432	0.1630
84	H	-0.7985	4.6102	0.5200
85	C	3.1137	1.9503	-0.1200
86	H	2.5523	2.8718	-0.3356
87	C	4.5725	2.1766	-0.5167
88	H	4.9425	3.0612	0.0215
89	H	4.7178	2.3588	-1.5870
90	H	5.2099	1.3320	-0.2306
91	C	2.9912	1.6734	1.3785
92	H	3.4173	0.6994	1.6548
93	H	1.9466	1.7033	1.7092
94	H	3.5394	2.4469	1.9352
95	C	3.2791	-0.7158	-1.6522
96	H	2.5576	-1.4773	-1.9797
97	C	4.1681	-0.3778	-2.8429
98	H	4.9425	0.3561	-2.5888
99	H	3.5889	0.0110	-3.6902
100	H	4.6744	-1.2950	-3.1783
101	C	4.0582	-1.3007	-0.4749
102	H	4.4749	-2.2740	-0.7704
103	H	3.4250	-1.4644	0.4058
104	H	4.8968	-0.6609	-0.1753
105	C	0.0791	-0.2541	3.0531
106	O	0.1297	-0.6210	4.1420
107	O	0.0267	0.1228	1.9513

/db/nbandeira/Fe(NPiso)/L=Cl/0e-/1-Cl
Energy (POTENTIAL) = -4334.24062118 Eh

	Atom	X	Y	Z
1	Fe	-0.0013	-0.0019	0.0032
2	P	-0.8459	-2.2190	-0.7083
3	P	-1.6605	1.6686	-0.6524
4	P	2.1307	0.6770	-1.0699
5	Cl	0.0050	0.0138	2.2714
6	N	-0.2985	-0.0335	-2.7650
7	C	0.2674	-1.2998	-3.1182
8	C	1.0341	-1.4343	-4.2793
9	H	1.2089	-0.5647	-4.9103
10	C	1.5722	-2.6660	-4.6330
11	H	2.1740	-2.7446	-5.5391
12	C	1.3375	-3.8058	-3.8543
13	C	0.5566	-3.6596	-2.7046
14	H	0.3697	-4.5439	-2.0964
15	C	0.0340	-2.4238	-2.3054
16	C	1.9252	-5.1357	-4.2298
17	H	1.8041	-5.3365	-5.3030
18	H	1.4551	-5.9534	-3.6693
19	H	3.0042	-5.1609	-4.0154
20	C	-1.7192	0.0613	-2.9410
21	C	-2.3519	-0.6517	-3.9613
22	H	-1.7642	-1.3045	-4.6048
23	C	-3.7252	-0.5435	-4.1535
24	H	-4.2006	-1.1222	-4.9461
25	C	-4.4988	0.3030	-3.3517
26	C	-3.8497	1.0166	-2.3378
27	H	-4.4541	1.6607	-1.7001
28	C	-2.4756	0.9008	-2.1027
29	C	-5.9750	0.4565	-3.5792
30	H	-6.1721	1.2063	-4.3610
31	H	-6.4890	0.7884	-2.6682
32	H	-6.4287	-0.4865	-3.9109
33	C	0.4151	1.1189	-3.2346
34	C	-0.0761	1.8476	-4.3229
35	H	-0.9805	1.5124	-4.8272
36	C	0.5569	3.0093	-4.7470
37	H	0.1434	3.5666	-5.5882
38	C	1.7093	3.4728	-4.1020

39	C	2.2047	2.7211	-3.0331
40	H	3.0909	3.0921	-2.5254
41	C	1.5839	1.5493	-2.5821
42	C	2.3958	4.7312	-4.5487
43	H	3.1468	5.0585	-3.8190
44	H	1.6749	5.5476	-4.6920
45	H	2.9071	4.5781	-5.5109
46	C	-0.1743	-3.5970	0.3557
47	H	-0.3975	-4.5499	-0.1471
48	C	1.3370	-3.4247	0.4944
49	H	1.5651	-2.4982	1.0411
50	H	1.8626	-3.3952	-0.4672
51	H	1.7502	-4.2608	1.0771
52	C	-0.8028	-3.6163	1.7513
53	H	-0.2442	-4.3278	2.3770
54	H	-1.8474	-3.9369	1.7482
55	H	-0.7402	-2.6298	2.2306
56	C	-2.6366	-2.6004	-1.1203
57	H	-2.9788	-1.6640	-1.5796
58	C	-2.7801	-3.7250	-2.1394
59	H	-2.3751	-4.6725	-1.7547
60	H	-2.2787	-3.4970	-3.0877
61	H	-3.8478	-3.8827	-2.3538
62	C	-3.5122	-2.8632	0.1040
63	H	-4.5644	-2.7175	-0.1797
64	H	-3.2971	-2.1927	0.9439
65	H	-3.4093	-3.8985	0.4523
66	C	-3.0451	1.9297	0.5635
67	H	-3.8279	2.5073	0.0507
68	C	-3.6127	0.5798	0.9909
69	H	-2.8504	-0.0127	1.5146
70	H	-3.9822	-0.0069	0.1410
71	H	-4.4545	0.7349	1.6817
72	C	-2.5792	2.7319	1.7787
73	H	-3.3757	2.7246	2.5369
74	H	-2.3730	3.7796	1.5339
75	H	-1.6805	2.2925	2.2329
76	C	-1.1258	3.3553	-1.2480
77	H	-0.5250	3.1093	-2.1323
78	C	-2.2852	4.2354	-1.6991
79	H	-2.9249	4.5341	-0.8568

80	H	-2.9118	3.7327	-2.4484
81	H	-1.8913	5.1547	-2.1577
82	C	-0.2034	4.0596	-0.2537
83	H	0.3711	4.8379	-0.7764
84	H	0.5135	3.3691	0.2096
85	H	-0.7617	4.5488	0.5530
86	C	3.1574	1.9317	-0.1368
87	H	2.5903	2.8603	-0.3026
88	C	4.5944	2.1542	-0.6105
89	H	4.9966	3.0408	-0.0986
90	H	4.6899	2.3244	-1.6882
91	H	5.2411	1.3084	-0.3493
92	C	3.1300	1.6391	1.3636
93	H	3.6427	0.6981	1.6049
94	H	2.1071	1.5709	1.7527
95	H	3.6506	2.4472	1.8982
96	C	3.2246	-0.7338	-1.6355
97	H	2.4887	-1.4920	-1.9353
98	C	4.0929	-0.4257	-2.8494
99	H	4.8894	0.2925	-2.6195
100	H	3.5029	-0.0287	-3.6851
101	H	4.5715	-1.3554	-3.1918
102	C	4.0266	-1.3165	-0.4727
103	H	4.4300	-2.2951	-0.7699
104	H	3.4128	-1.4702	0.4234
105	H	4.8765	-0.6811	-0.1960

/db/nbandeira/Fe(NPiso)/L=Cl/1e-/1-NCMe+Cl-
Energy (POTENTIAL) = -4466.88688474991977 Eh

	Atom	X	Y	Z
1	Fe	-0.3091	1.4462	2.7758
2	P	-1.0323	-0.6841	1.9364
3	P	-1.8704	3.0830	2.1366
4	P	1.7833	2.1159	1.8220
5	N	-0.5123	1.5344	-0.1086
6	C	0.0706	0.2864	-0.4675
7	C	0.8639	0.1906	-1.6159
8	H	1.0268	1.0787	-2.2246
9	C	1.4404	-1.0191	-1.9864
10	H	2.0601	-1.0660	-2.8830
11	C	1.2166	-2.1765	-1.2327
12	C	0.4096	-2.0686	-0.0955
13	H	0.2370	-2.9715	0.4888
14	C	-0.1514	-0.8564	0.3242
15	C	1.8458	-3.4871	-1.6125
16	H	1.8551	-3.6265	-2.7021
17	H	1.3129	-4.3334	-1.1601
18	H	2.8912	-3.5348	-1.2707
19	C	-1.9228	1.6510	-0.2796
20	C	-2.5555	1.0005	-1.3419
21	H	-1.9619	0.3934	-2.0242
22	C	-3.9289	1.1206	-1.5327
23	H	-4.4033	0.5963	-2.3634
24	C	-4.7009	1.9203	-0.6840
25	C	-4.0502	2.5779	0.3675
26	H	-4.6554	3.1931	1.0329
27	C	-2.6788	2.4427	0.6090
28	C	-6.1877	2.0432	-0.8621
29	H	-6.4821	1.8739	-1.9061
30	H	-6.5479	3.0343	-0.5561
31	H	-6.7180	1.2996	-0.2473
32	C	0.2335	2.6999	-0.4505
33	C	-0.1891	3.5063	-1.5133
34	H	-1.0726	3.2174	-2.0806
35	C	0.4863	4.6778	-1.8346
36	H	0.1276	5.2961	-2.6585
37	C	1.6184	5.0667	-1.1099
38	C	2.0375	4.2425	-0.0607

39	H	2.9057	4.5635	0.5083
40	C	1.3681	3.0654	0.2979
41	C	2.3703	6.3207	-1.4553
42	H	3.0200	6.6382	-0.6298
43	H	1.6850	7.1455	-1.6930
44	H	3.0084	6.1654	-2.3388
45	C	-0.4040	-2.1647	2.8973
46	H	-0.5739	-3.0696	2.2954
47	C	1.0925	-1.9850	3.1362
48	H	1.2701	-1.1099	3.7765
49	H	1.6619	-1.8482	2.2094
50	H	1.4985	-2.8671	3.6538
51	C	-1.1120	-2.3453	4.2410
52	H	-0.5170	-3.0249	4.8697
53	H	-2.1075	-2.7867	4.1402
54	H	-1.2300	-1.4037	4.7930
55	C	-2.8128	-1.0799	1.4571
56	H	-3.1487	-0.1272	1.0266
57	C	-2.9327	-2.1568	0.3843
58	H	-2.5115	-3.1149	0.7241
59	H	-2.4278	-1.8745	-0.5476
60	H	-3.9954	-2.3270	0.1517
61	C	-3.7317	-1.4047	2.6361
62	H	-4.7723	-1.2013	2.3425
63	H	-3.5251	-0.8268	3.5444
64	H	-3.6742	-2.4692	2.8978
65	C	-3.3042	3.3307	3.3061
66	H	-4.0522	3.9699	2.8150
67	C	-3.9338	1.9838	3.6410
68	H	-3.2428	1.3583	4.2218
69	H	-4.2383	1.4254	2.7474
70	H	-4.8276	2.1320	4.2662
71	C	-2.8435	4.0289	4.5860
72	H	-3.6391	3.9669	5.3434
73	H	-2.6237	5.0910	4.4290
74	H	-1.9473	3.5502	5.0068
75	C	-1.3480	4.8138	1.6339
76	H	-0.7246	4.6150	0.7530
77	C	-2.4992	5.7124	1.2004
78	H	-3.1591	5.9674	2.0420
79	H	-3.1093	5.2444	0.4157

80	H	-2.1038	6.6567	0.7956
81	C	-0.4549	5.4809	2.6781
82	H	0.1270	6.2883	2.2095
83	H	0.2536	4.7716	3.1252
84	H	-1.0369	5.9270	3.4938
85	C	2.7809	3.3601	2.8268
86	H	2.2406	4.2983	2.6314
87	C	4.2530	3.5920	2.4824
88	H	4.6150	4.4616	3.0517
89	H	4.4368	3.7969	1.4222
90	H	4.8790	2.7381	2.7666
91	C	2.6319	3.0569	4.3178
92	H	3.0711	2.0850	4.5829
93	H	1.5797	3.0437	4.6247
94	H	3.1505	3.8287	4.9065
95	C	2.9636	0.7754	1.2342
96	H	2.2649	0.0144	0.8596
97	C	3.8861	1.1534	0.0812
98	H	4.6362	1.8979	0.3751
99	H	3.3254	1.5525	-0.7737
100	H	4.4244	0.2571	-0.2640
101	C	3.7267	0.1576	2.4052
102	H	4.1417	-0.8151	2.1024
103	H	3.0854	-0.0143	3.2783
104	H	4.5669	0.7850	2.7264
105	C	-0.2390	1.1585	5.9132
106	N	-0.2294	1.2742	4.7600
107	C	-0.3121	0.9931	7.3456
108	H	0.4835	0.3215	7.6941
109	H	-1.3045	0.5503	7.5587
110	H	-0.2124	1.9646	7.8478
111	Cl	-3.3896	-0.3621	6.7240

/db/nbandeira/Fe(NPiso)/1_with_vacancy_+2e-
Energy (POTENTIAL) = -3872.88030638 Eh

	Atom	X	Y	Z
1	Fe	-0.2132	-0.0596	0.4070
2	P	2.1341	-0.0735	0.6200
3	P	-1.1418	-2.0719	0.7393
4	P	-1.1267	1.9955	0.7960
5	N	0.0054	-0.1207	2.7228
6	C	2.1602	0.9183	2.1678
7	C	1.0528	0.8157	3.0285
8	C	0.9738	1.6269	4.1594
9	H	0.1059	1.5416	4.8125
10	C	1.9826	2.5464	4.4419
11	H	1.9000	3.1790	5.3269
12	C	3.1058	2.6546	3.6154
13	C	3.1798	1.8169	2.4950
14	H	4.0591	1.8869	1.8541
15	C	4.1903	3.6572	3.8942
16	H	4.0569	4.5605	3.2790
17	H	5.1834	3.2503	3.6602
18	H	4.1847	3.9720	4.9458
19	C	3.1672	-1.5729	1.1469
20	H	2.4149	-2.2016	1.6464
21	C	3.7445	-2.3675	-0.0211
22	H	3.0047	-2.5790	-0.8013
23	H	4.1222	-3.3332	0.3482
24	H	4.5928	-1.8422	-0.4824
25	C	4.2677	-1.2534	2.1532
26	H	4.9960	-0.5358	1.7460
27	H	4.8168	-2.1747	2.4034
28	H	3.8682	-0.8382	3.0861
29	C	3.2276	0.8586	-0.5820
30	H	4.2717	0.7993	-0.2350
31	C	2.7997	2.3178	-0.7024
32	H	1.7758	2.3724	-1.0956
33	H	3.4617	2.8425	-1.4079
34	H	2.8170	2.8616	0.2485
35	C	3.1103	0.2206	-1.9708
36	H	3.4793	-0.8079	-2.0165
37	H	3.6865	0.8123	-2.6982
38	H	2.0601	0.2183	-2.3016

39	C	-0.2233	-2.5370	2.2660
40	C	0.2936	-1.4890	3.0605
41	C	1.1086	-1.7910	4.1547
42	H	1.5063	-0.9811	4.7644
43	C	1.4254	-3.1116	4.4650
44	H	2.0712	-3.3205	5.3193
45	C	0.9174	-4.1695	3.7025
46	C	0.0886	-3.8537	2.6181
47	H	-0.3023	-4.6754	2.0174
48	C	1.2724	-5.5964	4.0143
49	H	2.2622	-5.8558	3.6073
50	H	0.5454	-6.2940	3.5784
51	H	1.3122	-5.7733	5.0979
52	C	-0.9541	-3.5659	-0.3671
53	H	-1.2884	-4.4575	0.1839
54	C	-1.8241	-3.4146	-1.6138
55	H	-2.8956	-3.4628	-1.3862
56	H	-1.6009	-4.2237	-2.3257
57	H	-1.6279	-2.4587	-2.1238
58	C	0.5082	-3.7349	-0.7589
59	H	0.8539	-2.8662	-1.3374
60	H	0.6348	-4.6312	-1.3855
61	H	1.1638	-3.8374	0.1153
62	C	-2.9265	-2.1398	1.3359
63	H	-2.8651	-1.5443	2.2577
64	C	-3.8825	-1.4085	0.3997
65	H	-3.4767	-0.4230	0.1331
66	H	-4.8509	-1.2529	0.8993
67	H	-4.0752	-1.9670	-0.5266
68	C	-3.4161	-3.5364	1.6992
69	H	-3.5381	-4.1723	0.8104
70	H	-4.3981	-3.4752	2.1935
71	H	-2.7293	-4.0456	2.3900
72	C	-1.9931	1.2427	2.1902
73	C	-1.3273	0.3216	3.0669
74	C	-1.9754	-0.2223	4.1625
75	H	-1.4360	-0.9310	4.7914
76	C	-3.3222	0.0765	4.4437
77	H	-3.8142	-0.3625	5.3120
78	C	-4.0219	0.9574	3.5886
79	C	-3.3574	1.5312	2.5137

80	H	-3.9223	2.2047	1.8717
81	C	0.1472	4.5376	0.3251
82	H	0.6046	4.0128	-0.5223
83	H	0.8944	5.2480	0.7128
84	H	-0.6903	5.1302	-0.0636
85	C	-2.4798	2.5113	-0.4002
86	H	-3.1978	1.6834	-0.2920
87	C	-3.2287	3.8207	-0.1580
88	H	-3.6279	3.9065	0.8593
89	H	-4.0796	3.8880	-0.8539
90	H	-2.5941	4.6964	-0.3393
91	C	-1.9314	2.4568	-1.8272
92	H	-1.1608	3.2228	-1.9965
93	H	-2.7391	2.6314	-2.5551
94	H	-1.4841	1.4755	-2.0441
95	C	-0.2889	3.5818	1.4320
96	H	0.6236	3.1599	1.8789
97	C	-1.0550	4.2937	2.5405
98	H	-1.9731	4.7673	2.1677
99	H	-0.4299	5.0848	2.9858
100	H	-1.3364	3.5971	3.3414
101	C	-5.4738	1.2597	3.8427
102	H	-5.6377	1.6102	4.8733
103	H	-6.0969	0.3607	3.7126
104	H	-5.8518	2.0307	3.1582

/db/nbandeira/Fe(NPiso)/BIH/0e-/BIH
Energy (POTENTIAL) = -689.53956096799789 Eh

	Atom	X	Y	Z
1	C	1.3577	-3.0862	-1.4175
2	C	2.6477	-3.5971	-1.1490
3	C	1.0535	-1.8095	-0.9721
4	H	2.9032	-4.5998	-1.4931
5	C	3.5800	-2.8465	-0.4431
6	C	2.0047	-1.0434	-0.2537
7	H	4.5668	-3.2603	-0.2334
8	C	3.2634	-1.5511	0.0251
9	H	3.9900	-0.9718	0.5942
10	H	0.6218	-3.6848	-1.9536
11	N	-0.0887	-1.0471	-1.1011
12	N	1.4292	0.1764	0.0377
13	C	1.9553	1.0952	1.0047
14	H	1.8331	0.7446	2.0454
15	H	3.0251	1.2574	0.8188
16	H	1.4465	2.0626	0.9059
17	C	-1.3588	-1.5658	-1.5166
18	H	-2.0334	-0.7343	-1.7582
19	H	-1.2335	-2.1714	-2.4237
20	H	-1.8442	-2.1917	-0.7463
21	C	-0.0028	0.1122	-0.2263
22	H	-0.3348	1.0224	-0.7580
23	C	-0.8399	-0.0163	1.0408
24	C	-1.7315	0.9945	1.4024
25	C	-0.7093	-1.1409	1.8669
26	C	-2.4857	0.8931	2.5746
27	C	-1.4599	-1.2465	3.0364
28	C	-2.3501	-0.2281	3.3934
29	H	-1.8365	1.8704	0.7590
30	H	-0.0180	-1.9387	1.5920
31	H	-3.1791	1.6893	2.8467
32	H	-1.3525	-2.1255	3.6725
33	H	-2.9370	-0.3120	4.3085

/db/nbandeira/Fe(NPiso)/L=CO2/CO2
Energy (POTENTIAL) = -188.11766132012451 Eh

	Atom	X	Y	Z
1	C	-0.0000	0.0000	0.0000
2	O	0.0000	-0.0000	-1.1593
3	O	0.0000	-0.0000	1.1593

/db/nbandeira/Fe(NPiso)/_Ir(ppy)2(dtb-bpy)_+/0e-/triplet_state
Energy (POTENTIAL) = -19596.21153441006027 Eh

	Atom	X	Y	Z
1	C	-1.4868	2.7648	-0.1884
2	H	-0.4823	3.1946	-0.2127
3	C	-2.5927	3.5759	-0.2898
4	C	-3.8986	2.9960	-0.2410
5	C	-3.9661	1.6288	-0.1027
6	H	-4.9335	1.1295	-0.0643
7	C	-2.7969	0.8241	-0.0090
8	C	-2.8057	-0.5902	0.1180
9	C	-3.9780	-1.3867	0.1884
10	H	-4.9452	-0.8848	0.1270
11	C	-3.9251	-2.7573	0.3364
12	C	-2.6315	-3.3458	0.4158
13	C	-1.5159	-2.5397	0.3332
14	H	-0.5158	-2.9778	0.3807
15	C	1.4391	1.5504	-0.0850
16	C	2.0899	2.2512	0.9480
17	H	1.8795	2.0041	1.9919
18	C	3.0051	3.2563	0.6556
19	H	3.5094	3.7901	1.4667
20	C	3.2855	3.5899	-0.6765
21	H	4.0039	4.3834	-0.9013
22	C	2.6515	2.9181	-1.7211
23	H	2.8844	3.1910	-2.7536
24	C	1.7300	1.9096	-1.4338
25	C	1.0084	1.1464	-2.4503
26	C	1.1112	1.3235	-3.8311
27	H	1.7803	2.0856	-4.2332
28	C	0.3576	0.5260	-4.6838
29	H	0.4328	0.6571	-5.7666
30	C	-0.4922	-0.4372	-4.1425
31	H	-1.1037	-1.0847	-4.7742
32	C	-0.5547	-0.5689	-2.7625
33	H	-1.1993	-1.3072	-2.2820
34	C	1.4222	-1.3545	0.2940
35	C	2.0913	-2.0627	-0.7221
36	H	1.9070	-1.8163	-1.7711
37	C	2.9916	-3.0741	-0.4062
38	H	3.5106	-3.6137	-1.2042

39	C	3.2384	-3.4067	0.9328
40	H	3.9453	-4.2051	1.1759
41	C	2.5854	-2.7279	1.9610
42	H	2.7922	-3.0004	2.9992
43	C	1.6783	-1.7131	1.6501
44	C	0.9389	-0.9423	2.6483
45	C	1.0070	-1.1182	4.0313
46	H	1.6598	-1.8854	4.4502
47	C	0.2399	-0.3132	4.8648
48	H	0.2882	-0.4434	5.9493
49	C	-0.5888	0.6562	4.3023
50	H	-1.2099	1.3095	4.9185
51	C	-0.6175	0.7863	2.9210
52	H	-1.2447	1.5286	2.4239
53	Ir	0.1027	0.1040	0.0882
54	N	-1.5551	1.4290	-0.0400
55	N	-1.5704	-1.2072	0.1785
56	N	0.1779	0.1972	-1.9468
57	N	0.1283	0.0130	2.1242
58	H	-2.4452	4.6518	-0.3986
59	H	-2.4888	-4.4193	0.5337
60	C	-5.1291	3.8899	-0.3346
61	C	-5.2123	-3.5794	0.4045
62	C	-4.9295	-5.0718	0.5929
63	H	-5.8839	-5.6243	0.6402
64	H	-4.3434	-5.4865	-0.2454
65	H	-4.3803	-5.2692	1.5299
66	C	-5.9961	-3.3929	-0.9042
67	H	-5.4020	-3.7347	-1.7703
68	H	-6.9312	-3.9811	-0.8754
69	H	-6.2651	-2.3356	-1.0700
70	C	-5.0840	4.6706	-1.6583
71	H	-4.1808	5.2999	-1.7328
72	H	-5.0940	3.9814	-2.5213
73	H	-5.9645	5.3333	-1.7368
74	C	-6.4316	3.0898	-0.2846
75	H	-7.2916	3.7784	-0.3535
76	H	-6.5046	2.3760	-1.1235
77	H	-6.5284	2.5260	0.6594
78	C	-5.1151	4.8778	0.8431
79	H	-5.9926	5.5469	0.7880

80	H	-5.1532	4.3395	1.8068
81	H	-4.2093	5.5081	0.8389
82	C	-6.0649	-3.0923	1.5867
83	H	-6.3414	-2.0294	1.4803
84	H	-6.9982	-3.6803	1.6482
85	H	-5.5201	-3.2112	2.5401

/db/nbandeira/Fe(NPiso)/_Ir(ppy)2(dtb-bpy)_+/1e-/Ir(ppy)2(dtb-bpy)_+1e-+1H+
Energy (POTENTIAL) = -19597.23307627491886 Eh

	Atom	X	Y	Z
1	C	-1.6366	2.7455	-0.3448
2	H	-0.6302	3.1710	-0.3611
3	C	-2.7589	3.5450	-0.4705
4	C	-4.0387	2.9694	-0.4424
5	C	-4.0945	1.5840	-0.2892
6	H	-5.0545	1.0706	-0.2722
7	C	-2.9263	0.8316	-0.1660
8	C	-2.9175	-0.6356	0.0031
9	C	-4.0379	-1.3726	0.2645
10	H	-5.0047	-0.8723	0.3322
11	C	-3.9838	-2.8306	0.5390
12	C	-2.6542	-3.3835	0.1736
13	C	-1.5883	-2.5719	-0.0792
14	H	-0.5945	-2.9815	-0.2760
15	C	1.3948	1.4886	-0.0105
16	C	2.0014	2.0997	1.0971
17	H	1.7008	1.8140	2.1099
18	C	2.9886	3.0728	0.9364
19	H	3.4441	3.5342	1.8191
20	C	3.4031	3.4633	-0.3417
21	H	4.1771	4.2265	-0.4636
22	C	2.8239	2.8721	-1.4594
23	H	3.1492	3.1775	-2.4582
24	C	1.8317	1.8944	-1.2972
25	C	1.1660	1.2233	-2.4107
26	C	1.4217	1.4421	-3.7684
27	H	2.1769	2.1718	-4.0646
28	C	0.7175	0.7314	-4.7302
29	H	0.9159	0.8982	-5.7925
30	C	-0.2437	-0.1947	-4.3227
31	H	-0.8238	-0.7770	-5.0415
32	C	-0.4579	-0.3704	-2.9650
33	H	-1.1973	-1.0818	-2.5923
34	C	1.3558	-1.3030	0.2019
35	C	2.1495	-1.9112	-0.7821
36	H	2.0571	-1.6002	-1.8272
37	C	3.0615	-2.9161	-0.4558
38	H	3.6681	-3.3742	-1.2442

39	C	3.2084	-3.3429	0.8685
40	H	3.9236	-4.1315	1.1198
41	C	2.4384	-2.7553	1.8665
42	H	2.5553	-3.0887	2.9017
43	C	1.5233	-1.7447	1.5387
44	C	0.6782	-1.0689	2.5194
45	C	0.6558	-1.3252	3.8944
46	H	1.3044	-2.0979	4.3096
47	C	-0.1867	-0.5962	4.7222
48	H	-0.2067	-0.7939	5.7975
49	C	-1.0008	0.3904	4.1648
50	H	-1.6759	0.9936	4.7751
51	C	-0.9426	0.5978	2.7959
52	H	-1.5580	1.3575	2.3112
53	Ir	-0.0530	0.0990	-0.0315
54	N	-1.7137	1.4180	-0.1901
55	N	-1.6745	-1.2165	-0.0987
56	N	0.2257	0.3142	-2.0369
57	N	-0.1340	-0.1115	1.9966
58	H	-2.6196	4.6215	-0.5897
59	H	-2.5070	-4.4656	0.1497
60	C	-5.2835	3.8390	-0.5684
61	C	-4.3796	-3.1600	2.0459
62	C	-4.3773	-4.6777	2.2375
63	H	-4.7436	-4.9223	3.2500
64	H	-5.0405	-5.1747	1.5069
65	H	-3.3668	-5.1088	2.1385
66	C	-5.7883	-2.6292	2.3189
67	H	-6.5142	-3.0271	1.5872
68	H	-6.1141	-2.9432	3.3262
69	H	-5.8332	-1.5274	2.2875
70	C	-5.2178	4.6162	-1.8929
71	H	-4.3313	5.2710	-1.9426
72	H	-5.1867	3.9258	-2.7541
73	H	-6.1139	5.2533	-1.9942
74	C	-6.5690	3.0104	-0.5470
75	H	-7.4385	3.6830	-0.6424
76	H	-6.6068	2.2926	-1.3845
77	H	-6.6811	2.4513	0.3980
78	C	-5.3090	4.8247	0.6112
79	H	-6.2033	5.4686	0.5397

80	H	-5.3485	4.2856	1.5741
81	H	-4.4205	5.4790	0.6181
82	C	-3.3811	-2.5100	3.0046
83	H	-3.3729	-1.4108	2.8992
84	H	-3.6535	-2.7462	4.0485
85	H	-2.3542	-2.8784	2.8322
86	H	-4.7706	-3.3369	-0.0587

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/1e-/1-Cl+NCMe
Energy (POTENTIAL) = -4456.33950670902868 Eh

	Atom	X	Y	Z
1	Fe	-0.0321	-0.0789	0.0712
2	P	-0.7476	-2.2163	-0.7124
3	P	-1.6250	1.5229	-0.5651
4	P	2.0363	0.5396	-0.9525
5	Cl	0.0765	-0.1865	2.4509
6	N	-0.3242	-0.0541	-2.8191
7	C	0.2485	-1.3054	-3.1816
8	C	0.9855	-1.4228	-4.3643
9	H	1.1172	-0.5462	-4.9970
10	C	1.5455	-2.6404	-4.7359
11	H	2.1228	-2.7068	-5.6592
12	C	1.3578	-3.7822	-3.9486
13	C	0.6046	-3.6521	-2.7768
14	H	0.4547	-4.5431	-2.1677
15	C	0.0667	-2.4302	-2.3553
16	C	1.9687	-5.1006	-4.3321
17	H	1.9288	-5.2607	-5.4181
18	H	1.4565	-5.9375	-3.8401
19	H	3.0285	-5.1436	-4.0369
20	C	-1.7396	0.0528	-2.9542
21	C	-2.3983	-0.6264	-3.9830
22	H	-1.8203	-1.2453	-4.6679
23	C	-3.7786	-0.5304	-4.1311
24	H	-4.2719	-1.0828	-4.9321
25	C	-4.5346	0.2742	-3.2722
26	C	-3.8603	0.9541	-2.2505
27	H	-4.4547	1.5620	-1.5689
28	C	-2.4788	0.8469	-2.0536
29	C	-6.0201	0.4198	-3.4467
30	H	-6.2540	1.1826	-4.2055
31	H	-6.5053	0.7283	-2.5116
32	H	-6.4789	-0.5205	-3.7805
33	C	0.4058	1.1171	-3.1783
34	C	-0.0482	1.9103	-4.2382
35	H	-0.9262	1.5922	-4.7985
36	C	0.5809	3.1077	-4.5598
37	H	0.1960	3.7149	-5.3802
38	C	1.6942	3.5390	-3.8313

39	C	2.1537	2.7214	-2.7933
40	H	3.0083	3.0761	-2.2244
41	C	1.5408	1.5115	-2.4427
42	C	2.3893	4.8296	-4.1619
43	H	3.0122	5.1740	-3.3265
44	H	1.6684	5.6218	-4.4051
45	H	3.0461	4.7101	-5.0373
46	C	-0.1040	-3.6848	0.2617
47	H	-0.3879	-4.6067	-0.2688
48	C	1.4162	-3.6000	0.3762
49	H	1.6958	-2.7287	0.9840
50	H	1.9249	-3.5130	-0.5909
51	H	1.8027	-4.4980	0.8817
52	C	-0.6868	-3.7294	1.6770
53	H	-0.1578	-4.5010	2.2574
54	H	-1.7511	-3.9762	1.7029
55	H	-0.5439	-2.7662	2.1869
56	C	-2.5366	-2.6585	-1.1443
57	H	-2.9028	-1.7192	-1.5798
58	C	-2.6727	-3.7553	-2.1946
59	H	-2.2248	-4.7012	-1.8544
60	H	-2.2034	-3.4815	-3.1472
61	H	-3.7394	-3.9474	-2.3901
62	C	-3.4148	-2.9789	0.0637
63	H	-4.4714	-2.8507	-0.2158
64	H	-3.2211	-2.3362	0.9293
65	H	-3.2896	-4.0229	0.3805
66	C	-3.0237	1.7628	0.6517
67	H	-3.8191	2.3495	0.1693
68	C	-3.5758	0.4012	1.0573
69	H	-2.7882	-0.2015	1.5288
70	H	-3.9655	-0.1616	0.1999
71	H	-4.3952	0.5217	1.7829
72	C	-2.5412	2.5317	1.8818
73	H	-3.3189	2.5026	2.6602
74	H	-2.3390	3.5865	1.6621
75	H	-1.6308	2.0792	2.3002
76	C	-1.1876	3.2649	-1.1241
77	H	-0.6614	3.0747	-2.0685
78	C	-2.3889	4.1514	-1.4291
79	H	-2.9447	4.4189	-0.5191

80	H	-3.0876	3.6667	-2.1251
81	H	-2.0532	5.0905	-1.8958
82	C	-0.1888	3.9345	-0.1844
83	H	0.2614	4.8100	-0.6761
84	H	0.6225	3.2465	0.0856
85	H	-0.6567	4.2824	0.7448
86	C	3.1363	1.7420	-0.0065
87	H	2.5684	2.6818	-0.0829
88	C	4.5576	2.0072	-0.5073
89	H	4.9736	2.8647	0.0436
90	H	4.6238	2.2402	-1.5755
91	H	5.2176	1.1526	-0.3161
92	C	3.1739	1.3614	1.4742
93	H	3.7359	0.4308	1.6360
94	H	2.1684	1.2145	1.8881
95	H	3.6790	2.1549	2.0463
96	C	3.1687	-0.7979	-1.6474
97	H	2.4410	-1.5512	-1.9770
98	C	4.0085	-0.4130	-2.8601
99	H	4.7937	0.3113	-2.6105
100	H	3.3947	0.0140	-3.6634
101	H	4.5025	-1.3114	-3.2622
102	C	4.0138	-1.4398	-0.5484
103	H	4.4155	-2.3997	-0.9066
104	H	3.4325	-1.6442	0.3588
105	H	4.8691	-0.8142	-0.2649
106	C	-3.2518	-1.4849	4.2326
107	N	-3.6818	-2.4662	3.7910
108	C	-2.6967	-0.2557	4.7656
109	H	-1.7468	-0.0432	4.2512
110	H	-2.5174	-0.3560	5.8438
111	H	-3.3905	0.5770	4.5930

/db/nbandeira/Fe(NPiso)/L=CO2/H2O
Energy (POTENTIAL) = -76.32431195 Eh

	Atom	X	Y	Z
1	O	0.0000	-0.0000	-0.0645
2	H	0.0000	0.7616	0.5283
3	H	0.0000	-0.7616	0.5283

/db/nbandeira/Fe(NPiso)/L=CO2/2e-/1-CO2+2e-
Energy (POTENTIAL) = -4061.27922043 Eh

	Atom	X	Y	Z
1	Fe	-0.0168	0.0196	0.1107
2	P	-0.6031	-2.1247	-0.6407
3	P	-1.6168	1.5585	-0.5953
4	P	1.9682	0.6841	-1.0173
5	N	-0.2971	-0.0621	-2.8587
6	C	0.2733	-1.3225	-3.1906
7	C	0.9828	-1.4823	-4.3838
8	H	1.1250	-0.6239	-5.0387
9	C	1.4953	-2.7248	-4.7452
10	H	2.0515	-2.8259	-5.6781
11	C	1.2820	-3.8462	-3.9380
12	C	0.5824	-3.6653	-2.7390
13	H	0.4363	-4.5375	-2.1025
14	C	0.1013	-2.4191	-2.3242
15	C	1.7720	-5.2092	-4.3390
16	H	0.9454	-5.8279	-4.7211
17	H	2.2089	-5.7459	-3.4857
18	H	2.5300	-5.1453	-5.1302
19	C	-1.7118	0.0433	-2.9823
20	C	-2.3799	-0.6555	-3.9918
21	H	-1.8151	-1.3251	-4.6391
22	C	-3.7494	-0.5004	-4.1778
23	H	-4.2525	-1.0657	-4.9637
24	C	-4.4782	0.3927	-3.3857
25	C	-3.7961	1.0741	-2.3712
26	H	-4.3757	1.7459	-1.7403
27	C	-2.4306	0.8923	-2.1181
28	C	-5.9449	0.6236	-3.6172
29	H	-6.1048	1.3817	-4.3996
30	H	-6.4431	0.9819	-2.7069
31	H	-6.4477	-0.2949	-3.9479
32	C	0.4107	1.0937	-3.2967
33	C	-0.0574	1.8280	-4.3930
34	H	-0.9458	1.4865	-4.9220
35	C	0.5807	2.9951	-4.7929
36	H	0.1907	3.5574	-5.6425
37	C	1.7162	3.4535	-4.1138
38	C	2.1795	2.7013	-3.0306

39	H	3.0452	3.0806	-2.4957
40	C	1.5475	1.5283	-2.5951
41	C	2.4109	4.7176	-4.5346
42	H	3.2072	4.9901	-3.8302
43	H	1.7050	5.5585	-4.5943
44	H	2.8650	4.6072	-5.5306
45	C	0.0619	-3.6044	0.3088
46	H	-0.3057	-4.5051	-0.2063
47	C	1.5885	-3.6044	0.3152
48	H	1.9576	-2.7586	0.9084
49	H	2.0384	-3.5378	-0.6821
50	H	1.9561	-4.5276	0.7881
51	C	-0.4074	-3.6646	1.7637
52	H	0.0177	-4.5662	2.2304
53	H	-1.4927	-3.7147	1.8749
54	H	-0.0486	-2.7968	2.3304
55	C	-2.4244	-2.5172	-0.9385
56	H	-2.7752	-1.5912	-1.4126
57	C	-2.6711	-3.6699	-1.9050
58	H	-2.2559	-4.6158	-1.5258
59	H	-2.2392	-3.4817	-2.8957
60	H	-3.7550	-3.8155	-2.0336
61	C	-3.2290	-2.7022	0.3469
62	H	-4.2931	-2.5168	0.1374
63	H	-2.9106	-2.0163	1.1411
64	H	-3.1490	-3.7327	0.7193
65	C	-3.0943	1.9719	0.4786
66	H	-3.7077	2.6842	-0.0927
67	C	-3.9343	0.7429	0.8161
68	H	-3.3787	0.0892	1.4971
69	H	-4.2149	0.1578	-0.0680
70	H	-4.8628	1.0628	1.3149
71	C	-2.6495	2.6682	1.7650
72	H	-3.5185	2.7960	2.4280
73	H	-2.2293	3.6631	1.5823
74	H	-1.9060	2.0685	2.3077
75	C	-1.0267	3.2516	-1.1704
76	H	-0.3785	2.9810	-2.0114
77	C	-2.1158	4.1728	-1.7047
78	H	-2.7846	4.5236	-0.9058
79	H	-2.7266	3.6813	-2.4747

80	H	-1.6583	5.0636	-2.1626
81	C	-0.1470	3.9455	-0.1294
82	H	0.5626	4.6227	-0.6273
83	H	0.4340	3.2281	0.4661
84	H	-0.7381	4.5518	0.5689
85	C	2.9963	1.9863	-0.1274
86	H	2.4341	2.9035	-0.3573
87	C	4.4474	2.2073	-0.5611
88	H	4.8086	3.1492	-0.1208
89	H	4.5888	2.2764	-1.6448
90	H	5.1050	1.4101	-0.1950
91	C	2.9340	1.7886	1.3869
92	H	3.4888	0.8929	1.6991
93	H	1.9052	1.6743	1.7474
94	H	3.3921	2.6545	1.8886
95	C	3.1300	-0.7073	-1.5148
96	H	2.4212	-1.5049	-1.7745
97	C	3.9980	-0.4505	-2.7407
98	H	4.7628	0.3147	-2.5572
99	H	3.3988	-0.1351	-3.6042
100	H	4.5188	-1.3797	-3.0193
101	C	3.9512	-1.1926	-0.3210
102	H	4.3369	-2.2025	-0.5233
103	H	3.3602	-1.2438	0.6018
104	H	4.8141	-0.5439	-0.1302
105	C	-0.7568	-0.3515	1.8161
106	O	-1.6729	-0.6302	2.5815
107	O	0.4819	-0.1555	2.0645

/db/nbandeira/Fe(NPiso)/BIH/1e-/BIH+
Energy (POTENTIAL) = -689.36539451065141 Eh

	Atom	X	Y	Z
1	C	1.4108	-3.1221	-1.5490
2	C	2.7273	-3.5394	-1.4629
3	C	1.0753	-1.9182	-0.9073
4	H	3.0247	-4.4678	-1.9489
5	C	3.7063	-2.7902	-0.7574
6	C	2.0614	-1.1691	-0.1818
7	H	4.7299	-3.1611	-0.7245
8	C	3.3946	-1.6054	-0.1136
9	H	4.1490	-1.0342	0.4230
10	H	0.6656	-3.7020	-2.0891
11	N	-0.0901	-1.2575	-0.8248
12	N	1.4583	-0.0929	0.3489
13	C	2.0754	0.9723	1.0967
14	H	2.9426	0.5858	1.6414
15	H	2.3973	1.7822	0.4264
16	H	1.3536	1.3701	1.8190
17	C	-1.3649	-1.6534	-1.3659
18	H	-1.9081	-0.7629	-1.7030
19	H	-1.2091	-2.3173	-2.2215
20	H	-1.9658	-2.1733	-0.6063
21	C	0.0553	-0.0552	-0.0234
22	H	-0.1360	0.8290	-0.6590
23	C	-0.8771	-0.0220	1.1700
24	C	-1.8213	0.9979	1.2911
25	C	-0.7942	-1.0232	2.1446
26	C	-2.6863	1.0203	2.3876
27	C	-1.6575	-0.9990	3.2372
28	C	-2.6044	0.0231	3.3593
29	H	-1.8805	1.7749	0.5282
30	H	-0.0555	-1.8207	2.0518
31	H	-3.4225	1.8185	2.4803
32	H	-1.5926	-1.7780	3.9967
33	H	-3.2787	0.0402	4.2157

/db/nbandeira/Fe(NPiso)/BIH/1e-/BI+
Energy (POTENTIAL) = -688.74255152645094 Eh

	Atom	X	Y	Z
1	C	1.4422	-2.8840	-2.0484
2	C	2.7902	-3.0368	-2.3542
3	C	1.1383	-2.0502	-0.9717
4	H	3.0759	-3.6775	-3.1875
5	C	3.7961	-2.3826	-1.6151
6	C	2.1385	-1.4003	-0.2364
7	H	4.8393	-2.5323	-1.8908
8	C	3.4915	-1.5520	-0.5422
9	H	4.2688	-1.0501	0.0307
10	H	0.6654	-3.3856	-2.6222
11	N	-0.0695	-1.6877	-0.4031
12	N	1.4947	-0.6604	0.7393
13	C	2.1683	0.2096	1.6843
14	H	2.6273	-0.3839	2.4836
15	H	2.9427	0.7736	1.1540
16	H	1.4471	0.9095	2.1134
17	C	-1.3601	-2.1920	-0.8320
18	H	-2.0956	-2.0308	-0.0400
19	H	-1.6824	-1.6786	-1.7454
20	H	-1.2721	-3.2662	-1.0253
21	C	0.1707	-0.8514	0.6200
22	C	-0.8515	-0.2423	1.4716
23	C	-1.8852	0.5100	0.8944
24	C	-0.7954	-0.4131	2.8627
25	C	-2.8551	1.0889	1.7092
26	C	-1.7728	0.1653	3.6690
27	C	-2.8006	0.9161	3.0940
28	H	-1.9184	0.6551	-0.1851
29	H	-0.0006	-1.0103	3.3087
30	H	-3.6535	1.6792	1.2609
31	H	-1.7330	0.0255	4.7487
32	H	-3.5627	1.3687	3.7282

/db/nbandeira/Fe(NPiso)/L=Cl/2e-/1-Cl+NCMe
Energy (POTENTIAL) = -4466.93422870 Eh

	Atom	X	Y	Z
1	Fe	-0.0297	-0.1152	0.0354
2	P	-0.7673	-2.2263	-0.7603
3	P	-1.6281	1.4896	-0.5325
4	P	2.0227	0.5765	-1.0248
5	Cl	0.1428	-0.3075	2.4323
6	N	-0.3465	-0.0256	-2.8216
7	C	0.2502	-1.2615	-3.1891
8	C	1.0525	-1.3371	-4.3336
9	H	1.2162	-0.4308	-4.9151
10	C	1.6115	-2.5476	-4.7334
11	H	2.2400	-2.5828	-5.6252
12	C	1.3605	-3.7228	-4.0126
13	C	0.5627	-3.6306	-2.8686
14	H	0.3698	-4.5445	-2.3069
15	C	0.0298	-2.4139	-2.4140
16	C	1.9566	-5.0358	-4.4398
17	H	1.8841	-5.1754	-5.5277
18	H	1.4536	-5.8811	-3.9521
19	H	3.0249	-5.0923	-4.1791
20	C	-1.7573	0.0604	-2.9374
21	C	-2.4137	-0.6150	-3.9708
22	H	-1.8294	-1.2082	-4.6727
23	C	-3.8059	-0.5387	-4.0993
24	H	-4.3039	-1.0884	-4.8999
25	C	-4.5592	0.2415	-3.2249
26	C	-3.8813	0.9356	-2.2040
27	H	-4.4757	1.5378	-1.5171
28	C	-2.4966	0.8436	-2.0252
29	C	-6.0552	0.3394	-3.3401
30	H	-6.3813	1.3831	-3.4630
31	H	-6.5522	-0.0450	-2.4364
32	H	-6.4288	-0.2342	-4.1983
33	C	0.3587	1.1523	-3.2053
34	C	-0.1564	1.9811	-4.1899
35	H	-1.0999	1.7070	-4.6627
36	C	0.5112	3.1689	-4.5755
37	H	0.0839	3.8245	-5.3351
38	C	1.7668	3.4673	-3.9812

39	C	2.2898	2.6140	-3.0245
40	H	3.2527	2.8778	-2.5926
41	C	1.6041	1.4335	-2.5601
42	C	2.5171	4.7024	-4.4018
43	H	3.4503	4.8229	-3.8346
44	H	1.9112	5.6106	-4.2512
45	H	2.7744	4.6762	-5.4734
46	C	-0.1396	-3.7396	0.1621
47	H	-0.4529	-4.6384	-0.3915
48	C	1.3832	-3.7019	0.2631
49	H	1.6916	-2.8621	0.8992
50	H	1.8849	-3.5890	-0.7053
51	H	1.7503	-4.6286	0.7305
52	C	-0.7058	-3.8120	1.5830
53	H	-0.1910	-4.6132	2.1361
54	H	-1.7761	-4.0314	1.6151
55	H	-0.5313	-2.8667	2.1165
56	C	-2.5666	-2.6533	-1.1717
57	H	-2.9220	-1.7124	-1.6118
58	C	-2.7242	-3.7522	-2.2164
59	H	-2.2995	-4.7067	-1.8697
60	H	-2.2420	-3.4907	-3.1660
61	H	-3.7939	-3.9226	-2.4182
62	C	-3.4445	-2.9552	0.0416
63	H	-4.5006	-2.7984	-0.2266
64	H	-3.2259	-2.3210	0.9077
65	H	-3.3459	-4.0033	0.3552
66	C	-3.0292	1.7585	0.6806
67	H	-3.8149	2.3570	0.1960
68	C	-3.6037	0.4078	1.0914
69	H	-2.8265	-0.2032	1.5700
70	H	-3.9942	-0.1545	0.2341
71	H	-4.4255	0.5417	1.8124
72	C	-2.5412	2.5202	1.9130
73	H	-3.3128	2.4866	2.6977
74	H	-2.3394	3.5758	1.6986
75	H	-1.6272	2.0679	2.3240
76	C	-1.1292	3.2175	-1.0683
77	H	-0.5314	2.9879	-1.9604
78	C	-2.2857	4.1127	-1.4937
79	H	-2.9193	4.4005	-0.6414

80	H	-2.9237	3.6208	-2.2412
81	H	-1.9004	5.0410	-1.9450
82	C	-0.2002	3.9020	-0.0677
83	H	0.3857	4.6837	-0.5753
84	H	0.5091	3.1904	0.3762
85	H	-0.7484	4.3851	0.7512
86	C	3.0568	1.8597	-0.0939
87	H	2.5263	2.7903	-0.3486
88	C	4.5244	2.0500	-0.4818
89	H	4.9152	2.9542	0.0124
90	H	4.6864	2.1685	-1.5585
91	H	5.1448	1.2091	-0.1473
92	C	2.9543	1.6659	1.4178
93	H	3.4971	0.7661	1.7426
94	H	1.9163	1.5472	1.7519
95	H	3.4008	2.5272	1.9411
96	C	3.2175	-0.8233	-1.4747
97	H	2.5054	-1.5893	-1.8153
98	C	4.1673	-0.5544	-2.6344
99	H	4.9832	0.1256	-2.3576
100	H	3.6274	-0.1141	-3.4837
101	H	4.6246	-1.4968	-2.9775
102	C	3.9339	-1.3797	-0.2474
103	H	4.3292	-2.3864	-0.4545
104	H	3.2619	-1.4614	0.6174
105	H	4.7831	-0.7520	0.0528
106	C	-3.1757	-1.4339	4.2608
107	N	-3.6650	-2.3866	3.8181
108	C	-2.5477	-0.2403	4.7931
109	H	-1.6015	-0.0702	4.2552
110	H	-2.3480	-0.3612	5.8656
111	H	-3.2035	0.6274	4.6450

/db/nbandeira/Fe(NPiso)/L=Cl/0e-/1-NCMe+Cl-
Energy (POTENTIAL) = -4466.76716424 Eh

	Atom	X	Y	Z
1	Fe	-0.2984	1.4266	2.6661
2	P	-1.0737	-0.7925	1.9417
3	P	-1.9415	3.1656	2.1502
4	P	1.8928	2.1387	1.8075
5	N	-0.4968	1.5303	0.0354
6	C	0.0823	0.2844	-0.3848
7	C	0.8733	0.2247	-1.5343
8	H	1.0608	1.1312	-2.1067
9	C	1.4226	-0.9819	-1.9549
10	H	2.0416	-1.0013	-2.8525
11	C	1.1773	-2.1675	-1.2546
12	C	0.3736	-2.0949	-0.1126
13	H	0.1807	-3.0167	0.4346
14	C	-0.1647	-0.8899	0.3509
15	C	1.7771	-3.4734	-1.6892
16	H	1.9686	-3.4852	-2.7697
17	H	1.1202	-4.3172	-1.4415
18	H	2.7389	-3.6474	-1.1826
19	C	-1.9126	1.6393	-0.1944
20	C	-2.5073	0.9721	-1.2676
21	H	-1.8976	0.3462	-1.9169
22	C	-3.8706	1.0969	-1.5079
23	H	-4.3159	0.5567	-2.3441
24	C	-4.6729	1.9137	-0.7019
25	C	-4.0617	2.5846	0.3618
26	H	-4.6861	3.2100	0.9988
27	C	-2.6972	2.4507	0.6443
28	C	-6.1437	2.0544	-0.9683
29	H	-6.3252	2.4530	-1.9768
30	H	-6.6191	2.7281	-0.2449
31	H	-6.6493	1.0798	-0.9109
32	C	0.2371	2.6993	-0.3713
33	C	-0.2152	3.4769	-1.4414
34	H	-1.1167	3.1840	-1.9762
35	C	0.4602	4.6330	-1.8135
36	H	0.0792	5.2288	-2.6436
37	C	1.6152	5.0403	-1.1354
38	C	2.0664	4.2428	-0.0805

39	H	2.9552	4.5670	0.4544
40	C	1.4003	3.0780	0.3196
41	C	2.3486	6.2885	-1.5328
42	H	3.1212	6.5491	-0.7989
43	H	1.6608	7.1400	-1.6276
44	H	2.8402	6.1593	-2.5086
45	C	-0.4071	-2.2322	2.9197
46	H	-0.5531	-3.1361	2.3107
47	C	1.0850	-2.0099	3.1530
48	H	1.2482	-1.1262	3.7863
49	H	1.6509	-1.8797	2.2231
50	H	1.5071	-2.8765	3.6819
51	C	-1.1200	-2.4344	4.2567
52	H	-0.5158	-3.1141	4.8752
53	H	-2.1067	-2.8916	4.1422
54	H	-1.2561	-1.5033	4.8228
55	C	-2.8636	-1.1142	1.4948
56	H	-3.1798	-0.1463	1.0841
57	C	-3.0092	-2.1747	0.4089
58	H	-2.6182	-3.1478	0.7405
59	H	-2.4964	-1.8955	-0.5197
60	H	-4.0765	-2.3065	0.1763
61	C	-3.7587	-1.4325	2.6933
62	H	-4.7995	-1.2070	2.4199
63	H	-3.5217	-0.8662	3.6026
64	H	-3.7139	-2.5002	2.9424
65	C	-3.3571	3.3804	3.3320
66	H	-4.1053	4.0038	2.8211
67	C	-3.9719	2.0260	3.6691
68	H	-3.3091	1.4280	4.3098
69	H	-4.2243	1.4389	2.7779
70	H	-4.8998	2.1811	4.2390
71	C	-2.9179	4.1068	4.6036
72	H	-3.7275	4.0472	5.3453
73	H	-2.7119	5.1685	4.4294
74	H	-2.0247	3.6489	5.0515
75	C	-1.3550	4.8630	1.6483
76	H	-0.7170	4.6421	0.7837
77	C	-2.4876	5.7682	1.1790
78	H	-3.1669	6.0343	2.0009
79	H	-3.0773	5.3044	0.3766

80	H	-2.0644	6.7033	0.7833
81	C	-0.4780	5.5215	2.7117
82	H	0.1151	6.3215	2.2463
83	H	0.2201	4.8132	3.1760
84	H	-1.0733	5.9753	3.5126
85	C	2.8446	3.3644	2.8530
86	H	2.2943	4.2991	2.6673
87	C	4.3130	3.5995	2.4987
88	H	4.6764	4.4562	3.0848
89	H	4.4850	3.8295	1.4418
90	H	4.9394	2.7387	2.7596
91	C	2.6935	3.0281	4.3367
92	H	3.1118	2.0422	4.5807
93	H	1.6438	3.0432	4.6509
94	H	3.2336	3.7767	4.9343
95	C	3.0244	0.7667	1.2269
96	H	2.3109	0.0207	0.8502
97	C	3.9448	1.1471	0.0734
98	H	4.7072	1.8766	0.3724
99	H	3.3857	1.5611	-0.7753
100	H	4.4655	0.2444	-0.2793
101	C	3.7752	0.1352	2.3985
102	H	4.1925	-0.8303	2.0789
103	H	3.1252	-0.0541	3.2616
104	H	4.6113	0.7589	2.7361
105	C	-0.2570	1.1948	5.8444
106	N	-0.2555	1.3198	4.6953
107	C	-0.2874	1.0189	7.2709
108	H	-0.1761	1.9891	7.7725
109	H	0.5235	0.3461	7.5798
110	H	-1.2739	0.5668	7.4978
111	Cl	-3.3017	-0.3107	6.5957

/db/nbandeira/Fe(NPiso)/_Ir(ppy)2(dtb-bpy)_+/1e-/Ir(ppy)2(dtb-bpy)+_+1e-
Energy (POTENTIAL) = -19596.40354413244495 Eh

	Atom	X	Y	Z
1	C	-1.5349	2.7711	-0.1379
2	H	-0.5251	3.1925	-0.1587
3	C	-2.6427	3.5910	-0.2180
4	C	-3.9458	3.0064	-0.1821
5	C	-4.0127	1.6350	-0.0765
6	H	-4.9809	1.1357	-0.0485
7	C	-2.8407	0.8285	-0.0013
8	C	-2.8498	-0.5905	0.1078
9	C	-4.0247	-1.3884	0.1607
10	H	-4.9932	-0.8870	0.1097
11	C	-3.9719	-2.7635	0.2765
12	C	-2.6814	-3.3571	0.3437
13	C	-1.5638	-2.5426	0.2812
14	H	-0.5586	-2.9730	0.3252
15	C	1.4751	1.4828	-0.1173
16	C	2.1805	2.1706	0.8848
17	H	1.9713	1.9569	1.9382
18	C	3.1455	3.1278	0.5703
19	H	3.6768	3.6485	1.3746
20	C	3.4423	3.4291	-0.7643
21	H	4.1991	4.1808	-1.0076
22	C	2.7670	2.7626	-1.7813
23	H	3.0004	2.9979	-2.8242
24	C	1.7972	1.8003	-1.4632
25	C	1.0401	1.0521	-2.4632
26	C	1.1729	1.1749	-3.8510
27	H	1.8938	1.8830	-4.2629
28	C	0.3915	0.3984	-4.6950
29	H	0.4935	0.4908	-5.7799
30	C	-0.5231	-0.4974	-4.1388
31	H	-1.1613	-1.1288	-4.7607
32	C	-0.6135	-0.5776	-2.7578
33	H	-1.3086	-1.2610	-2.2669
34	C	1.4567	-1.2872	0.3246
35	C	2.1811	-1.9813	-0.6595
36	H	2.0009	-1.7653	-1.7178
37	C	3.1290	-2.9473	-0.3210
38	H	3.6760	-3.4727	-1.1116

39	C	3.3887	-3.2518	1.0206
40	H	4.1320	-4.0106	1.2828
41	C	2.6937	-2.5796	2.0205
42	H	2.8982	-2.8176	3.0688
43	C	1.7412	-1.6083	1.6781
44	C	0.9657	-0.8534	2.6590
45	C	1.0610	-0.9788	4.0496
46	H	1.7637	-1.6946	4.4793
47	C	0.2656	-0.1951	4.8739
48	H	0.3385	-0.2896	5.9610
49	C	-0.6251	0.7102	4.2952
50	H	-1.2729	1.3474	4.9010
51	C	-0.6790	0.7924	2.9124
52	H	-1.3543	1.4827	2.4040
53	Ir	0.0355	0.1049	0.0859
54	N	-1.6004	1.4387	-0.0247
55	N	-1.6160	-1.2134	0.1599
56	N	0.1442	0.1698	-1.9430
57	N	0.0923	0.0381	2.1168
58	H	-2.4984	4.6696	-0.3045
59	H	-2.5413	-4.4333	0.4403
60	C	-5.1797	3.8997	-0.2545
61	C	-5.2620	-3.5844	0.3262
62	C	-4.9839	-5.0829	0.4680
63	H	-5.9398	-5.6343	0.4988
64	H	-4.3990	-5.4727	-0.3830
65	H	-4.4344	-5.3112	1.3978
66	C	-6.0540	-3.3585	-0.9712
67	H	-5.4658	-3.6757	-1.8507
68	H	-6.9905	-3.9452	-0.9549
69	H	-6.3214	-2.2963	-1.1046
70	C	-5.1402	4.7102	-1.5602
71	H	-4.2376	5.3417	-1.6228
72	H	-5.1509	4.0402	-2.4383
73	H	-6.0219	5.3733	-1.6227
74	C	-6.4813	3.0970	-0.2209
75	H	-7.3429	3.7853	-0.2739
76	H	-6.5537	2.4015	-1.0750
77	H	-6.5760	2.5118	0.7102
78	C	-5.1687	4.8623	0.9438
79	H	-6.0478	5.5308	0.9046

80	H	-5.2043	4.3032	1.8958
81	H	-4.2640	5.4943	0.9525
82	C	-6.1077	-3.1319	1.5267
83	H	-6.3806	-2.0653	1.4538
84	H	-7.0429	-3.7186	1.5768
85	H	-5.5579	-3.2805	2.4731

/db/nbandeira/Fe(NPiso)/1_with_vacancy
Energy (POTENTIAL) = -3872.67903567 Eh

	Atom	X	Y	Z
1	Fe	-0.0383	-0.0283	0.3739
2	P	2.3320	-0.1137	0.6684
3	P	-1.2421	-2.1052	0.7160
4	P	-1.2567	2.0011	0.8046
5	N	-0.0140	-0.0887	2.6201
6	C	2.2075	0.9119	2.1832
7	C	1.0384	0.8493	2.9677
8	C	0.9017	1.6835	4.0758
9	H	0.0011	1.6354	4.6849
10	C	1.9080	2.5881	4.4020
11	H	1.7771	3.2382	5.2673
12	C	3.0827	2.6687	3.6464
13	C	3.2133	1.8108	2.5487
14	H	4.1281	1.8599	1.9578
15	C	4.1615	3.6585	3.9753
16	H	4.1110	4.5239	3.2973
17	H	5.1591	3.2141	3.8614
18	H	4.0610	4.0330	5.0014
19	C	3.2441	-1.6544	1.2208
20	H	2.4508	-2.2615	1.6785
21	C	3.8483	-2.4511	0.0676
22	H	3.1469	-2.6176	-0.7575
23	H	4.1533	-3.4355	0.4501
24	H	4.7468	-1.9604	-0.3293
25	C	4.2999	-1.3446	2.2771
26	H	5.0662	-0.6564	1.8920
27	H	4.8029	-2.2808	2.5601
28	H	3.8688	-0.9084	3.1859
29	C	3.3673	0.8488	-0.5353
30	H	4.3940	0.8903	-0.1405
31	C	2.8008	2.2581	-0.6885
32	H	1.7858	2.2160	-1.1096
33	H	3.4250	2.8254	-1.3934
34	H	2.7574	2.8205	0.2508
35	C	3.3662	0.1644	-1.9054
36	H	3.8698	-0.8059	-1.9113
37	H	3.8883	0.8125	-2.6237
38	H	2.3388	0.0212	-2.2727

39	C	-0.2455	-2.5148	2.1944
40	C	0.2961	-1.4660	2.9607
41	C	1.1182	-1.7555	4.0487
42	H	1.5330	-0.9452	4.6455
43	C	1.4160	-3.0755	4.3710
44	H	2.0655	-3.2802	5.2224
45	C	0.8922	-4.1395	3.6268
46	C	0.0588	-3.8341	2.5457
47	H	-0.3468	-4.6566	1.9568
48	C	1.2331	-5.5609	3.9658
49	H	2.2705	-5.7897	3.6796
50	H	0.5769	-6.2664	3.4418
51	H	1.1473	-5.7417	5.0458
52	C	-0.9559	-3.4654	-0.5048
53	H	-1.2690	-4.4051	-0.0264
54	C	-1.8016	-3.2383	-1.7574
55	H	-2.8755	-3.3435	-1.5658
56	H	-1.5271	-3.9873	-2.5135
57	H	-1.6209	-2.2433	-2.1910
58	C	0.5277	-3.5395	-0.8494
59	H	0.8671	-2.6138	-1.3379
60	H	0.6996	-4.3674	-1.5519
61	H	1.1543	-3.7143	0.0335
62	C	-3.0090	-2.1453	1.3017
63	H	-2.9567	-1.5642	2.2327
64	C	-3.9744	-1.4326	0.3600
65	H	-3.6294	-0.4230	0.1091
66	H	-4.9495	-1.3370	0.8582
67	H	-4.1321	-1.9846	-0.5744
68	C	-3.4619	-3.5605	1.6462
69	H	-3.5542	-4.1899	0.7504
70	H	-4.4532	-3.5126	2.1199
71	H	-2.7812	-4.0550	2.3520
72	C	-2.0439	1.2947	2.2990
73	C	-1.3428	0.3242	3.0391
74	C	-1.9389	-0.2590	4.1571
75	H	-1.3984	-1.0089	4.7317
76	C	-3.2331	0.0904	4.5277
77	H	-3.6837	-0.3888	5.3972
78	C	-3.9644	1.0335	3.7964
79	C	-3.3448	1.6260	2.6921

80	H	-3.9120	2.3552	2.1177
81	C	0.0645	4.4194	0.1833
82	H	0.4942	3.8539	-0.6508
83	H	0.8255	5.1349	0.5254
84	H	-0.7831	4.9994	-0.1992
85	C	-2.6149	2.4135	-0.3995
86	H	-3.3219	1.5846	-0.2444
87	C	-3.3631	3.7294	-0.1931
88	H	-3.7602	3.8550	0.8202
89	H	-4.2161	3.7566	-0.8864
90	H	-2.7331	4.5977	-0.4166
91	C	-2.0723	2.2984	-1.8259
92	H	-1.3077	3.0579	-2.0370
93	H	-2.8955	2.4469	-2.5393
94	H	-1.6370	1.3076	-2.0195
95	C	-0.3317	3.5286	1.3594
96	H	0.5913	3.1067	1.7803
97	C	-1.0459	4.3031	2.4616
98	H	-1.9931	4.7355	2.1143
99	H	-0.4001	5.1311	2.7894
100	H	-1.2539	3.6760	3.3377
101	C	-5.3612	1.4093	4.1960
102	H	-5.3507	2.0330	5.1024
103	H	-5.9621	0.5184	4.4224
104	H	-5.8658	1.9766	3.4044

/db/nbandeira/Fe(NPiso)/L=Cl/0e-/1-Cl+NCMe
Energy (POTENTIAL) = -4466.79551675 Eh

	Atom	X	Y	Z
1	Fe	0.0152	-0.1480	0.0423
2	P	-0.8164	-2.3365	-0.7574
3	P	-1.6608	1.5427	-0.5172
4	P	2.1352	0.6044	-1.0028
5	Cl	0.0645	-0.2370	2.3155
6	N	-0.2985	-0.0524	-2.7111
7	C	0.2725	-1.2972	-3.1294
8	C	1.0265	-1.3725	-4.3036
9	H	1.1911	-0.4734	-4.8947
10	C	1.5635	-2.5844	-4.7232
11	H	2.1531	-2.6172	-5.6401
12	C	1.3410	-3.7609	-3.9982
13	C	0.5747	-3.6728	-2.8324
14	H	0.3969	-4.5862	-2.2658
15	C	0.0524	-2.4600	-2.3688
16	C	1.9263	-5.0707	-4.4419
17	H	1.9028	-5.1683	-5.5354
18	H	1.3846	-5.9193	-4.0054
19	H	2.9788	-5.1538	-4.1301
20	C	-1.7216	0.0384	-2.8740
21	C	-2.3552	-0.6340	-3.9216
22	H	-1.7660	-1.2492	-4.5998
23	C	-3.7309	-0.5332	-4.0971
24	H	-4.2064	-1.0805	-4.9118
25	C	-4.5072	0.2665	-3.2507
26	C	-3.8574	0.9414	-2.2115
27	H	-4.4630	1.5499	-1.5409
28	C	-2.4797	0.8307	-1.9931
29	C	-5.9876	0.4082	-3.4582
30	H	-6.2007	1.1265	-4.2647
31	H	-6.4867	0.7714	-2.5511
32	H	-6.4435	-0.5482	-3.7467
33	C	0.4034	1.1248	-3.1365
34	C	-0.0978	1.8927	-4.1927
35	H	-1.0030	1.5723	-4.7051
36	C	0.5278	3.0729	-4.5750
37	H	0.1075	3.6599	-5.3923
38	C	1.6821	3.5162	-3.9193

39	C	2.1859	2.7271	-2.8817
40	H	3.0733	3.0820	-2.3647
41	C	1.5726	1.5359	-2.4732
42	C	2.3625	4.7922	-4.3237
43	H	3.1131	5.0975	-3.5841
44	H	1.6380	5.6098	-4.4390
45	H	2.8735	4.6733	-5.2910
46	C	-0.1318	-3.7612	0.2336
47	H	-0.3618	-4.6889	-0.3116
48	C	1.3811	-3.5973	0.3659
49	H	1.6142	-2.7082	0.9694
50	H	1.8981	-3.5051	-0.5963
51	H	1.7997	-4.4687	0.8901
52	C	-0.7442	-3.8424	1.6338
53	H	-0.1838	-4.5867	2.2185
54	H	-1.7923	-4.1508	1.6323
55	H	-0.6672	-2.8796	2.1562
56	C	-2.6084	-2.7072	-1.1752
57	H	-2.9600	-1.7506	-1.5830
58	C	-2.7505	-3.7766	-2.2525
59	H	-2.3279	-4.7384	-1.9265
60	H	-2.2652	-3.4896	-3.1932
61	H	-3.8189	-3.9367	-2.4616
62	C	-3.4736	-3.0439	0.0379
63	H	-4.5291	-2.8999	-0.2345
64	H	-3.2677	-2.4179	0.9133
65	H	-3.3540	-4.0946	0.3313
66	C	-3.0363	1.7386	0.7197
67	H	-3.8299	2.3302	0.2406
68	C	-3.5844	0.3642	1.0901
69	H	-2.8047	-0.2513	1.5576
70	H	-3.9740	-0.1790	0.2205
71	H	-4.4059	0.4736	1.8133
72	C	-2.5631	2.4928	1.9624
73	H	-3.3453	2.4381	2.7335
74	H	-2.3790	3.5537	1.7601
75	H	-1.6490	2.0511	2.3821
76	C	-1.1428	3.2553	-1.0483
77	H	-0.5414	3.0474	-1.9421
78	C	-2.3111	4.1401	-1.4659
79	H	-2.9553	4.3992	-0.6138

80	H	-2.9314	3.6604	-2.2353
81	H	-1.9263	5.0807	-1.8875
82	C	-0.2263	3.9317	-0.0297
83	H	0.3401	4.7338	-0.5242
84	H	0.4972	3.2320	0.4093
85	H	-0.7901	4.3858	0.7937
86	C	3.1577	1.8268	-0.0228
87	H	2.5841	2.7578	-0.1485
88	C	4.5918	2.0780	-0.4903
89	H	4.9924	2.9387	0.0652
90	H	4.6825	2.3048	-1.5581
91	H	5.2422	1.2222	-0.2748
92	C	3.1375	1.4721	1.4642
93	H	3.6544	0.5235	1.6637
94	H	2.1166	1.3842	1.8540
95	H	3.6576	2.2591	2.0299
96	C	3.2347	-0.7703	-1.6411
97	H	2.5014	-1.5164	-1.9754
98	C	4.0955	-0.3983	-2.8426
99	H	4.8865	0.3157	-2.5829
100	H	3.4981	0.0321	-3.6564
101	H	4.5804	-1.3069	-3.2300
102	C	4.0442	-1.4039	-0.5106
103	H	4.4554	-2.3629	-0.8572
104	H	3.4339	-1.6074	0.3780
105	H	4.8892	-0.7756	-0.2042
106	C	-3.1163	-1.4331	4.2702
107	N	-3.4623	-2.4429	3.8197
108	C	-2.6756	-0.1660	4.8224
109	H	-1.7258	0.1225	4.3529
110	H	-2.5339	-0.2533	5.9073
111	H	-3.4222	0.6126	4.6200

/db/nbandeira/Fe(NPiso)/L=CO2/1e-/1-CO2H+1e-
Energy (POTENTIAL) = -4061.59801853 Eh

	Atom	X	Y	Z
1	Fe	-0.0498	-0.0211	-0.4216
2	P	-0.7878	-2.2793	-0.6581
3	P	-1.7057	1.7693	-0.6682
4	P	2.1120	0.7738	-0.9456
5	N	-0.2690	-0.0286	-2.5928
6	C	0.2864	-1.3002	-3.0444
7	C	1.0103	-1.3898	-4.2302
8	H	1.2267	-0.4970	-4.8126
9	C	1.4549	-2.6298	-4.6815
10	H	2.0316	-2.6803	-5.6051
11	C	1.1572	-3.8055	-3.9850
12	C	0.4371	-3.6928	-2.7906
13	H	0.2133	-4.6015	-2.2328
14	C	0.0215	-2.4554	-2.2925
15	C	1.5799	-5.1485	-4.5033
16	H	0.7879	-5.5838	-5.1318
17	H	1.7724	-5.8522	-3.6836
18	H	2.4841	-5.0716	-5.1198
19	C	-1.7055	0.0640	-2.8628
20	C	-2.2873	-0.6742	-3.8904
21	H	-1.6860	-1.3545	-4.4897
22	C	-3.6499	-0.5540	-4.1498
23	H	-4.0909	-1.1515	-4.9479
24	C	-4.4565	0.3158	-3.4085
25	C	-3.8521	1.0551	-2.3853
26	H	-4.4764	1.7211	-1.7903
27	C	-2.4901	0.9414	-2.0951
28	C	-5.9183	0.4696	-3.7088
29	H	-6.0736	1.2445	-4.4752
30	H	-6.4808	0.7721	-2.8166
31	H	-6.3471	-0.4638	-4.0948
32	C	0.4421	1.1273	-3.1357
33	C	-0.0268	1.7718	-4.2792
34	H	-0.9274	1.4189	-4.7771
35	C	0.6386	2.8878	-4.7755
36	H	0.2473	3.3876	-5.6616
37	C	1.7883	3.3826	-4.1494
38	C	2.2497	2.7169	-3.0096

39	H	3.1320	3.1100	-2.5095
40	C	1.5960	1.5938	-2.4930
41	C	2.5127	4.5798	-4.6898
42	H	3.1559	5.0373	-3.9281
43	H	1.8089	5.3384	-5.0560
44	H	3.1526	4.2910	-5.5374
45	C	-0.1227	-3.6978	0.3520
46	H	-0.5606	-4.5928	-0.1186
47	C	1.4022	-3.7931	0.2908
48	H	1.8655	-2.9461	0.8060
49	H	1.8001	-3.8329	-0.7289
50	H	1.7128	-4.7131	0.8062
51	C	-0.5803	-3.6525	1.8120
52	H	-0.1584	-4.5251	2.3306
53	H	-1.6654	-3.6933	1.9313
54	H	-0.2109	-2.7586	2.3273
55	C	-2.6084	-2.5884	-0.9803
56	H	-2.9485	-1.6355	-1.4067
57	C	-2.8272	-3.6889	-2.0140
58	H	-2.4347	-4.6563	-1.6693
59	H	-2.3701	-3.4537	-2.9824
60	H	-3.9088	-3.8077	-2.1747
61	C	-3.4155	-2.8575	0.2873
62	H	-4.4816	-2.7328	0.0512
63	H	-3.1724	-2.1719	1.1071
64	H	-3.2753	-3.8883	0.6367
65	C	-3.0647	1.9786	0.5761
66	H	-3.8615	2.5396	0.0651
67	C	-3.5998	0.6135	0.9952
68	H	-2.8219	0.0298	1.5033
69	H	-3.9769	0.0328	0.1445
70	H	-4.4337	0.7512	1.6986
71	C	-2.6031	2.7905	1.7862
72	H	-3.3957	2.7662	2.5477
73	H	-2.4227	3.8421	1.5385
74	H	-1.6941	2.3694	2.2338
75	C	-1.1888	3.4501	-1.2855
76	H	-0.5765	3.2013	-2.1620
77	C	-2.3715	4.2893	-1.7548
78	H	-3.0284	4.5717	-0.9204
79	H	-2.9725	3.7684	-2.5121

80	H	-1.9953	5.2173	-2.2096
81	C	-0.2999	4.1937	-0.2893
82	H	0.2674	4.9691	-0.8227
83	H	0.4205	3.5312	0.2054
84	H	-0.8869	4.6910	0.4914
85	C	2.9908	2.0990	0.0297
86	H	2.4443	2.9986	-0.2893
87	C	4.4681	2.2922	-0.3175
88	H	4.8072	3.2275	0.1500
89	H	4.6644	2.3725	-1.3923
90	H	5.0897	1.4832	0.0822
91	C	2.7998	1.9523	1.5369
92	H	3.2648	1.0376	1.9250
93	H	1.7400	1.9600	1.8206
94	H	3.2790	2.8083	2.0328
95	C	3.2327	-0.6444	-1.4305
96	H	2.5081	-1.4229	-1.7118
97	C	4.0975	-0.3506	-2.6523
98	H	4.8666	0.4035	-2.4435
99	H	3.5046	-0.0124	-3.5111
100	H	4.6099	-1.2783	-2.9458
101	C	4.0452	-1.1784	-0.2522
102	H	4.4567	-2.1588	-0.5304
103	H	3.4379	-1.3119	0.6488
104	H	4.8900	-0.5244	-0.0074
105	C	0.4081	-0.2801	1.4134
106	O	-0.4053	0.2549	2.1262
107	O	1.4722	-0.9327	1.8367
108	H	1.5088	-0.9214	2.8157

/db/nbandeira/Fe(NPiso)/L=Cl/1e-/1-Cl+NCMe
Energy (POTENTIAL) = -4466.89254868127591 Eh

	Atom	X	Y	Z
1	Fe	-0.0321	-0.0789	0.0712
2	P	-0.7476	-2.2163	-0.7124
3	P	-1.6250	1.5229	-0.5651
4	P	2.0363	0.5396	-0.9525
5	Cl	0.0765	-0.1865	2.4509
6	N	-0.3242	-0.0541	-2.8191
7	C	0.2485	-1.3054	-3.1816
8	C	0.9855	-1.4228	-4.3643
9	H	1.1172	-0.5462	-4.9970
10	C	1.5455	-2.6404	-4.7359
11	H	2.1228	-2.7068	-5.6592
12	C	1.3578	-3.7822	-3.9486
13	C	0.6046	-3.6521	-2.7768
14	H	0.4547	-4.5431	-2.1677
15	C	0.0667	-2.4302	-2.3553
16	C	1.9687	-5.1006	-4.3321
17	H	1.9288	-5.2607	-5.4181
18	H	1.4565	-5.9375	-3.8401
19	H	3.0285	-5.1436	-4.0369
20	C	-1.7396	0.0528	-2.9542
21	C	-2.3983	-0.6264	-3.9830
22	H	-1.8203	-1.2453	-4.6679
23	C	-3.7786	-0.5304	-4.1311
24	H	-4.2719	-1.0828	-4.9321
25	C	-4.5346	0.2742	-3.2722
26	C	-3.8603	0.9541	-2.2505
27	H	-4.4547	1.5620	-1.5689
28	C	-2.4788	0.8469	-2.0536
29	C	-6.0201	0.4198	-3.4467
30	H	-6.2540	1.1826	-4.2055
31	H	-6.5053	0.7283	-2.5116
32	H	-6.4789	-0.5205	-3.7805
33	C	0.4058	1.1171	-3.1783
34	C	-0.0482	1.9103	-4.2382
35	H	-0.9262	1.5922	-4.7985
36	C	0.5809	3.1077	-4.5598
37	H	0.1960	3.7149	-5.3802
38	C	1.6942	3.5390	-3.8313

39	C	2.1537	2.7214	-2.7933
40	H	3.0083	3.0761	-2.2244
41	C	1.5408	1.5115	-2.4427
42	C	2.3893	4.8296	-4.1619
43	H	3.0122	5.1740	-3.3265
44	H	1.6684	5.6218	-4.4051
45	H	3.0461	4.7101	-5.0373
46	C	-0.1040	-3.6848	0.2617
47	H	-0.3879	-4.6067	-0.2688
48	C	1.4162	-3.6000	0.3762
49	H	1.6958	-2.7287	0.9840
50	H	1.9249	-3.5130	-0.5909
51	H	1.8027	-4.4980	0.8817
52	C	-0.6868	-3.7294	1.6770
53	H	-0.1578	-4.5010	2.2574
54	H	-1.7511	-3.9762	1.7029
55	H	-0.5439	-2.7662	2.1869
56	C	-2.5366	-2.6585	-1.1443
57	H	-2.9028	-1.7192	-1.5798
58	C	-2.6727	-3.7553	-2.1946
59	H	-2.2248	-4.7012	-1.8544
60	H	-2.2034	-3.4815	-3.1472
61	H	-3.7394	-3.9474	-2.3901
62	C	-3.4148	-2.9789	0.0637
63	H	-4.4714	-2.8507	-0.2158
64	H	-3.2211	-2.3362	0.9293
65	H	-3.2896	-4.0229	0.3805
66	C	-3.0237	1.7628	0.6517
67	H	-3.8191	2.3495	0.1693
68	C	-3.5758	0.4012	1.0573
69	H	-2.7882	-0.2015	1.5288
70	H	-3.9655	-0.1616	0.1999
71	H	-4.3952	0.5217	1.7829
72	C	-2.5412	2.5317	1.8818
73	H	-3.3189	2.5026	2.6602
74	H	-2.3390	3.5865	1.6621
75	H	-1.6308	2.0792	2.3002
76	C	-1.1876	3.2649	-1.1241
77	H	-0.6614	3.0747	-2.0685
78	C	-2.3889	4.1514	-1.4291
79	H	-2.9447	4.4189	-0.5191

80	H	-3.0876	3.6667	-2.1251
81	H	-2.0532	5.0905	-1.8958
82	C	-0.1888	3.9345	-0.1844
83	H	0.2614	4.8100	-0.6761
84	H	0.6225	3.2465	0.0856
85	H	-0.6567	4.2824	0.7448
86	C	3.1363	1.7420	-0.0065
87	H	2.5684	2.6818	-0.0829
88	C	4.5576	2.0072	-0.5073
89	H	4.9736	2.8647	0.0436
90	H	4.6238	2.2402	-1.5755
91	H	5.2176	1.1526	-0.3161
92	C	3.1739	1.3614	1.4742
93	H	3.7359	0.4308	1.6360
94	H	2.1684	1.2145	1.8881
95	H	3.6790	2.1549	2.0463
96	C	3.1687	-0.7979	-1.6474
97	H	2.4410	-1.5512	-1.9770
98	C	4.0085	-0.4130	-2.8601
99	H	4.7937	0.3113	-2.6105
100	H	3.3947	0.0140	-3.6634
101	H	4.5025	-1.3114	-3.2622
102	C	4.0138	-1.4398	-0.5484
103	H	4.4155	-2.3997	-0.9066
104	H	3.4325	-1.6442	0.3588
105	H	4.8691	-0.8142	-0.2649
106	C	-3.2518	-1.4849	4.2326
107	N	-3.6818	-2.4662	3.7910
108	C	-2.6967	-0.2557	4.7656
109	H	-1.7468	-0.0432	4.2512
110	H	-2.5174	-0.3560	5.8438
111	H	-3.3905	0.5770	4.5930

/db/nbandeira/Fe(NPiso)/L=CO2/1e-/1-CO2+1e-
Energy (POTENTIAL) = -4061.17775504 Eh

	Atom	X	Y	Z
1	Fe	-0.0541	0.0102	0.0228
2	P	-0.6721	-2.2475	-0.6546
3	P	-1.7117	1.6610	-0.6211
4	P	2.0865	0.7260	-0.9894
5	N	-0.2867	-0.0531	-2.7212
6	C	0.2843	-1.3088	-3.1119
7	C	1.0034	-1.4258	-4.3025
8	H	1.1740	-0.5445	-4.9180
9	C	1.4923	-2.6620	-4.7156
10	H	2.0577	-2.7275	-5.6458
11	C	1.2483	-3.8195	-3.9701
12	C	0.5381	-3.6847	-2.7721
13	H	0.3625	-4.5800	-2.1763
14	C	0.0779	-2.4474	-2.3123
15	C	1.7148	-5.1688	-4.4360
16	H	0.8891	-5.7256	-4.9049
17	H	2.0818	-5.7771	-3.5985
18	H	2.5178	-5.0799	-5.1783
19	C	-1.7059	0.0386	-2.9156
20	C	-2.3307	-0.6876	-3.9320
21	H	-1.7445	-1.3712	-4.5435
22	C	-3.6930	-0.5431	-4.1722
23	H	-4.1604	-1.1308	-4.9631
24	C	-4.4626	0.3586	-3.4294
25	C	-3.8256	1.0729	-2.4096
26	H	-4.4304	1.7547	-1.8137
27	C	-2.4668	0.9115	-2.1150
28	C	-5.9215	0.5638	-3.7192
29	H	-6.0585	1.3060	-4.5206
30	H	-6.4579	0.9312	-2.8350
31	H	-6.3973	-0.3676	-4.0529
32	C	0.4150	1.1060	-3.1972
33	C	-0.0769	1.8153	-4.2984
34	H	-0.9780	1.4691	-4.8010
35	C	0.5553	2.9698	-4.7411
36	H	0.1439	3.5122	-5.5930
37	C	1.7079	3.4425	-4.1029
38	C	2.1981	2.7131	-3.0167

39	H	3.0817	3.0972	-2.5148
40	C	1.5751	1.5504	-2.5427
41	C	2.3949	4.6927	-4.5720
42	H	3.1876	4.9993	-3.8782
43	H	1.6825	5.5237	-4.6693
44	H	2.8520	4.5415	-5.5612
45	C	0.0272	-3.6757	0.3268
46	H	-0.3374	-4.5900	-0.1659
47	C	1.5536	-3.6520	0.3077
48	H	1.9236	-2.7626	0.8329
49	H	1.9843	-3.6587	-0.7000
50	H	1.9348	-4.5345	0.8417
51	C	-0.4357	-3.6941	1.7847
52	H	-0.0413	-4.6044	2.2591
53	H	-1.5211	-3.7017	1.9064
54	H	-0.0328	-2.8380	2.3406
55	C	-2.4949	-2.5822	-0.9386
56	H	-2.8317	-1.6487	-1.4090
57	C	-2.7444	-3.7293	-1.9112
58	H	-2.3554	-4.6822	-1.5236
59	H	-2.2931	-3.5465	-2.8941
60	H	-3.8285	-3.8482	-2.0562
61	C	-3.2934	-2.7645	0.3505
62	H	-4.3579	-2.5955	0.1335
63	H	-2.9957	-2.0645	1.1397
64	H	-3.1983	-3.7879	0.7362
65	C	-3.1716	2.0006	0.4842
66	H	-3.8290	2.6772	-0.0812
67	C	-3.9379	0.7237	0.8218
68	H	-3.3536	0.0935	1.5004
69	H	-4.1977	0.1296	-0.0623
70	H	-4.8752	0.9934	1.3306
71	C	-2.7439	2.7229	1.7622
72	H	-3.6042	2.7788	2.4447
73	H	-2.4104	3.7488	1.5731
74	H	-1.9409	2.1882	2.2884
75	C	-1.0719	3.3274	-1.1733
76	H	-0.4279	3.0575	-2.0183
77	C	-2.1672	4.2506	-1.6925
78	H	-2.8402	4.5804	-0.8890
79	H	-2.7688	3.7719	-2.4773

80	H	-1.7071	5.1500	-2.1282
81	C	-0.1894	3.9972	-0.1209
82	H	0.4461	4.7509	-0.6073
83	H	0.4697	3.2832	0.3908
84	H	-0.7802	4.5115	0.6462
85	C	3.1222	2.0275	-0.1228
86	H	2.5670	2.9493	-0.3527
87	C	4.5644	2.2121	-0.5985
88	H	4.9609	3.1414	-0.1631
89	H	4.6709	2.2862	-1.6860
90	H	5.2109	1.3948	-0.2577
91	C	3.0843	1.8438	1.3943
92	H	3.5546	0.9011	1.7044
93	H	2.0608	1.8504	1.7849
94	H	3.6407	2.6653	1.8693
95	C	3.1879	-0.7024	-1.4915
96	H	2.4511	-1.4761	-1.7478
97	C	4.0546	-0.4658	-2.7224
98	H	4.8580	0.2564	-2.5321
99	H	3.4648	-0.1067	-3.5754
100	H	4.5245	-1.4156	-3.0191
101	C	3.9953	-1.2135	-0.2988
102	H	4.3703	-2.2234	-0.5185
103	H	3.3970	-1.2746	0.6190
104	H	4.8643	-0.5781	-0.0909
105	C	-0.5880	-0.2970	1.9002
106	O	-1.5156	-0.5729	2.6106
107	O	0.6296	-0.0544	1.9633

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/2e-/1-NCMe+Cl-
Energy (POTENTIAL) = -4456.34947219861624 Eh

	Atom	X	Y	Z
1	Fe	-0.3137	1.4408	2.7667
2	P	-0.9841	-0.6999	1.9498
3	P	-1.9048	3.0658	2.1086
4	P	1.7724	2.0884	1.7998
5	N	-0.5247	1.5015	-0.1114
6	C	0.0748	0.2685	-0.4650
7	C	0.8535	0.1819	-1.6247
8	H	0.9900	1.0710	-2.2383
9	C	1.4533	-1.0242	-1.9962
10	H	2.0658	-1.0648	-2.8985
11	C	1.2636	-2.1770	-1.2360
12	C	0.4701	-2.0790	-0.0797
13	H	0.3337	-2.9798	0.5178
14	C	-0.1133	-0.8779	0.3350
15	C	1.8780	-3.4929	-1.6247
16	H	2.5334	-3.3851	-2.4986
17	H	1.1061	-4.2369	-1.8739
18	H	2.4748	-3.9153	-0.8029
19	C	-1.9402	1.5901	-0.2750
20	C	-2.5770	0.8816	-1.2800
21	H	-1.9794	0.2315	-1.9212
22	C	-3.9711	0.9857	-1.4849
23	H	-4.4611	0.4038	-2.2666
24	C	-4.7131	1.9190	-0.7022
25	C	-4.0667	2.6469	0.2796
26	H	-4.6594	3.3549	0.8624
27	C	-2.6693	2.4841	0.5862
28	C	-6.1834	2.1028	-0.9619
29	H	-6.3756	2.4478	-1.9914
30	H	-6.6286	2.8348	-0.2740
31	H	-6.7330	1.1541	-0.8466
32	C	0.2016	2.6770	-0.4461
33	C	-0.2621	3.5065	-1.4751
34	H	-1.1623	3.2098	-2.0122
35	C	0.3971	4.6867	-1.7958
36	H	0.0100	5.3203	-2.5957
37	C	1.5508	5.0687	-1.0995
38	C	2.0039	4.2298	-0.0775

39	H	2.8867	4.5460	0.4712
40	C	1.3485	3.0426	0.2807
41	C	2.2759	6.3416	-1.4375
42	H	3.0924	6.5352	-0.7300
43	H	1.5972	7.2065	-1.4185
44	H	2.7105	6.2969	-2.4476
45	C	-0.3518	-2.1789	2.9139
46	H	-0.5139	-3.0860	2.3128
47	C	1.1423	-1.9969	3.1623
48	H	1.3144	-1.1157	3.7964
49	H	1.7135	-1.8632	2.2362
50	H	1.5490	-2.8744	3.6879
51	C	-1.0679	-2.3606	4.2528
52	H	-0.4850	-3.0498	4.8830
53	H	-2.0680	-2.7900	4.1439
54	H	-1.1793	-1.4195	4.8080
55	C	-2.7613	-1.1080	1.4826
56	H	-3.0733	-0.1715	1.0014
57	C	-2.8867	-2.2306	0.4596
58	H	-2.5135	-3.1864	0.8585
59	H	-2.3407	-2.0081	-0.4650
60	H	-3.9468	-2.3732	0.1963
61	C	-3.6915	-1.3679	2.6681
62	H	-4.7274	-1.1495	2.3674
63	H	-3.4702	-0.7628	3.5546
64	H	-3.6623	-2.4229	2.9714
65	C	-3.3562	3.3601	3.2598
66	H	-4.0518	4.0333	2.7364
67	C	-4.0765	2.0497	3.5546
68	H	-3.4741	1.4059	4.2104
69	H	-4.3134	1.4935	2.6393
70	H	-5.0208	2.2481	4.0868
71	C	-2.9388	4.0300	4.5678
72	H	-3.7837	4.0267	5.2745
73	H	-2.6345	5.0736	4.4301
74	H	-2.1070	3.4924	5.0458
75	C	-1.2888	4.8170	1.7442
76	H	-0.6457	4.6241	0.8756
77	C	-2.3812	5.7816	1.3037
78	H	-3.0544	6.0446	2.1332
79	H	-2.9893	5.3505	0.4954

80	H	-1.9425	6.7205	0.9286
81	C	-0.4026	5.3944	2.8453
82	H	0.2931	6.1410	2.4320
83	H	0.1970	4.6118	3.3326
84	H	-0.9869	5.8954	3.6279
85	C	2.7962	3.3323	2.7856
86	H	2.2420	4.2672	2.6126
87	C	4.2583	3.5803	2.4098
88	H	4.6271	4.4502	2.9750
89	H	4.4188	3.7902	1.3470
90	H	4.8975	2.7303	2.6766
91	C	2.6932	3.0185	4.2784
92	H	3.1669	2.0580	4.5261
93	H	1.6497	2.9691	4.6092
94	H	3.2043	3.8007	4.8606
95	C	2.9618	0.7575	1.1969
96	H	2.2662	-0.0095	0.8300
97	C	3.8642	1.1451	0.0312
98	H	4.6159	1.8914	0.3164
99	H	3.2861	1.5460	-0.8109
100	H	4.4017	0.2535	-0.3283
101	C	3.7511	0.1435	2.3525
102	H	4.1755	-0.8222	2.0395
103	H	3.1251	-0.0413	3.2338
104	H	4.5874	0.7805	2.6656
105	C	-0.2604	1.2485	5.9037
106	N	-0.2414	1.3280	4.7459
107	C	-0.3485	1.1201	7.3405
108	H	0.4617	0.4822	7.7182
109	H	-1.3281	0.6545	7.5584
110	H	-0.2819	2.1062	7.8197
111	Cl	-3.3937	-0.3328	6.6590

/db/nbandeira/Fe(NPiso)/L=Cl/Cl-
Energy (POTENTIAL) = -461.46795119 Eh

	Atom	X	Y	Z
1	Cl	0.0000	0.0000	0.0000

/db/nbandeira/Fe(NPiso)/L=NCMe/NCMe
Energy (POTENTIAL) = -132.55828395 Eh

	Atom	X	Y	Z
1	C	-0.0001	0.0000	-0.1674
2	N	0.0002	-0.0000	-1.3258
3	C	-0.0001	0.0000	1.2847
4	H	1.0307	-0.0000	1.6616
5	H	-0.5153	-0.8926	1.6620
6	H	-0.5153	0.8926	1.6620

/db/nbandeira/Fe(NPiso)/L=Cl/1e-/1-Cl
Energy (POTENTIAL) = -4334.34566254 Eh

	Atom	X	Y	Z
1	Fe	0.0014	0.0067	0.0245
2	P	-0.7292	-2.1554	-0.6551
3	P	-1.6016	1.5902	-0.6380
4	P	2.0384	0.5641	-1.0819
5	Cl	0.0896	0.0006	2.3943
6	N	-0.3681	-0.0868	-2.8630
7	C	0.1882	-1.3540	-3.1920
8	C	0.8938	-1.5223	-4.3856
9	H	1.0173	-0.6718	-5.0545
10	C	1.4355	-2.7594	-4.7238
11	H	1.9901	-2.8665	-5.6571
12	C	1.2590	-3.8674	-3.8901
13	C	0.5387	-3.6853	-2.7028
14	H	0.4025	-4.5494	-2.0528
15	C	0.0217	-2.4451	-2.3160
16	C	1.8408	-5.2103	-4.2322
17	H	2.1386	-5.2602	-5.2873
18	H	1.1230	-6.0192	-4.0381
19	H	2.7349	-5.4194	-3.6250
20	C	-1.7862	0.0210	-2.9607
21	C	-2.4760	-0.6986	-3.9394
22	H	-1.9200	-1.3488	-4.6136
23	C	-3.8607	-0.6054	-4.0509
24	H	-4.3781	-1.1899	-4.8130
25	C	-4.5895	0.2361	-3.2057
26	C	-3.8840	0.9560	-2.2324
27	H	-4.4570	1.5929	-1.5591
28	C	-2.4984	0.8542	-2.0718
29	C	-6.0789	0.3839	-3.3394
30	H	-6.3329	1.2561	-3.9616
31	H	-6.5564	0.5332	-2.3618
32	H	-6.5286	-0.4985	-3.8127
33	C	0.3566	1.0665	-3.2848
34	C	-0.1204	1.8184	-4.3645
35	H	-1.0090	1.4774	-4.8939
36	C	0.4968	3.0056	-4.7412
37	H	0.0939	3.5816	-5.5754
38	C	1.6202	3.4682	-4.0481

39	C	2.1052	2.6890	-2.9925
40	H	2.9681	3.0680	-2.4525
41	C	1.5062	1.4887	-2.5886
42	C	2.2972	4.7532	-4.4331
43	H	2.9563	5.1132	-3.6328
44	H	1.5644	5.5406	-4.6561
45	H	2.9134	4.6198	-5.3356
46	C	-0.0536	-3.5854	0.3541
47	H	-0.3457	-4.5280	-0.1337
48	C	1.4683	-3.4891	0.4222
49	H	1.7598	-2.5866	0.9768
50	H	1.9487	-3.4495	-0.5626
51	H	1.8739	-4.3590	0.9608
52	C	-0.5987	-3.5830	1.7851
53	H	-0.0389	-4.3193	2.3822
54	H	-1.6560	-3.8545	1.8446
55	H	-0.4653	-2.5970	2.2527
56	C	-2.5364	-2.6004	-0.9938
57	H	-2.9067	-1.6836	-1.4713
58	C	-2.7268	-3.7559	-1.9697
59	H	-2.2885	-4.6889	-1.5845
60	H	-2.2789	-3.5492	-2.9493
61	H	-3.8022	-3.9361	-2.1239
62	C	-3.3711	-2.8285	0.2658
63	H	-4.4347	-2.6803	0.0262
64	H	-3.1155	-2.1440	1.0828
65	H	-3.2638	-3.8572	0.6343
66	C	-2.9689	1.9115	0.5956
67	H	-3.7625	2.4862	0.0957
68	C	-3.5388	0.5877	1.0927
69	H	-2.7623	0.0202	1.6236
70	H	-3.9213	-0.0361	0.2753
71	H	-4.3687	0.7718	1.7926
72	C	-2.4509	2.7358	1.7739
73	H	-3.2318	2.7977	2.5473
74	H	-2.1936	3.7622	1.4885
75	H	-1.5676	2.2625	2.2257
76	C	-1.1652	3.2997	-1.2923
77	H	-0.6673	3.0556	-2.2388
78	C	-2.3640	4.1832	-1.6157
79	H	-2.8959	4.5049	-0.7089

80	H	-3.0836	3.6715	-2.2699
81	H	-2.0292	5.0926	-2.1385
82	C	-0.1346	4.0078	-0.4164
83	H	0.3584	4.8085	-0.9877
84	H	0.6427	3.3120	-0.0751
85	H	-0.5851	4.4681	0.4722
86	C	3.1633	1.7901	-0.2005
87	H	2.5915	2.7268	-0.2841
88	C	4.5686	2.0444	-0.7497
89	H	4.9975	2.9209	-0.2401
90	H	4.6019	2.2418	-1.8266
91	H	5.2375	1.1987	-0.5507
92	C	3.2425	1.4445	1.2873
93	H	3.8135	0.5204	1.4549
94	H	2.2487	1.3034	1.7309
95	H	3.7591	2.2526	1.8278
96	C	3.1516	-0.7941	-1.7716
97	H	2.4159	-1.5604	-2.0491
98	C	3.9452	-0.4444	-3.0254
99	H	4.7399	0.2851	-2.8251
100	H	3.3028	-0.0390	-3.8173
101	H	4.4243	-1.3542	-3.4200
102	C	4.0429	-1.3985	-0.6875
103	H	4.4325	-2.3687	-1.0307
104	H	3.5005	-1.5745	0.2491
105	H	4.9070	-0.7622	-0.4611

/db/nbandeira/Fe(NPiso)/_Ir(ppy)2(dtb-bpy)_+/0e-/Ir(ppy)2(dtb-bpy)_+1H+
Energy (POTENTIAL) = -19597.03088083895636 Eh

	Atom	X	Y	Z
1	C	-1.6858	2.8051	-0.2245
2	H	-0.6693	3.1784	-0.0787
3	C	-2.7552	3.6708	-0.3830
4	C	-4.0506	3.1647	-0.5606
5	C	-4.1770	1.7743	-0.5747
6	H	-5.1540	1.3153	-0.7128
7	C	-3.0604	0.9549	-0.4127
8	C	-3.1331	-0.5184	-0.4260
9	C	-4.3198	-1.2310	-0.6077
10	H	-5.2673	-0.7083	-0.7414
11	C	-4.2854	-2.6211	-0.6224
12	C	-3.0656	-3.2697	-0.4438
13	C	-1.9234	-2.4995	-0.2631
14	H	-0.9410	-2.9563	-0.1230
15	C	1.2601	1.3944	0.0642
16	C	1.8535	1.9592	1.2034
17	H	1.5087	1.6701	2.2007
18	C	2.8850	2.8929	1.0948
19	H	3.3288	3.3179	2.0013
20	C	3.3577	3.2897	-0.1607
21	H	4.1659	4.0222	-0.2420
22	C	2.7926	2.7438	-1.3081
23	H	3.1634	3.0540	-2.2892
24	C	1.7565	1.8052	-1.1987
25	C	1.1062	1.1802	-2.3468
26	C	1.4239	1.4122	-3.6891
27	H	2.2173	2.1175	-3.9416
28	C	0.7339	0.7452	-4.6914
29	H	0.9807	0.9227	-5.7418
30	C	-0.2743	-0.1524	-4.3384
31	H	-0.8448	-0.7031	-5.0891
32	C	-0.5488	-0.3417	-2.9935
33	H	-1.3246	-1.0375	-2.6705
34	C	1.0960	-1.3846	0.2313
35	C	1.8644	-2.0426	-0.7409
36	H	1.7873	-1.7449	-1.7911
37	C	2.7331	-3.0789	-0.3961
38	H	3.3202	-3.5760	-1.1757

39	C	2.8620	-3.4881	0.9357
40	H	3.5430	-4.3019	1.2012
41	C	2.1179	-2.8511	1.9228
42	H	2.2202	-3.1718	2.9636
43	C	1.2453	-1.8095	1.5758
44	C	0.4294	-1.0800	2.5418
45	C	0.4348	-1.2746	3.9276
46	H	1.0831	-2.0371	4.3617
47	C	-0.3743	-0.4941	4.7416
48	H	-0.3690	-0.6402	5.8252
49	C	-1.1916	0.4744	4.1573
50	H	-1.8465	1.1123	4.7542
51	C	-1.1625	0.6197	2.7792
52	H	-1.7825	1.3633	2.2765
53	Ir	-0.2440	0.0778	-0.0295
54	N	-1.8300	1.4756	-0.2318
55	N	-1.9558	-1.1628	-0.2625
56	N	0.1177	0.3024	-2.0249
57	N	-0.3775	-0.1310	1.9933
58	H	-2.5603	4.7450	-0.3627
59	H	-2.9892	-4.3594	-0.4460
60	C	-5.2356	4.1069	-0.7298
61	C	-3.8010	-3.5832	3.0077
62	C	-3.0313	-4.7853	3.2875
63	H	-3.6499	-5.6325	3.6223
64	H	-2.6282	-5.0622	2.2825
65	H	-2.1555	-4.5972	3.9285
66	C	-5.2202	-3.6910	2.7028
67	H	-5.4741	-4.6532	2.2276
68	H	-5.6977	-3.7283	3.7122
69	H	-5.6295	-2.8215	2.1692
70	C	-5.0070	4.9587	-1.9892
71	H	-4.0843	5.5591	-1.9156
72	H	-4.9342	4.3214	-2.8879
73	H	-5.8537	5.6541	-2.1270
74	C	-6.5565	3.3504	-0.8774
75	H	-7.3811	4.0748	-0.9886
76	H	-6.5604	2.7007	-1.7697
77	H	-6.7739	2.7289	0.0087
78	C	-5.3206	5.0176	0.5058
79	H	-6.1739	5.7103	0.3995

80	H	-5.4716	4.4229	1.4238
81	H	-4.4077	5.6238	0.6328
82	C	-3.1550	-2.2833	3.0958
83	H	-3.6278	-1.5081	2.4744
84	H	-3.3223	-1.9903	4.1618
85	H	-2.0631	-2.3449	2.9683
86	H	-5.2066	-3.1909	-0.7700

/db/nbandeira/Fe(NPiso)/L=NCMe/0e-/1-NCMe
Energy (POTENTIAL) = -4005.27028908 Eh

	Atom	X	Y	Z
1	Fe	-0.3214	1.4520	2.6442
2	P	-1.0857	-0.7771	1.9189
3	P	-1.9428	3.1873	2.1309
4	P	1.8982	2.1422	1.8294
5	N	-0.4914	1.5292	0.0343
6	C	0.0863	0.2834	-0.3921
7	C	0.8780	0.2219	-1.5399
8	H	1.0726	1.1277	-2.1111
9	C	1.4201	-0.9890	-1.9604
10	H	2.0412	-1.0110	-2.8564
11	C	1.1657	-2.1749	-1.2639
12	C	0.3589	-2.1004	-0.1235
13	H	0.1558	-3.0208	0.4236
14	C	-0.1688	-0.8913	0.3391
15	C	1.7587	-3.4832	-1.7008
16	H	1.9631	-3.4888	-2.7790
17	H	1.0910	-4.3227	-1.4675
18	H	2.7125	-3.6700	-1.1839
19	C	-1.9079	1.6391	-0.1993
20	C	-2.5010	0.9657	-1.2701
21	H	-1.8892	0.3416	-1.9190
22	C	-3.8656	1.0797	-1.5073
23	H	-4.3080	0.5353	-2.3423
24	C	-4.6741	1.8889	-0.6992
25	C	-4.0656	2.5681	0.3604
26	H	-4.6920	3.1908	0.9984
27	C	-2.6982	2.4496	0.6372
28	C	-6.1468	2.0144	-0.9617
29	H	-6.3344	2.4161	-1.9679
30	H	-6.6284	2.6790	-0.2341
31	H	-6.6410	1.0337	-0.9087
32	C	0.2446	2.7008	-0.3617
33	C	-0.1970	3.4757	-1.4379
34	H	-1.0892	3.1772	-1.9852
35	C	0.4755	4.6367	-1.7999
36	H	0.1029	5.2301	-2.6352
37	C	1.6165	5.0522	-1.1032
38	C	2.0579	4.2567	-0.0426

39	H	2.9367	4.5870	0.5049
40	C	1.3953	3.0859	0.3459
41	C	2.3452	6.3073	-1.4871
42	H	3.1137	6.5654	-0.7482
43	H	1.6530	7.1558	-1.5767
44	H	2.8403	6.1891	-2.4624
45	C	-0.4307	-2.1901	2.9425
46	H	-0.6332	-3.1163	2.3843
47	C	1.0748	-2.0178	3.1278
48	H	1.2859	-1.1245	3.7323
49	H	1.6217	-1.9317	2.1820
50	H	1.4781	-2.8846	3.6708
51	C	-1.1018	-2.2856	4.3142
52	H	-0.5496	-3.0159	4.9231
53	H	-2.1401	-2.6221	4.2630
54	H	-1.0756	-1.3257	4.8460
55	C	-2.8688	-1.1276	1.4583
56	H	-3.1943	-0.1720	1.0264
57	C	-2.9949	-2.2104	0.3927
58	H	-2.6016	-3.1744	0.7470
59	H	-2.4743	-1.9455	-0.5356
60	H	-4.0587	-2.3535	0.1512
61	C	-3.7701	-1.4287	2.6548
62	H	-4.8146	-1.2575	2.3579
63	H	-3.5634	-0.7966	3.5264
64	H	-3.6867	-2.4788	2.9616
65	C	-3.3364	3.3676	3.3427
66	H	-4.1238	3.9643	2.8596
67	C	-3.8893	1.9883	3.6887
68	H	-3.1298	1.3715	4.1898
69	H	-4.2446	1.4448	2.8048
70	H	-4.7382	2.0950	4.3793
71	C	-2.8767	4.1043	4.6010
72	H	-3.6626	4.0305	5.3662
73	H	-2.6983	5.1696	4.4184
74	H	-1.9600	3.6671	5.0219
75	C	-1.3793	4.8875	1.6184
76	H	-0.7562	4.6708	0.7416
77	C	-2.5324	5.7782	1.1710
78	H	-3.1980	6.0373	2.0062
79	H	-3.1325	5.3060	0.3814

80	H	-2.1284	6.7174	0.7654
81	C	-0.4899	5.5557	2.6650
82	H	0.0768	6.3688	2.1896
83	H	0.2327	4.8583	3.1078
84	H	-1.0743	5.9944	3.4820
85	C	2.8561	3.3614	2.8750
86	H	2.3059	4.2980	2.6987
87	C	4.3233	3.5956	2.5160
88	H	4.6916	4.4470	3.1067
89	H	4.4901	3.8335	1.4598
90	H	4.9487	2.7313	2.7670
91	C	2.7079	3.0140	4.3567
92	H	3.1175	2.0223	4.5917
93	H	1.6590	3.0386	4.6743
94	H	3.2565	3.7526	4.9589
95	C	3.0183	0.7695	1.2335
96	H	2.2971	0.0302	0.8586
97	C	3.9300	1.1558	0.0747
98	H	4.6963	1.8817	0.3727
99	H	3.3657	1.5764	-0.7672
100	H	4.4463	0.2544	-0.2875
101	C	3.7791	0.1266	2.3924
102	H	4.1923	-0.8360	2.0591
103	H	3.1375	-0.0707	3.2598
104	H	4.6191	0.7463	2.7278
105	C	-0.2762	1.1997	5.8340
106	N	-0.2740	1.3037	4.6837
107	C	-0.2779	1.0682	7.2696
108	H	0.6649	1.4600	7.6741
109	H	-0.3789	0.0093	7.5421
110	H	-1.1175	1.6362	7.6913

/db/nbandeira/Fe(NPiso)/L=CO2/CO
Energy (POTENTIAL) = -113.00905754 Eh

	Atom	X	Y	Z
1	C	0.0000	0.0000	0.1860
2	O	0.0000	0.0000	1.3140

/db/nbandeira/Fe(NPiso)/L=CO2/2e-/1-CO2H+2e-
Energy (POTENTIAL) = -4061.72421889 Eh

	Atom	X	Y	Z
1	Fe	-0.0437	-0.0063	-0.3375
2	P	-0.7784	-2.2322	-0.6685
3	P	-1.6963	1.6984	-0.6092
4	P	2.0885	0.7422	-0.9675
5	N	-0.2828	-0.0134	-2.5829
6	C	0.2732	-1.2760	-3.0505
7	C	0.9979	-1.3570	-4.2383
8	H	1.2064	-0.4602	-4.8172
9	C	1.4625	-2.5896	-4.6919
10	H	2.0426	-2.6301	-5.6144
11	C	1.1845	-3.7695	-3.9951
12	C	0.4557	-3.6667	-2.8048
13	H	0.2458	-4.5778	-2.2448
14	C	0.0200	-2.4369	-2.3064
15	C	1.6372	-5.1054	-4.5102
16	H	0.8869	-5.5324	-5.1935
17	H	1.7816	-5.8227	-3.6922
18	H	2.5776	-5.0204	-5.0698
19	C	-1.7142	0.0762	-2.8543
20	C	-2.2944	-0.6395	-3.8997
21	H	-1.6882	-1.3025	-4.5135
22	C	-3.6589	-0.5241	-4.1561
23	H	-4.0981	-1.1073	-4.9661
24	C	-4.4673	0.3252	-3.3955
25	C	-3.8637	1.0443	-2.3562
26	H	-4.4923	1.6924	-1.7462
27	C	-2.5028	0.9282	-2.0642
28	C	-5.9315	0.4802	-3.6898
29	H	-6.0984	1.3034	-4.4016
30	H	-6.5009	0.7139	-2.7811
31	H	-6.3484	-0.4304	-4.1385
32	C	0.4262	1.1328	-3.1399
33	C	-0.0620	1.7976	-4.2652
34	H	-0.9869	1.4711	-4.7355
35	C	0.6150	2.8991	-4.7792
36	H	0.2066	3.4163	-5.6480
37	C	1.8022	3.3526	-4.1943
38	C	2.2828	2.6639	-3.0759

39	H	3.1949	3.0261	-2.6066
40	C	1.6141	1.5614	-2.5345
41	C	2.5439	4.5314	-4.7550
42	H	3.2446	4.9504	-4.0221
43	H	1.8529	5.3250	-5.0687
44	H	3.1259	4.2375	-5.6418
45	C	-0.1202	-3.6701	0.3249
46	H	-0.5220	-4.5791	-0.1505
47	C	1.4072	-3.7117	0.2968
48	H	1.8148	-2.8333	0.8082
49	H	1.8262	-3.7479	-0.7152
50	H	1.7507	-4.6084	0.8335
51	C	-0.5902	-3.6285	1.7815
52	H	-0.1454	-4.4792	2.3185
53	H	-1.6746	-3.7015	1.8943
54	H	-0.2503	-2.7111	2.2761
55	C	-2.5897	-2.6023	-1.0155
56	H	-2.9448	-1.6603	-1.4545
57	C	-2.7906	-3.7157	-2.0376
58	H	-2.3784	-4.6721	-1.6840
59	H	-2.3325	-3.4813	-3.0060
60	H	-3.8686	-3.8620	-2.2038
61	C	-3.4124	-2.8710	0.2427
62	H	-4.4787	-2.7593	-0.0015
63	H	-3.1834	-2.1800	1.0625
64	H	-3.2667	-3.8981	0.6020
65	C	-3.1004	1.9502	0.5829
66	H	-3.8938	2.4847	0.0400
67	C	-3.6226	0.5884	1.0287
68	H	-2.8437	0.0458	1.5801
69	H	-3.9465	-0.0300	0.1822
70	H	-4.4872	0.7211	1.6959
71	C	-2.6870	2.7969	1.7860
72	H	-3.5049	2.7939	2.5219
73	H	-2.4968	3.8421	1.5170
74	H	-1.7946	2.3793	2.2686
75	C	-1.1884	3.3894	-1.2230
76	H	-0.5869	3.1424	-2.1077
77	C	-2.3582	4.2546	-1.6758
78	H	-3.0048	4.5438	-0.8354
79	H	-2.9760	3.7449	-2.4277

80	H	-1.9761	5.1802	-2.1322
81	C	-0.2724	4.1107	-0.2349
82	H	0.2873	4.8983	-0.7598
83	H	0.4564	3.4314	0.2246
84	H	-0.8354	4.5896	0.5751
85	C	3.0345	2.0768	-0.0527
86	H	2.5018	2.9850	-0.3728
87	C	4.5114	2.2531	-0.4084
88	H	4.8733	3.1838	0.0532
89	H	4.7019	2.3251	-1.4848
90	H	5.1258	1.4357	-0.0133
91	C	2.8605	1.9535	1.4598
92	H	3.3054	1.0289	1.8489
93	H	1.8041	1.9716	1.7534
94	H	3.3612	2.8019	1.9494
95	C	3.2327	-0.6641	-1.4384
96	H	2.5120	-1.4361	-1.7444
97	C	4.1534	-0.3997	-2.6236
98	H	4.9352	0.3328	-2.3878
99	H	3.5998	-0.0409	-3.5009
100	H	4.6525	-1.3389	-2.9059
101	C	3.9789	-1.1989	-0.2168
102	H	4.3901	-2.1918	-0.4501
103	H	3.3197	-1.2999	0.6533
104	H	4.8199	-0.5535	0.0647
105	C	0.2083	-0.0775	1.5396
106	O	-0.4510	0.4458	2.4237
107	O	1.2846	-0.8261	1.9170
108	H	1.3385	-0.8023	2.8922

/db/nbandeira/Fe(NPiso)/NCMe_substitution_/0e-/1-Cl+NCMe
Energy (POTENTIAL) = -4456.35144525 Eh

	Atom	X	Y	Z
1	Fe	0.0152	-0.1480	0.0423
2	P	-0.8164	-2.3365	-0.7574
3	P	-1.6608	1.5427	-0.5172
4	P	2.1352	0.6044	-1.0028
5	Cl	0.0645	-0.2370	2.3155
6	N	-0.2985	-0.0524	-2.7111
7	C	0.2725	-1.2972	-3.1294
8	C	1.0265	-1.3725	-4.3036
9	H	1.1911	-0.4734	-4.8947
10	C	1.5635	-2.5844	-4.7232
11	H	2.1531	-2.6172	-5.6401
12	C	1.3410	-3.7609	-3.9982
13	C	0.5747	-3.6728	-2.8324
14	H	0.3969	-4.5862	-2.2658
15	C	0.0524	-2.4600	-2.3688
16	C	1.9263	-5.0707	-4.4419
17	H	1.9028	-5.1683	-5.5354
18	H	1.3846	-5.9193	-4.0054
19	H	2.9788	-5.1538	-4.1301
20	C	-1.7216	0.0384	-2.8740
21	C	-2.3552	-0.6340	-3.9216
22	H	-1.7660	-1.2492	-4.5998
23	C	-3.7309	-0.5332	-4.0971
24	H	-4.2064	-1.0805	-4.9118
25	C	-4.5072	0.2665	-3.2507
26	C	-3.8574	0.9414	-2.2115
27	H	-4.4630	1.5499	-1.5409
28	C	-2.4797	0.8307	-1.9931
29	C	-5.9876	0.4082	-3.4582
30	H	-6.2007	1.1265	-4.2647
31	H	-6.4867	0.7714	-2.5511
32	H	-6.4435	-0.5482	-3.7467
33	C	0.4034	1.1248	-3.1365
34	C	-0.0978	1.8927	-4.1927
35	H	-1.0030	1.5723	-4.7051
36	C	0.5278	3.0729	-4.5750
37	H	0.1075	3.6599	-5.3923
38	C	1.6821	3.5162	-3.9193

39	C	2.1859	2.7271	-2.8817
40	H	3.0733	3.0820	-2.3647
41	C	1.5726	1.5359	-2.4732
42	C	2.3625	4.7922	-4.3237
43	H	3.1131	5.0975	-3.5841
44	H	1.6380	5.6098	-4.4390
45	H	2.8735	4.6733	-5.2910
46	C	-0.1318	-3.7612	0.2336
47	H	-0.3618	-4.6889	-0.3116
48	C	1.3811	-3.5973	0.3659
49	H	1.6142	-2.7082	0.9694
50	H	1.8981	-3.5051	-0.5963
51	H	1.7997	-4.4687	0.8901
52	C	-0.7442	-3.8424	1.6338
53	H	-0.1838	-4.5867	2.2185
54	H	-1.7923	-4.1508	1.6323
55	H	-0.6672	-2.8796	2.1562
56	C	-2.6084	-2.7072	-1.1752
57	H	-2.9600	-1.7506	-1.5830
58	C	-2.7505	-3.7766	-2.2525
59	H	-2.3279	-4.7384	-1.9265
60	H	-2.2652	-3.4896	-3.1932
61	H	-3.8189	-3.9367	-2.4616
62	C	-3.4736	-3.0439	0.0379
63	H	-4.5291	-2.8999	-0.2345
64	H	-3.2677	-2.4179	0.9133
65	H	-3.3540	-4.0946	0.3313
66	C	-3.0363	1.7386	0.7197
67	H	-3.8299	2.3302	0.2406
68	C	-3.5844	0.3642	1.0901
69	H	-2.8047	-0.2513	1.5576
70	H	-3.9740	-0.1790	0.2205
71	H	-4.4059	0.4736	1.8133
72	C	-2.5631	2.4928	1.9624
73	H	-3.3453	2.4381	2.7335
74	H	-2.3790	3.5537	1.7601
75	H	-1.6490	2.0511	2.3821
76	C	-1.1428	3.2553	-1.0483
77	H	-0.5414	3.0474	-1.9421
78	C	-2.3111	4.1401	-1.4659
79	H	-2.9553	4.3992	-0.6138

80	H	-2.9314	3.6604	-2.2353
81	H	-1.9263	5.0807	-1.8875
82	C	-0.2263	3.9317	-0.0297
83	H	0.3401	4.7338	-0.5242
84	H	0.4972	3.2320	0.4093
85	H	-0.7901	4.3858	0.7937
86	C	3.1577	1.8268	-0.0228
87	H	2.5841	2.7578	-0.1485
88	C	4.5918	2.0780	-0.4903
89	H	4.9924	2.9387	0.0652
90	H	4.6825	2.3048	-1.5581
91	H	5.2422	1.2222	-0.2748
92	C	3.1375	1.4721	1.4642
93	H	3.6544	0.5235	1.6637
94	H	2.1166	1.3842	1.8540
95	H	3.6576	2.2591	2.0299
96	C	3.2347	-0.7703	-1.6411
97	H	2.5014	-1.5164	-1.9754
98	C	4.0955	-0.3983	-2.8426
99	H	4.8865	0.3157	-2.5829
100	H	3.4981	0.0321	-3.6564
101	H	4.5804	-1.3069	-3.2300
102	C	4.0442	-1.4039	-0.5106
103	H	4.4554	-2.3629	-0.8572
104	H	3.4339	-1.6074	0.3780
105	H	4.8892	-0.7756	-0.2042
106	C	-3.1163	-1.4331	4.2702
107	N	-3.4623	-2.4429	3.8197
108	C	-2.6756	-0.1660	4.8224
109	H	-1.7258	0.1225	4.3529
110	H	-2.5339	-0.2533	5.9073
111	H	-3.4222	0.6126	4.6200

/db/nbandeira/Fe(NPiso)/L=CO2/2e-/1-CO+H2O
Energy (POTENTIAL) = -4062.22115560 Eh

	Atom	X	Y	Z
1	Fe	-0.1389	0.0783	-0.6130
2	P	-0.8217	-2.1666	-0.6362
3	P	-1.7425	1.7653	-0.7483
4	P	2.0551	0.7531	-1.0618
5	N	-0.3386	-0.0422	-2.6467
6	C	0.2178	-1.3353	-3.0643
7	C	0.9157	-1.4712	-4.2594
8	H	1.1038	-0.6076	-4.8931
9	C	1.3766	-2.7266	-4.6505
10	H	1.9338	-2.8168	-5.5830
11	C	1.1276	-3.8673	-3.8806
12	C	0.4272	-3.7060	-2.6792
13	H	0.2352	-4.5845	-2.0633
14	C	-0.0105	-2.4527	-2.2488
15	C	1.5780	-5.2264	-4.3284
16	H	0.7545	-5.7579	-4.8294
17	H	1.8951	-5.8434	-3.4778
18	H	2.4094	-5.1569	-5.0405
19	C	-1.7828	0.0398	-2.9142
20	C	-2.3675	-0.7090	-3.9299
21	H	-1.7673	-1.3884	-4.5315
22	C	-3.7353	-0.5998	-4.1709
23	H	-4.1822	-1.2045	-4.9601
24	C	-4.5404	0.2639	-3.4209
25	C	-3.9314	1.0121	-2.4057
26	H	-4.5530	1.6714	-1.8003
27	C	-2.5653	0.9101	-2.1378
28	C	-6.0072	0.4016	-3.7031
29	H	-6.1792	1.1790	-4.4633
30	H	-6.5628	0.6932	-2.8031
31	H	-6.4293	-0.5345	-4.0896
32	C	0.3849	1.0820	-3.2522
33	C	-0.0960	1.7011	-4.4026
34	H	-1.0237	1.3673	-4.8622
35	C	0.6007	2.7712	-4.9560
36	H	0.2038	3.2577	-5.8471
37	C	1.7904	3.2349	-4.3832
38	C	2.2577	2.5929	-3.2313

39	H	3.1701	2.9657	-2.7708
40	C	1.5730	1.5201	-2.6533
41	C	2.5482	4.3788	-4.9899
42	H	3.2543	4.8172	-4.2742
43	H	1.8672	5.1666	-5.3374
44	H	3.1248	4.0376	-5.8629
45	C	-0.1172	-3.4389	0.5224
46	H	-0.5579	-4.3935	0.1932
47	C	1.4038	-3.5103	0.4317
48	H	1.8454	-2.5579	0.7473
49	H	1.7807	-3.7480	-0.5687
50	H	1.7650	-4.2864	1.1216
51	C	-0.5120	-3.1783	1.9793
52	H	-0.2759	-4.0752	2.5691
53	H	-1.5720	-2.9556	2.1269
54	H	0.0741	-2.3523	2.3984
55	C	-2.6283	-2.5850	-0.9300
56	H	-3.0377	-1.6598	-1.3582
57	C	-2.7961	-3.7080	-1.9494
58	H	-2.3457	-4.6476	-1.5985
59	H	-2.3646	-3.4605	-2.9261
60	H	-3.8712	-3.8885	-2.0950
61	C	-3.3940	-2.9041	0.3507
62	H	-4.4627	-2.9742	0.1033
63	H	-3.2832	-2.1350	1.1228
64	H	-3.0882	-3.8721	0.7692
65	C	-3.0406	1.9870	0.5517
66	H	-3.8575	2.5468	0.0718
67	C	-3.5662	0.6301	1.0069
68	H	-2.7800	0.0407	1.4971
69	H	-3.9755	0.0403	0.1778
70	H	-4.3728	0.7811	1.7382
71	C	-2.5183	2.8083	1.7305
72	H	-3.2717	2.7951	2.5304
73	H	-2.3435	3.8557	1.4629
74	H	-1.5882	2.3960	2.1452
75	C	-1.2485	3.4319	-1.4148
76	H	-0.6677	3.1613	-2.3070
77	C	-2.4527	4.2541	-1.8608
78	H	-3.0817	4.5500	-1.0099
79	H	-3.0758	3.7166	-2.5877

80	H	-2.0959	5.1745	-2.3455
81	C	-0.3284	4.2055	-0.4713
82	H	0.2234	4.9598	-1.0491
83	H	0.4063	3.5599	0.0236
84	H	-0.8909	4.7324	0.3082
85	C	2.9486	2.1134	-0.1475
86	H	2.4230	3.0068	-0.5159
87	C	4.4335	2.2712	-0.4805
88	H	4.7724	3.2376	-0.0808
89	H	4.6513	2.2661	-1.5544
90	H	5.0412	1.4919	-0.0076
91	C	2.7306	2.0351	1.3617
92	H	3.0792	1.0875	1.7925
93	H	1.6761	2.1695	1.6289
94	H	3.2949	2.8479	1.8412
95	C	3.1717	-0.6955	-1.4381
96	H	2.4466	-1.4901	-1.6667
97	C	4.0535	-0.5050	-2.6672
98	H	4.8100	0.2758	-2.5185
99	H	3.4668	-0.2529	-3.5594
100	H	4.5813	-1.4483	-2.8707
101	C	3.9662	-1.1262	-0.2047
102	H	4.3079	-2.1611	-0.3465
103	H	3.3859	-1.0911	0.7260
104	H	4.8574	-0.5038	-0.0656
105	C	-0.0109	0.1580	1.1224
106	O	0.0554	0.2116	2.2679
107	O	2.7796	-1.0252	3.2440
108	H	1.8984	-0.6649	3.0834
109	H	2.7304	-1.9420	2.9455

/db/nbandeira/Fe(NPiso)/L=NCMe/1e-/1-NCMe
Energy (POTENTIAL) = -4005.40462845962793 Eh

	Atom	X	Y	Z
1	Fe	-0.3137	1.4546	2.7779
2	P	-1.0402	-0.6723	1.9323
3	P	-1.8674	3.0954	2.1277
4	P	1.7838	2.1132	1.8312
5	N	-0.5076	1.5360	-0.1092
6	C	0.0712	0.2857	-0.4677
7	C	0.8639	0.1822	-1.6149
8	H	1.0363	1.0680	-2.2244
9	C	1.4261	-1.0351	-1.9855
10	H	2.0451	-1.0892	-2.8820
11	C	1.1874	-2.1912	-1.2347
12	C	0.3826	-2.0751	-0.0960
13	H	0.1958	-2.9757	0.4882
14	C	-0.1599	-0.8557	0.3242
15	C	1.7979	-3.5108	-1.6138
16	H	1.9647	-3.5789	-2.6968
17	H	1.1599	-4.3503	-1.3080
18	H	2.7742	-3.6472	-1.1234
19	C	-1.9183	1.6547	-0.2808
20	C	-2.5514	1.0014	-1.3431
21	H	-1.9567	0.3944	-2.0246
22	C	-3.9243	1.1147	-1.5311
23	H	-4.3973	0.5861	-2.3600
24	C	-4.7001	1.9102	-0.6793
25	C	-4.0515	2.5677	0.3716
26	H	-4.6587	3.1760	1.0414
27	C	-2.6768	2.4417	0.6080
28	C	-6.1828	2.0441	-0.8830
29	H	-6.4120	2.4552	-1.8769
30	H	-6.6315	2.7052	-0.1310
31	H	-6.6824	1.0666	-0.8167
32	C	0.2421	2.7004	-0.4469
33	C	-0.1717	3.5046	-1.5152
34	H	-1.0503	3.2141	-2.0894
35	C	0.5068	4.6747	-1.8338
36	H	0.1559	5.2903	-2.6632
37	C	1.6332	5.0652	-1.1003
38	C	2.0442	4.2428	-0.0470

39	H	2.9094	4.5634	0.5268
40	C	1.3714	3.0663	0.3085
41	C	2.3818	6.3232	-1.4387
42	H	3.1214	6.5682	-0.6661
43	H	1.6991	7.1778	-1.5447
44	H	2.9175	6.2181	-2.3941
45	C	-0.4263	-2.1440	2.9161
46	H	-0.6628	-3.0634	2.3596
47	C	1.0842	-2.0249	3.1026
48	H	1.3162	-1.1515	3.7276
49	H	1.6331	-1.9203	2.1598
50	H	1.4685	-2.9165	3.6202
51	C	-1.0800	-2.2267	4.2980
52	H	-0.5426	-2.9717	4.9038
53	H	-2.1291	-2.5308	4.2637
54	H	-1.0182	-1.2654	4.8250
55	C	-2.8186	-1.0758	1.4465
56	H	-3.1587	-0.1269	1.0110
57	C	-2.9346	-2.1592	0.3803
58	H	-2.5129	-3.1152	0.7252
59	H	-2.4297	-1.8814	-0.5528
60	H	-3.9970	-2.3317	0.1478
61	C	-3.7340	-1.3957	2.6275
62	H	-4.7790	-1.2333	2.3252
63	H	-3.5421	-0.7720	3.5080
64	H	-3.6440	-2.4480	2.9270
65	C	-3.2886	3.3253	3.3160
66	H	-4.0640	3.9379	2.8338
67	C	-3.8727	1.9626	3.6717
68	H	-3.1187	1.3364	4.1692
69	H	-4.2338	1.4201	2.7895
70	H	-4.7204	2.0837	4.3630
71	C	-2.8227	4.0501	4.5788
72	H	-3.6091	3.9910	5.3459
73	H	-2.6206	5.1122	4.4009
74	H	-1.9141	3.5928	4.9969
75	C	-1.3623	4.8272	1.6146
76	H	-0.7499	4.6288	0.7256
77	C	-2.5259	5.7160	1.1934
78	H	-3.1779	5.9677	2.0422
79	H	-3.1416	5.2417	0.4170

80	H	-2.1425	6.6623	0.7820
81	C	-0.4586	5.5036	2.6438
82	H	0.1124	6.3118	2.1636
83	H	0.2602	4.8003	3.0837
84	H	-1.0314	5.9502	3.4656
85	C	2.7820	3.3511	2.8421
86	H	2.2456	4.2919	2.6484
87	C	4.2556	3.5782	2.5013
88	H	4.6209	4.4428	3.0759
89	H	4.4414	3.7884	1.4424
90	H	4.8773	2.7197	2.7812
91	C	2.6273	3.0431	4.3316
92	H	3.0562	2.0657	4.5936
93	H	1.5741	3.0408	4.6359
94	H	3.1524	3.8072	4.9247
95	C	2.9584	0.7699	1.2393
96	H	2.2562	0.0138	0.8616
97	C	3.8819	1.1492	0.0875
98	H	4.6336	1.8913	0.3835
99	H	3.3223	1.5516	-0.7665
100	H	4.4183	0.2525	-0.2597
101	C	3.7194	0.1435	2.4070
102	H	4.1297	-0.8296	2.0992
103	H	3.0783	-0.0298	3.2797
104	H	4.5627	0.7656	2.7302
105	C	-0.2714	1.1877	5.9147
106	N	-0.2696	1.2909	4.7604
107	C	-0.2755	1.0570	7.3553
108	H	0.6576	1.4598	7.7709
109	H	-0.3635	-0.0013	7.6351
110	H	-1.1233	1.6107	7.7801

/db/nbandeira/Fe(NPiso)/L=NCMe/2e-/1-NCMe
Energy (POTENTIAL) = -4005.45348021416612 Eh

	Atom	X	Y	Z
1	Fe	-0.3176	1.4435	2.7499
2	P	-1.0008	-0.6870	1.9222
3	P	-1.8694	3.1042	2.0930
4	P	1.7712	2.0842	1.8158
5	N	-0.5115	1.5073	-0.1284
6	C	0.0772	0.2695	-0.4827
7	C	0.8601	0.1727	-1.6394
8	H	1.0110	1.0596	-2.2529
9	C	1.4441	-1.0409	-2.0091
10	H	2.0581	-1.0886	-2.9100
11	C	1.2362	-2.1939	-1.2524
12	C	0.4396	-2.0861	-0.0993
13	H	0.2856	-2.9848	0.4978
14	C	-0.1262	-0.8773	0.3140
15	C	1.8370	-3.5165	-1.6395
16	H	2.4762	-3.4206	-2.5267
17	H	1.0575	-4.2597	-1.8659
18	H	2.4482	-3.9327	-0.8250
19	C	-1.9285	1.6053	-0.2790
20	C	-2.5754	0.9017	-1.2825
21	H	-1.9812	0.2623	-1.9377
22	C	-3.9717	0.9886	-1.4647
23	H	-4.4641	0.4129	-2.2494
24	C	-4.7180	1.8900	-0.6493
25	C	-4.0651	2.6140	0.3310
26	H	-4.6596	3.2988	0.9393
27	C	-2.6600	2.4770	0.6061
28	C	-6.1976	2.0447	-0.8726
29	H	-6.4211	2.3944	-1.8942
30	H	-6.6413	2.7615	-0.1679
31	H	-6.7248	1.0840	-0.7530
32	C	0.2266	2.6788	-0.4536
33	C	-0.2118	3.5028	-1.4973
34	H	-1.0982	3.2025	-2.0553
35	C	0.4490	4.6856	-1.8041
36	H	0.0810	5.3140	-2.6169
37	C	1.5801	5.0767	-1.0766
38	C	2.0114	4.2410	-0.0421
39	H	2.8766	4.5643	0.5305
40	C	1.3564	3.0496	0.2994

41	C	2.3076	6.3524	-1.3980
42	H	3.0673	6.5808	-0.6395
43	H	1.6158	7.2047	-1.4561
44	H	2.8170	6.2851	-2.3714
45	C	-0.3832	-2.1571	2.9092
46	H	-0.6046	-3.0781	2.3489
47	C	1.1238	-2.0290	3.1126
48	H	1.3437	-1.1502	3.7348
49	H	1.6781	-1.9228	2.1731
50	H	1.5110	-2.9157	3.6373
51	C	-1.0535	-2.2479	4.2822
52	H	-0.5235	-2.9934	4.8944
53	H	-2.1017	-2.5538	4.2314
54	H	-1.0022	-1.2872	4.8124
55	C	-2.7764	-1.1012	1.4483
56	H	-3.0896	-0.1715	0.9549
57	C	-2.8969	-2.2363	0.4387
58	H	-2.5176	-3.1862	0.8456
59	H	-2.3550	-2.0208	-0.4898
60	H	-3.9568	-2.3876	0.1800
61	C	-3.7089	-1.3450	2.6344
62	H	-4.7474	-1.1591	2.3217
63	H	-3.4998	-0.6931	3.4903
64	H	-3.6580	-2.3866	2.9781
65	C	-3.2801	3.3748	3.2984
66	H	-4.0366	4.0008	2.8016
67	C	-3.9094	2.0317	3.6455
68	H	-3.1776	1.3834	4.1484
69	H	-4.2687	1.5078	2.7510
70	H	-4.7632	2.1703	4.3278
71	C	-2.8275	4.0932	4.5685
72	H	-3.6310	4.0631	5.3210
73	H	-2.5894	5.1478	4.3907
74	H	-1.9410	3.6139	5.0090
75	C	-1.3101	4.8628	1.6715
76	H	-0.6884	4.6671	0.7878
77	C	-2.4484	5.7789	1.2428
78	H	-3.1013	6.0444	2.0878
79	H	-3.0689	5.3032	0.4699
80	H	-2.0553	6.7199	0.8251
81	C	-0.4063	5.4977	2.7249
82	H	0.2277	6.2747	2.2705
83	H	0.2575	4.7538	3.1883

84	H	-0.9777	5.9757	3.5308
85	C	2.7869	3.3176	2.8229
86	H	2.2351	4.2545	2.6545
87	C	4.2524	3.5684	2.4633
88	H	4.6178	4.4304	3.0425
89	H	4.4207	3.7923	1.4043
90	H	4.8885	2.7140	2.7235
91	C	2.6651	2.9876	4.3109
92	H	3.1281	2.0204	4.5531
93	H	1.6166	2.9438	4.6279
94	H	3.1751	3.7593	4.9080
95	C	2.9631	0.7575	1.2086
96	H	2.2679	-0.0044	0.8295
97	C	3.8740	1.1545	0.0525
98	H	4.6190	1.9039	0.3474
99	H	3.3015	1.5562	-0.7932
100	H	4.4193	0.2673	-0.3063
101	C	3.7441	0.1307	2.3626
102	H	4.1666	-0.8339	2.0430
103	H	3.1138	-0.0599	3.2396
104	H	4.5814	0.7616	2.6852
105	C	-0.3649	1.2178	5.8775
106	N	-0.3106	1.3086	4.7208
107	C	-0.4392	1.1072	7.3191
108	H	0.5106	1.4183	7.7748
109	H	-0.6477	0.0682	7.6083
110	H	-1.2430	1.7493	7.7037