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Supporting Information

Dissection of Light-Induced Charge Accumulation at a Highly Active Iron Porphyrin: Insights in the Photocatalytic CO_2 Reduction

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A.A. Conceptualization:Lead; Formal analysis:Equal; Supervision:Lead; Writing – original draft:Equal; Writing – review & editing:Equal

SUPPORTING INFORMATION

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Dissection of the Light Induced Charge Accumulation at Iron Porphyrin for a Highly Active Photocatalytic CO_2 Reduction

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Abstract: Using light energy to drive multielectron catalytic reduction of CO_2 to produce a fuel is a contemporary research thrust. Recent efforts in the design of porphyrin-based catalysts have positioned them among the most performant electrocatalysts for CO_2 reduction. Powering these catalysts with the help of photosensitizers to realize light-driven catalysis comes along with a couple of unsolved challenges that need to be addressed with much vigor. We have designed an iron porphyrin catalyst decorated with urea functions (**UrFe**) acting as a multipoint hydrogen bonding scaffold towards the CO_2 substrate. When powered by a molecular photosensitizer in presence of an electron donor and water, a spectacular photocatalytic activity reaching unreported TONs and TOFs as high as 7270 and 3720 h^{-1} respectively are observed. Importantly, we have spectroscopically characterized all the photo-reduced Fe^{II}, Fe^{I} and Fe^{0} states and compared with the electrochemically generated ones. While the Fe^{0} redox state has been widely accepted as the catalytically active species, we show here that the Fe^{I} species is already involved in the CO_2 activation which represents the rate determining step in the photocatalytic cycle. DFT calculations bring support to our experimental findings that constitute ahis new paradigm in the catalytic reduction of CO_2.

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SUPPORTING INFORMATION

Table of Contents

SUPPORTING INFORMATION

SUPPORTING INFORMATION

1. Experimental Procedures

General Materials

The syntheses of **UrFe**, **F_{20}TPPFe** and **TPPFe** were previously reported by our group.[1] 1,3-dimethyl-2-phenyl-2,3-dihydro-1*H*-benzo[*d*]imidazole (BIH) was prepared as found in the literature.[2] Solvents, photosensitizers and electrolyte salts were purchased from Sigma Aldrich or Carlo Erba (N,N-dimethylformammide).

Photocatalysis

Photocatalysis experiments were performed in 41.5 mL glass vials hermetically closed with a septum and containing 6.5 mL of solution and an 8 mm stir bar. The reaction mixture was first purged with CO_2 during 30 min, while kept in the dark, and then irradiated with LED light source (SugarCube).

The gas phase was automatically injected and analyzed by a Micro GC Fusion Gas Analyser (Inficon). In module A (PLOT column with molecular sieve and 10 m length) a 9 s backflush is applied to separate H_2, O_2, N_2, CH_4 and CO. Module B (RT-Q-bond column of 12 m) allows the detection of heavier molecules, such as CO_2, H_2O vapor and C_2 products. The setup is equipped of an Ar carrier gas with 99.999% purity and a TCD detector.

For experiments with limited amount of CO_2, the reaction vial was first degassed with Ar, then different amounts of a solution of 10 mL of DMF previously purged for 20 min with CO_2 were injected. The solubility of CO_2 in DMF was taken to be 230 mM[ref].

To quantify products, calibration was manually performed injecting fixed aliquots (100 or 500 µL) of reference gasses in the same vial used in a typical run, filled with 6.5 mL of the same solvent mixture and an 8 mm stirring bar, and purged for 30 min with CO_2. Calibration curves were fitted with 10 points choosing the same range of area peaks obtained experimentally.

Turnover numbers (TON) were calculated from chromatograms quantification as the number of moles of product over the number of moles of catalyst.

Turnover frequencies (TOF) were calculated from the slope of the TON evolution over time, considering the initial linear region, but cutting out the point zero linked to artefacts of catalysis activation (small inflection due to bubble formation).

Labeled $^{13}CO_2$ photocatalysis was done as described above, but purging with a $^{13}CO_2$ bottle of Sigma Aldrich. ^{13}CO was detected by manual sampling (50 µL) from the headspace of the reaction cells into a TraceGC Ultra / ISQ GC/MS system (Thermo Scientific) equipped with a TraceGOLD TG-5MS 30 m, 0.25 mm diameter column (Thermo Scientific) kept at 313 K using helium carrier gas.

Photoaccumulation

Photoaccumulation experiments were conducted in a 1 cm optical path quartz cuvette hermetically closed with a septum. To probe the sample a Agilent Technologies Cary 60 UV-Vis spectrophotometer was used, adapted with a liquid nitrogen dewar and thermostated around the cuvette to perform measurements down to -196°C. This apparatus is connected to the temperature controller (CoolSpek UV USP-203 by Unisoku), able to regulate the flux of liquid nitrogen and to heat the cuvette. During the measurement, the sample is irradiated with a blue LED light source (SugarCube). The solution is stirred during the measurement. Spectra acquisition is operated through the CaryWin software, in the Scanning Kinetics mode.

UV-vis spectroelectrochemistry

UV-vis spectroelectrochemical measurements were done in a quartz cuvette with Pt honeycomb electrode (PINE research) and a Pt wire pseudo-reference electrode. To probe the sample the spectrophotometer Agilent Technologies Cary 50 UV-Vis was used. The potentials were applied through the pontentiostat Metrohm Autolab 204 in the chronoamperometry method.

IR-spectroelectrochemistry

Infrared spectroelectrochemical measurements were recorded with an FT-IR Thermo Scientific Nicolet 6700 spectrometer, with ATR diamond accessory. A home-made PTFE electrochemical cell fitted ATR crystal was filled with 1 mL of THF solution containing 1 mM catalyst and 0.1 M $TBAPF_6$ in a three-electrode system including a GC working electrode, Pt counter electrode and $Ag/AgNO_3$ (10 mM) reference electrode (+0.54 V vs. NHE) under a continuous flow of Argon or CO_2. Applied potential was varied by 200 mV steps and three infrared spectra were recorded for each potential applied.

2. Electrochemical data

Table S1 Electrochemical potentials in Volts of the studied compounds vs NHE in 0.1 M $TBAPF_6$ Ar-saturated DMF_{dry} solution.

Entry	Compound	$E^{1/2}$ (M/M^{-})	$E^{1/2}$ (M^{-}/M^{2-})	$E^{1/2}$ (M^{2-}/M^{3-})	Ref.
1	UrFe	0.23	-0.63	-1.12	[1]
2	TPPFe	0.09	-0.79	-1.42	[1]
3	F_{20}TPPFe	0.25	-0.59	-1.11	[1]
4	$Ru(bpy)_3^{2+}$ [a]	-1.09			[3]
5	$Ir(ppy)_3^{+}$ [a]	-1.95			[3]

[a] In acetonitrile solution.

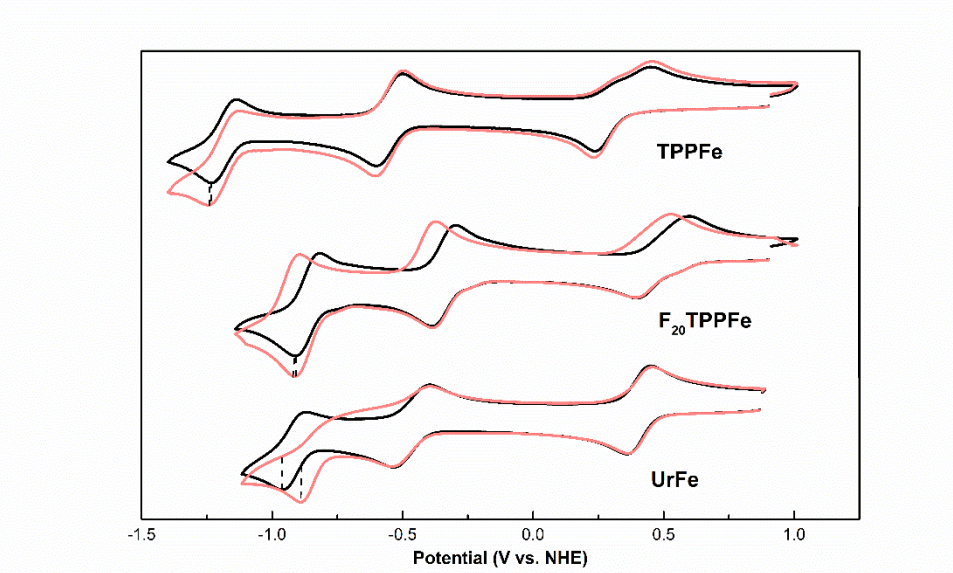


Figure S1. Cyclic voltammograms of the studied iron porphyrins in Ar (black) and CO_2 (red) atmospheres, 1 mM catalyst, 0.1 M $TBAPF_6$ in DMF_{dry}, 100 mV s^{-1}.

3. Photocatalysis

Table S2 Photocatalysis experiments performed with 20 µM catalyst, 1 mM Ru(bpy)32+, BIH as SED in DMF/H2O 9:1 under LED irradiation (100 W m-2) for 2h.

	Catalyst	[SED] (mM)	LED type	CO (µmol)	H_2 (µmol)	Selectivity (CO %)	TON_{CO}	TOF_{CO} (h^{-1})
1	**UrFe**[a]	50	Blue	8	0.7	92	63	46
2	**UrFe**[b]	100	Blue	2.7	0.6	82	21	14.6
3	-	50	Blue	50	0.4	99	-	-
4	**UrFe**[c]	50	White	0	-	-	0	-
5	**UrFe**[d]	50	White	0.9	0	100	7	3.5
6	**UrFe**[e]	50	Blue	65	0.1	100	623	497

[a] In ACN/H_2O 9:1 solvent mixture. [b] Sodium ascorbate used as SED in ACN/H_2O 6:4. [c] No photosensitizer in the reaction mixture. [d] $Ir(ppy)_3$ is used as photosensitizer and TEA as electron donor. [e] No water in the solvent mixture.

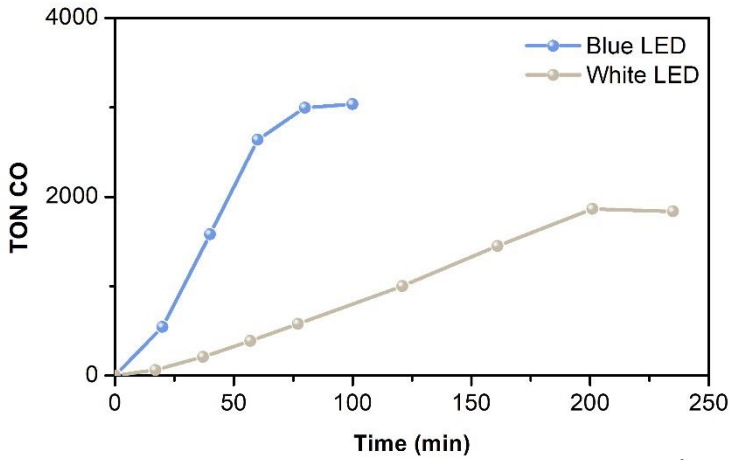


Figure S2 Time evolution of CO produced under light irradiation with a blue LED (blue dots, λem=460 nm 100 W m^{-2}) and white LED (grey dots, λ> 405 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 μM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 50 mM in CO_2-saturated DMF/H_2O 9:1

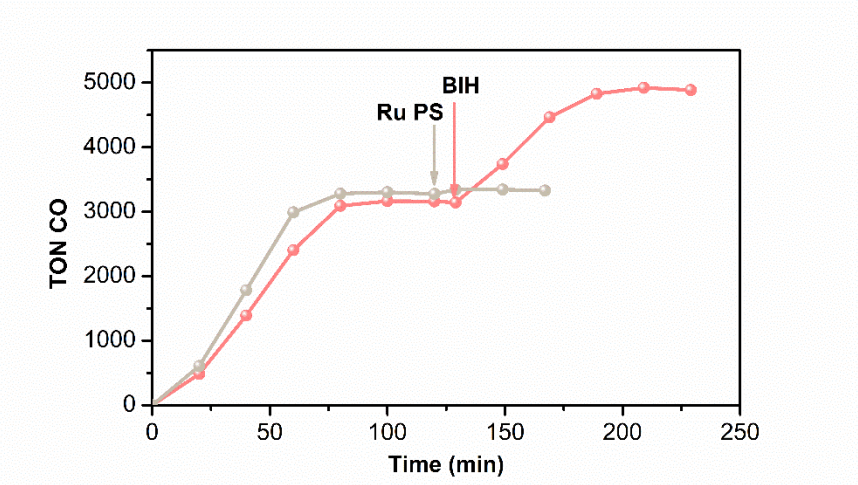


Figure S3 Time evolution of CO produced under light irradiation with a blue LED (λem=460 nm 100 W m-2) of TPPFe-Ur as catalyst with 20 μM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 50 mM in CO_2-saturated DMF/H2O 9:1. The arrows indicate the point of reinjection of 1 mL of 2 mM $[Ru(bpy)_3]^{2+}$(beige) or 1 mL of 0.2 M BIH (red).

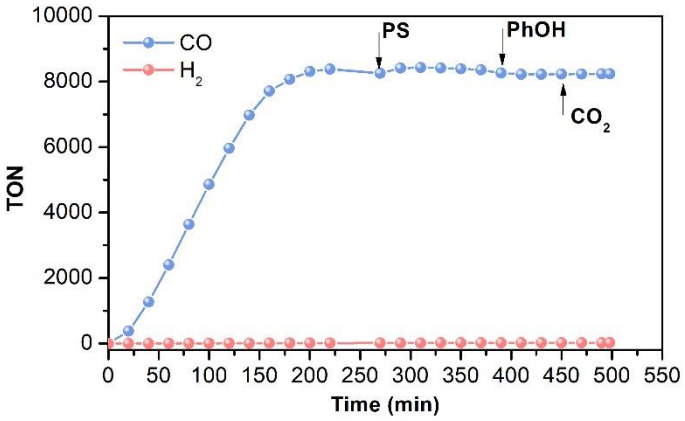


Figure S4 Time evolution of CO (blue) and H_2 (red) produced under light irradiation with a blue LED (λ_{em}=460 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 µM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 250 mM in CO_2-saturated DMF/H_2O 9:1. The arrows indicate the re-injections of the photosensitizer (PS), of a proton source (PhOH) and rebubbling of CO_2.

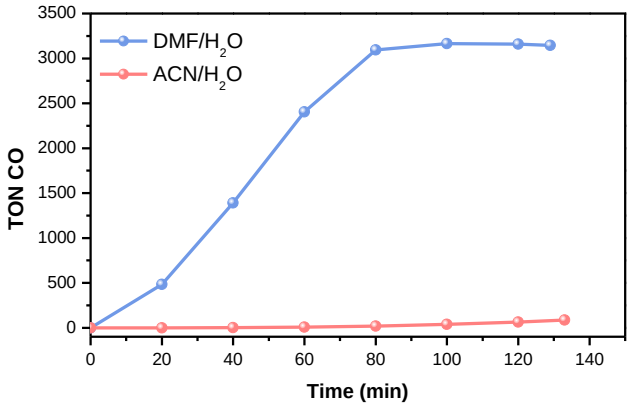


Figure S5 Time evolution of CO produced under light irradiation with a blue LED (λ_{em}=460 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 µM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 50 mM in CO_2-saturated DMF/H_2O 9:1 (blue) and CO_2-saturated ACN/H_2O 9:1 (red).

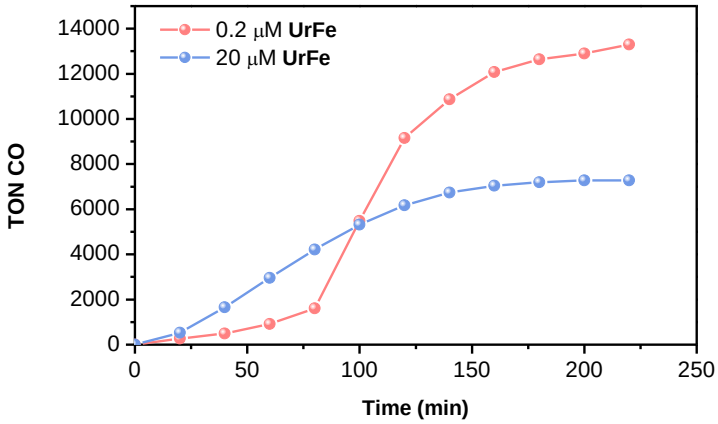


Figure S6. Time evolution of CO produced under light irradiation with a blue LED (λ_{em}=460 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 µM concentration (blue) and 0.2 µM concentration (red); $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 250 mM in CO_2-saturated DMF/H_2O 9:1.

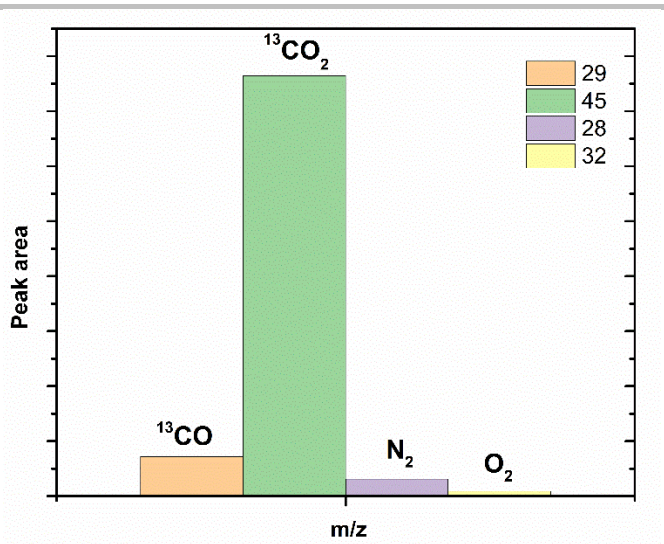


Figure S7 GC/MS analysis of 50 µL of gas mixture produced upon 1 h irradiation with blue LED (λ_{em}=460 nm 100 W m^{-2}) of 20 µM **UrFe** catalyst; 1 mM $[Ru(bpy)_3]^{2+}$ photosensitizer, 50 mM BIH sacrificial electron donor $^{13}CO_2$-saturated DMF/H_2O 9:1.

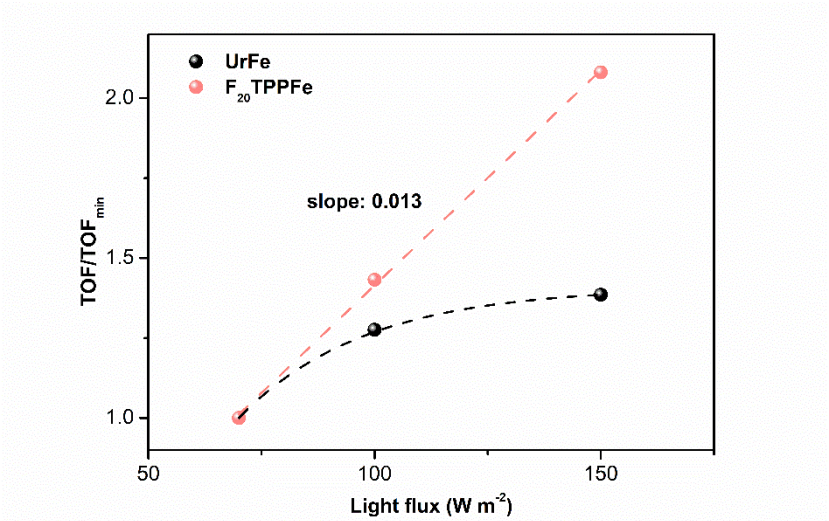


Figure S8 Dependency of the reaction kinetics (TOF) on the light flow for **UrFe** (red) and for F_{20}TPPFe (black). 20 µM catalyst, 1 mM $[Ru(bpy)_3]^{2+}$ photosensitizer, 50 mM BIH sacrificial electron donor in CO_2-saturated DMF/H_2O 9:1, blue LED irradiation (λem=460 nm).

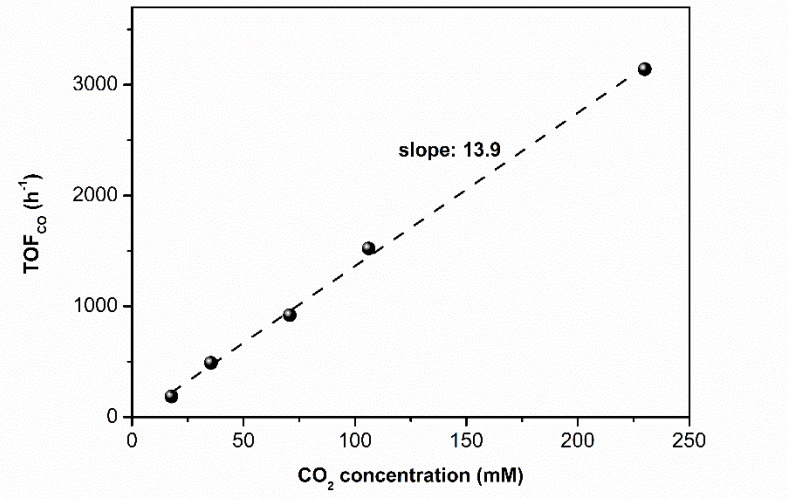


Figure S9 Dependency of the reaction kinetics (TOF) on the amount of CO_2 added for **UrFe** 20 µM catalyst, 1 mM $[Ru(bpy)_3]^{2+}$ photosensitizer, 50 mM BIH sacrificial electron donor in DMF/H_2O 9:1, blue LED irradiation (λem=460 nm 100 W m^{-2})..

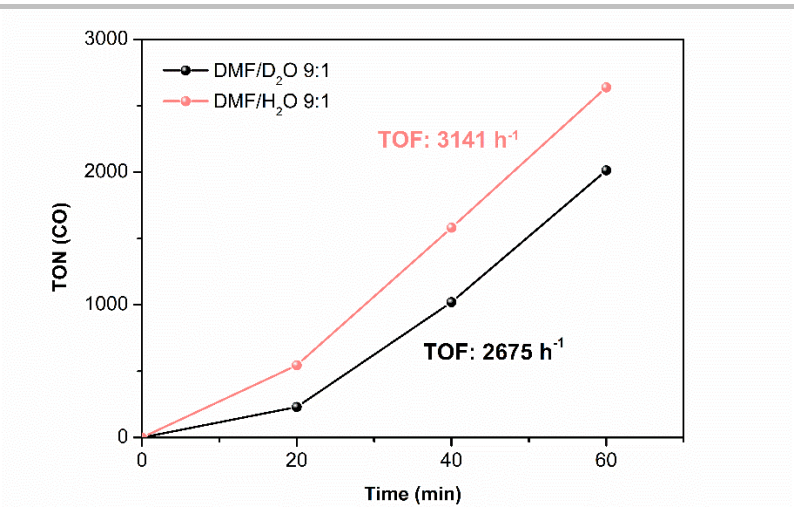


Figure S10 Time evolution of CO produced under light irradiation with a blue LED (λem=460 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 μM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 50 mM in CO_2-saturated DMF/H_2O 9:1 (red) and CO_2-saturated DMF/D_2O 9:1 (black).

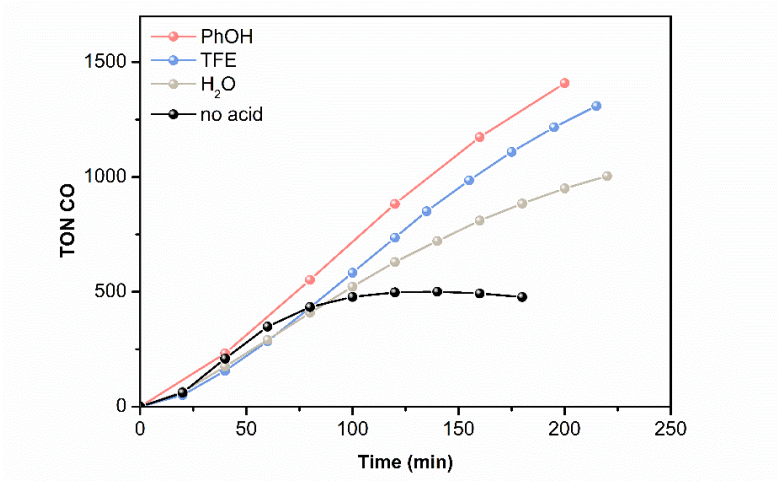


Figure S11. Time evolution of CO produced under light irradiation with a white LED (λ>405 nm, 100 W m^{-2}) of **UrFe** as catalyst with 20 μM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 50 mM in CO_2-saturated DMF and 100 mM PhOH (red), 100 mM TFE (blue), 100 mM H2O (grey) or in absence of proton (black).

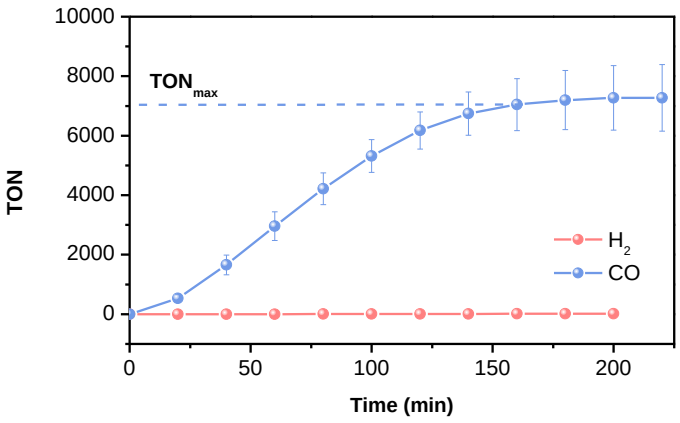


Figure S12 Time evolution of CO (blue) and H_2 (red) produced under light irradiation with a blue LED (λem=460 nm 100 W m^{-2}) of **UrFe** as catalyst with 20 μM concentration; $[Ru(bpy)_3]^{2+}$ photosensitizer 1 mM, BIH sacrificial electron donor 250 mM in CO_2-saturated DMF/H_2O 9:1. The data is the average of 3 runs, error bars represent the standard error.

4. UV-vis spectroscopy

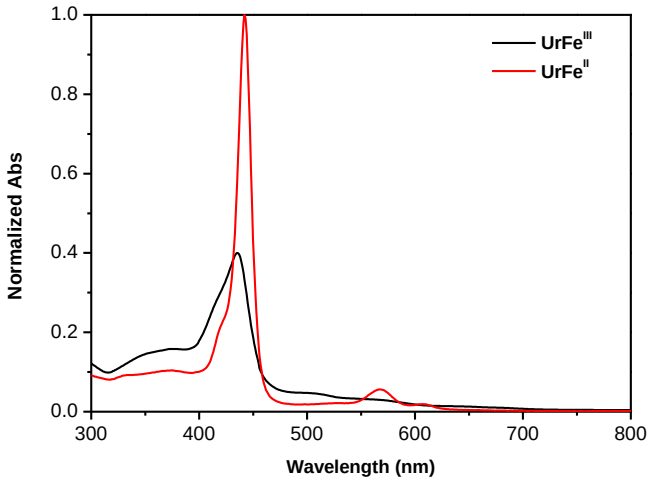


Figure S13 UV-vis reference spectra of **UrFe**^{III} (black) in Ar-saturated DMF, and chemically prepared **UrFe**^{II} (red) with ZnHg amalgam in N_2-saturated DMF.

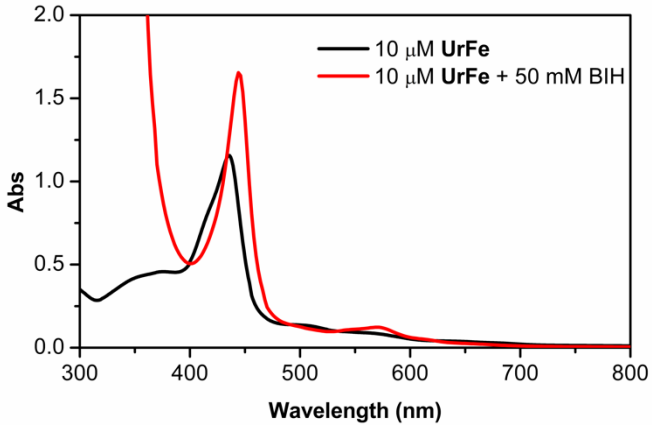


Figure S14 UV-vis reference spectra of **UrFe** in Ar-saturated DMF before (black) and after the addition of 50 mM of BIH (red).

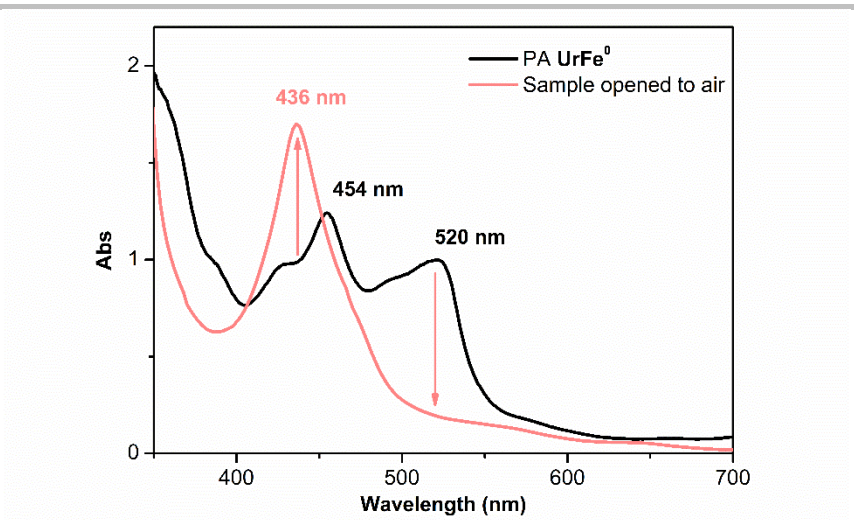


Figure S15 UV-vis spectra of photoaccumulated (blue LED irradiation) **UrFe** 10 µM, $[Ru(bpy)_3]^{2+}$ 30 µM, BIH 7 mM in N_2-saturated DMF_{dry} at -35 °C before (black) and after (red) opening the sample to the air.

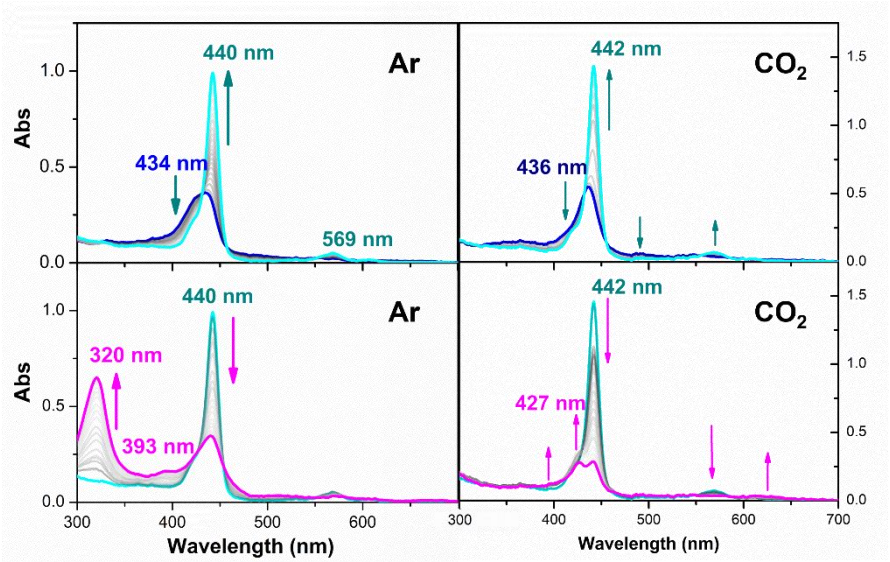


Figure S16 UV-vis spectral evolution in spectroelectrochemistry experiment with **UrFe** 40 µM in Ar-saturated DMF_{dry} (left) and CO_2-saturated DMF_{dry} (right), 0.2 M $TBAPF_6$, Pt Working Electrode, Pt Counter Electrode and Ag pseudo-Reference Electrode; Room Temperature. Top: Fe^{III} to Fe^{II} reduction; Bottom: Fe^{II} to Fe^{I} reduction

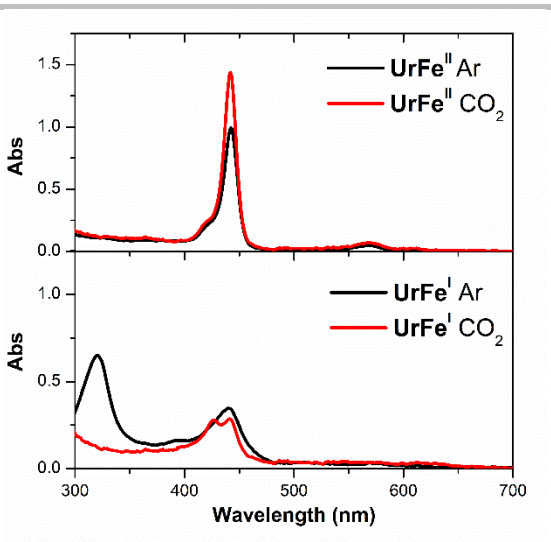


Figure S17 UV-vis spectra obtained in spectroelectrochemistry experiment with **UrFe** 40 µM in 0.2 M $TBAPF_6$ DMF_{dry} solution in Ar (black) and CO_2 (red) atmosphere. Top: **UrFe^{II}**, bottom: **UrFe^{I}**. Pt Working Electrode, Pt Counter Electrode and Ag pseudo-Reference Electrode; Room Temperature. (See Figure S17)

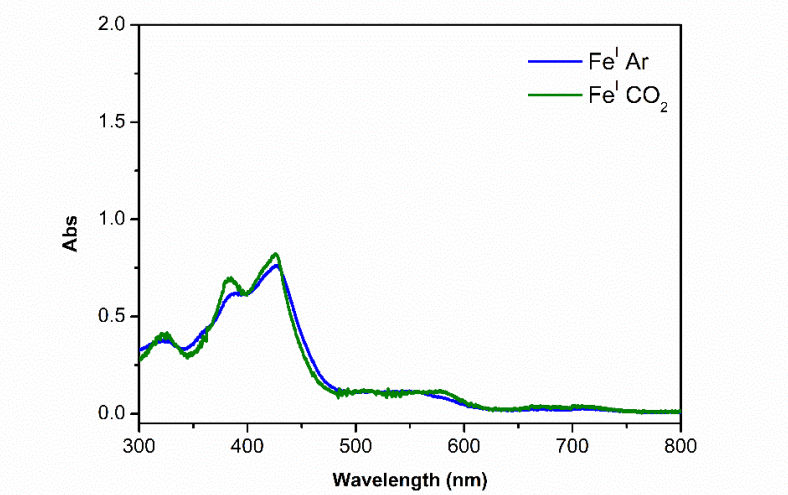


Figure S18 UV-vis spectral evolution in spectroelectrochemistry experiment with $F_{20}TPPFe$ 40 µM in DMF_{dry}, 0.2 M $TBAPF_6$, Pt Working Electrode, Pt Counter Electrode and Pt pseudo-Reference Electrode; Room Temperature.

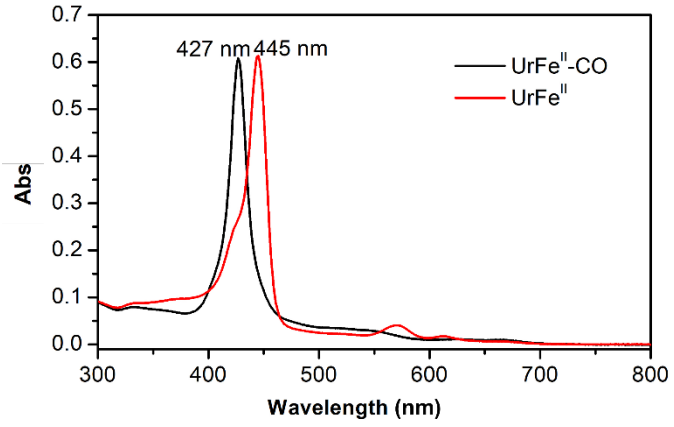


Figure S19 UV-vis reference spectra of chemically prepared **UrFe^{II}** in N_2-saturated DMF (red) and with CO-saturated DMF (black).

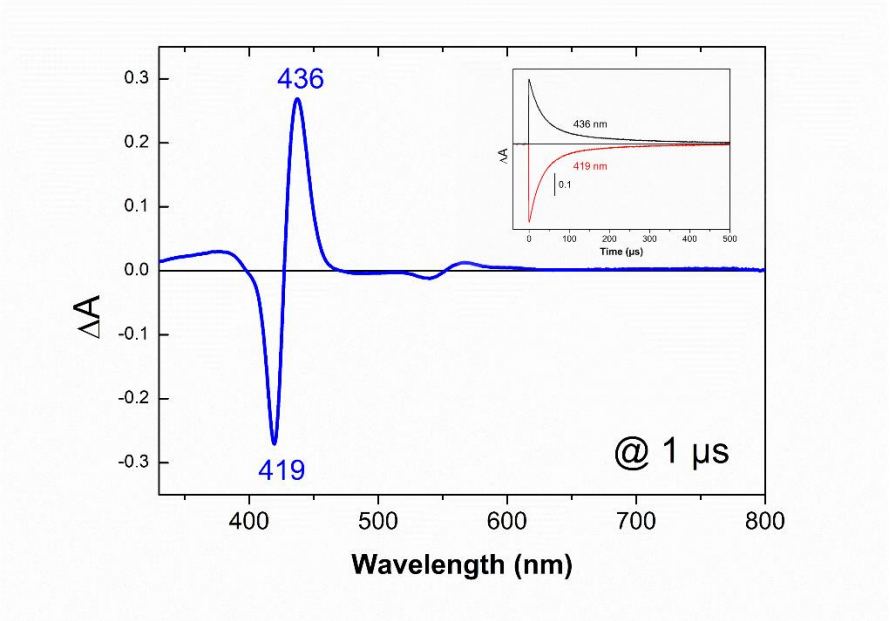


Figure S20 UV-vis laser flash photolysis of UrFe (OD 420=1), in CO-saturated ACN/H_2O 9/1, 25 mM NaAsc, exc 460 nm, 15 mJ

5. Infrared spectroscopy

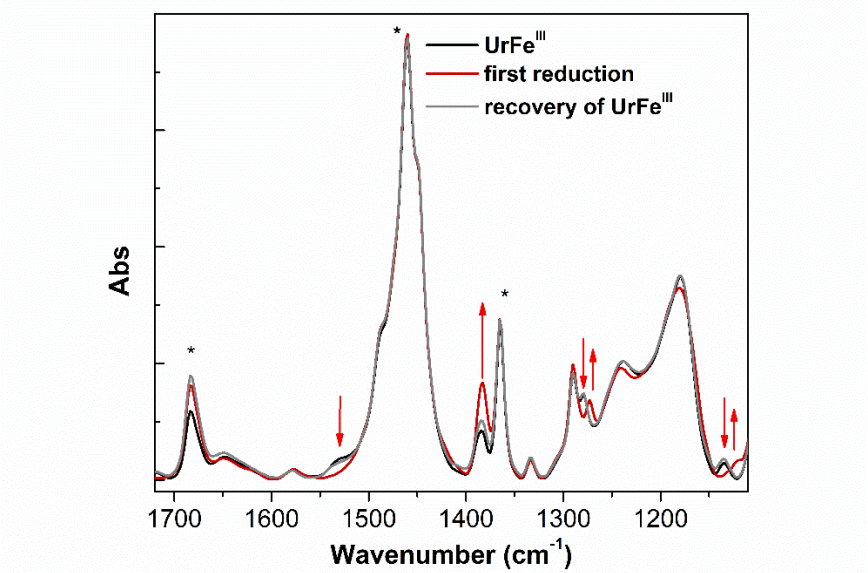


Figure S21 IR reversible conversion of Fe^{III} to Fe^{II} in spectroelectrochemistry experiment with **UrFe** 1 mM in Ar-saturated THF, 0.1 M $TBAPF_6$, GC Working Electrode, Pt Counter Electrode and $AgNO_3$/Ag Reference Electrode; Room Temperature. Peaks with asterisk are due to the solvent.

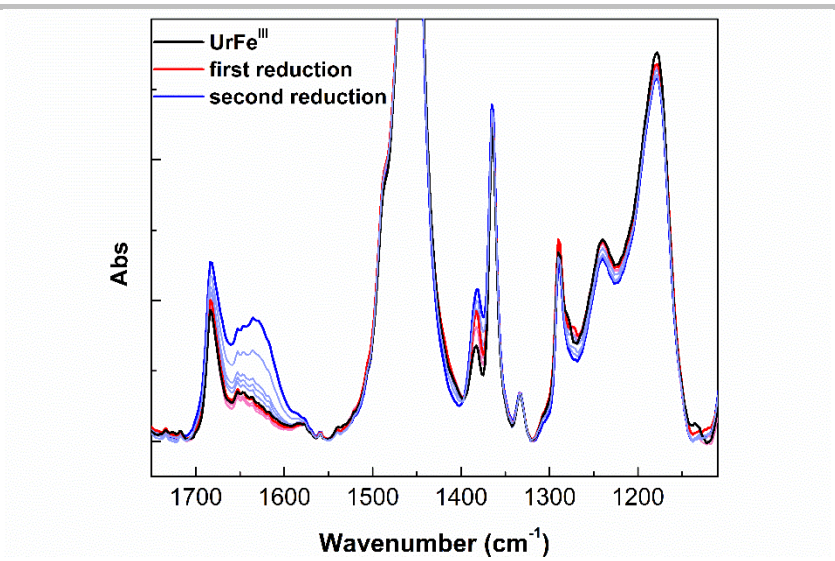
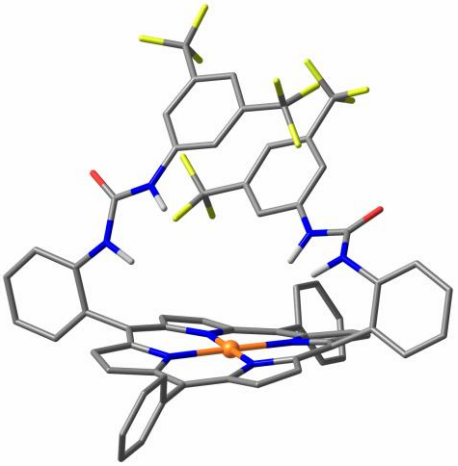


Figure S22 IR spectral evolution in spectroelectrochemistry experiment with **UrFe** 1 mM in CO_2-saturated THF. Black: **UrFe^{III}**, Red: **UrFe^{II}**, Blue: **UrFe^{I}**

6. Computational study

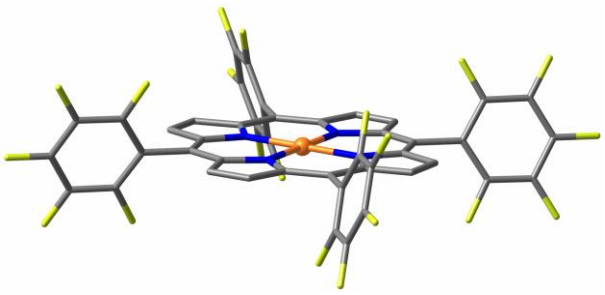
DFT calculations were performed using the Gaussian 16 program package. [4] PBE0[5] functional was used to predict geometries and relative energies. [6,7] B3LYP[8] was used for the calculation of vibrational spectra. In both cases, dispersion correction with Becke-Johnson damping (D3BJ) [9] was introduced to better reproduce the weak interactions occurring at the 2nd sphere coordination and solvent effects (DMF) were included using the CPCM approach. [10] Lanld2z with ECP[11] and 6-31G(d) [12] basis sets were chosen for Fe and main group atoms respectively. To speed up the calculations, the two arms at the opposite of the coordination face of the porphyrin were replaced with protons. The corresponding model porphyrin is denoted **ααUr**. The F_{20}TPPFe was optimized as is. The geometry of intermediates were optimized as singlet, open singlet (S=1) and triplet (S=3) for formally Fe(II) species, and as doublet (S=2) for Fe(I) species. Only the most stable configurations are detailed herein. IR spectra were generated by convoluting the theoretical stick spectra with a Gaussian fit (half-width $W_{1/2}$= 15 cm^{-1}). Figures, charges and spin analysis were performed using ChemCraft program. [13]

αaUrFe(I)



	NPA charges	spin density
CO_2	-	-
Fe	0.67	2.00
Por	-1.67	-1.00

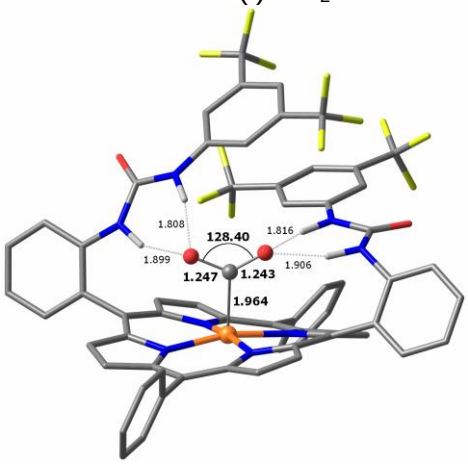
F_{20}TPPFe(I)



	NPA charges	spin density
CO_2	-	-
Fe	0.73	1.98
Por	-1.73	-0. 98

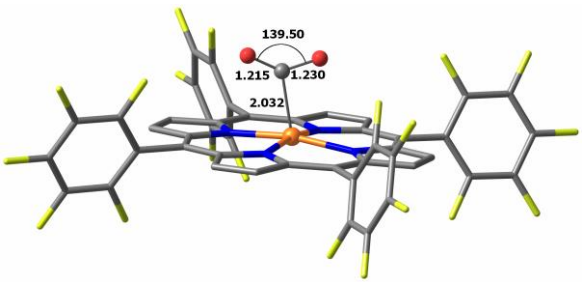
Figure S23 PBE0 geometries, partial charges and spin densities of **αaUrFe^{I}** and **F_{20}TPPFe^{I}**

αaUrFe(I)-CO_2



	NPA charges	spin density
CO_2	-0.63	-0.33
Fe	0.38	1.42
Por	-0.75	-0.09

F_{20}TPPFe(I)-CO_2



	NPA charges	spin density
CO_2	-0.45	-0.27
Fe	0.34	1.40
Por	-0.89	-0. 13

Figure S24 PBE0 geometries, partial charges and spin densities of **αaUrFe^{I}-CO_2** and **F_{20}TPPFe^{I}-CO_2**

Table S3 Predicted CO_2 binding energies, dissociation and association constant, and expected half-wave potential change[4] in the Fe(I) oxidation state at 298K

	ΔG coord (kcal/mol)	**k_D** (M^{-1})	**k_A** (M^{-1})	**ΔE** (V)
ααUrFe(I)	0.78	0.87	1.16	0.006
F_{20}TPPFe(I)	10.46	$1.09\ 10^{7}$	$9.19\ 10^{8}$	0.000

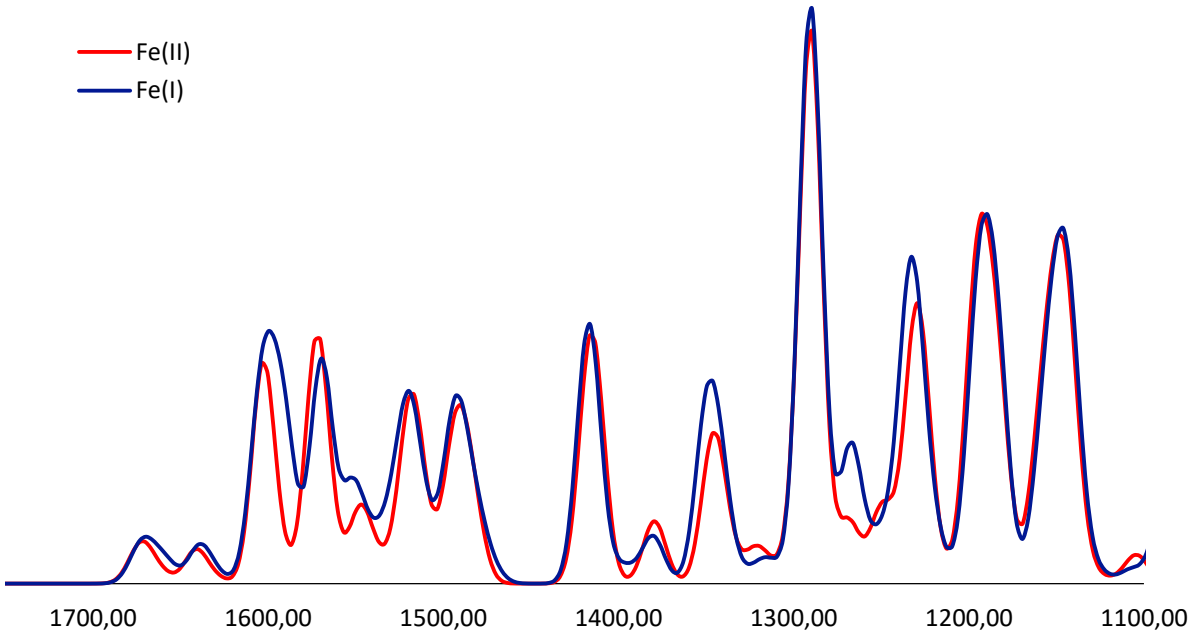


Figure S25 Theoretical IR band spectra (gaussian fit $w_{1/2}$=15 cm^{-1}) obtained for Red: **ααUrFe^{II}**, Blue: **ααUrFe^{I}**

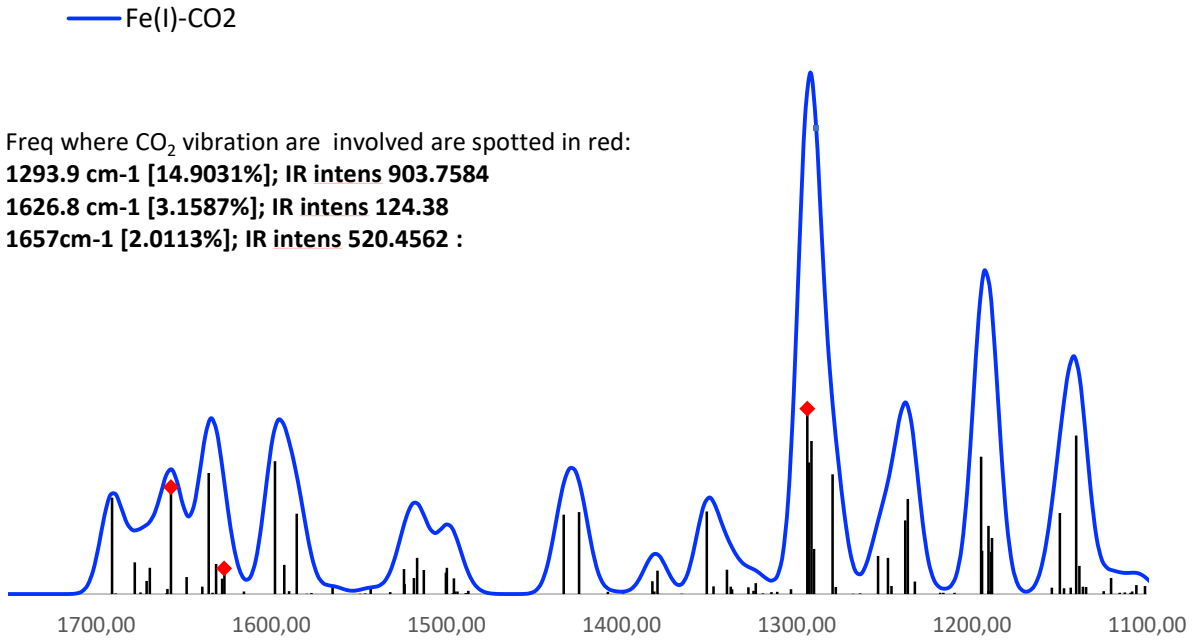


Figure S26 Theoretical IR stick and band spectrum (gaussian fit $w_{1/2}$=15 cm^{-1}) obtained for **ααUrFe^{I}-CO_2**

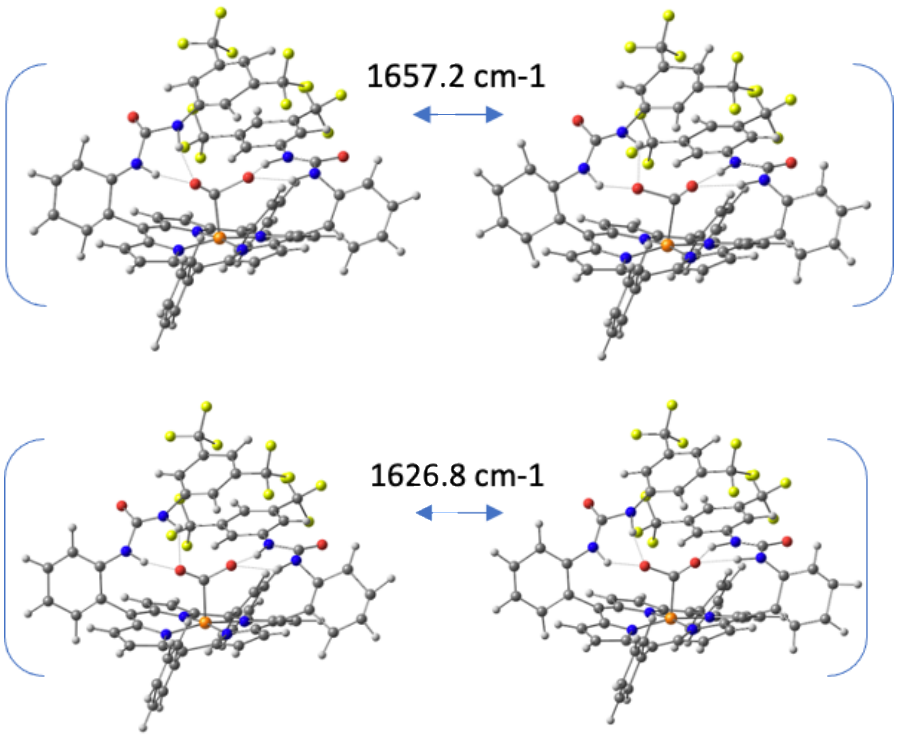


Figure S27 Vibration modes associated with the CO_2 fragment in **ααUrFe^{I}-CO_2**

Table S4 xyz coordinates (charge, spin multiplicity) and energetics (E (G) at 298K) at the PBE0 level

ααUrFe^{II} (0,3)
-4290.147976 (-4289.390599) Hartrees

C	0.699866000000	0.663492000000	3.108864000000
C	0.498759000000	-0.660109000000	3.499933000000
C	1.076032000000	-1.739592000000	2.828643000000
C	0.701163000000	-3.109721000000	3.046463000000
H	0.002137000000	-3.450056000000	3.796915000000
C	1.362739000000	-3.851001000000	2.117761000000
H	1.324981000000	-4.920627000000	1.963808000000
C	2.171719000000	-2.937730000000	1.359710000000
C	3.027647000000	-3.335044000000	0.329672000000
C	3.950400000000	-2.482108000000	-0.270605000000
C	4.986833000000	-2.920953000000	-1.165232000000
H	5.130741000000	-3.941040000000	-1.494186000000
C	5.743913000000	-1.829230000000	-1.450205000000
H	6.630126000000	-1.776666000000	-2.066212000000
C	5.117029000000	-0.707358000000	-0.800457000000
C	5.491839000000	0.622885000000	-0.997549000000
C	4.726503000000	1.695618000000	-0.536895000000
C	4.941758000000	3.060430000000	-0.943245000000
H	5.754254000000	3.399459000000	-1.570038000000
C	3.922726000000	3.791111000000	-0.421617000000
H	3.738234000000	4.852138000000	-0.519636000000
C	3.110092000000	2.881974000000	0.342508000000
C	2.015796000000	3.281398000000	1.107758000000
C	1.335431000000	2.428978000000	1.979402000000
C	0.374804000000	2.879861000000	2.948237000000
H	0.048406000000	3.903896000000	3.064363000000
C	0.008577000000	1.790890000000	3.673754000000
H	-0.685206000000	1.743853000000	4.500545000000
C	-0.420225000000	-0.958217000000	4.629828000000
C	-1.789352000000	-0.684089000000	4.541842000000
H	-2.187379000000	-0.234100000000	3.638879000000
C	-2.639112000000	-0.987485000000	5.601969000000
H	-3.700656000000	-0.771981000000	5.517690000000
C	-2.132753000000	-1.570682000000	6.761812000000
H	-2.796894000000	-1.807604000000	7.588211000000
C	-0.770819000000	-1.850693000000	6.856505000000
H	-0.368025000000	-2.304235000000	7.757792000000
C	0.079496000000	-1.548652000000	5.796541000000
C	2.785943000000	-4.687690000000	-0.242089000000
C	3.594616000000	-5.799495000000	-0.015358000000
H	4.493966000000	-5.687621000000	0.583757000000
C	3.232480000000	-7.047444000000	-0.519780000000
H	3.862959000000	-7.910748000000	-0.329063000000
C	2.057279000000	-7.187435000000	-1.254494000000
H	1.769952000000	-8.161065000000	-1.640643000000
C	1.252206000000	-6.080829000000	-1.515980000000
H	0.346166000000	-6.172027000000	-2.104615000000
C	1.618949000000	-4.834750000000	-1.018724000000
C	-0.411574000000	-3.499871000000	-0.748087000000
C	-1.877537000000	-1.620773000000	-0.049795000000
C	-3.099216000000	-2.276829000000	-0.240163000000
H	-3.111098000000	-3.282206000000	-0.634604000000
C	-4.282206000000	-1.609825000000	0.044247000000
C	-4.289788000000	-0.306423000000	0.529416000000
H	-5.222209000000	0.216211000000	0.706411000000
C	-3.070134000000	0.325385000000	0.739920000000
C	-1.869275000000	-0.318947000000	0.463949000000
H	-0.926277000000	0.200088000000	0.614957000000
C	6.698719000000	0.924468000000	-1.812205000000
C	6.747334000000	0.615499000000	-3.176488000000
H	5.887079000000	0.147978000000	-3.647917000000
C	7.879894000000	0.914204000000	-3.928920000000
H	7.901812000000	0.671970000000	-4.987733000000
C	8.977374000000	1.528302000000	-3.328426000000
H	9.860737000000	1.761455000000	-3.916138000000
C	8.935780000000	1.845257000000	-1.972110000000
H	9.787363000000	2.324223000000	-1.497099000000
C	7.803238000000	1.546866000000	-1.219375000000
C	1.519161000000	4.679451000000	0.962039000000
C	1.975510000000	5.714954000000	1.775729000000
H	2.728689000000	5.493660000000	2.526912000000
C	1.469301000000	7.004918000000	1.641612000000
H	1.828119000000	7.801237000000	2.286513000000
C	0.500481000000	7.260467000000	0.674277000000
H	0.099295000000	8.263248000000	0.557403000000
C	0.041333000000	6.247172000000	-0.161254000000
H	-0.707703000000	6.448557000000	-0.915929000000
C	0.545259000000	4.951689000000	-0.020306000000
C	-1.095400000000	3.708353000000	-1.393061000000
C	-2.363129000000	1.814123000000	-2.374485000000
C	-2.231949000000	0.500623000000	-2.844445000000
H	-1.244857000000	0.063983000000	-2.963885000000
C	-3.357898000000	-0.260089000000	-3.119489000000
C	-4.636936000000	0.257886000000	-2.938248000000
H	-5.513720000000	-0.349347000000	-3.124817000000
C	-4.755499000000	1.563490000000	-2.481246000000
C	-3.642703000000	2.352842000000	-2.210070000000
H	-3.753682000000	3.365273000000	-1.849126000000
N	1.525706000000	1.075808000000	2.086634000000
N	1.984027000000	-1.653044000000	1.798932000000
N	4.041410000000	-1.129227000000	-0.057339000000
N	3.606392000000	1.605807000000	0.253190000000
N	0.851778000000	-3.672285000000	-1.281394000000
H	1.416002000000	-2.833184000000	-1.333849000000
N	-0.658337000000	-2.182792000000	-0.411444000000
H	0.142618000000	-1.574431000000	-0.302909000000
N	0.153358000000	3.890922000000	-0.849037000000
H	0.735362000000	3.068029000000	-0.756035000000
N	-1.193602000000	2.496037000000	-2.053298000000
H	-0.347064000000	1.952024000000	-2.149367000000
O	-1.211991000000	-4.410994000000	-0.606205000000
O	-2.006968000000	4.518745000000	-1.317944000000
Fe	2.786596000000	-0.023783000000	1.017923000000
H	1.141829000000	-1.765964000000	5.869353000000
H	7.770367000000	1.792002000000	-0.161101000000
C	-3.063085000000	1.716761000000	1.300281000000
F	-4.107449000000	2.436852000000	0.863503000000
F	-3.138812000000	1.711720000000	2.646341000000
F	-1.945125000000	2.385162000000	0.976912000000
C	-5.600817000000	-2.285858000000	-0.189174000000
F	-5.475903000000	-3.453934000000	-0.831555000000
F	-6.238405000000	-2.532485000000	0.969408000000
F	-6.425174000000	-1.510076000000	-0.919702000000
C	-6.115322000000	2.110846000000	-2.166483000000
F	-6.446168000000	1.890473000000	-0.877676000000
F	-6.183189000000	3.437121000000	-2.359695000000
F	-7.073352000000	1.542286000000	-2.914452000000
C	-3.198566000000	-1.654564000000	-3.648613000000
F	-3.223638000000	-1.680836000000	-4.992602000000
F	-2.034664000000	-2.209846000000	-3.269584000000
F	-4.185842000000	-2.461868000000	-3.225687000000

ααUrFe^{I} (-1,2)
-4290.27915891 (-4477.90691) Hartrees

C	0.662060000000	-0.653280000000	-3.116500000000
C	0.448740000000	0.654380000000	-3.501620000000
C	1.039660000000	1.754220000000	-2.847700000000
C	0.701480000000	3.107220000000	-3.091730000000
H	0.003230000000	3.449830000000	-3.842790000000
C	1.407290000000	3.867490000000	-2.184880000000
H	1.404480000000	4.942850000000	-2.067980000000
C	2.181140000000	2.964080000000	-1.412310000000
C	3.049240000000	3.364920000000	-0.368720000000
C	3.944490000000	2.499110000000	0.236270000000
C	4.975400000000	2.926920000000	1.150340000000
H	5.127460000000	3.947960000000	1.473540000000
C	5.716540000000	1.830880000000	1.446450000000
H	6.596540000000	1.774900000000	2.072250000000

C	5.093560000000	0.705510000000	0.796550000000
C	5.464290000000	-0.609350000000	1.002210000000
C	4.713680000000	-1.702650000000	0.527520000000
C	4.931450000000	-3.048660000000	0.923330000000
H	5.736710000000	-3.388200000000	1.560240000000
C	3.917970000000	-3.797010000000	0.372380000000
H	3.750140000000	-4.862480000000	0.454380000000
C	3.112320000000	-2.897790000000	-0.379420000000
C	2.009350000000	-3.298730000000	-1.161820000000
C	1.333610000000	-2.437280000000	-2.011920000000
C	0.357140000000	-2.879160000000	-2.977080000000
H	0.038020000000	-3.904720000000	-3.102490000000
C	-0.025720000000	-1.786490000000	-3.680520000000
H	-0.731060000000	-1.735940000000	-4.498130000000
C	-0.489220000000	0.948610000000	-4.617080000000
C	-1.857810000000	0.678860000000	-4.505820000000
H	-2.239010000000	0.234720000000	-3.592600000000
C	-2.727000000000	0.971950000000	-5.553900000000
H	-3.786960000000	0.756130000000	-5.449190000000
C	-2.242060000000	1.544910000000	-6.727640000000
H	-2.920310000000	1.774640000000	-7.544790000000
C	-0.881230000000	1.823420000000	-6.847050000000
H	-0.493620000000	2.268440000000	-7.759530000000
C	-0.013350000000	1.529780000000	-5.799070000000
C	2.785830000000	4.708820000000	0.209080000000
C	3.597700000000	5.829620000000	0.043600000000
H	4.524400000000	5.730500000000	-0.515420000000
C	3.212450000000	7.069300000000	0.554280000000
H	3.850710000000	7.936250000000	0.409600000000
C	2.003250000000	7.196340000000	1.233590000000
H	1.696120000000	8.162910000000	1.623030000000
C	1.187240000000	6.084280000000	1.436230000000
H	0.253740000000	6.164580000000	1.981980000000
C	1.581820000000	4.848490000000	0.934590000000
C	-0.459230000000	3.516920000000	0.654280000000
C	-1.903260000000	1.630370000000	-0.074160000000
C	-3.130470000000	2.257650000000	0.175230000000
H	-3.144250000000	3.270890000000	0.549140000000
C	-4.309880000000	1.555070000000	-0.026910000000
C	-4.311280000000	0.243250000000	-0.488000000000
H	-5.237640000000	-0.306990000000	-0.599820000000
C	-3.088900000000	-0.359880000000	-0.759380000000
C	-1.890900000000	0.318900000000	-0.566220000000
H	-0.944260000000	-0.178140000000	-0.762870000000
C	6.657590000000	-0.909530000000	1.837210000000
C	6.686750000000	-0.601320000000	3.202480000000
H	5.818500000000	-0.132870000000	3.658280000000
C	7.807780000000	-0.895860000000	3.974760000000
H	7.812080000000	-0.650710000000	5.033410000000
C	8.916030000000	-1.509440000000	3.394360000000
H	9.790470000000	-1.740140000000	3.996520000000
C	8.895190000000	-1.829010000000	2.037650000000
H	9.755160000000	-2.307580000000	1.576910000000
C	7.774120000000	-1.533220000000	1.267040000000
C	1.514760000000	-4.696170000000	-1.016870000000
C	1.955470000000	-5.740060000000	-1.828290000000
H	2.699070000000	-5.524690000000	-2.591050000000
C	1.449140000000	-7.029990000000	-1.681540000000
H	1.797630000000	-7.830290000000	-2.327730000000
C	0.493180000000	-7.280470000000	-0.700550000000
H	0.091330000000	-8.282130000000	-0.574460000000
C	0.045480000000	-6.261340000000	0.135620000000
H	-0.696950000000	-6.455770000000	0.898870000000
C	0.552260000000	-4.969300000000	-0.020850000000
C	-1.040540000000	-3.704980000000	1.394210000000
C	-2.271820000000	-1.779590000000	2.366050000000
C	-2.122200000000	-0.456050000000	2.802170000000
H	-1.131570000000	-0.015880000000	2.865510000000
C	-3.234960000000	0.307510000000	3.117350000000
C	-4.520370000000	-0.215530000000	3.007890000000
H	-5.388620000000	0.393170000000	3.226240000000
C	-4.657450000000	-1.528410000000	2.578440000000
C	-3.556900000000	-2.321610000000	2.269340000000
H	-3.681990000000	-3.340770000000	1.932090000000
N	1.516250000000	-1.074010000000	-2.100080000000
N	1.953900000000	1.667310000000	-1.808530000000
N	4.016550000000	1.137000000000	0.030230000000
N	3.591230000000	-1.613400000000	-0.276710000000
N	0.822940000000	3.672760000000	1.141200000000
H	1.401910000000	2.843570000000	1.068610000000
N	-0.680950000000	2.228680000000	0.201650000000
H	0.136630000000	1.694130000000	-0.074720000000
N	0.179900000000	-3.895170000000	0.799160000000
H	0.739590000000	-3.067360000000	0.626000000000
N	-1.116990000000	-2.466550000000	2.010740000000
H	-0.270080000000	-1.915560000000	2.041180000000
O	-1.295100000000	4.408800000000	0.652710000000
O	-1.948450000000	-4.524470000000	1.401780000000
Fe	2.766810000000	0.028240000000	-1.035360000000
H	1.047370000000	1.747830000000	-5.891410000000
H	7.757410000000	-1.782770000000	0.209360000000
C	-3.077110000000	-1.762100000000	-1.291290000000
F	-4.104300000000	-2.484950000000	-0.816610000000
F	-3.181230000000	-1.786460000000	-2.635140000000
F	-1.946460000000	-2.411960000000	-0.976810000000
C	-5.630100000000	2.207720000000	0.255760000000
F	-5.503470000000	3.374340000000	0.900990000000
F	-6.310670000000	2.452270000000	-0.879360000000
F	-6.419010000000	1.415140000000	1.007750000000
C	-6.027360000000	-2.086150000000	2.334790000000
F	-6.389190000000	-1.951610000000	1.042380000000
F	-6.095780000000	-3.396870000000	2.617200000000
F	-6.964740000000	-1.464770000000	3.066480000000
C	-3.052160000000	1.710440000000	3.614620000000
F	-3.021440000000	1.759820000000	4.958370000000
F	-1.903950000000	2.256250000000	3.178890000000
F	-4.054850000000	2.512730000000	3.219960000000

ααUrFe^{I}-CO$_2$ (-1,2)

-4478.68994942 (-4289.515802) Hartrees

C	-0.310010000000	-1.109340000000	2.660280000000
C	0.229200000000	0.104060000000	3.089100000000
C	-0.263130000000	1.330790000000	2.641740000000
C	0.314780000000	2.603370000000	2.971170000000
H	1.113170000000	2.760730000000	3.681900000000
C	-0.327420000000	3.533660000000	2.214300000000
H	-0.158890000000	4.601180000000	2.181890000000
C	-1.328620000000	2.833470000000	1.460600000000
C	-2.208660000000	3.469820000000	0.576780000000
C	-3.367450000000	2.866920000000	0.100870000000
C	-4.424900000000	3.571650000000	-0.575670000000
H	-4.387240000000	4.608710000000	-0.878890000000
C	-5.463390000000	2.703760000000	-0.683880000000
H	-6.444250000000	2.889070000000	-1.097800000000
C	-5.011180000000	1.442500000000	-0.151020000000
C	-5.758250000000	0.264670000000	-0.187270000000
C	-5.217830000000	-0.978050000000	0.151410000000
C	-5.849220000000	-2.231450000000	-0.175850000000
H	-6.848960000000	-2.338590000000	-0.572430000000
C	-4.926610000000	-3.203300000000	0.051340000000
H	-5.021400000000	-4.268950000000	-0.107280000000
C	-3.759670000000	-2.549940000000	0.578320000000
C	-2.597000000000	-3.216000000000	0.957600000000
C	-1.549550000000	-2.593970000000	1.639960000000
C	-0.473500000000	-3.313670000000	2.264410000000
H	-0.335910000000	-4.385110000000	2.217850000000
C	0.282080000000	-2.394450000000	2.919370000000
H	1.182810000000	-2.557930000000	3.491700000000
C	1.410710000000	0.075550000000	3.989390000000
C	2.629630000000	0.645780000000	3.601680000000
H	2.709270000000	1.123750000000	2.631320000000
C	3.740830000000	0.589050000000	4.437000000000
H	4.677650000000	1.026830000000	4.104130000000
C	3.650320000000	-0.036710000000	5.678630000000
H	4.517370000000	-0.083900000000	6.331610000000
C	2.441060000000	-0.603160000000	6.078910000000
H	2.360020000000	-1.087990000000	7.047840000000
C	1.331020000000	-0.549280000000	5.240560000000
C	-1.810090000000	4.828770000000	0.123860000000

C	-2.500370000000	5.990810000000	0.471590000000
H	-3.402530000000	5.908400000000	1.071610000000
C	-2.019280000000	7.242780000000	0.095670000000
H	-2.560370000000	8.139380000000	0.383260000000
C	-0.836230000000	7.339360000000	-0.633910000000
H	-0.452760000000	8.313740000000	-0.923130000000
C	-0.145920000000	6.190520000000	-1.011260000000
H	0.764800000000	6.252560000000	-1.596540000000
C	-0.630050000000	4.937310000000	-0.642900000000
C	-7.152840000000	0.301700000000	-0.700750000000
C	-7.428130000000	0.639450000000	-2.031100000000
H	-6.606000000000	0.879560000000	-2.699950000000
C	-8.738560000000	0.655920000000	-2.500740000000
H	-8.935720000000	0.916550000000	-3.536890000000
C	-9.792110000000	0.330740000000	-1.648290000000
H	-10.814470000000	0.342870000000	-2.015470000000
C	-9.528030000000	-0.013620000000	-0.324080000000
H	-10.343810000000	-0.268740000000	0.346610000000
C	-8.217460000000	-0.029200000000	0.145640000000
C	-2.376880000000	-4.630030000000	0.547610000000
C	-2.967940000000	-5.713020000000	1.194830000000
H	-3.652550000000	-5.519880000000	2.016450000000
C	-2.668350000000	-7.020530000000	0.818880000000
H	-3.129200000000	-7.856090000000	1.337060000000
C	-1.763580000000	-7.242720000000	-0.216600000000
H	-1.517120000000	-8.258220000000	-0.514420000000
C	-1.174420000000	-6.177550000000	-0.891460000000
H	-0.477970000000	-6.350230000000	-1.702390000000
C	-1.480900000000	-4.865250000000	-0.520810000000
N	-1.429720000000	-1.250510000000	1.873400000000
N	-1.301070000000	1.498150000000	1.750630000000
N	-3.730280000000	1.562700000000	0.329780000000
N	-3.957890000000	-1.194040000000	0.645740000000
N	0.020420000000	3.748960000000	-1.034760000000
C	1.286130000000	3.434140000000	-0.575140000000
H	-0.603140000000	2.943170000000	-1.102390000000
N	1.457300000000	2.068680000000	-0.503520000000
C	2.561720000000	1.374580000000	-0.046760000000
C	3.802130000000	1.965940000000	0.213430000000
H	3.920600000000	3.031270000000	0.072800000000
C	4.861170000000	1.172510000000	0.648280000000
C	4.728220000000	-0.198610000000	0.817980000000
H	5.567100000000	-0.804930000000	1.139180000000
C	3.485400000000	-0.775520000000	0.565470000000
C	2.409960000000	-0.008000000000	0.152450000000
H	1.444970000000	-0.473540000000	-0.016670000000
H	0.618900000000	1.510360000000	-0.682430000000
N	-0.978180000000	-3.746790000000	-1.189680000000
C	0.240070000000	-3.627550000000	-1.814700000000
H	-1.458090000000	-2.867710000000	-0.992360000000
N	0.404030000000	-2.345910000000	-2.307360000000
C	1.587910000000	-1.724650000000	-2.669200000000
C	1.506420000000	-0.369560000000	-3.026690000000
H	0.542410000000	0.130970000000	-3.016430000000
C	2.657810000000	0.345250000000	-3.319440000000
C	3.911710000000	-0.255900000000	-3.261440000000
H	4.811830000000	0.311960000000	-3.472190000000
C	3.980220000000	-1.601990000000	-2.918360000000
C	2.841250000000	-2.348470000000	-2.640840000000
H	2.910240000000	-3.390850000000	-2.364620000000
H	-0.387910000000	-1.710970000000	-2.149410000000
O	2.132900000000	4.265050000000	-0.273510000000
O	1.059530000000	-4.530910000000	-1.935410000000
Fe	-2.524010000000	0.136460000000	1.003100000000
H	0.388840000000	-0.990260000000	5.555010000000
H	-8.010400000000	-0.296310000000	1.178610000000
C	3.328700000000	-2.246540000000	0.803180000000
F	4.280810000000	-2.954600000000	0.167010000000
F	3.446290000000	-2.546210000000	2.111200000000
F	2.141960000000	-2.713080000000	0.393020000000
C	6.155600000000	1.834090000000	1.012430000000
F	6.393860000000	2.927650000000	0.272430000000
F	6.154320000000	2.234350000000	2.302580000000
F	7.204100000000	1.009510000000	0.865750000000
C	5.336840000000	-2.231800000000	-2.804810000000
F	6.059020000000	-2.049920000000	-3.926530000000
F	6.049010000000	-1.684230000000	-1.802280000000
F	5.278210000000	-3.550850000000	-2.577420000000
C	2.575820000000	1.790820000000	-3.710680000000
F	2.978180000000	1.975850000000	-4.982130000000
F	1.333500000000	2.283980000000	-3.612980000000
F	3.374570000000	2.556990000000	-2.944700000000
C	-1.655560000000	0.112840000000	-0.757830000000
O	-1.062080000000	1.097610000000	-1.231220000000
O	-1.802260000000	-1.019110000000	-1.261130000000

F_{20}TPPFe^{I} (-1,2)

-4016.83072779 (-4016.488052) Hartrees

C	-1.153280000000	2.804080000000	0.002970000000
C	-2.473120000000	2.370370000000	0.001830000000
C	-2.850580000000	1.033400000000	0.000750000000
C	-4.214600000000	0.590390000000	-0.001870000000
H	-5.081390000000	1.237570000000	-0.014060000000
C	-4.185730000000	-0.768830000000	0.005950000000
H	-5.024230000000	-1.452260000000	0.017960000000
C	-2.804210000000	-1.153480000000	0.003470000000
C	-2.370510000000	-2.473320000000	0.001870000000
C	-1.033560000000	-2.850770000000	0.000550000000
C	-0.590500000000	-4.214760000000	-0.002550000000
H	-1.237630000000	-5.081590000000	-0.014970000000
C	0.768700000000	-4.185840000000	0.006230000000
H	1.452110000000	-5.024350000000	0.018750000000
C	1.153360000000	-2.804300000000	0.003320000000
C	2.473200000000	-2.370570000000	0.001840000000
C	2.850650000000	-1.033580000000	0.000330000000
C	4.214670000000	-0.590540000000	-0.002430000000
H	5.081470000000	-1.237710000000	-0.014650000000
C	4.185800000000	0.768680000000	0.005450000000
H	5.024320000000	1.452090000000	0.017450000000
C	2.804280000000	1.153330000000	0.002860000000
C	2.370550000000	2.473170000000	0.001220000000
C	1.033610000000	2.850570000000	-0.000070000000
C	0.590570000000	4.214560000000	-0.002800000000
H	1.237740000000	5.081370000000	-0.015060000000
C	-0.768640000000	4.185640000000	0.005620000000
H	-1.452050000000	5.024150000000	0.018050000000
C	-3.544360000000	3.396660000000	0.000970000000
C	-3.836360000000	4.142560000000	-1.139110000000
F	-3.148720000000	3.939950000000	-2.263330000000
C	-4.833530000000	5.108430000000	-1.152130000000
F	-5.088750000000	5.805440000000	-2.257570000000
C	-5.575150000000	5.341130000000	-0.001690000000
F	-6.534900000000	6.260330000000	-0.002900000000
C	-5.311980000000	4.611760000000	1.150030000000
F	-6.021110000000	4.837780000000	2.254100000000
C	-4.303710000000	3.657390000000	1.139700000000
C	-3.396880000000	-3.544480000000	0.000630000000
C	-3.657620000000	-4.304350000000	1.138980000000
F	-2.981150000000	-4.073920000000	2.264670000000
C	-4.612140000000	-5.312480000000	1.148870000000
F	-4.838140000000	-6.022190000000	2.252570000000
C	-5.341670000000	-5.574910000000	-0.002910000000
F	-6.261010000000	-6.534520000000	-0.004530000000
C	-5.109000000000	-4.832710000000	-1.152980000000
F	-5.806250000000	-5.087170000000	-2.258440000000
C	-4.142940000000	-3.835730000000	-1.139550000000
C	3.544490000000	-3.396840000000	0.001060000000
C	3.836690000000	-4.142650000000	-1.139020000000
F	3.149120000000	-3.940110000000	-2.263300000000
C	4.833980000000	-5.108390000000	-1.151990000000
F	5.089380000000	-5.805340000000	-2.257430000000
C	5.575530000000	-5.341050000000	-0.001500000000
F	6.535400000000	-6.260110000000	-0.002670000000
C	5.312150000000	-4.611780000000	1.150240000000
F	6.021240000000	-4.837730000000	2.254350000000
C	4.303770000000	-3.657530000000	1.139860000000
C	3.396780000000	3.544440000000	0.000310000000
C	3.656810000000	4.304370000000	1.138790000000
F	2.979760000000	4.073890000000	2.264120000000

C	4.611130000000	5.312680000000	1.149140000000
F	4.836430000000	6.022440000000	2.252950000000
C	5.341210000000	5.575230000000	-0.002280000000
F	6.260360000000	6.535020000000	-0.003450000000
C	5.109210000000	4.833000000000	-1.152460000000
F	5.806890000000	5.087620000000	-2.257610000000
C	4.143300000000	3.835870000000	-1.139510000000
N	-0.041790000000	1.981640000000	0.001400000000
N	-1.981720000000	-0.042030000000	0.002450000000
N	0.041860000000	-1.981860000000	0.001970000000
N	1.981800000000	0.041860000000	0.001760000000
F	-3.940310000000	-3.147510000000	-2.263410000000
F	3.941270000000	3.147670000000	-2.263500000000
Fe	0.000040000000	-0.000070000000	0.001760000000
F	-4.072520000000	2.981220000000	2.265410000000
F	4.072470000000	-2.981360000000	2.265550000000

$F_{20}TPPFe^{I}$-CO_2 (-1,2)
-4205.2142678 (-4204.863734) Hartrees

C	2.818770000000	1.159590000000	-0.105550000000
C	3.434090000000	-0.088360000000	-0.090750000000
C	2.741770000000	-1.294710000000	-0.083950000000
C	3.382770000000	-2.584850000000	-0.108770000000
H	4.450700000000	-2.754390000000	-0.122620000000
C	2.389850000000	-3.508070000000	-0.119600000000
H	2.484240000000	-4.584640000000	-0.159870000000
C	1.147290000000	-2.778680000000	-0.080620000000
C	-0.103230000000	-3.389080000000	-0.077380000000
C	-1.314390000000	-2.703500000000	-0.067120000000
C	-2.599850000000	-3.355140000000	-0.081100000000
H	-2.761010000000	-4.424530000000	-0.081920000000
C	-3.533820000000	-2.372140000000	-0.088550000000
H	-4.610020000000	-2.475120000000	-0.115900000000
C	-2.814370000000	-1.124020000000	-0.075930000000
C	-3.431650000000	0.122600000000	-0.084430000000
C	-2.740870000000	1.330470000000	-0.102280000000
C	-3.381900000000	2.621380000000	-0.123380000000
H	-4.449720000000	2.792530000000	-0.122280000000
C	-2.387760000000	3.543110000000	-0.139720000000
H	-2.480080000000	4.620260000000	-0.171370000000
C	-1.145760000000	2.810270000000	-0.118040000000
C	0.105970000000	3.419330000000	-0.116270000000
C	1.318370000000	2.735100000000	-0.114150000000
C	2.603280000000	3.389920000000	-0.126750000000
H	2.762430000000	4.459670000000	-0.130910000000
C	3.538510000000	2.408170000000	-0.127640000000
H	4.614810000000	2.512150000000	-0.149110000000
C	4.917800000000	-0.133420000000	-0.088620000000
C	5.647380000000	0.183240000000	1.054860000000
F	5.013120000000	0.531900000000	2.173670000000
C	7.035030000000	0.149440000000	1.071570000000
F	7.707350000000	0.456270000000	2.177820000000
C	7.723530000000	-0.214260000000	-0.078290000000
F	9.050820000000	-0.252660000000	-0.073450000000
C	7.023580000000	-0.537960000000	-1.233200000000
F	7.685140000000	-0.883360000000	-2.334610000000
C	5.636220000000	-0.490950000000	-1.226960000000
C	-0.149250000000	-4.873210000000	-0.123980000000
C	-0.539300000000	-5.542990000000	-1.282240000000
F	-0.877330000000	-4.850640000000	-2.369770000000
C	-0.591400000000	-6.928340000000	-1.348640000000
F	-0.968210000000	-7.539420000000	-2.468840000000
C	-0.238960000000	-7.679410000000	-0.235140000000
F	-0.281760000000	-9.005560000000	-0.286970000000
C	0.159060000000	-7.041710000000	0.932040000000
F	0.495320000000	-7.761670000000	1.999200000000
C	0.197260000000	-5.654440000000	0.976300000000
C	-4.915120000000	0.165850000000	-0.079700000000
C	-5.643230000000	-0.147990000000	1.065650000000
F	-5.007620000000	-0.493400000000	2.184680000000
C	-7.030820000000	-0.113960000000	1.084300000000
F	-7.701500000000	-0.417680000000	2.192400000000
C	-7.721080000000	0.247050000000	-0.065370000000
F	-9.048340000000	0.285510000000	-0.058660000000
C	-7.022800000000	0.567970000000	-1.222050000000
F	-7.685930000000	0.910360000000	-2.323450000000
C	-5.635460000000	0.520980000000	-1.217760000000
C	0.150690000000	4.903930000000	-0.127570000000
C	0.495220000000	5.610770000000	-1.277090000000
F	0.792900000000	4.954330000000	-2.398010000000
C	0.543030000000	6.997960000000	-1.297940000000
F	0.875360000000	7.648180000000	-2.410110000000
C	0.234180000000	7.709640000000	-0.146150000000
F	0.273660000000	9.036920000000	-0.154950000000
C	-0.115830000000	7.032840000000	1.014840000000
F	-0.408440000000	7.716430000000	2.118080000000
C	-0.151210000000	5.645070000000	1.012340000000
N	1.466300000000	1.373870000000	-0.102970000000
N	1.377650000000	-1.428930000000	-0.060890000000
N	-1.461330000000	-1.342100000000	-0.059810000000
N	-1.377560000000	1.460740000000	-0.101210000000
F	0.584110000000	-5.077540000000	2.112840000000
F	-0.487050000000	5.022620000000	2.141620000000
Fe	0.001010000000	0.014520000000	0.089260000000
F	4.991120000000	-0.802790000000	-2.350570000000
F	-4.992350000000	0.829420000000	-2.343440000000
C	-0.017770000000	-0.394770000000	2.079360000000
O	-0.065940000000	-1.496740000000	2.587970000000
O	0.031800000000	0.788060000000	2.413100000000

Table S5 xyz coordinates (charge, spin multiplicity) and energetics (E (G) at 298K) at the B3LYP level

αα$UrFe^{II}$ (0,3)
-4294.81524272 (-4294.054410) Hartrees

C	0.557662000000	0.677508000000	3.140869000000
C	0.323250000000	-0.651303000000	3.501749000000
C	0.925640000000	-1.731112000000	2.848316000000
C	0.548065000000	-3.106766000000	3.049636000000
H	-0.189744000000	-3.448072000000	3.759801000000
C	1.271920000000	-3.853876000000	2.167520000000
H	1.248446000000	-4.923884000000	2.021938000000
C	2.118697000000	-2.942668000000	1.444066000000
C	3.024323000000	-3.340865000000	0.457066000000
C	3.947656000000	-2.477898000000	-0.132105000000
C	5.017674000000	-2.908716000000	-0.995134000000
H	5.197469000000	-3.931746000000	-1.292409000000
C	5.750347000000	-1.800428000000	-1.298395000000
H	6.645049000000	-1.741466000000	-1.899391000000
C	5.082586000000	-0.673489000000	-0.691550000000
C	5.429096000000	0.662226000000	-0.917456000000
C	4.641622000000	1.731104000000	-0.478329000000
C	4.834869000000	3.097300000000	-0.903289000000
H	5.639613000000	3.439206000000	-1.536611000000
C	3.808563000000	3.826318000000	-0.383323000000
H	3.615303000000	4.883589000000	-0.493069000000
C	3.005054000000	2.919381000000	0.398736000000
C	1.910578000000	3.319947000000	1.166639000000
C	1.233558000000	2.467010000000	2.042588000000
C	0.269889000000	2.910864000000	3.015533000000
H	-0.048237000000	3.934561000000	3.145537000000
C	-0.122234000000	1.810459000000	3.716931000000
H	-0.828341000000	1.759558000000	4.531441000000
C	-0.658230000000	-0.952088000000	4.584506000000
C	-2.020341000000	-0.658556000000	4.425995000000
H	-2.362964000000	-0.191177000000	3.511076000000
C	-2.931723000000	-0.964240000000	5.437198000000
H	-3.984179000000	-0.734117000000	5.298520000000

C	-2.494877000000	-1.568568000000	6.618258000000
H	-3.205248000000	-1.806558000000	7.404570000000
C	-1.140157000000	-1.866830000000	6.783379000000
H	-0.792013000000	-2.335008000000	7.699491000000
C	-0.228341000000	-1.562780000000	5.772075000000
C	2.823217000000	-4.703647000000	-0.121457000000
C	3.614289000000	-5.816063000000	0.170339000000
H	4.466563000000	-5.702168000000	0.833314000000
C	3.291264000000	-7.068299000000	-0.359491000000
H	3.906054000000	-7.930351000000	-0.119746000000
C	2.174268000000	-7.211438000000	-1.184850000000
H	1.918662000000	-8.185631000000	-1.590421000000
C	1.388485000000	-6.102518000000	-1.507790000000
H	0.529722000000	-6.194564000000	-2.162761000000
C	1.716285000000	-4.853913000000	-0.984839000000
C	-0.304665000000	-3.491124000000	-0.749017000000
C	-1.754730000000	-1.582798000000	-0.063846000000
C	-2.982668000000	-2.237258000000	-0.241611000000
H	-2.999702000000	-3.248777000000	-0.613629000000
C	-4.165539000000	-1.553841000000	0.018991000000
C	-4.165111000000	-0.236380000000	0.472510000000
H	-5.093124000000	0.298496000000	0.625161000000
C	-2.939187000000	0.394615000000	0.671437000000
C	-1.738071000000	-0.264942000000	0.417168000000
H	-0.793050000000	0.250163000000	0.556149000000
C	6.638418000000	0.971432000000	-1.735177000000
C	6.701767000000	0.628775000000	-3.094017000000
H	5.855547000000	0.130346000000	-3.557191000000
C	7.834372000000	0.933455000000	-3.849765000000
H	7.867403000000	0.665195000000	-4.901693000000
C	8.917692000000	1.587303000000	-3.257947000000
H	9.798997000000	1.824515000000	-3.846596000000
C	8.861539000000	1.937584000000	-1.906970000000
H	9.699847000000	2.446018000000	-1.439699000000
C	7.728736000000	1.633150000000	-1.151251000000
C	1.400760000000	4.716968000000	1.002517000000
C	1.777507000000	5.748676000000	1.865679000000
H	2.478721000000	5.528827000000	2.665150000000
C	1.255453000000	7.034168000000	1.716512000000
H	1.551520000000	7.824773000000	2.398775000000
C	0.352572000000	7.291195000000	0.683260000000
H	-0.058077000000	8.288315000000	0.554443000000
C	-0.023939000000	6.282099000000	-0.202515000000
H	-0.718205000000	6.482884000000	-1.006843000000
C	0.493966000000	4.991057000000	-0.045954000000
C	-1.065284000000	3.714029000000	-1.496083000000
C	-2.261558000000	1.759111000000	-2.478811000000
C	-2.079799000000	0.434616000000	-2.909609000000
H	-1.078314000000	0.028292000000	-3.002677000000
C	-3.178878000000	-0.373964000000	-3.171764000000
C	-4.479432000000	0.105893000000	-3.013587000000
H	-5.331786000000	-0.537629000000	-3.180938000000
C	-4.648194000000	1.421281000000	-2.594123000000
C	-3.562484000000	2.259394000000	-2.340947000000
H	-3.710903000000	3.274258000000	-2.006546000000
N	1.409198000000	1.100352000000	2.132465000000
N	1.892757000000	-1.645980000000	1.861938000000
N	3.998709000000	-1.108990000000	0.047731000000
N	3.518617000000	1.639027000000	0.321640000000
N	0.954710000000	-3.687792000000	-1.303994000000
H	1.524713000000	-2.852421000000	-1.370939000000
N	-0.534425000000	-2.163914000000	-0.416794000000
H	0.276443000000	-1.568179000000	-0.297470000000
N	0.174131000000	3.937033000000	-0.928313000000
H	0.770351000000	3.125713000000	-0.822518000000
N	-1.113758000000	2.493435000000	-2.161821000000
H	-0.249019000000	1.971941000000	-2.227727000000
O	-1.114523000000	-4.396333000000	-0.589172000000
O	-2.005532000000	4.498213000000	-1.438929000000
Fe	2.700677000000	-0.003253000000	1.088467000000
H	0.825068000000	-1.794422000000	5.899199000000
H	7.684565000000	1.904092000000	-0.100452000000
C	-2.934387000000	1.806503000000	1.184900000000
F	-3.951059000000	2.533403000000	0.672509000000
F	-3.074191000000	1.854894000000	2.533777000000
F	-1.784693000000	2.452249000000	0.888131000000
C	-5.490252000000	-2.224060000000	-0.214762000000
F	-5.373900000000	-3.399249000000	-0.863356000000
F	-6.137726000000	-2.470119000000	0.948615000000
F	-6.317015000000	-1.437737000000	-0.950876000000
C	-6.026701000000	1.932588000000	-2.287193000000
F	-6.298835000000	1.853376000000	-0.958163000000
F	-6.175293000000	3.231408000000	-2.629701000000
F	-6.988687000000	1.231390000000	-2.923116000000
C	-2.969290000000	-1.782963000000	-3.650664000000
F	-2.981057000000	-1.862919000000	-5.001357000000
F	-1.783761000000	-2.291193000000	-3.240390000000
F	-3.939036000000	-2.613607000000	-3.203302000000

ααUrFe^{I} (-1,2)

-4294.92547712 (-4294.167651) Hartrees

C	0.523485000000	-0.648208000000	-3.185609000000
C	0.290741000000	0.667720000000	-3.533993000000
C	0.910464000000	1.761141000000	-2.886783000000
C	0.583500000000	3.124406000000	-3.113243000000
H	-0.144141000000	3.479845000000	-3.827875000000
C	1.352309000000	3.876337000000	-2.244919000000
H	1.370910000000	4.951003000000	-2.132290000000
C	2.151061000000	2.963013000000	-1.505497000000
C	3.072124000000	3.348146000000	-0.500298000000
C	3.941082000000	2.463879000000	0.112837000000
C	4.993615000000	2.871869000000	1.020908000000
H	5.187589000000	3.893990000000	1.314292000000
C	5.685014000000	1.753848000000	1.357259000000
H	6.556041000000	1.679926000000	1.991748000000
C	5.019665000000	0.628104000000	0.733273000000
C	5.345043000000	-0.694226000000	0.971103000000
C	4.572805000000	-1.778012000000	0.494605000000
C	4.757535000000	-3.132139000000	0.893724000000
H	5.539897000000	-3.486438000000	1.548991000000
C	3.747623000000	-3.867792000000	0.308495000000
H	3.567698000000	-4.931164000000	0.381477000000
C	2.969691000000	-2.957086000000	-0.463284000000
C	1.880243000000	-3.341648000000	-1.278322000000
C	1.217220000000	-2.469084000000	-2.124397000000
C	0.232873000000	-2.888206000000	-3.100407000000
H	-0.088001000000	-3.909378000000	-3.246391000000
C	-0.164791000000	-1.779286000000	-3.771279000000
H	-0.882227000000	-1.712154000000	-4.575482000000
C	-0.699137000000	0.979846000000	-4.606523000000
C	-2.064049000000	0.705194000000	-4.435692000000
H	-2.400755000000	0.242261000000	-3.516024000000
C	-2.984019000000	1.014455000000	-5.439065000000
H	-4.037384000000	0.794419000000	-5.288479000000
C	-2.554865000000	1.609286000000	-6.627496000000
H	-3.270896000000	1.851334000000	-7.407734000000
C	-1.198065000000	1.892044000000	-6.806635000000
H	-0.854113000000	2.352148000000	-7.728840000000
C	-0.279715000000	1.581367000000	-5.803280000000
C	2.870042000000	4.712584000000	0.072084000000
C	3.680893000000	5.820262000000	-0.182240000000
H	4.561004000000	5.697035000000	-0.806709000000
C	3.348742000000	7.078525000000	0.330218000000
H	3.983547000000	7.933641000000	0.117628000000
C	2.195145000000	7.236450000000	1.100227000000
H	1.930074000000	8.214717000000	1.490468000000
C	1.383942000000	6.135663000000	1.390102000000
H	0.496327000000	6.238540000000	2.003648000000
C	1.725772000000	4.883004000000	0.885980000000
C	-0.327677000000	3.548176000000	0.673869000000
C	-1.774845000000	1.637502000000	-0.019420000000
C	-3.004683000000	2.259420000000	0.245098000000
H	-3.020133000000	3.270544000000	0.618839000000
C	-4.185142000000	1.545732000000	0.065188000000
C	-4.182396000000	0.229323000000	-0.390903000000
H	-5.104353000000	-0.329560000000	-0.478215000000
C	-2.956824000000	-0.368945000000	-0.676615000000
C	-1.758115000000	0.320489000000	-0.506224000000
H	-0.811697000000	-0.168797000000	-0.713742000000

C	6.516924000000	-1.015007000000	1.837996000000	C	-2.216135000000	3.481076000000	0.634093000000
C	6.524647000000	-0.687286000000	3.202231000000	C	-3.378513000000	2.881085000000	0.157039000000
H	5.660313000000	-0.188738000000	3.631030000000	C	-4.447448000000	3.587906000000	-0.510773000000
C	7.622998000000	-0.998756000000	4.005640000000	H	-4.417706000000	4.628370000000	-0.799360000000
H	7.610400000000	-0.737580000000	5.060155000000	C	-5.483806000000	2.713760000000	-0.629653000000
C	8.730336000000	-1.650304000000	3.457951000000	H	-6.464290000000	2.900110000000	-1.041144000000
H	9.584975000000	-1.894081000000	4.082543000000	C	-5.026563000000	1.441960000000	-0.111502000000
C	8.731100000000	-1.989469000000	2.102393000000	C	-5.767023000000	0.257450000000	-0.157512000000
H	9.588424000000	-2.495865000000	1.667730000000	C	-5.222625000000	-0.989235000000	0.171899000000
C	7.632766000000	-1.675482000000	1.301122000000	C	-5.849877000000	-2.247313000000	-0.165399000000
C	1.363945000000	-4.737778000000	-1.137698000000	H	-6.848260000000	-2.354725000000	-0.562440000000
C	1.703155000000	-5.760672000000	-2.026435000000	C	-4.923835000000	-3.222375000000	0.055749000000
H	2.386355000000	-5.534785000000	-2.840094000000	H	-5.019118000000	-4.285792000000	-0.110929000000
C	1.167346000000	-7.043367000000	-1.890312000000	C	-3.751341000000	-2.574080000000	0.588235000000
H	1.435425000000	-7.823890000000	-2.595961000000	C	-2.581415000000	-3.241894000000	0.949939000000
C	0.287346000000	-7.311172000000	-0.840632000000	C	-1.520800000000	-2.625463000000	1.620759000000
H	-0.133845000000	-8.305432000000	-0.722112000000	C	-0.431129000000	-3.347663000000	2.229801000000
C	-0.053606000000	-6.313970000000	0.074084000000	H	-0.293468000000	-4.417761000000	2.176737000000
H	-0.732906000000	-6.519992000000	0.890223000000	C	0.337435000000	-2.430302000000	2.878407000000
C	0.479102000000	-5.028682000000	-0.072979000000	H	1.246515000000	-2.599472000000	3.432455000000
C	-1.019732000000	-3.738985000000	1.429857000000	C	1.488626000000	0.040321000000	3.952597000000
C	-2.156118000000	-1.762487000000	2.445650000000	C	2.700421000000	0.625696000000	3.554676000000
C	-1.941903000000	-0.437938000000	2.861733000000	H	2.759229000000	1.127214000000	2.597806000000
H	-0.933655000000	-0.039615000000	2.900204000000	C	3.830804000000	0.555006000000	4.367768000000
C	-3.018434000000	0.378741000000	3.184207000000	H	4.758519000000	1.002356000000	4.024538000000
C	-4.329273000000	-0.091249000000	3.098443000000	C	3.767019000000	-0.099389000000	5.599841000000
H	-5.166247000000	0.557920000000	3.314226000000	H	4.646839000000	-0.158250000000	6.234123000000
C	-4.530790000000	-1.404425000000	2.685959000000	C	2.564262000000	-0.678751000000	6.012686000000
C	-3.467159000000	-2.251068000000	2.374217000000	H	2.503302000000	-1.183906000000	6.972396000000
H	-3.640423000000	-3.264680000000	2.047887000000	C	1.435503000000	-0.610877000000	5.195385000000
N	1.399757000000	-1.092734000000	-2.187946000000	C	-1.823065000000	4.847706000000	0.181190000000
N	1.876803000000	1.660171000000	-1.887991000000	C	-2.506679000000	6.009930000000	0.552327000000
N	3.960094000000	1.083983000000	-0.056910000000	H	-3.395776000000	5.923724000000	1.169723000000
N	3.467307000000	-1.671042000000	-0.340888000000	C	-2.033191000000	7.267372000000	0.172443000000
N	0.956443000000	3.717878000000	1.176163000000	H	-2.568007000000	8.161693000000	0.477447000000
H	1.526208000000	2.879694000000	1.135774000000	C	-0.864462000000	7.369675000000	-0.585108000000
N	-0.548113000000	2.244645000000	0.248684000000	H	-0.487922000000	8.345677000000	-0.876852000000
H	0.268888000000	1.716054000000	-0.043525000000	C	-0.181710000000	6.219873000000	-0.985326000000
N	0.197874000000	-3.981690000000	0.831549000000	H	0.715312000000	6.284939000000	-1.590080000000
H	0.799416000000	-3.177507000000	0.693275000000	C	-0.658682000000	4.962325000000	-0.613053000000
N	-1.031856000000	-2.509255000000	2.083443000000	C	-7.167251000000	0.293755000000	-0.671955000000
H	-0.160759000000	-1.994684000000	2.102665000000	C	-7.444303000000	0.638869000000	-2.003276000000
O	-1.164014000000	4.444488000000	0.643404000000	H	-6.623372000000	0.885599000000	-2.669854000000
O	-1.972443000000	-4.511600000000	1.414367000000	C	-8.757717000000	0.655720000000	-2.474026000000
Fe	2.672715000000	-0.005325000000	-1.115060000000	H	-8.955300000000	0.921918000000	-3.508412000000
H	0.774537000000	1.802989000000	-5.941854000000	C	-9.813223000000	0.323217000000	-1.621413000000
H	7.633125000000	-1.940168000000	0.247665000000	H	-10.835412000000	0.335527000000	-1.988301000000
C	-2.947669000000	-1.781079000000	-1.188570000000	C	-9.547530000000	-0.028449000000	-0.295972000000
F	-3.942405000000	-2.520133000000	-0.647358000000	H	-10.362484000000	-0.288619000000	0.373376000000
F	-3.123288000000	-1.834177000000	-2.533019000000	C	-8.233793000000	-0.043998000000	0.174374000000
F	-1.784298000000	-2.412437000000	-0.920063000000	C	-2.364180000000	-4.655967000000	0.518627000000
C	-5.507339000000	2.186972000000	0.377725000000	C	-2.940111000000	-5.749401000000	1.168096000000
F	-5.380120000000	3.343602000000	1.057847000000	H	-3.610719000000	-5.566784000000	2.002760000000
F	-6.209005000000	2.461295000000	-0.748221000000	C	-2.640802000000	-7.055521000000	0.774943000000
F	-6.292612000000	1.366740000000	1.122870000000	H	-3.088850000000	-7.897063000000	1.294199000000
C	-5.927785000000	-1.905257000000	2.456079000000	C	-1.751496000000	-7.266431000000	-0.280559000000
F	-6.274256000000	-1.825072000000	1.144425000000	H	-1.506340000000	-8.278196000000	-0.590928000000
F	-6.066968000000	-3.203224000000	2.807202000000	C	-1.178399000000	-6.189958000000	-0.958175000000
F	-6.848223000000	-1.197479000000	3.144456000000	H	-0.496930000000	-6.352349000000	-1.782624000000
C	-2.769803000000	1.783249000000	3.656662000000	C	-1.484890000000	-4.879744000000	-0.569913000000
F	-2.701674000000	1.854942000000	5.006864000000	N	-1.392200000000	-1.276009000000	1.859401000000
F	-1.605548000000	2.283783000000	3.181667000000	N	-1.281994000000	1.491104000000	1.776468000000
F	-3.756588000000	2.624829000000	3.272494000000	N	-3.738863000000	1.566021000000	0.370953000000
				N	-3.955542000000	-1.211330000000	0.668978000000
αα$UrFe^{I}$-CO_2 (-1,2)				N	-0.006871000000	3.771758000000	-1.029365000000
-4483.54448453 (-4482.767888) Hartrees				C	1.255074000000	3.441149000000	-0.548883000000
				H	-0.632248000000	2.969865000000	-1.113469000000
C	-0.254970000000	-1.136253000000	2.636000000000	N	1.415247000000	2.069516000000	-0.476390000000
C	0.287298000000	0.077196000000	3.069253000000	C	2.525116000000	1.360302000000	-0.039422000000
C	-0.218760000000	1.311401000000	2.649055000000	C	3.777120000000	1.941864000000	0.201933000000
C	0.358389000000	2.588037000000	2.983089000000	H	3.900668000000	3.005610000000	0.068476000000
H	1.171351000000	2.740887000000	3.676250000000	C	4.841510000000	1.135442000000	0.608896000000
C	-0.304417000000	3.528812000000	2.250546000000	C	4.699904000000	-0.239068000000	0.767162000000
H	-0.135975000000	4.595442000000	2.227919000000	H	5.539481000000	-0.855003000000	1.062525000000
C	-1.321711000000	2.837868000000	1.502084000000	C	3.445822000000	-0.806296000000	0.532114000000

C	2.364602000000	-0.025690000000	0.149549000000	C	3.287596000000	-2.281878000000	0.753182000000
H	1.394387000000	-0.480549000000	-0.007045000000	F	4.239169000000	-2.991240000000	0.097331000000
H	0.572771000000	1.517242000000	-0.657284000000	F	3.417091000000	-2.603719000000	2.064746000000
N	-0.995399000000	-3.749445000000	-1.245584000000	F	2.089960000000	-2.746295000000	0.343981000000
C	0.234040000000	-3.612369000000	-1.857790000000	C	6.149201000000	1.785005000000	0.957009000000
H	-1.484672000000	-2.875550000000	-1.049279000000	F	6.388079000000	2.889718000000	0.217695000000
N	0.389585000000	-2.321931000000	-2.350055000000	F	6.174115000000	2.181065000000	2.259100000000
C	1.577546000000	-1.678609000000	-2.684469000000	F	7.197301000000	0.949825000000	0.789009000000
C	1.486741000000	-0.314911000000	-3.018961000000	C	5.340950000000	-2.149300000000	-2.771312000000
H	0.519894000000	0.176512000000	-3.006398000000	F	6.089589000000	-1.930270000000	-3.880180000000
C	2.638142000000	0.417314000000	-3.282216000000	F	6.036207000000	-1.618281000000	-1.735456000000
C	3.899701000000	-0.174528000000	-3.215400000000	F	5.294847000000	-3.482780000000	-2.577345000000
H	4.796232000000	0.405891000000	-3.400258000000	C	2.548802000000	1.871783000000	-3.648576000000
C	3.977591000000	-1.529175000000	-2.895543000000	F	2.973341000000	2.088590000000	-4.917617000000
C	2.838737000000	-2.292894000000	-2.650090000000	F	1.293701000000	2.357934000000	-3.562280000000
H	2.913644000000	-3.337017000000	-2.390501000000	F	3.333154000000	2.638766000000	-2.851674000000
H	-0.411361000000	-1.697256000000	-2.198491000000	C	-1.685919000000	0.091280000000	-0.770979000000
O	2.106370000000	4.268407000000	-0.232945000000	O	-1.081960000000	1.083631000000	-1.233276000000
O	1.067925000000	-4.509261000000	-1.972240000000	O	-1.856918000000	-1.024279000000	-1.315706000000
Fe	-2.508355000000	0.125375000000	1.011362000000				
H	0.502367000000	-1.062727000000	5.518350000000				
H	-8.026211000000	-0.317095000000	1.204953000000				

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