

Operando Elucidation on the Working State of Immobilized Fluorinated-Iron Porphyrin for Selective Aqueous Electroreduction of CO₂ to CO

Xiaofei Lu,^{†,1} Hassan Ait Ahsaine,^{†,1} Busra Dereli,[‡] Angel T. Garcia-Esparza,^{||} Marco Reinhard,^{||} Tatsuya Shingawa,[†] Duanxing Li,[†] Karim Adil,[§] Mohamed Rachid Tchalala,[§] Thomas Kroll,^{||} Mohamed Eddaoudi,^{§,*} Dimosthenis Sokaras,^{||,*} Luigi Cavallo,^{‡,*} Kazuhiro Takanabe^{†,*}

[†]Department of Chemical System Engineering, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

[‡]KAUST Catalysis Center (KCC) and Physical Sciences and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), 4700 KAUST, Thuwal 23955-6900, Saudi Arabia

[§]Functional Materials Design, Discovery and Development Research Group (FMD3), Advanced Membranes and Porous Materials Center (AMPMC), Division of Physical Sciences and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, KSA

^{||}Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA

Corresponding Author *E-mail: mohamed.eddaoudi@kaust.edu.sa (M. E.); dsokaras@slac.stanford.edu (D.S.); luigi.cavallo@kaust.edu.sa (L.C.); takanabe@chemsys.t.u-tokyo.ac.jp (K.T.)

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S1. Surface Structures of Catalysts.

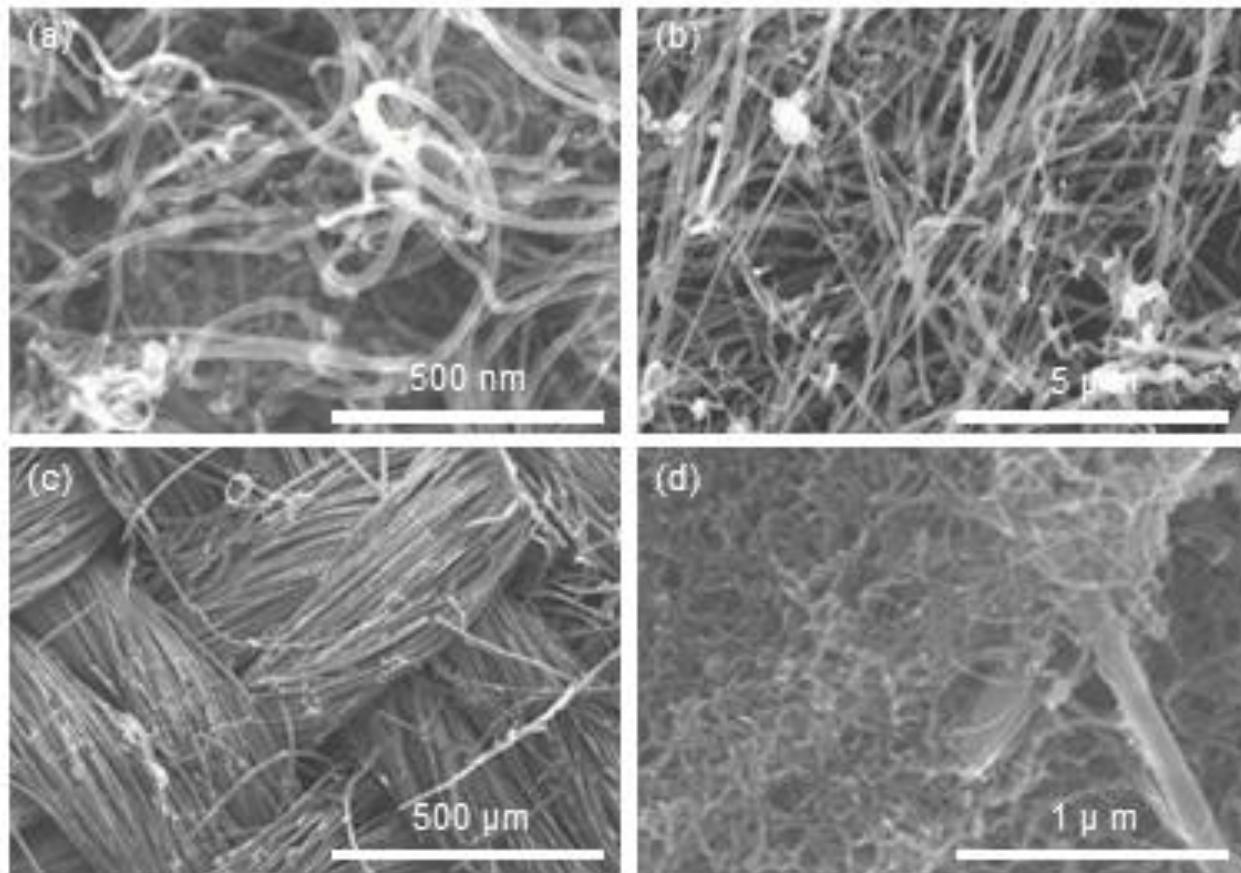


Figure S1. Ex-situ characterization of samples. Scanning electron microscopy (SEM) images of (a) multiwall carbon nanotubes (CNTs), (b) carbon fiber (CF), (c) carbon cloth (CC), and (d) fluorinated iron tetraphenylporphyrin (FeF₂₀TPP) supported on CNT-CF/CC.

S2. Additional DFT Calculations

We tested the sensitivity of Fe spin states to the choice of functional for all FeTPP species at five different density functionals (**Tables S1-S5**). Fluctuations between the spin states over the tested functionals are usually not larger than 2 kcal/mol (**Tables S1-S4**), which is acceptable within the associated error of DFT for chemical accuracy. Hybrid functionals with relatively large Hartree-Fock (HF) exchange contribution are biased toward high spin state (which is obvious in some instances in the tabulated data), while the local functionals are generally biased toward low spin. Therefore, we chose to apply TPSSh with a relatively small HF exchange percentage (HF = 10%) for electronic energy calculations.

The choice of this functional was further confirmed to have produced similar ground-state electronic structures as in the seminal work by Römel et al.¹ For FeF₂₀TPP, we predicted a similar trend in terms of spin-state energies and spin density distribution (see **Figure 3** in the **main text**) to the parent FeTPP system at the M06/def2SVP|def2TZVP level of theory. Since there is only a quantitative difference and not a qualitative one, we continued with TPSSh single-point calculations for M06 optimized structures in the case of FeF₂₀TPP.

Table S1. Spin-corrected relative electronic energies (in kcal/mol) of FeTPP for formal Fe(III) at various DF levels.

Total Spin	PBE0-D3BJ	τ -HCTH	TPSSh	M06-L	M06
S=1/2	16.0	18.9	14.8	17.7	19.2
S=3/2	0.0	0.0	0.0	2.0	0.4
S=5/2	5.9	4.8	13.0	0.0	0.0

Table S2. Spin-corrected relative electronic energies (in kcal/mol) of FeTPP for formal Fe(II) at various DF levels.

Total Spin	PBE0-D3BJ	τ -HCTH	TPSSh	M06-L	M06
S=0	30.5	30.5	24.6	25.0	29.9
S=1	1.9	0.0	0.0	2.2	0.9
S=2	0.0	2.4	8.5	0.0	0.0

Table S3. Spin-corrected relative electronic energies (in kcal/mol) of FeTPP for formal “Fe(I)” at various DF levels.

Total Spin	PBE0-D3BJ	τ -HCTH	TPSSh	M06-L	M06
S=1/2	0.0	0.0	0.0	0.0	0.0
S=3/2	5.3	11.4	8.6	8.6	5.8

Table S4. Spin-corrected relative electronic energies (in kcal/mol) of FeTPP for formal “Fe(0)” at various DF levels.

Total Spin	PBE0-D3BJ	τ -HCTH	TPSSh	M06-L	M06
S=0	0.0	0.0	0.0	0.5	0.0
S=1	15.4	5.1	11.0	0.0	8.1
S=2	12.1	14.2	15.4	5.5	7.8

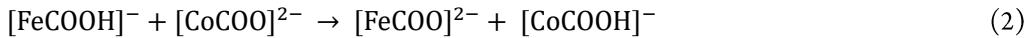
Table S5. Relative electronic energies with iron spin density for FeTPP intermediates at TPSSh//M06/def2-SVP|def2-TZVP.

Complex	ΔE	S_{Fe}
$^2[Fe]^+$	14.9	2.18
$^4[Fe]^+$	0.0	2.98
$^6[Fe]^+$	12.8	4.36
Complex	ΔE	S_{Fe}
$^1[Fe]$	24.6	0.00
$^3[Fe]$	0.0	2.18
$^5[Fe]$	8.5	3.83
Complex	ΔE	S_{Fe}
$^2[Fe]^-$	0.0	2.02
$^4[Fe]^-$	6.2	2.16
Complex	ΔE	S_{Fe}
$^1[Fe]^{2-}$	0.0	1.89
$^3[Fe]^{2-}$	8.0	2.02
$^5[Fe]^{2-}$	12.2	2.20
Complex	ΔE	S_{Fe}
$^2[FeCO_2]^-$	0.0	1.37
$^4[FeCO_2]^-$	13.6	2.08
Complex	ΔE	S_{Fe}
$^1[FeCO_2]^{2-}$	0.0	1.35
$^3[FeCO_2]^{2-}$	12.8	1.34
$^5[FeCO_2]^{2-}$	8.0	3.38
Complex	ΔE	S_{Fe}
$^2[FeCO_2]^{3-}$	0.0	1.31

$^4[\text{FeCO}_2]^{3-}$	3.4	1.40
Complex	ΔE	S_{Fe}
$^2[\text{FeCOOH}]$	0.0	1.14
$^4[\text{FeCOOH}]$	38.4	1.20
Complex	ΔE	S_{Fe}
$^1[\text{FeCOOH}]^-$	0.0	0.00
$^3[\text{FeCOOH}]^-$	13.6	1.15
$^5[\text{FeCOOH}]^-$	17.7	3.85
Complex	ΔE	S_{Fe}
$^2[\text{FeCOOH}]^{2-}$	0.0	0.30
$^4[\text{FeCOOH}]^{2-}$	12.7	1.18
Complex	ΔE	S_{Fe}
$^2[\text{FeCO}]^-$	0.0	0.01
$^4[\text{FeCO}]^-$	37.2	0.06
Complex	ΔE	S_{Fe}
$^1[\text{FeCO}]$	0.0	0.00
$^3[\text{FeCO}]$	18.1	2.04
$^5[\text{FeCO}]$	29.0	3.78
Complex	ΔE	S_{Fe}
$^2[\text{FeCO}]^+$	0.0	0.02
$^4[\text{FeCO}]^+$	44.4	0.03

S3. Isodesmic Proton-Exchange Reaction Scheme.

The pK_a of the nonfluorinated carboxylic acid [FeCOOH] is calculated with respect to the pK_a of the reference acids [CoCOOH] and $[CoCOOH]^-$ ($pK_a[(CoCOOH)] = 3.5$ and $pK_a[CoCOOH]^- = 8.6$), which was obtained from Römelt *et al.*² The solvation free energy of the acid-base reaction (ΔG_{soln}) is predicted as -0.7 kcal/mol and 10.6 kcal/mol for equations 1 and 2, respectively, at the TPSSh//M06/def2SVP|def2TZVP level. The corresponding pK_a values are calculated as 2.8 and 16.4 , respectively.

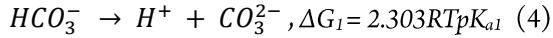


$$pK_a[FeCOOH] = \frac{\Delta G_{soln}}{2.303RT} + pK_a[CoCOOH]^- \quad (3)$$

The associated pK_a value using the gas-phase optimized structures is predicted as 3.6 and 17.4 for equations 1 and 2, respectively. We applied the same protocol for the fluorinated species in gas phase, resulting in pK_a values of 0.7 and 15.8 for equations 1 and 2, respectively (see the **main text**).

S4. Correction Term to HCO_3^- Proton Source.

We assessed the accuracy of the DFT method for predicting the pK_a of HCO_3^- , which was used as the acid source in PT reactions. To this end, we applied the isodesmic proton-exchange reaction scheme using acetic acid with a well-known pK_a value ($\text{pK}_a[\text{CH}_3\text{COOH}] = 4.7$) as the reference acid.



The predicted ΔG_{rxn} was 22.6 kcal/mol (equation 6), which deviates by 17.7 kcal/mol from the experimental value ($\Delta G_{exp} = 4.9$ kcal/mol) based on pK_a ($[\text{CH}_3\text{COOH}] = 4.7$). Thus, the prediction of $\text{pK}_a[\text{HCO}_3^-]$ at the TPSSh//M06/def2SVP|def2TZVP level is drastically erroneous, which prompted us to subtract roughly 17.7 kcal/mol from the reaction energies for each $\text{HCO}_3^-/\text{CO}_3^{2-}$ acid-base pair involved.

S5. Calculation of Electroactive Surface Concentration

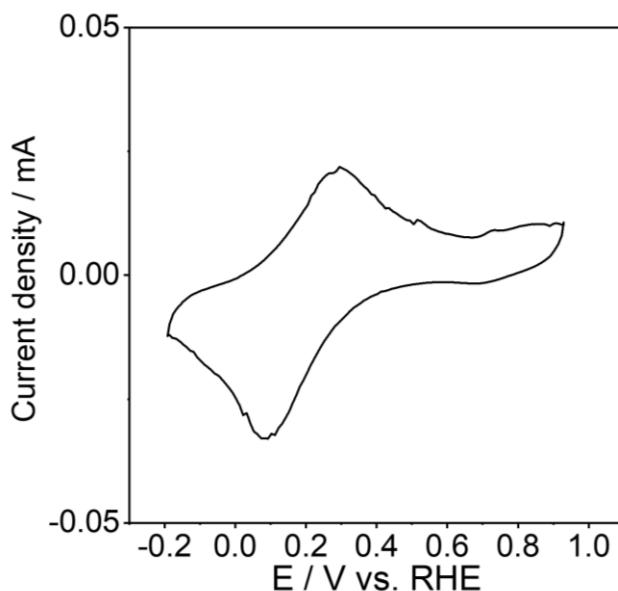


Figure S2. Cyclic voltammograms of FeF₂₀TPP/CNT-CF in Ar saturated HClO₄ solution (pH 1.4) at the scan rates of 20 mV s⁻¹.

$$\Gamma = \frac{Q}{nFA}$$

Γ is the surface concentration of FeF₂₀TPP (mol cm⁻²), n is the number of electrons exchanged (1 electron), F is the Faraday constant (96500 C mol⁻¹) and A is the electrode surface (0.28 cm⁻²). Q is the charge calculated from the integration of the electrochemical wave (C), which was determined by dividing the integral of redox peak in the cyclic voltammograms by the scan rate (20 mV s⁻¹). With this equation, the surface concentration of electroactive FeF₂₀TPP was determined to be 2.3 x 10⁻⁸ mol cm⁻². Because the loaded total amount of FeF₂₀TPP was 3.9 x 10⁻⁸ mol cm⁻², this value indicates approximately 60% of FeF₂₀TPP being active in the prepared electrode.

S6. Electronic States for FeF₂₀TPP Species and Spin Density Analysis.

Table S6. Spin densities on Fe, porphyrin, and CO₂/CO fragments and electronic states for studied FeF₂₀TPP species.

Species	Spin state	Spin density			NPA charge		^c S _{Fe}	^d S _{tot}
		Fe	F ₂₀ TPP	CO ₂ /CO	^a Fe-CO	^b q(F ₂₀ TPP)		
[Fe(III)F ₂₀ (TPP)] ⁺	⁴ HS	2.97	0.03		1.00	0.00	3/2	3/2
[Fe(II)F ₂₀ (TPP)]	³ IS	2.19	-0.19		0.77	-0.77	1	1
[Fe(II)F ₂₀ (TPP [·])] ⁻	² BS(2,1)	2.06	-1.06		0.69	-1.69	1	1/2
[Fe(II)F ₂₀ (TPP ^{··})] ²⁻	¹ BS(2,2)	1.91	-1.91		0.61	-2.61	1	0
[Fe(II)F ₂₀ (TPP [·])COO] ⁻	² BS(2,1)	1.79	-0.75	-0.04	0.30	-1.30	1	1/2
[Fe(II)F ₂₀ (TPP ^{··})COO] ²⁻	¹ BS(2,2)	1.79	-1.71	-0.08	0.27	-2.27	1	0
[Fe(II) F ₂₀ (TPP [·])COO] ³⁻	² BS(2,1)	1.74	-0.62	-0.12	0.27	-3.27	1	1/2
[Fe(II)F ₂₀ (TPP [·])COOH]	² LS	1.15	-0.06	-0.09	0.40	-0.40	1/2	1/2
[Fe(II)F ₂₀ (TPP ^{··})COOH] ⁻	¹ LS	0.00	0.00	0.00	0.00	-1.00	0	0
[Fe(II)F ₂₀ (TPP [·])COOH] ²⁻	² LS	0.27	0.75	-0.03	0.17	-2.17	0	1/2
[Fe(II)F ₂₀ (TPP [·])CO] ⁺	² LS	-0.02	1.02	0.00	0.37	0.63	0	1/2
[Fe(II)F ₂₀ (TPP ^{··})CO]	¹ LS	0.00	0.00	0.00	0.34	-0.34	0	0
[Fe(II)F ₂₀ (TPP [·])CO] ⁻	² LS	0.02	0.99	-0.01	0.31	-1.31	0	1/2

^aq(Fe-CO): Sum of NPA charges on Fe and CO₂/COOH/CO fragments. ^bq(F₂₀TPP): NPA charge on F₂₀TPP fragment. ^cS_{Fe}:

total spin for Fe center in the associated complex. ^dS_{tot}: total spin for the entire system. HS (high spin), IS (intermediate spin), LS (low spin), and BS (broken symmetry) solutions.

S7. Electrocatalytic Performance of Immobilized Molecular Catalysts.

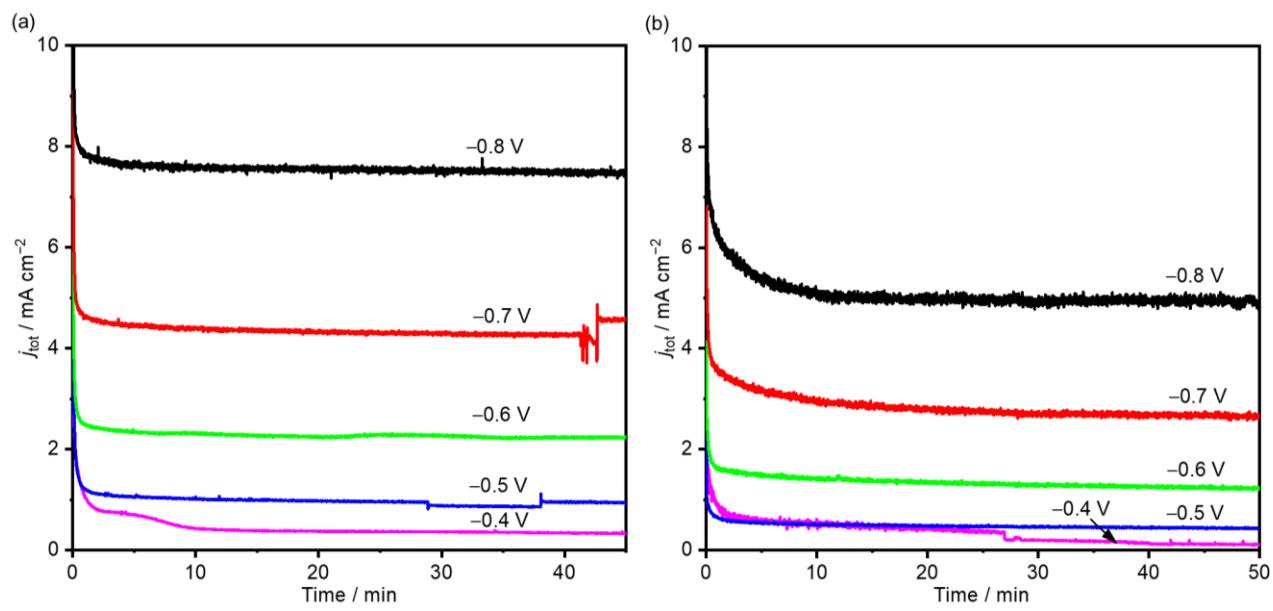


Figure S3. Electrocatalytic CO_2 reduction reaction over TPP-based electrocatalysts. Representative chronoamperometry (CA) profiles over (a) 15 wt.% fluoridized iron tetraphenylporphyrin ($\text{FeF}_{20}\text{TPP}$) supported on the mixture of multiwall carbon nanotubes (CNTs) and carbon fiber (CF), which were deposited on carbon cloth (CC), and (b) 15 wt.% iron tetraphenylporphyrin (FeTPP) supported on CNT-CF/CC were recorded in the potential range from -0.4 to -0.8 V vs. reversible hydrogen electrode (RHE) in CO_2 -saturated aqueous solution of 0.5 M NaHCO_3 at pH 7.2 at 25 °C. The numbers in the figures denote the applied potential on the RHE scale.

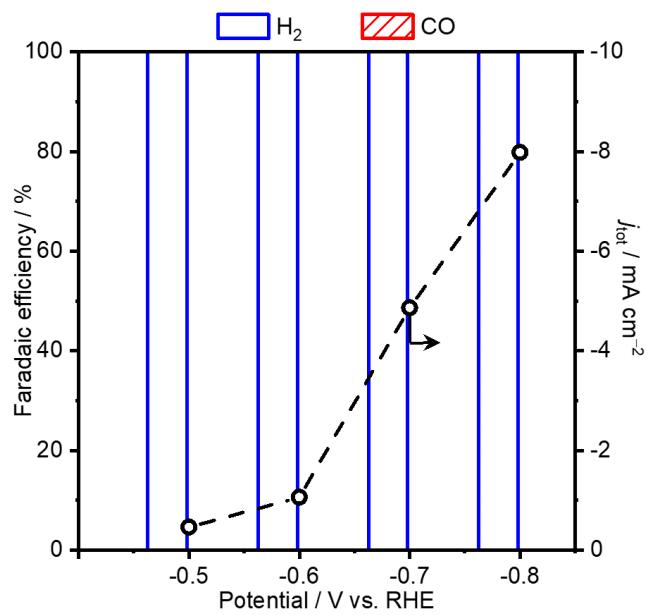


Figure S4. Electrocatalytic CO_2 reduction reaction without molecular catalysts. The electrocatalytic performance of CNT-CF/CC was assessed by CA in the potential window between -0.5 and -0.8 V vs. RHE at the denoted potential for 50 min in CO_2 -saturated aqueous solution of 0.5 M NaHCO_3 at pH 7.2 at 25°C .

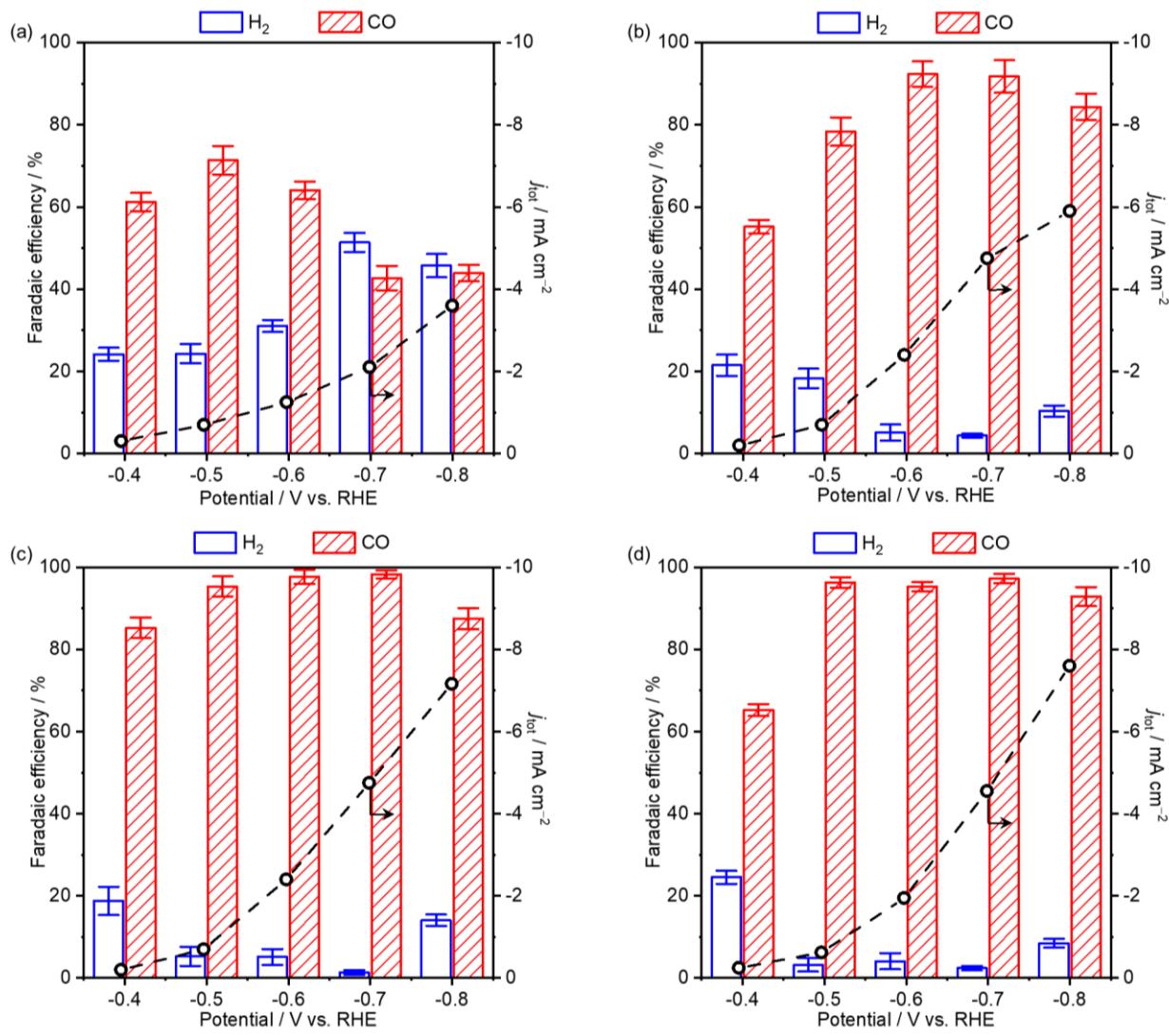


Figure S5. Electrocatalytic CO₂ reduction reaction at various loading of FeF₂₀TPP. The electrocatalytic performance of (a) 5, (b) 10, (c) 20, and (d) 30 wt.% FeF₂₀TPP/CNT-CF/CC was assessed by CA at the denoted potential for 50 min in CO₂-saturated aqueous solution of 0.5 M NaHCO₃ at pH 7.2 at 25 °C.

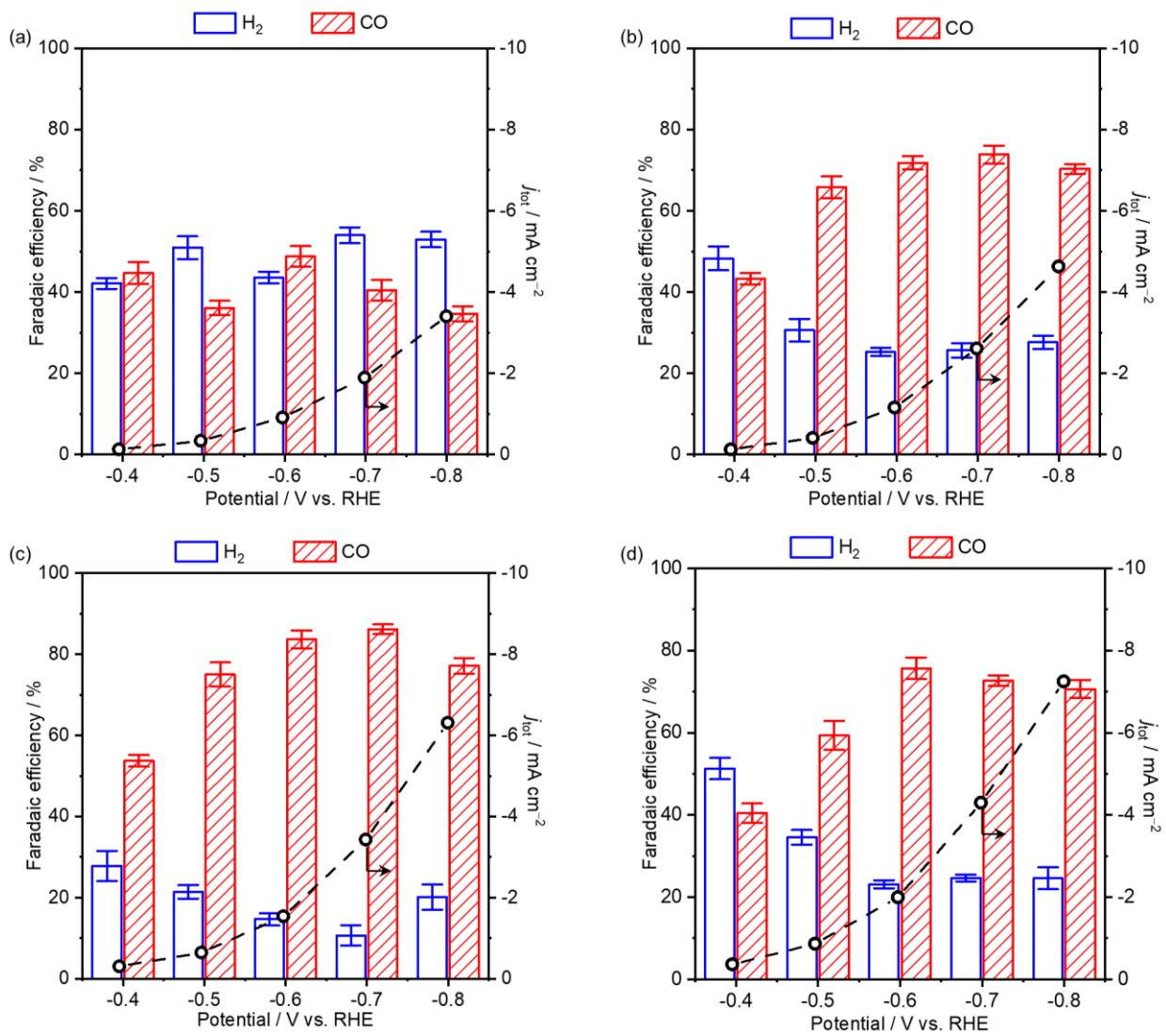


Figure S6. Electrocatalytic CO₂ reduction reaction at various loading of FeTPP. The electrocatalytic performance of (a) 5, (b) 10, (c) 20, and (d) 30 wt.% FeTPP/CNT-CF/CC was assessed by CA at the denoted potential for 50 min in CO₂-saturated aqueous solution of 0.5 M NaHCO₃ at pH 7.2 at 25 °C.

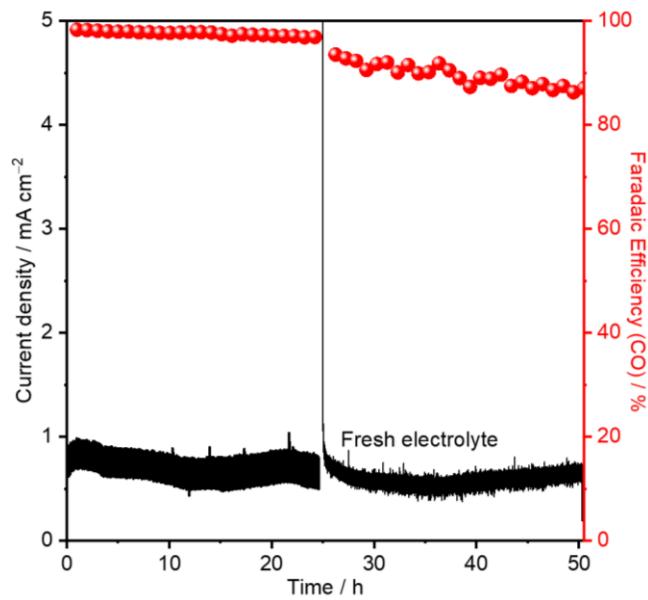


Figure S7. Long-term stability testing of immobilized FeF₂₀TPP for electrocatalytic CO₂ reduction reaction. The CA profile over 15 wt.% FeF₂₀TPP/CNT-CF/CC for electrocatalytic CO₂ reduction reaction was recorded at -0.5 V vs. RHE in CO₂-saturated aqueous solution of 0.5 M NaHCO₃ at pH 7.2 at 25 °C.

S8. Ex-situ and In-operando Characterization of the Molecular Catalysts.

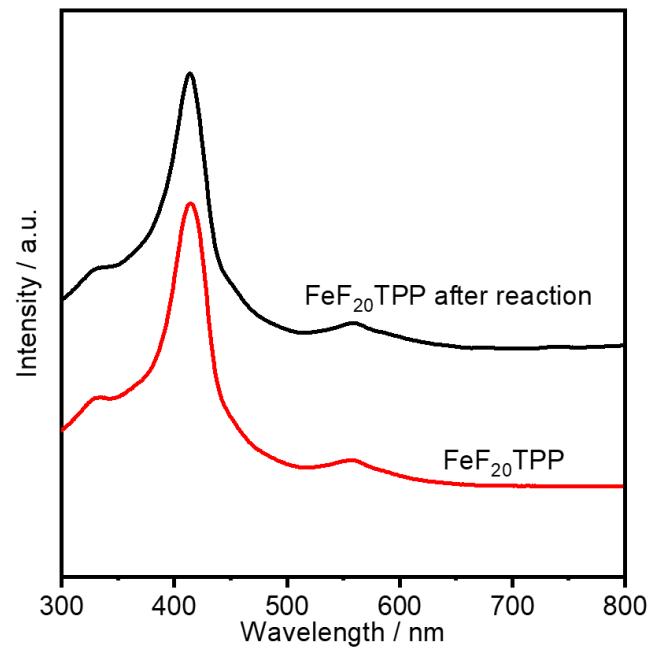


Figure S8. UV-Vis absorption spectra of pre- and post-reaction FeF₂₀TPP. The figure shows ex-situ UV-Vis spectra of pristine FeF₂₀TPP and that extracted from the electrode FeF₂₀TPP/CNT-CF/CC employed for stability testing for 50 h. The latter is denoted as “FeF₂₀TPP after reaction” in the figure.

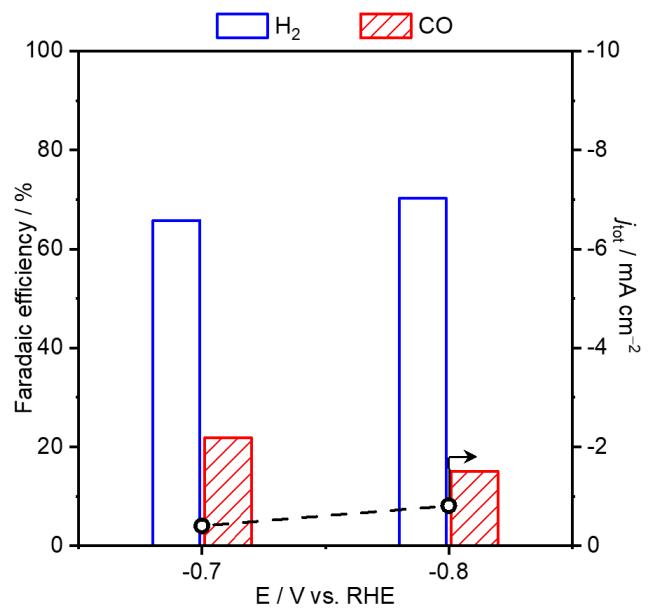


Figure S9. Electrocatalytic CO₂ reduction reaction in bicarbonate solution without the supply of CO₂. Catalytic testing was performed over 15 wt.% FeF₂₀TPP/CNT-CF/CC by CA at the denoted potential for 50 min in Ar-saturated aqueous solution of 0.5 M NaHCO₃ at pH 8.3 and 25 °C.

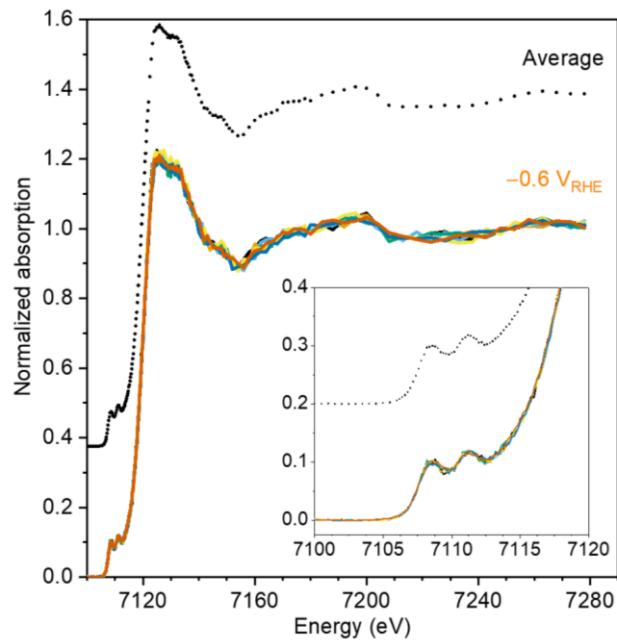


Figure S10. The normalized Fe K-edge XAS spectra of 15 wt.% FeF₂₀TPP/CNT-CF at -0.6 V vs RHE. The figure shows seven consecutive overlapping scans up to a k value of $\sim 6 \text{ \AA}^{-1}$ from various electrode spots (i.e. approximately 150 eV above the absorption edge) and the average spectra. The inset shows the magnified pre-edge region showing a well-resolved doublet under the cathodic conditions for electrocatalytic CO₂ reduction.

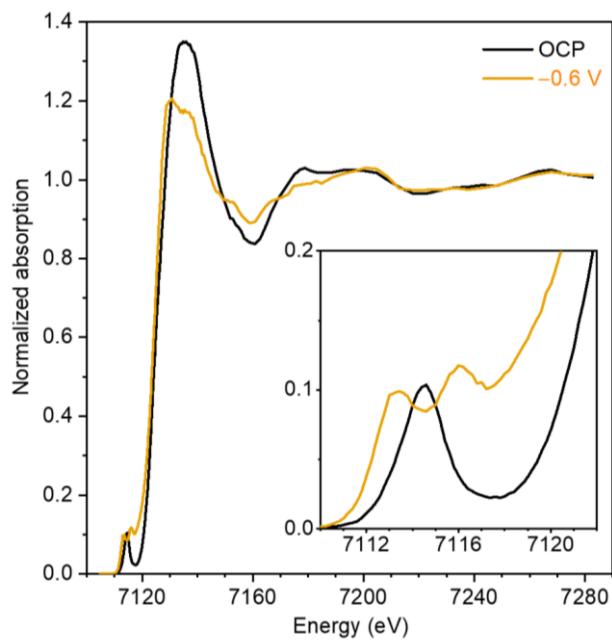


Figure S11. The normalized Fe K-edge XAS of 15 wt.% $\text{FeF}_{20}\text{TPP}/\text{CNT-CF}$ under open circuit potential and -0.6 V vs RHE up to a k value of $\sim 6 \text{ \AA}^{-1}$. The figure shows the full data range recorded for Figure 6 of the main manuscript. The inset shows the magnified pre-edge region of the spectra under rest and operation conditions for electrocatalytic CO_2 reduction.

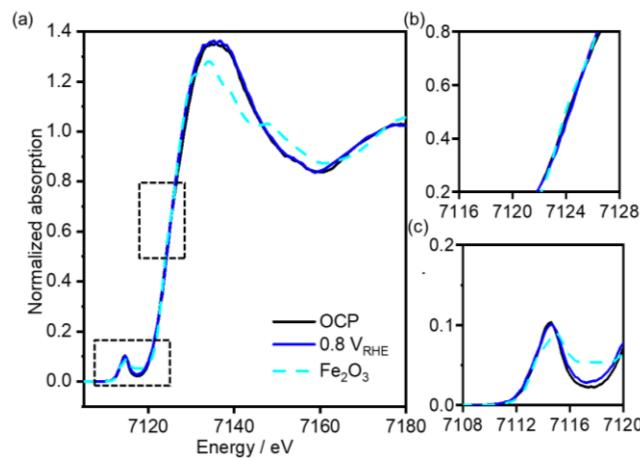


Figure S12. In-operando x-ray absorption spectra of $\text{FeF}_{20}\text{TPP}$. (a) Normalized Fe K-edge x-ray absorption near edge structure (XANES) spectra of $\text{FeF}_{20}\text{TPP}/\text{CNT-CF}$ deposited on carbon paper recorded at open-circuit potential (OCP) and $+0.8\text{V}$ vs. RHE in CO_2 -saturated aqueous solution of 0.5 M NaHCO_3 at $\text{pH } 7.2$. The spectra at the latter potential were recorded after the measurement at -0.6 V vs. RHE displayed in **Figure 6** of the main text. The spectra at the white line and the pre-edge are magnified in panels (b) and (c), respectively.

S9. The Spin Density Distributions of all Open-shell Intermediates Involved in the Catalytic Cycle

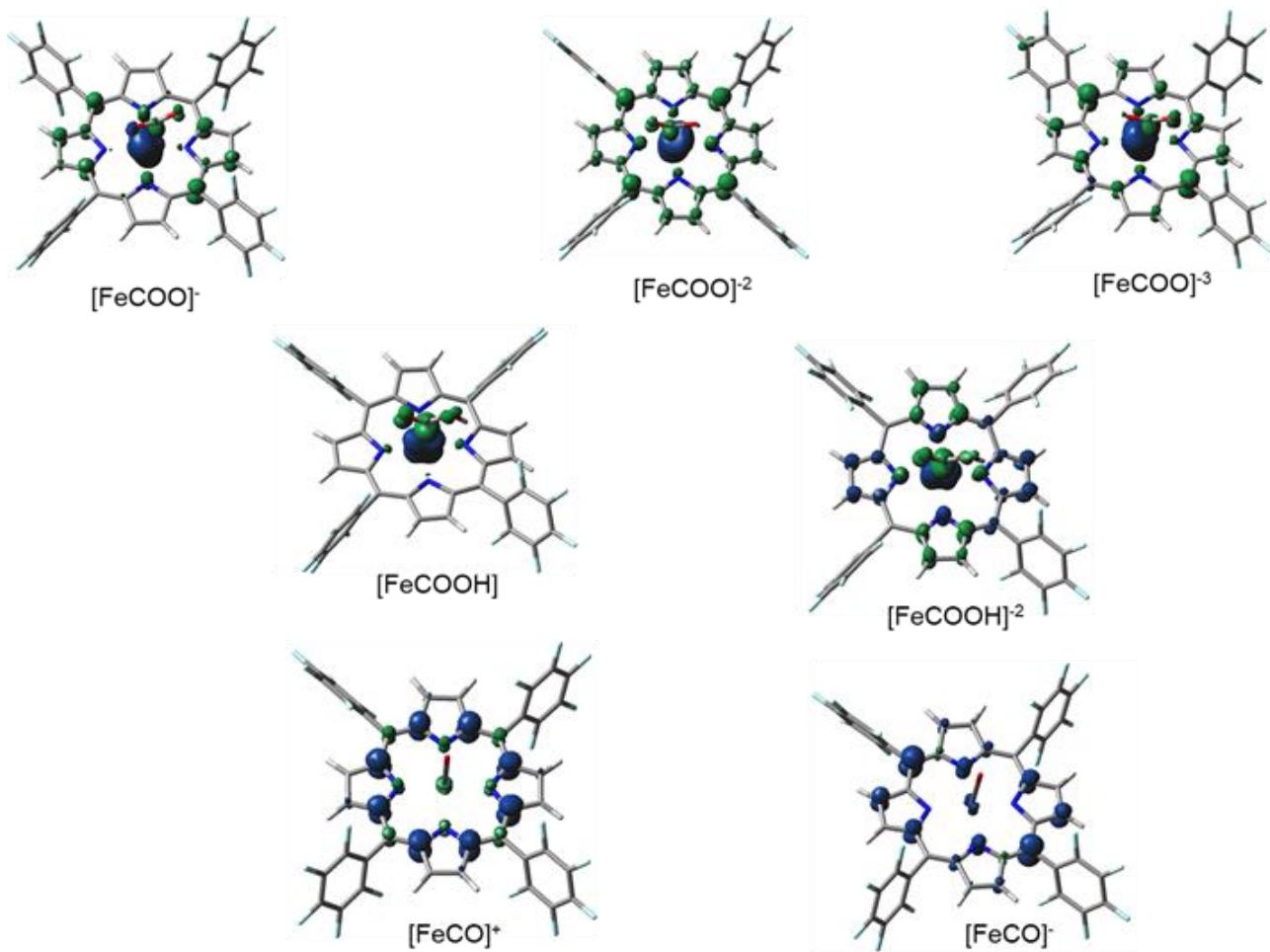


Figure S13. Mulliken spin density distributions (surfaces with 0.006 au isovalue) for all open-shell CO_2 , COOH and CO bound complexes at M06/def2-SVP|def2-TZVP.

S10. Influence of Explicit H₂O Molecule on [Fe(II)F₂₀(TPP[·])COO]⁻/[Fe(II) F₂₀(TPP^{··})COO]²⁻ Redox Potential.

The model of the oxidized and reduced forms of CO₂adducts in the presence of one explicit H₂O molecule (**Figure S10**) shows that the reduction potential is shifted by 0.24 V, which shows the significance of the second coordination sphere around the Fe-porphyrin system. Since the addition of explicit H₂O suggests a change in the cavity shape of [Fe(II)F₂₀(TPP[·])COO]⁻and [Fe(II)F₂₀(TPP^{··})COO]²⁻ structures, it might be crucial to perform the geometry optimizations in the condensed phase. Therefore, the calibrated redox potential (-0.64 V) for [Fe(II)F₂₀(TPP[·])COO]⁻/[Fe(II)F₂₀(TPP^{··})COO]²⁻ with one explicit H₂O was obtained using SMD optimized structures in water.

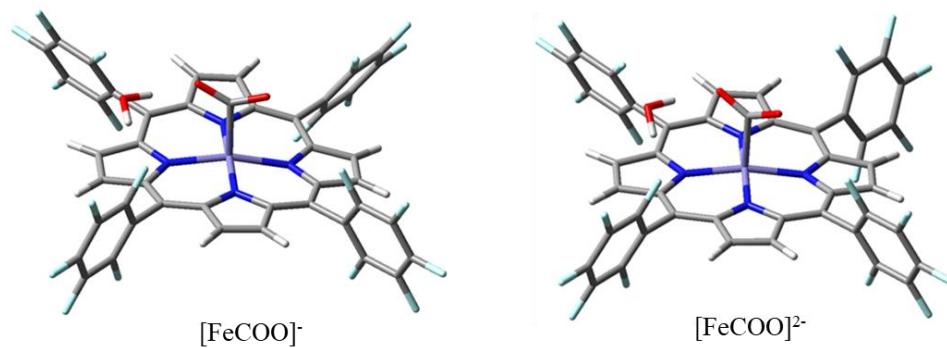
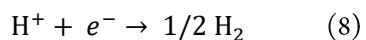
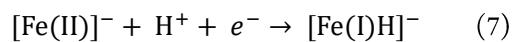


Figure S14. [FeCOO]⁻ and [FeCOO]²⁻ structures with one H₂O molecule stabilizing Fe bound CO₂ at TPSSh//M06/def2SVP|def2TZVP with SMD model.

S11. Formation of Fe-H species

The formation of Fe-H species is endergonic by 15.4 kcal/mol (equation 7), which is not favored in comparison to CO₂ activation ($\Delta G_{[\text{PFeCOOH}^-]} = -57.6$), thereby ruling out competition for HER.



S12. Energies for All Ground State Structures.

Table S7. Energies for all ground state FeTPP structures.

Species	E _{gas}	G _{gas}	E _{water}
⁴ [Fe(III)] ⁺	-3173.303407	-3172.776407	-3175.108458
³ [Fe(II)]	-3173.523787	-3172.996624	-3175.267218
² [Fe(I)] ⁻	-3173.583297	-3173.058568	-3175.376878
¹ [Fe(0)] ²⁻	-3173.528268	-3173.006535	-3175.47154
² [FeCOO] ⁻	-3361.929369	-3361.395511	-3363.814416
¹ [FeCOO] ²⁻	-3361.878048	-3361.347235	-3363.911402
² [FeCOO] ³⁻	-3361.726573	-3361.201560	-3363.99061
² [FeCOOH]	-3362.444431	-3361.897048	-3364.283364
¹ [FeCOOH] ⁻	-3362.512255	-3361.966486	-3364.412719
² [FeCOOH] ²⁻	-3362.462424	-3361.921584	-3364.502597
² [FeCO] ⁺	-3286.473995	-3285.940250	-3288.33237
¹ [FeCO]	-3286.709407	-3286.175045	-3288.519197
² [FeCO] ⁻	-3286.763488	-3286.234367	-3288.621871

Table S8. Energies for all ground state FeF₂₀TPP structures.

Species	E _{gas}	G _{gas}	E _{water}
⁴ [Fe(III)] ⁺	-5155.877745	-5155.523756	-5158.049386
³ [Fe(II)]	-5156.124644	-5155.771762	-5158.217212
² [Fe(I)] ⁻	-5156.213611	-5155.863199	-5158.338046
¹ [Fe(0)] ²⁻	-5156.18648	-5155.837854	-5158.443059
² [FeCOO] ⁻	-5156.186480	-5155.696203	-5346.765466
¹ [FeCOO] ²⁻	-5344.537537	-5344.182911	-5346.870947
² [FeCOO] ³⁻	-5344.413017	-5344.063907	-5346.955302
² [FeCOOH]	-5345.042085	-5344.668257	-5347.229893
¹ [FeCOOH] ⁻	-5345.135653	-5344.763188	-5347.371584
² [FeCOOH] ²⁻	-5345.113719	-5344.746277	-5347.467352
² [FeCO] ⁺	-5269.043388	-5268.686210	-5271.263262
¹ [FeCO]	-5269.309246	-5268.949299	-5271.107367
² [FeCO] ⁻	-5269.392677	-5269.038715	-5271.581577
¹ [FeH] ⁻	-5156.765698	-5156.407219	-5158.908699

Table S9. Energies for all optimized organic species.

Species	E _{gas}	G _{gas}	E _{water}
CO ₂	-188.361047	-188.369621	-188.4408745
CO	-113.164267	-113.178261	-113.216298
H ₂ O	-76.324429	-76.321161	-76.36467726
H ₂	-1.166944	-1.168378	-1.172738978
HCO ₃ ⁻	-264.12433	-264.122879	-264.3500997
CO ₃ ²⁻	-263.287276	-263.296436	-263.8381552

For the DFT optimized Cartesian coordinates, see coordinates.xyz file attached below.

References

- (1) Römelt, C.; Ye, S.; Bill, E.; Weyhermüller, T.; van Gastel, M.; Neese, F. Electronic Structure and Spin Multiplicity of Iron Tetraphenylporphyrins in Their Reduced States as Determined by a Combination of Resonance Raman Spectroscopy and Quantum Chemistry. *Inorg. Chem.* **2018**, *57*, 2141-2148.
- (2) Göttle, A. J.; Koper, M. T. Proton-Coupled Electron Transfer in the Electrocatalysis of CO₂ Reduction: Prediction of Sequential Vs. Concerted Pathways Using DFT. *Chem. Sci.* **2017**, *8*, 458-465.

The DFT optimized Cartesian coordinates

TPP Ligand

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[Fe]⁺¹

Fe	0.000001	-0.000002	-0.011399
N	-0.204614	-1.950765	-0.010931
N	1.950758	-0.204610	-0.011073
N	0.204615	1.950760	-0.010928
N	-1.950755	0.204607	-0.011115
C	-1.384985	-2.681734	-0.008924
C	0.798326	-2.910887	-0.009924
C	2.681725	-1.384981	-0.008526
C	2.910880	0.798329	-0.010779
C	1.384984	2.681732	-0.008897
C	-0.798326	2.910883	-0.009942
C	-2.681723	1.384978	-0.008585
C	-2.910880	-0.798330	-0.010842
C	-1.112722	-4.080011	-0.013301
H	-1.874572	-4.857711	-0.021869
C	0.241676	-4.222163	-0.002707
H	0.825552	-5.141031	0.008078
C	4.080002	-1.112721	-0.013347
H	4.857699	-1.874578	-0.021624
C	4.222159	0.241683	-0.003643
H	5.141030	0.825567	0.006571
C	1.112720	4.080009	-0.013280
H	1.874570	4.857710	-0.021834
C	-0.241678	4.222160	-0.002713
H	-0.825557	5.141028	0.008059
C	-4.080000	1.112720	-0.013439
H	-4.857697	1.874577	-0.021735
C	-4.222158	-0.241683	-0.003737
H	-5.141030	-0.825567	0.006457
C	2.166936	-2.674885	-0.007449
C	2.674885	2.166939	-0.008547
C	-2.166935	2.674882	-0.007496
C	-2.674885	-2.166941	-0.008602
C	3.103620	-3.830355	0.001149
C	3.315744	-4.579397	-1.161630
C	4.195117	-5.659328	-1.150333
H	4.358420	-6.236245	-2.064649
C	4.866986	-6.001342	0.021601
H	5.556406	-6.849828	0.029457
C	4.659043	-5.260661	1.183505

H	5.181739	-5.528368	2.105787
C	3.782323	-4.178718	1.174269
H	3.615450	-3.595141	2.086161
C	3.830391	3.103588	-0.000778
C	4.578670	3.315531	-1.164079
C	5.658684	4.194814	-1.153594
H	6.235004	4.357975	-2.068312
C	6.001543	4.866767	0.018043
H	6.850095	5.556114	0.025262
C	5.261627	4.658999	1.180466
H	5.530004	5.181758	2.102519
C	4.179603	3.782370	1.172044
H	3.596632	3.615625	2.084349
C	-3.103618	3.830353	0.001081
C	-3.315710	4.579400	-1.161701
C	-4.195082	5.659333	-1.150423
H	-4.358360	6.236253	-2.064742
C	-4.866980	6.001344	0.021494
H	-5.556398	6.849832	0.029335
C	-4.659069	5.260659	1.183402
H	-5.181788	5.528365	2.105671
C	-3.782351	4.178715	1.174185
H	-3.615502	3.595135	2.086081
C	-3.830393	-3.103587	-0.000855
C	-4.578648	-3.315531	-1.164172
C	-5.658665	-4.194810	-1.153709
H	-6.234965	-4.357971	-2.068439
C	-6.001552	-4.866758	0.017923
H	-6.850106	-5.556102	0.025126
C	-5.261661	-4.658990	1.180362
H	-5.530059	-5.181745	2.102410
C	-4.179633	-3.782364	1.171961
H	-3.596682	-3.615618	2.084278
H	-4.305451	-2.786866	-2.083871
H	-2.787095	4.306883	-2.081631
H	4.305495	2.786863	-2.083782
H	2.787152	-4.306878	-2.081572

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[Fe]

Fe	0.000000	-0.000001	-0.000112
N	-0.000108	1.990683	-0.000066
N	-1.992771	-0.000109	-0.000026
N	0.000108	-1.990685	-0.000064
N	1.992772	0.000108	-0.000070

C	1.092847	2.825130	0.004047		H	-4.931762	-5.777768	2.069697
C	-1.093152	2.825013	-0.004116		C	-3.749691	-4.222095	1.157116
C	-2.828411	1.090221	0.002851		H	-3.173212	-4.015093	2.065122
C	-2.828294	-1.090528	-0.002832		C	3.483957	-3.479734	-0.000589
C	-1.092847	-2.825131	0.004074		C	3.750223	-4.221694	-1.157070
C	1.093152	-2.825014	-0.004136		C	4.733879	-5.207797	-1.156849
C	2.828411	-1.090222	0.002790		H	4.932530	-5.777233	-2.069572
C	2.828294	1.090527	-0.002896		C	5.465643	-5.465538	0.000717
C	0.680474	4.197170	-0.002432		H	6.238373	-6.239720	0.001192
H	1.353805	5.053164	-0.010207		C	5.208658	-4.732479	1.157628
C	-0.680926	4.197098	0.002399		H	5.777283	-4.931499	2.070773
H	-1.354344	5.053022	0.010215		C	4.224507	-3.746882	1.156576
C	-4.208720	0.677509	-0.003232		H	4.018354	-3.169073	2.063930
H	-5.062896	1.353079	-0.011783		C	3.483571	3.480119	0.000532
C	-4.208648	-0.677963	0.003330		C	4.224102	3.747393	-1.156616
H	-5.062755	-1.353619	0.011932		C	5.208127	4.733116	-1.157627
C	-0.680474	-4.197171	-0.002413		H	5.776738	4.932234	-2.070759
H	-1.353806	-5.053165	-0.010172		C	5.465002	5.466178	-0.000693
C	0.680925	-4.197099	0.002389		H	6.237633	6.240459	-0.001139
H	1.354344	-5.053023	0.010191		C	4.733248	5.208320	1.156853
C	4.208720	-0.677510	-0.003326		H	4.931807	5.777764	2.069590
H	5.062897	-1.353079	-0.011895		C	3.749717	4.222092	1.157033
C	4.208648	0.677962	0.003236		H	3.173260	4.015086	2.065052
H	5.062755	1.353619	0.011818		H	4.018030	3.169587	-2.063990
C	-2.432307	2.425844	-0.001005		H	3.173763	-4.014775	-2.065108
C	-2.432043	-2.426109	0.001017		H	-4.018079	-3.169581	-2.063898
C	2.432307	-2.425845	-0.001056		H	-3.173811	4.014764	-2.065046
C	2.432043	2.426109	0.000961			77		
C	-3.483956	3.479733	-0.000518			[Fe] ⁻¹		
C	-3.750249	4.221688	-1.156996		Fe	0.000725	0.000002	-0.000065
C	-4.733903	5.207792	-1.156756		N	-1.984919	-0.000074	-0.000062
H	-4.932575	5.777224	-2.069477		N	0.000578	2.008924	0.001583
C	-5.465640	5.465540	0.000825		N	1.986847	0.000070	-0.000066
H	-6.238368	6.239724	0.001316		N	0.000730	-2.008926	-0.001729
C	-5.208628	4.732486	1.157734		C	-2.825153	-1.099518	-0.015344
H	-5.777231	4.931512	2.070891		C	-2.825246	1.099294	0.015268
C	-4.224479	3.746887	1.156664		C	-1.091112	2.846578	-0.014463
H	-4.018305	3.169082	2.064015		C	1.092358	2.846520	0.000350
C	-3.483572	-3.480120	0.000610		C	2.827109	1.099607	-0.000717
C	-4.224130	-3.747389	-1.156520		C	2.827205	-1.099386	0.000628
C	-5.208157	-4.733109	-1.157511		C	1.092584	-2.846429	-0.000415
H	-5.776791	-4.932224	-2.070630		C	-1.090886	-2.846670	0.014402
C	-5.465007	-5.466174	-0.000573		C	-4.205089	-0.677167	-0.004196
H	-6.237639	-6.240453	-0.001002		H	-5.063564	-1.348299	0.000359
C	-4.733225	-5.208321	1.156956					

C	-4.205148	0.676827	0.004154		H	4.829061	-5.885085	-2.037289
H	-5.063691	1.347872	-0.000362		C	3.698605	-4.285853	-1.134136
C	-0.685940	4.210863	-0.019235		H	3.067085	-4.125085	-2.014276
H	-1.356850	5.069467	-0.015822		C	-3.491790	-3.478441	0.001890
C	0.687423	4.210694	-0.021792		C	-3.710841	-4.273608	1.135088
H	1.358606	5.068886	-0.041870		C	-4.697461	-5.256308	1.143321
C	4.207000	0.677162	0.006819		H	-4.853578	-5.861936	2.042008
H	5.065515	1.348093	0.020544		C	-5.489748	-5.464828	0.014942
C	4.207060	-0.676822	-0.006881		H	-6.266820	-6.235817	0.020771
H	5.065645	-1.347665	-0.020575		C	-5.282904	-4.683707	-1.120322
C	0.687755	-4.210635	0.021824		H	-5.895842	-4.841591	-2.013736
H	1.359019	-5.068762	0.041955		C	-4.291435	-3.704649	-1.126126
C	-0.685607	-4.210921	0.019268		H	-4.122356	-3.092203	-2.018250
H	-1.356435	-5.069590	0.015909		H	-3.088323	-4.105403	2.020251
C	-2.439713	2.428058	0.001508		H	4.143656	-3.076016	2.003873
C	2.441127	2.428286	0.002821		H	3.066808	4.125147	2.014351
C	2.441321	-2.428100	-0.002902		H	-4.122591	3.091786	2.018248
C	-2.439520	-2.428248	-0.001579			77		
C	-3.492065	3.478168	-0.001871			[Fe] ⁻²		
C	-4.291713	3.704259	1.126150		Fe	0.000013	-0.000020	0.001343
C	-5.283253	4.683255	1.120408		N	0.003707	2.010731	0.001527
H	-5.896191	4.841046	2.013838		N	2.010850	-0.003707	0.001675
C	-5.490154	5.464425	-0.014804		N	-0.003676	-2.010771	0.001546
H	-6.267283	6.235356	-0.020586		N	-2.010816	0.003678	0.001689
C	-4.697849	5.256029	-1.143203		C	-1.095154	2.852695	-0.013333
H	-4.854011	5.861707	-2.041848		C	1.105483	2.848758	0.016557
C	-3.711167	4.273401	-1.135031		C	2.852648	1.095160	-0.013658
H	-3.088625	4.105291	-2.020193		C	2.848686	-1.105485	0.017553
C	3.492359	3.479596	0.006509		C	1.095188	-2.852731	-0.013307
C	3.698290	4.286032	1.134204		C	-1.105454	-2.848799	0.016588
C	4.682847	5.270792	1.143081		C	-2.852612	-1.095190	-0.013637
H	4.828647	5.885270	2.037478		C	-2.848655	1.105454	0.017583
C	5.485828	5.470495	0.020674		C	-0.678189	4.216648	0.001015
H	6.261170	6.243224	0.026961		H	-1.341208	5.081697	0.020005
C	5.291732	4.678549	-1.109329		C	0.693475	4.214187	0.000690
H	5.912934	4.829656	-1.998194		H	1.359486	5.076900	-0.019349
C	4.302520	3.697215	-1.115692		C	4.216596	0.678140	0.001623
H	4.143388	3.076477	-2.003900		H	5.081649	1.341211	0.020638
C	3.492637	-3.479325	-0.006496		C	4.214124	-0.693475	0.001704
C	4.302819	-3.696799	1.115702		H	5.076842	-1.359561	-0.017775
C	5.292105	-4.678070	1.109407		C	0.678231	-4.216685	0.001051
H	5.913320	-4.829060	1.998283		H	1.341254	-5.081731	0.020042
C	5.486244	-5.470089	-0.020528		C	-0.693435	-4.214228	0.000697
H	6.261647	-6.242758	-0.026763		H	-1.359438	-5.076945	-0.019363
C	4.683227	-5.270539	-1.142945					

C	-4.216560	-0.678177	0.001631		H	-4.666052	6.083455	-1.918677
H	-5.081609	-1.341257	0.020630		C	-3.613456	4.406377	-1.065451
C	-4.214092	0.693438	0.001726		H	-2.919900	4.314159	-1.907774
H	-5.076813	1.359521	-0.017756		H	-4.307448	2.938351	1.908424
C	2.450044	2.441121	0.001133		H	-2.938760	-4.307585	1.907275
C	2.441204	-2.449956	0.002126		H	4.307497	-2.938358	1.908406
C	-2.450017	-2.441151	0.001158		H	2.938670	4.307526	1.907286
C	-2.441172	2.449925	0.002134					
C	3.498772	3.485550	-0.000248	80				
C	3.631376	4.395249	1.063777		[FeCO ₂] ⁻¹			
C	4.614827	5.381157	1.062704		C	-4.232273	0.684969	-0.378224
H	4.691945	6.069845	1.912079		C	-2.864229	1.087904	-0.292247
C	5.508717	5.486711	-0.003621		N	-2.035669	0.000201	-0.276108
H	6.285143	6.259809	-0.004910		C	-2.864451	-1.087327	-0.292273
C	5.397454	4.591558	-1.068300		C	-4.232413	-0.684110	-0.378258
H	6.085006	4.664313	-1.918980		C	-2.451560	2.425077	-0.124023
C	4.407265	3.612480	-1.066063		C	-3.501099	3.477728	-0.096054
H	4.315036	2.918798	-1.908284		C	-4.213255	3.812303	-1.255195
C	3.485988	-3.498333	0.000639		C	-5.197729	4.797200	-1.232137
C	4.395611	-3.630827	1.064738		C	-5.488741	5.469720	-0.046117
C	5.381885	-4.613933	1.063569		C	-4.788849	5.146377	1.114919
H	6.070504	-4.691007	1.913004		C	-3.807372	4.157869	1.089534
C	5.487930	-5.507480	-0.002985		Fe	-0.018653	-0.000001	0.060158
H	6.261330	-6.283604	-0.004378		N	-0.025827	1.970224	-0.030018
C	4.592904	-5.396245	-1.067783		C	1.068689	2.813348	-0.029289
H	4.666074	-6.083502	-1.918665		C	0.646769	4.187301	0.105834
C	3.613483	-4.406416	-1.065449		C	-0.706759	4.183005	0.117263
H	2.919921	-4.314206	-1.907768		C	-1.126847	2.804695	0.012424
C	-3.498784	-3.485541	-0.000253		C	2.385699	2.430295	-0.210465
C	-3.631472	-4.395239	1.063763		C	3.446180	3.471940	-0.213220
C	-4.615001	-5.381070	1.062666		C	4.368784	3.548918	0.838793
H	-4.692176	-6.069768	1.912028		C	5.365618	4.521330	0.844867
C	-5.508898	-5.486532	-0.003662		C	5.459497	5.436855	-0.202785
H	-6.285387	-6.259566	-0.004967		C	4.550002	5.370119	-1.256426
C	-5.397574	-4.591355	-1.068314		C	3.555090	4.394571	-1.261158
H	-6.085142	-4.664026	-1.918988		C	-2.452058	-2.424592	-0.124091
C	-4.407308	-3.612355	-1.066055		C	-3.501810	-3.477030	-0.096148
H	-4.315040	-2.918645	-1.908249		C	-4.214080	-3.811391	-1.255282
C	-3.485952	3.498304	0.000645		C	-5.198757	-4.796085	-1.232243
C	-4.395568	3.630811	1.064751		C	-5.489864	-5.468615	-0.046253
C	-5.381840	4.613919	1.063579		C	-4.789862	-5.145484	1.114776
H	-6.070452	4.691003	1.913018		C	-3.808182	-4.157177	1.089412
C	-5.487893	5.507454	-0.002984		N	-0.026235	-1.970222	-0.030067
H	-6.261294	6.283579	-0.004380		C	1.068118	-2.813561	-0.029355
C	-4.592876	5.396206	-1.067788		C	0.645928	-4.187433	0.105727

C	-0.707599	-4.182876	0.117126
C	-1.127419	-2.804478	0.012343
C	2.385201	-2.430761	-0.210509
C	2.777420	-1.090506	-0.392565
C	4.122958	-0.685765	-0.629017
C	4.123094	0.684948	-0.629043
C	2.777645	1.089962	-0.392542
N	1.950336	-0.000186	-0.308740
C	3.445490	-3.472601	-0.213189
C	3.554322	-4.395262	-1.261107
C	4.549062	-5.370986	-1.256278
C	5.458456	-5.437869	-0.202560
C	5.364651	-4.522315	0.845075
C	4.367990	-3.549727	0.838904
C	0.487635	-0.000170	2.000700
O	-0.709230	0.000143	2.181137
O	1.579088	-0.000439	2.477878
H	4.967087	1.358534	-0.774851
H	4.966817	-1.359523	-0.774806
H	1.317714	5.044050	0.159525
H	-1.380325	5.037936	0.169067
H	-5.089967	1.356783	-0.397828
H	-5.090245	-1.355746	-0.397892
H	1.316705	-5.044316	0.159397
H	-1.381334	-5.037677	0.168882
H	-3.980472	-3.282011	-2.185164
H	-3.259779	-3.894289	2.000199
H	-5.014220	-5.663936	2.052512
H	-5.740712	-5.044328	-2.150550
H	-6.262666	-6.243577	-0.027016
H	4.285950	2.827306	1.658509
H	2.840914	4.334869	-2.089389
H	4.618305	6.081221	-2.086044
H	6.073635	4.567983	1.678528
H	6.242356	6.201955	-0.197823
H	-3.979722	3.282926	-2.185099
H	-3.259055	3.894816	2.000325
H	-5.013135	5.664822	2.052676
H	-5.739598	5.045609	-2.150449
H	-6.261383	6.244841	-0.026865
H	4.285208	-2.828087	1.658601
H	2.840225	-4.335444	-2.089398
H	4.617310	-6.082111	-2.085881
H	6.072589	-4.569085	1.678795
H	6.241179	-6.203107	-0.197523

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	[FeCO ₂] ⁻²		
C	-4.231190	0.682953	-0.419981
C	-2.861067	1.095534	-0.335956
N	-2.031859	0.000014	-0.324565
C	-2.861059	-1.095505	-0.335793
C	-4.231188	-0.682957	-0.419897
C	-2.464539	2.426084	-0.136616
C	-3.510775	3.471659	-0.100264
C	-4.338979	3.720038	-1.208540
C	-5.332063	4.695967	-1.171446
C	-5.522304	5.466069	-0.024324
C	-4.705141	5.240072	1.084698
C	-3.719333	4.257970	1.046222
Fe	-0.011909	0.000019	0.057376
N	-0.020588	1.986997	-0.024359
C	1.077244	2.832724	-0.012066
C	0.661593	4.187206	0.134214
C	-0.711045	4.182884	0.139682
C	-1.125276	2.822905	0.027252
C	2.410603	2.431763	-0.191294
C	3.467263	3.469491	-0.211061
C	4.492384	3.475097	0.750047
C	5.497760	4.438938	0.732664
C	5.504677	5.434017	-0.244947
C	4.492702	5.447723	-1.205579
C	3.492400	4.478778	-1.187873
C	-2.464544	-2.426032	-0.136294
C	-3.510758	-3.471633	-0.099777
C	-4.338828	-3.720322	-1.208084
C	-5.331895	-4.696261	-1.170852
C	-5.522242	-5.466071	-0.023551
C	-4.705193	-5.239788	1.085494
C	-3.719400	-4.257672	1.046877
N	-0.020587	-1.986957	-0.024433
C	1.077226	-2.832682	-0.012176
C	0.661599	-4.187149	0.134330
C	-0.711035	-4.182829	0.140054
C	-1.125285	-2.822873	0.027487
C	2.410578	-2.431780	-0.191627
C	2.791298	-1.097598	-0.368844
C	4.133671	-0.683649	-0.639459
C	4.133694	0.683688	-0.639289
C	2.791304	1.097593	-0.368645

N	1.961914	0.000004	-0.283203		C	-4.246523	0.492697	-0.511064
C	3.467200	-3.469524	-0.211576		C	-1.701665	2.994557	-0.063940
C	3.492072	-4.478910	-1.188279		C	-2.428598	4.273222	0.023261
C	4.492364	-5.447872	-1.206147		C	-3.202338	4.765633	-1.048854
C	5.504582	-5.434090	-0.245777		C	-3.889141	5.973411	-0.965525
C	5.497913	-4.438922	0.731752		C	-3.825663	6.750921	0.193795
C	4.492561	-3.475072	0.749298		C	-3.060346	6.285129	1.267942
C	0.388817	-0.000041	2.022433		C	-2.381022	5.073793	1.183632
O	-0.805969	0.000270	2.229831		Fe	-0.004482	0.008312	0.089913
O	1.476389	-0.000310	2.522087		N	0.550192	1.930654	-0.010212
H	4.975401	1.353910	-0.815385		C	1.829402	2.458269	-0.013287
H	4.975375	-1.353829	-0.815751		C	1.779758	3.863926	0.219425
H	1.326840	5.047642	0.206440		C	0.451074	4.214168	0.278050
H	-1.377678	5.044319	0.180180		C	-0.305040	3.020489	0.119587
H	-5.094791	1.348012	-0.421913		C	3.022512	1.726438	-0.237121
H	-5.094811	-1.347987	-0.421755		C	4.298111	2.438152	-0.332524
H	1.326879	-5.047560	0.206570		C	5.458024	2.011061	0.365814
H	-1.377697	-5.044234	0.180760		C	6.670777	2.682060	0.276277
H	-4.182928	-3.125680	-2.114340		C	6.807710	3.827405	-0.518629
H	-3.088323	-4.071367	1.922072		C	5.680527	4.271720	-1.220637
H	-4.846458	-5.829002	1.998799		C	4.467880	3.599894	-1.130534
H	-5.958508	-4.865353	-2.054206		C	-3.052205	-1.693465	-0.213149
H	-6.300606	-6.236510	0.006805		C	-4.329863	-2.407714	-0.248207
H	4.477807	2.699084	1.522409		C	-5.248828	-2.262533	-1.318368
H	2.704220	4.484018	-1.947973		C	-6.461652	-2.939795	-1.354973
H	4.488193	6.217653	-1.985657		C	-6.833368	-3.810218	-0.323374
H	6.280952	4.418673	1.499027		C	-5.946388	-3.971102	0.747888
H	6.293249	6.194606	-0.258107		C	-4.735926	-3.290319	0.784484
H	-4.183167	3.125171	-2.114662		N	-0.575635	-1.911962	0.008418
H	-3.088166	4.071896	1.921400		C	0.269817	-3.016317	0.069074
H	-4.846329	5.829508	1.997872		C	-0.490826	-4.204660	0.232518
H	-5.958769	4.864831	-2.054777		C	-1.816462	-3.845264	0.182579
H	-6.300683	6.236497	0.005913		C	-1.863352	-2.426151	0.031257
H	4.478166	-2.698989	1.521595		C	1.663779	-2.985281	-0.097240
H	2.703684	-4.484254	-1.948167		C	2.400592	-1.802146	-0.309192
H	4.487628	-6.217878	-1.986147		C	3.765652	-1.781836	-0.699434
H	6.281286	-4.418596	1.497930		C	4.146559	-0.460178	-0.754551
H	6.293138	-6.194691	-0.259069		C	3.010051	0.315408	-0.382118
					N	1.921340	-0.509496	-0.189449
					C	2.410582	-4.256229	-0.093117
					C	2.106799	-5.316003	-0.972569
[FeCO ₂] ⁻³					C	2.829608	-6.506242	-0.965269
C	-3.866290	1.810822	-0.453332		C	3.893631	-6.688038	-0.077599
C	-2.447480	1.828161	-0.336921		C	4.215486	-5.648696	0.801040
N	-1.954134	0.536252	-0.345913		C	3.489577	-4.461564	0.792921
C	-3.052975	-0.287179	-0.414293					

C	0.223674	-0.224954	2.068690	C	2.936491	0.692328	-0.316880
O	-0.783689	0.421228	2.287233	C	1.469034	2.645719	-0.111383
O	1.108286	-0.838691	2.603924	C	-0.688374	2.945718	-0.065148
H	5.117569	-0.060542	-1.048086	C	-4.046919	1.257985	-0.387674
H	4.370259	-2.659827	-0.933077	H	-4.797660	2.046677	-0.407993
H	2.642720	4.520857	0.327234	C	-4.235614	-0.087295	-0.428664
H	0.039387	5.219363	0.378352	H	-5.174881	-0.636063	-0.479046
H	-4.519819	2.683718	-0.429715	C	-1.264714	-4.063966	-0.030410
H	-5.264438	0.103378	-0.528917	H	-2.054519	-4.813764	-0.026118
H	-0.081071	-5.208112	0.354422	C	0.076520	-4.253412	0.028240
H	-2.676887	-4.513546	0.195047	H	0.624852	-5.191578	0.099571
H	-4.968590	-1.606290	-2.148835	C	4.038822	-1.261329	-0.378112
H	-4.073139	-3.408107	1.647486	H	4.789776	-2.048601	-0.429228
H	-6.215323	-4.628704	1.585241	C	4.228169	0.088131	-0.420531
H	-7.126325	-2.800525	-2.218112	H	5.167258	0.633549	-0.503380
H	-7.789011	-4.347298	-0.352727	C	1.252816	4.067125	-0.030493
H	5.370748	1.133196	1.013607	H	2.040763	4.818871	-0.020734
H	3.609836	3.954507	-1.710221	C	-0.089604	4.252854	0.013191
H	5.754563	5.154536	-1.869993	H	-0.641481	5.189703	0.074188
H	7.527795	2.314589	0.856549	C	-2.737317	-2.064094	-0.253480
H	7.764747	4.358453	-0.587893	C	2.055503	-2.744717	-0.109970
H	-3.243128	4.170902	-1.967231	C	2.732209	2.071181	-0.229924
H	-1.797928	4.705252	2.033832	C	-2.063319	2.736484	-0.139196
H	-3.005831	6.870213	2.194735	C	-3.929484	-2.954698	-0.267758
H	-4.472445	6.322805	-1.827146	C	-4.614854	-3.208329	-1.460973
H	-4.363241	7.704552	0.259863	C	-5.730799	-4.041896	-1.472872
H	3.734278	-3.654408	1.490798	H	-6.255655	-4.234038	-2.413261
H	1.287468	-5.174928	-1.684807	C	-6.175288	-4.631830	-0.291268
H	2.568306	-7.300334	-1.676480	H	-7.051793	-5.286155	-0.300292
H	5.039320	-5.772019	1.515387	C	-5.499488	-4.384157	0.902095
H	4.463835	-7.624969	-0.070661	H	-5.846118	-4.840790	1.833743

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[FeCOOH]

Fe	-0.016456	0.001573	-0.039677	C	3.092969	-4.784288	-1.147213
N	-1.956655	0.276388	-0.320157	C	3.947566	-5.882533	-1.086739
N	-0.282440	-1.968952	-0.112661	H	4.044004	-6.544127	-1.952547
N	1.954736	-0.275908	-0.228830	C	4.680053	-6.136040	0.071343
N	0.273301	1.969385	-0.114483	H	5.350740	-6.998777	0.118830
C	-2.631622	1.471201	-0.289535	C	4.554493	-5.286465	1.168801
C	-2.933762	-0.686819	-0.360321	H	5.123818	-5.481896	2.082153
C	-1.476790	-2.642360	-0.119915	C	3.700889	-4.187858	1.107473
C	0.679230	-2.947943	-0.048511	H	3.597480	-3.518212	1.968065
C	2.632337	-1.479589	-0.243255	C	3.922490	2.964440	-0.265963
				C	4.587747	3.213126	-1.471564

C	5.703045	4.046860	-1.505877		H	5.160191	0.682425	-0.571003
H	6.212078	4.234754	-2.455744		C	1.229060	4.077273	0.005241
C	6.166603	4.643090	-0.334777		H	2.009201	4.837839	0.024660
H	7.042212	5.298054	-0.361613		C	-0.127914	4.254527	0.066298
C	5.510085	4.402100	0.870505		H	-0.681262	5.188461	0.160313
H	5.870122	4.865585	1.793621		C	-4.056551	1.217908	-0.414540
C	4.395274	3.567619	0.904751		H	-4.814916	1.996898	-0.489919
H	3.875879	3.374801	1.849713		C	-4.230709	-0.125380	-0.463345
C	-2.970504	3.913758	-0.056062		H	-5.163037	-0.678786	-0.573304
C	-3.130867	4.776131	-1.146024		C	-1.225247	-4.078874	0.013203
C	-3.984336	5.873736	-1.059923		H	-2.004114	-4.840538	0.041164
H	-4.103102	6.538722	-1.920394		C	0.132909	-4.254779	0.051305
C	-4.687206	6.121929	0.117478		H	0.688898	-5.188423	0.131134
H	-5.357333	6.983802	0.185261		C	2.718714	2.084638	-0.259484
C	-4.533400	5.268135	1.208189		C	-2.096861	2.719856	-0.101599
H	-5.080697	5.459174	2.135862		C	-2.722121	-2.090260	-0.225662
C	-3.680539	4.170439	1.122218		C	2.096347	-2.712805	-0.136774
H	-3.554417	3.494704	1.974959		C	3.901756	2.985523	-0.272549
H	-2.576811	4.575735	-2.069458		C	4.594662	3.252631	-1.459387
H	4.218434	2.743444	-2.389597		C	5.703736	4.096426	-1.466469
H	2.516180	-4.580164	-2.055700		H	6.232397	4.292082	-2.405031
H	-4.261021	-2.742686	-2.387132		C	6.135917	4.693995	-0.284084
C	-0.065857	0.013788	1.921066		H	7.006112	5.358103	-0.288014
O	-1.093150	0.124766	2.512422		C	5.452200	4.439276	0.904152
O	1.121407	-0.106009	2.517020		H	5.786926	4.900748	1.838743
H	1.800366	-0.180366	1.825104		C	4.346417	3.592536	0.908853
					H	3.806628	3.384182	1.838664
					C	-3.014827	3.887911	-0.040949
					C	-3.087599	4.810340	-1.092954
					C	-3.957398	5.896566	-1.033495
					H	-4.002639	6.602737	-1.868856
					C	-4.772683	6.082202	0.082210
					H	-5.456914	6.935307	0.129209
					C	-4.708898	5.173991	1.137240
					H	-5.341167	5.313008	2.019998
					C	-3.836687	4.089614	1.075266
					H	-3.779777	3.374943	1.903169
					C	-3.902015	-2.995234	-0.262545
					C	-4.578313	-3.249180	-1.461842
					C	-5.686300	-4.093623	-1.494043
					H	-6.201797	-4.278582	-2.441985
					C	-6.133919	-4.705971	-0.324976
					H	-7.003116	-5.370866	-0.348862
					C	-5.466067	-4.466178	0.875074
					H	-5.811383	-4.941057	1.798993

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[FeCOOH]⁻¹

Fe	0.017712	-0.001295	-0.056152					
N	1.941534	-0.255653	-0.314286					
N	0.260701	1.987529	-0.122151					
N	-1.949548	0.255175	-0.218066					
N	-0.257701	-1.987580	-0.119535					
C	2.635739	-1.449645	-0.297759					
C	2.915821	0.721647	-0.380406					
C	1.448392	2.672153	-0.110090					
C	-0.710168	2.956045	-0.035918					
C	-2.646155	1.457579	-0.242662					
C	-2.928446	-0.726456	-0.327668					
C	-1.447842	-2.673940	-0.092372					
C	0.711983	-2.955110	-0.054218					
C	4.053962	-1.214590	-0.440644					
H	4.813128	-1.994749	-0.489458					
C	4.227206	0.125604	-0.488504					

C	-4.361443	-3.618130	0.904627	H	4.558195	-2.546390	-0.520636
H	-3.832779	-3.425410	1.844313	C	4.225402	-0.363207	-0.436972
C	3.017796	-3.876784	-0.052363	H	5.222851	0.066760	-0.527583
C	3.111802	-4.806378	-1.095767	C	1.683906	3.923794	0.039213
C	3.980584	-5.891972	-1.010752	H	2.536597	4.602698	0.055382
H	4.042892	-6.604812	-1.839395	C	0.344961	4.254866	0.044912
C	4.773079	-6.068001	0.122633	H	-0.097916	5.249667	0.101468
H	5.456852	-6.920177	0.190148	C	-2.967549	-1.777164	-0.176468
C	4.687869	-5.151408	1.169155	C	1.771895	-2.958725	-0.108994
H	5.303274	-5.282993	2.064921	C	2.965312	1.777494	-0.163599
C	3.816431	-4.067985	1.082444	C	-1.778597	2.946567	-0.146422
H	3.740942	-3.344599	1.901297	C	-4.238877	-2.532169	-0.191970
H	2.488507	-4.662641	-1.984824	C	-5.086190	-2.524978	-1.313995
H	-4.219681	-2.767940	-2.378128	C	-6.285668	-3.232811	-1.327645
H	-2.446836	4.659635	-1.968199	H	-6.919947	-3.206410	-2.221337
H	4.248545	2.782169	-2.386074	C	-6.673994	-3.984981	-0.219061
C	0.128574	-0.010614	1.883209	H	-7.615106	-4.545881	-0.228520
O	1.141534	-0.072684	2.517050	C	-5.843583	-4.011779	0.902780
O	-1.072579	0.059259	2.494650	H	-6.136734	-4.589803	1.786749
H	-1.738886	0.108150	1.788400	C	-4.649879	-3.295895	0.915306
				H	-4.007343	-3.306857	1.801760
				C	2.540916	-4.226347	-0.127160
				C	2.392229	-5.151932	-1.172359

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[FeCOOH]⁻²

Fe	-0.026484	0.003847	0.005243	C	3.122611	-6.337560	-1.200201
N	-1.923274	0.472077	-0.268574	H	2.990497	-7.036996	-2.033485
N	-0.500431	-1.960601	-0.061142	C	4.027951	-6.631360	-0.179854
N	1.928819	-0.479737	-0.178481	H	4.604744	-7.562650	-0.200949
N	0.490166	1.960161	-0.079210	C	4.188376	-5.724822	0.867443
C	-2.472462	1.750183	-0.268102	H	4.890140	-5.944535	1.679948
C	-3.005615	-0.389215	-0.320186	C	3.451721	-4.542065	0.893104
C	-1.762246	-2.508220	-0.026701	H	3.571298	-3.831727	1.717871
C	0.365567	-3.036392	-0.014117	C	4.233110	2.538524	-0.191324
C	2.477763	-1.765099	-0.232900	C	5.076030	2.527435	-1.316644
C	3.014507	0.386098	-0.289188	C	6.272273	3.240466	-1.339863
C	1.753961	2.506461	-0.034950	H	6.902796	3.211150	-2.236078
C	-0.372539	3.035590	-0.052137	C	6.661624	4.002202	-0.238201
C	-3.897422	1.679278	-0.403902	H	7.600109	4.567207	-0.255433
H	-4.566268	2.537701	-0.468925	C	5.834859	4.034512	0.886103
C	-4.228625	0.357612	-0.423507	H	6.127587	4.621999	1.763911
H	-5.227462	-0.075891	-0.471598	C	4.644480	3.313305	0.908110
C	-1.693123	-3.925045	0.066628	H	4.003412	3.331934	1.795643
H	-2.545798	-4.603844	0.081785	C	-2.552111	4.212349	-0.139482
C	-0.355357	-4.254616	0.093285	C	-2.443337	5.133858	-1.192202
H	0.086685	-5.248583	0.168863	C	-3.172588	6.320792	-1.194223
C	3.891978	-1.689604	-0.417379	H	-3.072842	7.018587	-2.033417

C	-4.035436	6.617632	-0.138777	H	-1.354976	-5.065745	-0.175547
H	-4.611699	7.549584	-0.138952	H	-5.064188	-1.348612	0.059133
C	-4.154718	5.714330	0.916872	H	-5.063413	1.351516	0.059066
H	-4.823542	5.937413	1.755826	H	1.348116	5.069424	-0.133009
C	-3.418835	4.530479	0.917120	H	-1.352105	5.066505	-0.175699
H	-3.503039	3.820482	1.746560	C	-3.482885	-3.477602	-0.068247
H	-1.768662	4.895339	-2.021085	C	-5.467515	-5.450953	-0.043481
H	4.765269	1.945087	-2.190512	C	-4.370566	-3.605463	-1.145937
H	1.685627	-4.916619	-1.974966	C	-3.601847	-4.350941	1.022053
H	-4.776870	-1.948141	-2.192068	C	-4.594781	-5.325447	1.036050
C	-0.083522	0.047603	1.946405	C	-5.350753	-4.592624	-1.135501
O	-1.038979	0.313223	2.618849	H	-4.274899	-2.933482	-2.005039
O	1.103318	-0.256418	2.514688	H	-2.919334	-4.248234	1.871990
H	1.719401	-0.413671	1.774248	H	-4.689057	-5.990941	1.898245
				H	-6.027769	-4.693704	-1.987910
				H	-6.242773	-6.221680	-0.033630
				C	-3.480867	3.479610	-0.068329
[FeCO] ⁺				C	-5.464260	5.454197	-0.043363
C	0.678915	4.211562	-0.130191	C	-3.599090	4.353105	1.021921
C	1.086115	2.837853	-0.121230	C	-4.368652	3.607943	-1.145879
N	-0.000130	2.002660	-0.100307	C	-5.348228	4.595712	-1.135339
C	-1.087017	2.836881	-0.097986	C	-4.591411	5.328232	1.036020
C	-0.681392	4.210526	-0.138408	H	-2.916475	4.250047	1.871734
C	2.431881	2.432834	-0.125956	H	-4.273558	2.935832	-2.004943
C	2.832919	1.085682	-0.126865	H	-6.025336	4.697146	-1.987633
C	4.201071	0.678986	-0.253207	H	-4.685112	5.993856	1.898177
C	4.200680	-0.681400	-0.253191	H	-6.239037	6.225407	-0.033433
C	2.832298	-1.087304	-0.126799	C	3.485007	3.473182	-0.145332
N	1.999904	-0.0000574	-0.071572	C	5.487232	5.428603	-0.175618
C	2.430486	-2.434227	-0.125807	C	4.376209	3.593688	0.930250
C	1.084495	-2.838474	-0.121054	C	3.611441	4.342628	-1.237949
N	-0.001280	-2.002664	-0.100176	C	4.612699	5.308499	-1.254367
C	-1.088636	-2.836268	-0.097801	C	5.364858	4.572391	0.917376
C	-0.683785	-4.210143	-0.138238	H	4.277495	2.921695	1.788997
C	0.676521	-4.211951	-0.130022	H	2.929461	4.242600	-2.088626
C	-2.434770	-2.432088	-0.083877	H	4.712654	5.971017	-2.118225
C	-2.837915	-1.085585	-0.092209	H	6.044542	4.667912	1.768289
N	-2.003596	0.0000570	-0.129762	H	6.269069	6.192626	-0.187496
C	-2.837294	1.087201	-0.092284	C	3.482989	-3.475203	-0.145275
C	-4.209279	0.681416	-0.014105	C	5.483979	-5.431882	-0.175782
C	-4.209670	-0.679005	-0.014075	C	3.608695	-4.344789	-1.237859
C	-2.433375	2.433474	-0.084041	C	4.374285	-3.596212	0.930175
Fe	-0.001280	0.000003	0.055570	C	5.362322	-4.575534	0.917187
H	5.050205	-1.352177	-0.364866	C	4.609342	-5.311290	-1.254391
H	5.050980	1.349273	-0.364906	H	2.926624	-4.244389	-2.088420

H	4.276133	-2.924111	1.788902	C	-3.721823	-4.234588	1.075824
H	6.042087	-4.671435	1.767993	C	-4.706010	-5.220042	1.086981
H	4.708732	-5.973923	-2.118226	C	-5.233429	-4.718682	-1.210633
H	6.265334	-6.196396	-0.187747	H	-4.063646	-3.145590	-2.126428
C	-0.032050	0.000068	1.819976	H	-3.124448	-4.038445	1.972623
O	-0.050005	0.000103	2.959690	H	-4.883994	-5.799569	1.997567
				H	-5.822503	-4.907733	-2.112854
79				H	-6.237162	-6.238399	-0.047771
[FeCO]				C	-3.480517	3.481402	-0.078132
C	0.676587	4.202951	-0.138129	C	-5.460953	5.467736	-0.056267
C	1.088895	2.825467	-0.121656	C	-3.718919	4.237014	1.075553
N	-0.001575	1.990968	-0.106100	C	-4.247639	3.735348	-1.220910
C	-1.092126	2.825191	-0.104963	C	-5.230991	4.721553	-1.210500
C	-0.680571	4.202566	-0.138697	C	-4.702465	5.223106	1.086823
C	2.425351	2.426901	-0.123313	H	-3.121330	4.040714	1.972173
C	2.821723	1.089655	-0.129385	H	-4.062508	3.147520	-2.126349
C	4.196981	0.677378	-0.210128	H	-5.820238	4.910796	-2.112567
C	4.196594	-0.679766	-0.210230	H	-4.879759	5.802973	1.997326
C	2.821097	-1.091271	-0.129367	H	-6.233345	6.242184	-0.047654
N	1.987747	-0.000577	-0.098043	C	3.481704	3.475512	-0.137253
C	2.423963	-2.428315	-0.123160	C	5.482308	5.441444	-0.162595
C	1.087293	-2.826113	-0.121275	C	4.253750	3.721107	1.003924
N	-0.002705	-1.990977	-0.105777	C	3.726612	4.227867	-1.291808
C	-1.093731	-2.824556	-0.104527	C	4.719904	5.204070	-1.304685
C	-0.682970	-4.202185	-0.138110	C	5.246863	4.697519	0.991908
C	0.674187	-4.203347	-0.137506	H	4.065252	3.134103	1.909146
C	-2.430438	-2.426468	-0.090244	H	3.126957	4.036220	-2.188102
C	-2.828043	-1.089696	-0.098012	H	4.902254	5.781504	-2.215755
N	-1.993389	0.000562	-0.114805	H	5.839835	4.880368	1.892831
C	-2.827401	1.091298	-0.098068	H	6.262469	6.208050	-0.172534
C	-4.204927	0.679764	-0.068391	C	3.479710	-3.477534	-0.137288
C	-4.205315	-0.677359	-0.068389	C	5.478980	-5.444825	-0.163121
C	-2.429033	2.427862	-0.090484	C	3.723916	-4.229981	-1.291943
Fe	-0.002236	0.000014	0.078787	C	4.251771	-3.723748	1.003737
H	5.047871	-1.355343	-0.280524	C	5.244226	-4.700829	0.991475
H	5.048627	1.352501	-0.280310	C	4.716543	-5.206852	-1.305066
H	1.348458	-5.058314	-0.152013	H	3.124215	-4.037889	-2.188110
H	-1.358900	-5.055645	-0.164331	H	4.063797	-3.136718	1.909052
H	-5.059596	-1.352087	-0.039450	H	5.837212	-4.884154	1.892292
H	-5.058828	1.354977	-0.039458	H	4.898337	-5.784352	-2.216206
H	1.351345	5.057534	-0.152802	H	6.258616	-6.211962	-0.173237
H	-1.356044	5.056382	-0.165022	C	-0.013726	0.000144	1.824379
C	-3.482522	-3.479407	-0.077948	O	-0.019446	0.000230	2.969496
C	-5.464264	-5.464455	-0.056308				
C	-4.249440	-3.733113	-1.220928				

[FeCO] ⁻¹			
C	0.689377	4.205170	-0.150739
C	1.094440	2.844708	-0.127054
N	0.000607	2.008458	-0.108220
C	-1.092637	2.845561	-0.112484
C	-0.687292	4.205247	-0.154919
C	2.446077	2.424385	-0.116802
C	2.832371	1.095744	-0.109367
C	4.212356	0.672743	-0.189241
C	4.211169	-0.680082	-0.189158
C	2.830534	-1.100610	-0.109362
N	1.998275	-0.001584	-0.083616
C	2.441813	-2.428375	-0.117004
C	1.089665	-2.846562	-0.127418
N	-0.002985	-2.008448	-0.108468
C	-1.097418	-2.843669	-0.113146
C	-0.694214	-4.204089	-0.156094
C	0.682451	-4.206258	-0.151650
C	-2.449424	-2.423812	-0.099780
C	-2.836923	-1.095808	-0.117526
N	-2.002096	0.001601	-0.146784
C	-2.835065	1.100715	-0.117241
C	-4.216951	0.680054	-0.064460
C	-4.218157	-0.672645	-0.064598
C	-2.445140	2.427831	-0.099223
Fe	-0.003494	-0.000008	0.084143
H	5.065018	-1.352631	-0.265387
H	5.067394	1.343748	-0.265600
H	1.350884	-5.066372	-0.163558
H	-1.365693	-5.061076	-0.196162
H	-5.075486	-1.342986	-0.013427
H	-5.073067	1.351961	-0.013239
H	1.359191	5.064208	-0.162329
H	-1.357399	5.063339	-0.194459
C	-3.498798	-3.475333	-0.076130
C	-5.496558	-5.462212	-0.025127
C	-4.350170	-3.671614	-1.171841
C	-3.664709	-4.303284	1.043134
C	-4.651493	-5.285082	1.070200
C	-5.341611	-4.650419	-1.146819
H	-4.221494	-3.036598	-2.054829
H	-3.001517	-4.160226	1.902717
H	-4.766467	-5.914814	1.958411
H	-5.995108	-4.783966	-2.015093
H	-6.273649	-6.232883	-0.004010
			83
[FeCO ₂ (H ₂ O)] ⁻¹			
Fe	-0.116649	-0.000023	-0.087459
N	-0.120769	1.982240	-0.125708
N	-2.115284	0.000244	-0.343310
N	1.836931	-0.000237	-0.471627
N	-0.121316	-1.982259	-0.125852
C	0.975277	2.812588	-0.106534
C	-2.946043	-1.091867	-0.314579

C	-1.209812	2.814721	-0.026778	C	3.363546	3.450926	-0.345658
C	-2.945712	1.092609	-0.314446	C	3.398773	4.456904	-1.319359
C	2.658139	1.090753	-0.596662	C	4.361770	3.426074	0.638464
C	-1.210582	-2.814496	-0.027166	C	4.404475	5.420671	-1.307785
C	2.657886	-1.091429	-0.596533	C	5.364848	4.393048	0.651820
C	0.974540	-2.812853	-0.106606	C	5.388010	5.393053	-0.320036
C	0.569454	4.181926	0.089012	H	-3.260325	3.951373	1.987765
C	-4.320913	-0.680118	-0.343426	H	-5.022878	5.702569	2.070558
C	-0.786989	4.185464	0.119905	H	-6.365866	6.221396	0.036262
C	-4.320698	0.681318	-0.343410	H	-5.932745	4.977648	-2.080351
C	3.989548	0.680571	-0.938368	H	-4.169647	3.227116	-2.156932
C	-0.788072	-4.185359	0.119326	H	4.342812	2.632269	1.394188
C	3.989399	-0.681608	-0.938235	H	6.176570	6.151096	-0.309307
C	0.568374	-4.182124	0.088706	H	4.421244	6.197177	-2.078131
H	1.240944	5.036126	0.165965	H	2.628094	4.475748	-2.097218
H	-5.183099	-1.345808	-0.327953	H	4.342219	-2.632879	1.394344
H	-1.450122	5.044177	0.217452	H	6.133429	-4.366918	1.429335
H	-5.182656	1.347311	-0.327918	H	6.175161	-6.152495	-0.308432
H	4.824088	1.350303	-1.143469	H	4.419811	-6.198505	-2.077272
H	-1.451366	-5.043975	0.216581	H	2.627078	-4.476675	-2.096681
H	4.823791	-1.351565	-1.143220	H	-6.367453	-6.219961	0.035595
H	1.239634	-5.036503	0.165667	H	-5.936015	-4.974123	-2.080120
C	2.292135	2.419985	-0.348812	H	-4.172438	-3.224112	-2.156627
C	-2.545758	-2.424539	-0.144930	O	1.229623	0.000032	2.415350
C	2.291530	-2.420556	-0.348666	O	-1.028991	0.000058	2.414636
C	-2.545072	2.425121	-0.144593	H	-5.022364	-5.703581	2.069166
C	0.099809	0.000045	1.921830	O	4.017327	-0.000366	2.306086
C	3.362722	-3.451713	-0.345275	H	3.041141	-0.000201	2.235572
C	3.397740	-4.457870	-1.318804	H	-3.259535	-3.952718	1.986525
C	4.360979	-3.426875	0.638807	H	6.134397	4.365905	1.428859
C	4.403224	-5.421864	-1.307060	H	4.161186	-0.000169	3.261456
C	5.363845	-4.394063	0.652329				
C	5.386775	-5.394274	-0.319324		83		
C	-3.599242	-3.473834	-0.090796	[FeCO ₂ (H ₂ O)] ⁻²			
C	-3.848756	-4.181345	1.092068	Fe	0.112201	-0.000001	-0.099787
C	-4.362882	-3.770995	-1.226956	N	0.114554	-1.998948	-0.129121
C	-4.836978	-5.162607	1.136580	N	2.089125	-0.000119	-0.362146
C	-5.351283	-4.751767	-1.182701	N	-1.830122	0.000104	-0.478512
C	-5.591226	-5.450091	-0.000084	N	0.114758	1.998935	-0.129123
C	-3.598294	3.474688	-0.090335	C	-0.983668	-2.828731	-0.083155
C	-3.848694	4.181044	1.093013	C	2.928531	1.100180	-0.357236
C	-4.360787	3.773167	-1.226913	C	1.205511	-2.828205	0.005034
C	-4.836735	5.162494	1.137601	C	2.928434	-1.100496	-0.356930
C	-5.348930	4.754199	-1.182606	C	-2.660898	-1.098920	-0.595519
C	-5.589810	5.451356	0.000511	C	1.205818	2.828109	0.004661

C	-2.660853	1.099208	-0.595088	C	-5.401917	-4.382762	0.642966
C	-0.983388	2.828807	-0.082795	C	-5.413476	-5.393998	-0.317062
C	-0.585447	-4.175694	0.149446	H	3.386336	-3.829226	2.020423
C	4.306238	0.677426	-0.456438	H	5.142623	-5.586339	2.101461
C	0.790902	-4.177367	0.192586	H	6.362552	-6.232251	0.025625
C	4.306175	-0.677892	-0.456261	H	5.813716	-5.103850	-2.129189
C	-3.995972	-0.677420	-0.950591	H	4.057027	-3.345858	-2.201836
C	0.791376	4.177286	0.192481	H	-4.385779	-2.616729	1.381007
C	-3.995923	0.677904	-0.950402	H	-6.202497	-6.151791	-0.308929
C	-0.584975	4.175769	0.149477	H	-4.421000	-6.217250	-2.052125
H	-1.255908	-5.029932	0.244478	H	-2.627886	-4.498426	-2.065236
H	5.168510	1.343748	-0.486696	H	-4.385472	2.617001	1.381725
H	1.453591	-5.033992	0.318348	H	-6.181444	4.346428	1.410435
H	5.168385	-1.344302	-0.486341	H	-6.201932	6.152377	-0.307904
H	-4.829249	-1.346406	-1.166306	H	-4.420419	6.217828	-2.051093
H	1.454164	5.033849	0.318139	H	-2.627479	4.498843	-2.064355
H	-4.829159	1.347005	-1.165918	H	6.363173	6.231661	0.024547
H	-1.255332	5.030083	0.244572	H	5.814140	5.103134	-2.130141
C	-2.313361	-2.415794	-0.339860	H	4.057279	3.345296	-2.202572
C	2.551815	2.417411	-0.146133	O	-1.137401	0.000000	2.407785
C	-2.313167	2.416013	-0.339226	O	1.106930	0.000068	2.463679
C	2.551570	-2.417647	-0.145592	H	5.143278	5.586030	2.100499
C	0.001082	0.000043	1.907441	O	-3.907962	-0.000020	2.317342
C	-3.383734	3.447267	-0.337440	H	-2.930634	0.000043	2.234045
C	-3.408535	4.468863	-1.297034	H	3.386821	3.829080	2.019675
C	-4.396234	3.417518	0.632746	H	-6.181844	-4.345962	1.409559
C	-4.414150	5.432702	-1.288972	H	-4.039301	-0.000229	3.274254
C	-5.401510	4.383206	0.643848				
C	-5.412978	5.394516	-0.316101	F₂₀TPP Ligand			
C	3.604864	3.467163	-0.096875	77			
C	3.921687	4.112190	1.106467	[Fe] ⁺¹			
C	4.298953	3.840343	-1.255525	C	3.418377	-2.465341	-0.261270
C	4.905914	5.097687	1.150493	C	2.453385	-3.424573	-0.264032
C	5.284240	4.825416	-1.213944	C	2.757626	-1.210682	-0.120457
C	5.590478	5.458005	-0.010005	C	1.203960	-2.758520	-0.105439
C	3.604513	-3.467498	-0.096146	N	1.383930	-1.384892	-0.058086
C	3.921215	-4.112458	1.107261	C	-0.001086	-3.429973	0.057179
C	4.298615	-3.840847	-1.254736	C	3.433778	-0.003797	0.000875
C	4.905347	-5.098048	1.151406	C	2.760155	1.204622	0.120977
C	5.283807	-4.826009	-1.213035	N	1.386909	1.381818	0.057127
C	5.589930	-5.458527	-0.009029	C	3.423550	2.457945	0.261239
C	-3.384046	-3.446933	-0.338233	C	1.209931	2.755878	0.103004
C	-3.408947	-4.468439	-1.297921	C	2.460698	3.419336	0.261891
C	-4.396556	-3.417164	0.631937	C	0.006400	3.429836	-0.060499
C	-4.414655	-5.432187	-1.289938	C	-1.197623	2.751593	-0.201335

N	-1.377584	1.381665	-0.094815		F	1.060395	-7.655513	2.208235	
C	-2.443076	3.407287	-0.421595		F	-1.099891	-7.711066	-1.954679	
C	-2.749661	1.202975	-0.176260		F	-0.025650	-9.029578	0.147561	
C	-3.406228	2.446052	-0.406739		F	-4.985577	1.148167	2.056024	
C	-3.427667	0.003729	0.001273		F	-7.678471	1.145580	2.055820	
C	-1.203529	-2.749191	0.199320		F	-9.027778	0.010681	0.005510	
N	-1.380549	-1.378776	0.094303		F	-7.684479	-1.127576	-2.046843	
C	-2.450205	-3.402330	0.420277		F	-4.991646	-1.136871	-2.051258	
C	-2.752139	-1.197094	0.177529		F	1.088271	4.957857	-2.174180	
C	-3.411191	-2.438896	0.407757		F	1.077567	7.650424	-2.216376	
H	4.495960	-2.600268	-0.336360		F	-1.081328	7.715794	1.947121	
H	2.579865	-4.502386	-0.351608		F	-0.004436	9.029386	-0.156821	
C	4.918274	-0.005448	0.002122		F	-1.082335	5.023270	1.994067	
C	-0.005875	-4.913189	0.082615		F	4.989872	0.445262	2.307088	
Fe	0.003518	-0.000049	-0.000372		F	7.685248	0.434418	2.308023	
H	4.501358	2.590547	0.337274		F	9.033972	-0.010175	0.006111	
H	2.589510	4.496959	0.348389		F	4.993312	-0.456196	-2.302730	
C	0.005030	4.913031	-0.087557		F	7.688708	-0.451590	-2.298396	
H	-2.567182	4.478798	-0.569368						
H	-4.479683	2.570133	-0.539767			77			
C	-4.910844	0.005474	0.002382			[Fe]			
H	-2.576575	-4.473711	0.567062			C	1.049671	-4.123526	0.019148
H	-4.484738	-2.560693	0.542129			C	-0.304567	-4.244317	-0.006693
C	-0.563481	-5.648156	-0.967488			C	1.336610	-2.719995	0.027951
C	0.543106	-5.619812	1.156330			C	-0.835826	-2.913936	0.004747
C	0.541886	-7.011571	1.188805			N	0.176327	-1.986371	0.017669
C	-0.019642	-7.721210	0.127093			C	-2.202667	-2.630392	0.022294
C	-0.574690	-7.040195	-0.956425			C	2.631305	-2.198705	0.048155
C	-5.633338	-0.576237	-1.043389			C	2.911212	-0.835446	0.034093
C	-5.630266	0.589057	1.049226			N	1.982685	0.173363	-0.002938
C	-7.022318	0.595820	1.060936			C	4.249937	-0.302933	0.033915
C	-7.025418	-0.579515	-1.052944			C	2.717711	1.330757	-0.035056
C	-7.719253	0.009026	0.004526			C	4.129378	1.045062	-0.005192
C	5.636665	0.219536	1.178582			C	2.200447	2.621414	-0.094163
C	5.638427	-0.231998	-1.172959			C	0.833283	2.904040	-0.096972
C	7.028873	0.220940	1.191653			N	-0.177825	1.977985	-0.025344
C	7.030652	-0.236596	-1.183307			C	0.300685	4.231815	-0.170750
C	7.725179	-0.008635	0.004850			C	-1.338217	2.711015	-0.031989
C	0.555511	5.617141	-1.162150			C	-1.053219	4.111697	-0.126366
C	-0.550377	5.650503	0.961961			C	-2.632446	2.191890	0.036579
C	0.557728	7.008865	-1.196120			C	-2.718709	-1.338218	0.053137
C	-0.001710	7.721029	-0.134993			N	-1.984179	-0.180558	0.028290
C	-0.558135	7.042552	0.949408			C	-4.128613	-1.051935	0.129933
F	-1.094289	-5.018472	-1.998689			C	-2.911986	0.828977	0.071115
F	1.077696	-4.962957	2.168980			C	-4.248529	0.296541	0.146103

H	1.791301	-4.921012	0.031542	F	4.415296	6.453481	1.931817
H	-0.894130	-5.159894	-0.027186	F	5.798824	6.922326	-0.347111
C	3.772271	-3.150304	0.080470	F	2.688847	4.396465	2.059503
C	-3.157733	-3.768446	0.009375	F	4.223787	-2.662141	2.337385
Fe	-0.000719	-0.004012	0.002970	F	6.288591	-4.383851	2.396108
H	5.164111	-0.894537	0.056891	F	6.948025	-5.784824	0.175727
H	4.924311	1.789502	-0.011084	F	3.459327	-3.746619	-2.174229
C	3.152393	3.760319	-0.158416	F	5.530016	-5.460738	-2.107771
H	0.888585	5.144950	-0.253725				
H	-1.796352	4.906983	-0.166155	77			
C	-3.768749	3.148130	0.073392	[Fe] ⁻¹			
H	-4.922037	-1.796507	0.178367	C	-4.229560	-0.572036	-0.007630
H	-5.160376	0.888789	0.209281	C	-4.191747	0.798863	0.021761
C	-3.906830	-4.063467	-1.131861	C	-2.876058	-1.011995	-0.018197
C	-3.344185	-4.577131	1.132485	C	-2.816108	1.163620	0.037172
C	-4.240379	-5.643217	1.125464	N	-2.008728	0.052626	0.007340
C	-4.974974	-5.914871	-0.026606	C	-2.355233	2.495600	0.073154
C	-4.809914	-5.123158	-1.160957	C	-2.489747	-2.367766	-0.030762
C	-4.614247	3.318181	-1.025164	C	-1.175932	-2.796315	-0.017736
C	-4.026656	3.913765	1.212769	N	-0.056667	-1.987256	-0.016104
C	-5.085337	4.817005	1.263595	C	-0.794384	-4.186914	-0.018354
C	-5.680072	4.214300	-0.995922	C	1.015913	-2.856719	-0.019327
C	-5.914069	4.965508	0.153658	C	0.558679	-4.224071	-0.009506
C	4.521945	-3.337722	1.243470	C	2.351350	-2.501314	-0.035236
C	4.136246	-3.885206	-1.049585	C	2.810930	-1.168474	-0.055885
C	5.596100	-4.223123	1.286823	N	2.004254	-0.057203	-0.022359
C	5.204968	-4.778070	-1.028719	C	4.184704	-0.803508	-0.128255
C	5.936325	-4.945310	0.145151	C	2.870955	1.007792	-0.056964
C	3.880550	4.026241	-1.320135	C	4.222363	0.567679	-0.130620
C	3.352417	4.602613	0.937495	C	2.485535	2.363635	-0.024787
C	4.777036	5.089342	-1.394762	C	-1.019654	2.850754	0.058288
C	4.955958	5.914776	-0.286910	N	0.052549	1.982139	0.011076
C	4.242196	5.672838	0.884671	C	-0.561896	4.217096	0.107508
F	-3.771773	-3.327416	-2.218762	C	1.171697	2.791185	0.013980
F	-2.660986	-4.342170	2.237306	C	0.790923	4.180413	0.078649
F	-4.400358	-6.391988	2.197821	H	-5.108406	-1.216953	-0.016718
F	-5.504264	-5.383342	-2.249951	H	-5.033607	1.491424	0.028454
F	-5.824224	-6.918714	-0.042964	C	-3.567566	-3.387070	-0.045706
F	-3.256300	3.793408	2.277617	C	-3.373230	3.573342	0.123274
F	-5.310242	5.526670	2.350620	Fe	-0.002118	-0.002524	-0.002724
F	-6.917378	5.814712	0.191096	H	-1.486319	-5.029138	-0.026905
F	-6.463675	4.358798	-2.045283	H	1.203096	-5.103126	0.000979
F	-4.415442	2.619569	-2.127119	C	3.372884	-3.576780	-0.040224
F	3.731293	3.258706	-2.383534	H	5.024707	-1.496288	-0.182440
F	5.451732	5.321474	-2.502442	H	5.099304	1.212791	-0.186695

C	3.562279	3.383588	-0.036637	[Fe] ⁻²	
H	-1.205782	5.094645	0.166518	C	-3.674512
H	1.483590	5.021543	0.109943	C	-2.795528
C	-3.638117	4.380304	-0.986241	C	-2.889645
C	-4.119780	3.817349	1.279364	C	-1.485351
C	-5.085974	4.819213	1.335057	N	-1.543044
C	-5.324077	5.609016	0.214026	C	-0.310657
C	-4.595568	5.392047	-0.951272	C	-3.432538
C	3.814870	4.165273	-1.167071	C	-2.667816
C	4.382003	3.592353	1.076207	N	-1.288820
C	5.406992	4.535518	1.070096	C	-3.227813
C	4.830550	5.118786	-1.193329	C	-0.986014
C	5.631301	5.301303	-0.070325	C	-2.175098
C	-3.877649	-4.139066	1.090191	C	0.306257
C	-4.331561	-3.622283	-1.191964	C	1.481271
C	-4.894311	-5.091865	1.089589	N	1.540044
C	-5.356606	-4.565233	-1.213710	C	2.789363
C	-5.638296	-5.302284	-0.067143	C	2.886229
C	3.609374	-4.358686	-1.173806	C	3.668568
C	4.158161	-3.837095	1.086379	C	3.431073
C	4.575978	-5.362183	-1.189603	C	0.982097
C	5.342859	-5.596101	-0.052612	N	1.285935
C	5.134010	-4.830998	1.091236	C	2.169530
F	-2.972864	4.204315	-2.113179	C	2.664660
F	-3.918675	3.097439	2.367123	C	3.222521
F	-5.773345	5.033189	2.445182	H	-4.764635
F	-4.824393	6.142109	-2.016863	H	-3.030754
F	-6.236323	6.564323	0.257935	C	-4.903966
F	4.197134	2.894257	2.180752	C	-0.441998
F	6.163921	4.716717	2.140007	Fe	-0.001461
F	6.598846	6.201541	-0.084431	H	-4.292908
F	5.046447	5.845192	-2.277900	H	-2.216830
F	3.083207	4.019158	-2.256583	C	0.440323
F	2.908835	-4.164952	-2.276543	H	3.022209
F	4.777318	-6.088132	-2.277389	H	4.756471
F	5.858366	-5.060745	2.174184	C	4.900758
F	6.263659	-6.544211	-0.057173	H	2.208969
F	3.986776	-3.139720	2.193375	H	4.286061
F	-3.200092	-3.965983	2.210406	C	-0.040121
F	-5.164600	-5.791453	2.179611	C	-0.974365
F	-6.606468	-6.201848	-0.078918	C	-1.109934
F	-4.093000	-2.948493	-2.301423	C	-0.695471
F	-6.060185	-4.772399	-2.314857	C	-0.154472
				C	5.595039
				C	5.684282
					0.000998
					1.078762

C	7.072288	0.116252	1.087488	C	-2.827548	1.180930	-0.162222
C	6.981032	1.152905	-1.076946	C	2.836542	0.964412	-0.335056
C	7.726077	0.698457	0.006358	C	-1.220577	-2.784660	0.018514
C	-5.602546	-0.919567	1.118207	C	2.761721	-1.211534	-0.256466
C	-5.679624	-0.098334	-1.113574	C	0.968350	-2.875185	-0.001529
C	-6.988832	-1.056807	1.127641	C	0.809068	4.159131	-0.064853
C	-7.067786	-0.215314	-1.120634	C	-4.255758	-0.542742	-0.181709
C	-7.727097	-0.699962	0.004100	C	-0.542982	4.211127	-0.028251
C	0.042679	-5.653929	-1.209563	C	-4.209029	0.826888	-0.185289
C	0.976933	-5.623193	0.978656	C	4.177027	0.511192	-0.456335
C	0.161341	-7.041162	-1.252825	C	-0.857904	-4.177563	0.096256
C	0.704249	-7.723754	-0.169239	C	4.131459	-0.859065	-0.412438
C	1.116712	-7.008833	0.950481	C	0.494208	-4.234958	0.095628
F	0.451284	5.164843	-2.081716	H	1.510314	4.993046	-0.098417
F	-1.355164	4.900088	2.275293	H	-5.139212	-1.181248	-0.177345
F	-1.609830	7.559628	2.317036	H	-1.178198	5.096705	-0.025577
F	0.225873	7.826738	-1.998786	H	-5.046029	1.524985	-0.183669
F	-0.814947	9.048306	0.190413	H	5.057348	1.146802	-0.549939
F	5.119304	-0.527952	2.149762	H	-1.561633	-5.009138	0.133160
F	7.781423	-0.301467	2.131236	H	4.963616	-1.559902	-0.477668
F	9.049682	0.819040	0.008395	H	1.127766	-5.120440	0.141620
F	7.605912	1.691623	-2.119112	C	2.473079	2.321010	-0.240512
F	4.946884	1.434276	-2.144854	C	-2.527478	-2.343617	-0.054814
F	-0.448778	-5.059916	-2.282915	C	2.306248	-2.538069	-0.108135
F	-0.216514	-7.721361	-2.330458	C	-2.357469	2.510233	-0.087221
F	1.619170	-7.661672	1.993401	C	0.555415	0.206682	2.134036
F	0.827256	-9.046487	-0.203164	C	3.320906	-3.618944	-0.090603
F	1.356953	-5.003682	2.081910	C	3.483829	-4.490039	-1.171517
F	-4.958910	-1.247107	2.224670	C	4.173345	-3.797995	1.003296
F	-7.619342	-1.504693	2.208412	C	4.441565	-5.501900	-1.166748
F	-9.050310	-0.820823	0.005273	C	5.143420	-4.797475	1.025842
F	-5.108009	0.339761	-2.221423	C	5.276536	-5.652756	-0.064123
F	-7.771045	0.110160	-2.200315	C	-3.615011	-3.353755	-0.025002
				C	-3.956804	-4.024709	1.151570
				C	-4.353647	-3.658171	-1.171220
				C	-4.984829	-4.964638	1.190376
[FeCO ₂] ⁻¹				C	-5.388356	-4.590569	-1.153814
Fe	-0.017980	-0.008363	0.057709	C	-5.704152	-5.245573	0.032958
N	0.045403	1.969272	-0.047336	C	-3.363322	3.599208	-0.073778
N	-2.035248	0.069250	-0.164406	C	-3.617032	4.346542	1.079842
N	1.966740	-0.096112	-0.241220	C	-4.109072	3.917116	-1.212734
N	-0.087467	-1.993605	-0.016839	C	-4.566500	5.366007	1.104687
C	1.175139	2.766429	-0.096430	C	-5.067989	4.927271	-1.208614
C	-2.904489	-0.990628	-0.153874	C	-5.296447	5.654603	-0.044130
C	-1.016995	2.847588	-0.034956	C	3.562600	3.327515	-0.262568

C	4.252367	3.639796	-1.435855	C	-1.476058	-3.989788	-0.068536
C	3.949998	3.990456	0.904829	C	3.339279	-2.699769	-0.220815
C	5.285885	4.573632	-1.454259	C	-3.961114	1.495836	-0.361447
C	4.977571	4.931568	0.907662	C	2.703460	3.290000	0.090252
C	5.648534	5.220944	-0.276722	C	-3.277462	2.682126	-0.348544
O	1.639345	0.478246	2.496388	C	1.516082	3.977522	0.070213
O	-0.603645	-0.047328	2.239206	H	-3.673181	-3.728238	-0.138956
F	6.625123	6.110963	-0.284453	H	5.100598	-1.363695	-0.171523
F	5.325433	5.547938	2.024727	H	-1.327278	-5.069206	-0.118068
F	3.338826	3.740893	2.046033	H	3.756341	-3.707569	-0.210031
F	5.921226	4.855449	-2.579918	H	-5.041015	1.350279	-0.405149
F	3.934383	3.049720	-2.573340	H	3.711861	3.705304	0.112331
F	2.718762	-4.375652	-2.242172	H	-3.688623	3.691231	-0.399980
F	4.571151	-6.313319	-2.203833	H	1.370165	5.058212	0.097234
F	6.190725	-6.606879	-0.050326	C	-3.305655	-0.902081	-0.173497
F	5.933626	-4.947365	2.075978	C	3.341417	0.884677	-0.043292
F	4.074722	-3.014416	2.059385	C	-0.880080	3.312846	-0.120976
F	-4.081825	-3.062035	-2.316720	C	0.924264	-3.327285	-0.120063
F	-3.301474	-3.784578	2.271528	C	-0.425637	0.204341	2.169583
F	-5.287216	-5.587199	2.317490	C	-1.267912	4.740059	-0.129153
F	-6.681513	-6.134268	0.059114	C	-0.986742	5.574321	-1.217747
F	-6.069007	-4.864131	-2.254428	C	-1.936109	5.328677	0.951771
F	-2.949333	4.102903	2.192143	C	-1.340893	6.921702	-1.233441
F	-3.914844	3.260543	-2.341313	C	-2.309738	6.671360	0.951412
F	-5.755676	5.209531	-2.303007	C	-2.007791	7.472756	-0.144425
F	-4.786393	6.056308	2.211557	C	4.764337	1.274307	0.009777
F	-6.200769	6.618179	-0.030786	C	5.341332	1.812798	1.168301

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[FeCO ₂] ⁻²				C	5.613596	1.132300	-1.096198
Fe	0.010383	-0.004227	0.059478	C	6.680543	2.191059	1.226334
N	-0.979880	-1.738012	-0.021696	C	6.958674	1.492072	-1.054703
N	1.771747	-1.012105	-0.208712	C	7.496024	2.027703	0.110916
N	-1.716166	0.989544	-0.235908	C	1.304409	-4.752833	-0.116614
N	1.010095	1.726467	-0.003084	C	1.091625	-5.574503	0.999792
C	-2.350512	-1.923131	-0.060748	C	1.895239	-5.365536	-1.230945
C	3.035833	-0.478052	-0.177621	C	1.441822	-6.922359	1.010274
C	-0.441194	-3.013112	-0.042504	C	2.266010	-6.708069	-1.235449
C	1.948901	-2.372696	-0.210566	C	2.035313	-7.493725	-0.111146
C	-2.986966	0.458031	-0.278448	C	-4.728736	-1.290232	-0.201556
C	2.381619	1.903696	0.037085	C	-5.527170	-1.106592	-1.339038
C	-1.894239	2.356377	-0.237562	C	-5.358050	-1.872546	0.908121
C	0.481110	3.004369	-0.012726	C	-6.873504	-1.462174	-1.371205
C	-2.667801	-3.309345	-0.080081	C	-6.698928	-2.248783	0.891276
C	4.020307	-1.512283	-0.200564	C	-7.463653	-2.039983	-0.252248
				O	-1.410082	0.715917	2.573544
				O	0.625568	-0.348900	2.295560

F	-8.745755	-2.388255	-0.275141	H	-4.901679	1.996288	0.009007
F	-7.266068	-2.786195	1.965876	H	1.904460	4.867148	-0.361182
F	-4.692789	-2.069830	2.031004	H	-3.271396	4.144229	-0.004383
F	-7.597248	-1.279878	-2.470984	H	4.854650	-1.985100	-0.238594
F	-5.014352	-0.595771	-2.445715	H	-4.138092	-3.252532	-0.140330
F	-0.378225	5.099065	-2.289871	H	3.210523	-4.126641	-0.240074
F	-1.065807	7.684492	-2.286052	H	-1.964274	-4.862244	-0.109390
F	-2.354271	8.754821	-0.151927	C	3.439552	0.496626	-0.217075
F	-2.936512	7.202283	1.995307	C	-3.473500	-0.477035	-0.086757
F	-2.228438	4.621671	2.026268	C	0.472489	-3.381430	-0.142582
F	5.152617	0.661773	-2.242182	C	-0.517976	3.415137	-0.116151
F	4.625146	1.966188	2.267116	C	0.334857	-0.352468	2.144461
F	7.197442	2.687169	2.345428	C	0.686462	-4.842633	-0.106334
F	8.776327	2.379567	0.159622	C	0.387845	-5.666938	-1.198150
F	7.731754	1.352603	-2.126685	C	1.198809	-5.479356	1.032639
F	0.560072	-5.082855	2.104141	C	0.584458	-7.046818	-1.165931
F	2.105045	-4.681233	-2.342600	C	1.415004	-6.856183	1.079469
F	2.815225	-7.256650	-2.314315	C	1.102501	-7.645089	-0.022459
F	1.237609	-7.667970	2.091113	C	-4.913195	-0.687181	-0.038878
F	2.378804	-8.777458	-0.106938	C	-5.553003	-1.417917	0.993364
				C	-5.798295	-0.184117	-1.025032
				C	-6.923782	-1.636403	1.034859
				C	-7.174138	-0.369076	-0.981058

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[FeCO₂]⁻³

Fe	-0.009420	0.005684	0.037482	C	-7.756550	-1.107214	0.048707
N	1.207759	1.607290	-0.048340	C	-0.715955	4.869067	-0.071072
N	-1.659119	1.217037	-0.235830	C	-0.258970	5.657044	1.003998
N	1.606469	-1.181577	-0.266065	C	-1.362358	5.576526	-1.104204
N	-1.237966	-1.588655	-0.045632	C	-0.436873	7.035561	1.052948
C	2.586572	1.633837	-0.148123	C	-1.562976	6.952999	-1.062868
C	-2.980035	0.848550	-0.174551	C	-1.095930	7.696267	0.017276
C	0.811093	2.941065	-0.103340	C	4.878536	0.708012	-0.247030
C	-1.656242	2.598825	-0.179349	C	5.715341	0.190326	-1.268068
C	2.937219	-0.821121	-0.277125	C	5.567360	1.463928	0.735065
C	-2.621296	-1.610513	-0.047253	C	7.092404	0.369915	-1.291827
C	1.602377	-2.568954	-0.217874	C	6.938941	1.677821	0.707500
C	-0.851972	-2.924983	-0.086541	C	7.724111	1.126085	-0.306202
C	3.047993	2.964890	-0.277955	O	1.139125	-1.113414	2.563938
C	-3.815445	2.001727	-0.090782	O	-0.541276	0.450324	2.291153
C	1.935214	3.781881	-0.244189	F	9.052351	1.309070	-0.323826
C	-2.986322	3.094291	-0.093312	F	7.538030	2.364297	1.686606
C	3.764541	-1.982824	-0.263143	F	4.916090	1.958852	1.778523
C	-3.091668	-2.949199	-0.086652	F	7.823049	-0.120057	-2.299979
C	2.930408	-3.071110	-0.244736	F	5.190465	-0.456886	-2.303817
C	-1.984350	-3.770613	-0.087570	F	-0.075034	-5.156576	-2.326871
H	4.085626	3.264755	-0.432875	F	0.303277	-7.802532	-2.228384

F	1.299941	-8.963651	0.015637	C	2.692342	-2.118718	0.200981
F	1.896754	-7.435954	2.178996	C	-2.102519	-2.701330	0.135972
F	1.483798	-4.790815	2.121038	C	-2.677182	2.116531	0.180738
F	-5.324079	0.449136	-2.091859	C	2.115299	2.680892	-0.014837
F	-4.852269	-1.886577	2.017855	C	3.864562	-3.030285	0.247077
F	-7.473712	-2.303141	2.055648	C	4.571919	-3.230964	1.434400
F	-9.082721	-1.298979	0.093089	C	5.678150	-4.074517	1.493893
F	-7.953383	0.099582	-1.962075	C	6.093450	-4.742350	0.343996
F	0.327043	5.098220	2.049153	C	5.404561	-4.562566	-0.853406
F	-1.773341	4.951661	-2.197963	C	4.302056	-3.711882	-0.890746
F	-2.162444	7.583691	-2.075887	C	-3.037290	-3.853813	0.089051
F	-0.015885	7.739555	2.106322	C	-3.137651	-4.767989	1.139816
F	-1.282063	9.019451	0.065235	C	-4.022984	-5.842186	1.090633
				C	-4.834859	-6.012495	-0.028700
				C	-4.757474	-5.113225	-1.090218
81				C	-3.864275	-4.047612	-1.020237
[FeCOOH]				C	-3.841899	3.035647	0.241833
Fe	0.013313	-0.007265	-0.023963	C	-4.033734	3.881080	1.337285
N	1.965859	0.234178	0.224316	C	-5.117514	4.752585	1.407273
N	0.244653	-1.979784	0.069865	C	-6.039306	4.786203	0.363225
N	-1.954181	-0.240731	0.209498	C	-5.873667	3.952180	-0.740578
N	-0.231405	1.964793	0.004444	C	-4.781768	3.089163	-0.790128
C	2.662571	1.413048	0.179919	C	3.040360	3.839708	-0.109592
C	2.921398	-0.745320	0.287358	C	3.152472	4.764166	0.931344
C	1.422887	-2.676621	0.071573	C	4.017809	5.852410	0.853027
C	-0.736207	-2.938215	0.021345	C	4.796485	6.028269	-0.288669
C	-2.650388	-1.426482	0.297381	C	4.706416	5.119844	-1.340886
C	-2.907463	0.747598	0.331169	C	-1.411711	2.662880	-0.012490
C	0.746086	2.916435	-0.108788	C	0.000328	-0.040440	-1.991327
C	4.073295	1.175272	0.296720	O	1.024547	0.101763	-2.576607
H	4.844279	1.944235	0.314608	O	-1.179941	-0.225053	-2.571482
C	4.235175	-0.170686	0.361487	H	-1.861085	-0.312285	-1.883924
H	5.167041	-0.729632	0.432412	F	-5.525462	-5.277334	-2.147256
C	1.181552	-4.094222	-0.018395	F	-5.674468	-7.022361	-0.083421
H	1.949755	-4.865924	-0.029632	F	-4.102127	-6.691702	2.094200
C	-0.161861	-4.256061	-0.066718	F	-3.811133	-3.206587	-2.036757
H	-0.724300	-5.186355	-0.131928	F	-2.383845	-4.627119	2.214083
C	-4.039246	-1.177805	0.526224	F	3.665824	-3.562850	-2.036032
H	-4.803283	-1.943204	0.656603	F	4.200874	-2.607505	2.537412
C	-4.197747	0.175021	0.555225	F	5.800497	-5.194533	-1.939192
H	-5.117792	0.736215	0.713275	F	7.135724	-5.542578	0.389106
C	-1.172376	4.070698	-0.199882	F	6.329420	-4.247693	2.626007
H	-1.942225	4.837834	-0.270686	F	-7.066349	5.604633	0.419783
C	0.171157	4.227894	-0.265109	F	-6.745888	3.987558	-1.726829
H	0.732647	5.151239	-0.399934	F	-4.647090	2.309519	-1.846967

F	-5.278749	5.539342	2.451213	C	-5.802488	3.859519	-1.554390
F	-3.176450	3.868535	2.340155	C	-6.202558	4.580732	-0.433222
F	3.769732	3.192469	-2.250405	C	-5.482393	4.473332	0.752860
F	2.426728	4.619793	2.024525	C	-4.365999	3.641177	0.808124
F	4.107891	6.710975	1.848407	C	-2.910558	-3.946495	-0.020823
F	5.617272	7.052015	-0.372781	C	-3.124156	-4.780897	-1.118968
F	5.443906	5.289698	-2.418970	C	-3.962384	-5.891304	-1.043543

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[FeCOOH]⁻¹

Fe	0.009551	0.000363	-0.010858	C	-4.419084	-5.366263	1.263934
N	-0.293724	1.956940	-0.158691	C	-3.573855	-4.263343	1.166631
N	-1.962896	-0.301556	-0.144003	C	3.954889	-2.919228	-0.147584
N	0.303896	-1.971586	-0.105023	C	4.740460	-3.064259	-1.293403
N	1.973917	0.287036	-0.149504	C	5.867012	-3.883243	-1.314503
C	0.654834	2.941657	-0.137573	C	6.227836	-4.585328	-0.168480
C	-1.489470	2.623252	-0.214563	C	5.462953	-4.462954	0.987840
C	-2.952597	0.646130	-0.207178	C	4.341879	-3.635441	0.987904
C	-2.629400	-1.501696	-0.140364	C	2.907557	3.934910	-0.012845
C	-0.645142	-2.962875	-0.103164	C	3.668713	4.356995	-1.104527
C	1.501834	-2.637636	-0.126796	C	4.492587	5.478081	-1.037367
C	2.961446	-0.659041	-0.142121	C	4.562224	6.208329	0.145288
C	2.634576	1.482946	-0.104108	C	3.811835	5.813542	1.249065
C	0.050713	4.249444	-0.204737	C	2.995897	4.686937	1.161925
H	0.589484	5.196808	-0.224392	C	0.089566	0.119389	1.903203
C	-1.288923	4.050675	-0.257953	O	0.823047	0.848323	2.518089
H	-2.076750	4.800552	-0.327317	O	-0.755671	-0.691493	2.606172
C	-4.255370	0.035668	-0.241013	H	-1.303023	-1.174609	1.973835
H	-5.204751	0.568893	-0.290885	F	-5.035324	-5.647887	2.398581
C	-4.054431	-1.306238	-0.197590	F	-5.409920	-7.231328	0.233016
H	-4.803383	-2.097965	-0.216993	F	-4.150955	-6.667116	-2.097588
C	-0.036766	-4.268461	-0.115719	F	-3.411328	-3.509242	2.237621
H	-0.570368	-5.218828	-0.114249	F	-2.526909	-4.533009	-2.269975
C	1.303646	-4.064497	-0.143755	F	-3.709538	3.564724	1.948269
H	2.094011	-4.814075	-0.177529	F	-4.330220	2.370743	-2.562893
C	4.268438	-0.049998	-0.101078	F	-5.866338	5.158277	1.816365
H	5.218336	-0.583908	-0.078557	F	-7.263267	5.365434	-0.495089
C	4.063212	1.288920	-0.071626	F	-6.485718	3.966155	-2.681697
H	4.810365	2.080654	-0.023186	F	7.293584	-5.365738	-0.178779
C	-2.746804	2.024659	-0.234887	F	5.809697	-5.128965	2.076087
C	-2.023588	-2.758285	-0.095426	F	3.644519	-3.544635	2.102688
C	2.759496	-2.037420	-0.137768	F	6.592454	-4.004576	-2.413708
C	2.031992	2.737847	-0.087767	F	4.429355	-2.417840	-2.401483
C	-3.940558	2.906649	-0.301249	F	2.299873	4.345017	2.224555
C	-4.680969	3.036877	-1.478101	F	3.625224	3.692075	-2.244976

F 3.883386 6.509212 2.371079

C -3.908520 -5.968899 0.977059

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C -4.828428 -6.062957 -0.061620

[FeCOOH]⁻²

C -4.853804 -5.075276 -1.042265

Fe 0.020894 -0.007539 -0.030098

C -3.959156 -4.011012 -0.977594

N 1.967852 0.246486 0.195040

C -3.869110 3.009557 0.271083

N 0.262551 -2.006708 0.059752

C -4.003402 3.952829 1.301037

N -1.961340 -0.257770 0.176549

C -5.089523 4.820521 1.381897

N -0.247896 1.989036 0.025627

C -6.099678 4.756446 0.427929

C 2.663658 1.439842 0.158834

C -6.006239 3.826492 -0.603340

C 2.938649 -0.732007 0.300216

C -4.904977 2.976952 -0.674621

C 1.455462 -2.693486 0.040682

C 3.019546 3.861284 -0.152511

C -0.714980 -2.973396 -0.002806

C 3.075166 4.857440 0.831241

C -2.652381 -1.459798 0.285145

C 3.930249 5.953213 0.734543

C -2.928716 0.729464 0.340523

C 4.778802 6.072776 -0.360505

C -1.439296 2.676179 -0.000459

C 4.758249 5.096771 -1.351683

C 0.727922 2.948197 -0.121966

C 3.886653 4.015150 -1.243157

C 4.061263 1.211631 0.323923

C 0.047895 -0.014697 -1.979619

H 4.827960 1.986512 0.366012

O 1.033089 0.114771 -2.644316

C 4.234023 -0.144608 0.406735

O -1.164611 -0.179410 -2.535258

H 5.172956 -0.691048 0.503364

H -1.801855 -0.259007 -1.801342

C 1.224832 -4.099844 -0.075196

F -5.719168 -5.174604 -2.045377

H 1.996167 -4.870598 -0.100618

F -5.673581 -7.086747 -0.119301

C -0.130877 -4.272921 -0.125662

F -3.897081 -6.899241 1.926364

H -0.680794 -5.210137 -0.218235

F -4.011009 -3.121616 -1.952304

C -4.020447 -1.220619 0.581023

F -2.212104 -4.830982 2.068632

H -4.770305 -1.992620 0.760172

F 3.735222 -3.622519 -2.004675

C -4.190903 0.144132 0.623315

F 4.251175 -2.543152 2.562906

H -5.107185 0.695055 0.840003

F 5.858331 -5.240153 -1.848859

C -1.212592 4.069078 -0.231331

F 7.210986 -5.505855 0.488084

H -1.989116 4.829306 -0.327295

F 6.393665 -4.137951 2.685556

C 0.142457 4.238521 -0.311400

F -7.143296 5.575896 0.499648

H 0.691541 5.165381 -0.482995

F -6.960563 3.778473 -1.526719

C 2.716723 -2.111674 0.201516

F -4.854919 2.140944 -1.696201

C -2.092029 -2.734916 0.106447

F -5.187673 5.692766 2.379700

C -2.705619 2.107374 0.194972

F -3.097391 4.034751 2.259746

C 2.102894 2.707206 -0.044018

F 3.894529 3.134912 -2.224363

C 3.891505 -3.006105 0.272210

F 2.319017 4.779420 1.912443

C 4.616896 -3.170980 1.458902

F 3.961611 6.875953 1.690331

C 5.733663 -3.999196 1.540745

F 5.601785 7.110762 -0.459946

C 6.151853 -4.707452 0.418993

F 5.559281 5.219342 -2.404304

C 5.451126 -4.573503 -0.774634

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C 4.344241 -3.728950 -0.838807

[FeCO]⁺¹

C -3.018093 -3.880957 0.055562

C -1.004824 -4.132752 0.119602

C -3.031281 -4.887903 1.031839

C -1.299084 -2.717291 -0.016939

N	-0.154859	-1.975498	-0.020334	C	-4.648969	-3.287512	0.858551
C	0.864845	-2.891488	0.084347	C	-3.902023	-4.029132	-1.291907
C	0.335042	-4.240266	0.189263	C	-4.948902	-4.944374	-1.354198
C	-2.604803	-2.219837	-0.137101	C	-5.703995	-4.195216	0.817927
C	-2.881593	-0.861225	-0.210770	C	-3.196402	3.731870	-0.054296
C	-4.224183	-0.334062	-0.383693	C	-5.078233	5.816156	0.004136
C	-4.117635	1.007341	-0.350216	C	-3.340242	4.603206	-1.137346
C	-2.708150	1.304927	-0.168300	C	-4.023709	3.926511	1.055206
N	-1.967095	0.161350	-0.114048	C	-4.958299	4.957109	1.096895
C	-2.217398	2.615861	-0.076665	C	-4.267959	5.641422	-1.117842
C	-0.859926	2.902537	-0.033585	C	-0.013839	0.027927	1.875062
N	0.162089	1.983048	-0.068687	O	-0.023983	0.041582	3.013240
C	1.305974	2.725001	-0.085595	F	6.861713	5.870939	-0.345022
C	1.008409	4.146193	-0.058053	F	5.461762	5.562345	1.948616
C	-0.331984	4.255848	-0.003116	F	3.412205	3.812843	2.048078
C	2.614425	2.223848	-0.137211	F	6.219607	4.425170	-2.538654
C	2.895063	0.864399	-0.145210	F	4.183193	2.663311	-2.440105
N	1.976195	-0.156104	-0.069805	F	4.376383	-6.521352	-1.855194
C	2.718580	-1.300411	-0.055115	F	2.599984	-4.502830	-2.000144
C	4.136219	-1.005859	-0.163876	F	5.907017	-6.818372	0.354387
C	4.246440	0.334720	-0.210708	F	5.667003	-5.090952	2.421113
C	2.223655	-2.607388	0.062892	F	3.899118	-3.061273	2.279144
Fe	0.002171	0.006174	0.106743	F	-3.053355	-3.966137	-2.301411
H	-4.907214	1.748937	-0.458719	F	-4.524035	-2.507897	1.916684
H	-5.119978	-0.936878	-0.523585	F	-6.553562	-4.275404	1.814930
H	-0.931532	5.163287	0.041937	F	-6.839543	-5.881726	-0.341571
H	1.748238	4.944315	-0.078890	F	-5.091983	-5.724627	-2.399600
H	5.152637	0.933561	-0.282713	F	-2.584514	4.449115	-2.209158
H	4.931019	-1.748820	-0.200475	F	-3.927355	3.113281	2.090892
H	-1.747467	-4.927433	0.164035	F	-4.386861	6.448487	-2.145983
H	0.934060	-5.142270	0.302276	F	-5.953661	6.788325	0.031489
C	3.742303	3.189149	-0.192442	F	-5.722348	5.123560	2.150626
C	5.869824	5.018657	-0.296513				
C	4.480940	3.368561	-1.364425				
C	4.094574	3.948767	0.925564				
C	5.147025	4.859156	0.886186				
C	5.538440	4.272210	-1.427396				
C	3.194951	-3.727846	0.138673				
C	5.045752	-5.835699	0.285406				
C	4.001624	-3.902667	1.266426				
C	3.341368	-4.633471	-0.915675				
C	4.254529	-5.682749	-0.853165				
C	4.921657	-4.943862	1.351047				
C	-3.730525	-3.186223	-0.190159				
C	-5.851561	-5.025165	-0.293499				

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[FeCO]

C	-0.669775	-4.203491	-0.112191
C	-1.081198	-2.825508	-0.101846
N	0.006330	-1.991337	-0.071945
C	1.094643	-2.824290	-0.056280
C	0.685643	-4.202611	-0.091811
C	-2.414583	-2.422651	-0.129953
C	-2.816016	-1.088363	-0.147857
C	-4.191574	-0.678293	-0.235947
C	-4.191710	0.677427	-0.235994

C	-2.816234	1.087774	-0.147939		C	-4.257346	3.725646	0.966770		
N	-1.983641	-0.000210	-0.107626		C	-5.254104	4.698251	0.954398		
C	-2.415081	2.422144	-0.130135		C	-4.703969	5.202815	-1.340432		
C	-1.081784	2.825289	-0.102020		C	-0.025240	0.000035	1.858124		
N	0.005917	1.991350	-0.072022		O	-0.042691	0.000040	3.000036		
C	1.094051	2.824535	-0.056359		F	6.392653	6.393922	0.080746		
C	0.684764	4.202767	-0.091975		F	4.899017	5.921234	2.288303		
C	-0.670656	4.203360	-0.112432		F	2.994712	4.022730	2.243806		
C	2.427653	2.422292	-0.018718		F	5.978053	4.956032	-2.175184		
C	2.830457	1.088476	-0.014881		F	4.081254	3.050501	-2.226982		
N	1.997315	0.000217	-0.038507		F	5.979013	-4.954596	-2.175462		
C	2.830687	-1.087864	-0.014876		F	4.081901	-3.049384	-2.227003		
C	4.208545	-0.677293	0.021619		F	6.393825	-6.392760	0.080259		
C	4.208401	0.678199	0.021617		F	4.900156	-5.920571	2.287900		
C	2.428163	-2.421766	-0.018695		F	2.995579	-4.022346	2.243684		
Fe	0.002881	0.000009	0.103007		F	-2.996046	-4.021484	-2.395176		
H	-5.047147	1.347949	-0.305808		F	-4.070015	-3.035639	2.075713		
H	-5.046882	-1.348983	-0.305722		F	-5.983856	-4.924774	2.027301		
H	-1.339886	5.062168	-0.137292		F	-6.412401	-6.361097	-0.226924		
H	1.355805	5.060492	-0.106331		F	-4.916266	-5.903439	-2.435997		
H	5.066585	1.348145	0.048982		F	-2.997289	4.020335	-2.395631		
H	5.066874	-1.347052	0.048998		F	-4.070221	3.035263	2.075669		
H	-1.338824	-5.062443	-0.136974		F	-4.917868	5.901940	-2.436493		
H	1.356857	-5.060199	-0.106162		F	-6.413597	6.359867	-0.227209		
C	3.477286	3.473785	0.007324		F	-5.984364	4.924114	2.027251		
C	5.463678	5.463566	0.057232							
C	4.262423	3.739922	-1.116333			79				
C	3.712553	4.231822	1.156165				[FeCO] ⁻¹			
C	4.693420	5.219898	1.192152				C	-0.587217	-4.228087	0.004936
C	5.249967	4.721867	-1.102530				C	-1.028918	-2.861456	-0.044900
C	3.478015	-3.473044	0.007257				N	0.055047	-2.003060	-0.061314
C	5.464721	-5.462528	0.056883				C	1.158058	-2.811342	-0.026657
C	3.713429	-4.231185	1.156001				C	0.768383	-4.200799	0.016816
C	4.263195	-3.738906	-1.116437				C	-2.358192	-2.485449	-0.077317
C	5.250901	-4.720690	-1.102769				C	-2.809988	-1.157203	-0.130359
C	4.694445	-5.219117	1.191845				C	-4.176044	-0.786834	-0.243299
C	-3.468297	-3.469980	-0.156700				C	-4.207978	0.584504	-0.260879
C	-5.474686	-5.439529	-0.204546				C	-2.855785	1.024271	-0.150869
C	-4.256805	-3.726275	0.966915				N	-1.998934	-0.039407	-0.092789
C	-3.712722	-4.225038	-1.305560				C	-2.475043	2.385215	-0.123230
C	-4.702716	-5.204030	-1.340049				C	-1.148924	2.809405	-0.098001
C	-5.253410	-4.699037	0.954549				N	-0.046073	2.000394	-0.082575
C	-3.469011	3.469255	-0.156941				C	1.037967	2.858560	-0.061056
C	-5.475734	5.438450	-0.204818				C	0.596442	4.226161	-0.066720
C	-3.713791	4.224008	-1.305924				C	-0.759245	4.199288	-0.082600

C	2.367688	2.482428	-0.065398	F	5.735673	5.165546	-2.345081
C	2.821621	1.154239	-0.079233	F	3.870218	3.234778	-2.352171
N	2.008993	0.036995	-0.052640	F	5.022847	-5.954978	-2.161183
C	2.866871	-1.027376	-0.057080	F	3.077520	-4.113549	-2.201166
C	4.223052	-0.589492	-0.114158	F	6.578990	-6.247706	0.040010
C	4.191391	0.781778	-0.118533	F	6.159406	-4.682958	2.212759
C	2.484203	-2.387333	-0.019971	F	4.203101	-2.851245	2.198104
Fe	0.002582	-0.000098	0.114973	F	-2.953067	-4.138314	-2.311586
H	-5.079520	1.231967	-0.355529	F	-3.971037	-3.109739	2.169937
H	-5.016899	-1.476386	-0.320334	F	-5.852842	-5.023877	2.174040
H	-1.445861	5.045515	-0.087049	F	-6.293975	-6.501512	-0.053446
H	1.248542	5.099741	-0.066662	F	-4.834966	-6.051525	-2.292183
H	5.036342	1.469675	-0.151640	F	-2.997858	4.099291	-2.336322
H	5.097993	-1.237986	-0.154758	F	-4.270632	2.855116	2.028226
H	-1.239452	-5.101195	0.030128	F	-4.952962	5.929801	-2.374706
H	1.454366	-5.046509	0.058881	F	-6.588759	6.224578	-0.232348
C	3.395683	3.554697	-0.066360	F	-6.237591	4.673748	1.962751
C	5.353769	5.579405	-0.065957				
C	4.106943	3.876991	-1.223929		78		
C	3.694833	4.275040	1.091529		[FeH] ⁻¹		
C	4.659272	5.280808	1.102236	Fe	0.001086	-0.002853	-0.066339
C	5.077787	4.875986	-1.234902	N	-2.003076	-0.113537	0.035398
C	3.556231	-3.407986	-0.000891	N	-0.107507	1.961874	0.000099
C	5.616658	-5.341327	0.025708	N	0.110931	-1.966051	0.032655
C	4.380413	-3.586165	1.115708	N	2.006750	0.109792	0.006363
C	3.805246	-4.230408	-1.104784	C	-2.778465	-1.243797	0.062072
C	4.812987	-5.192186	-1.100245	C	0.937684	2.864429	-0.066445
C	5.400784	-4.533772	1.138657	C	-2.899179	0.923481	0.083065
C	-3.389927	-3.553464	-0.070181	C	-1.248246	2.743335	0.000457
C	-5.368168	-5.559042	-0.059624	C	-0.935083	-2.870010	0.018416
C	-4.160859	-3.807226	1.066558	C	2.782625	1.239617	-0.027449
C	-3.642045	-4.331078	-1.202198	C	1.251849	-2.747551	0.036831
C	-4.615631	-5.328030	-1.206930	C	2.903862	-0.926408	0.049820
C	-5.140717	-4.797279	1.082987	C	-4.162515	-0.921065	0.151452
C	-3.549034	3.403205	-0.149497	C	0.441226	4.217632	-0.117312
C	-5.621226	5.323959	-0.207088	C	-4.238411	0.447604	0.167875
C	-3.763851	4.218276	-1.266065	C	-0.908058	4.143031	-0.071787
C	-4.413764	3.582699	0.936136	C	-0.439350	-4.224380	0.009151
C	-5.440340	4.523529	0.917247	C	4.169172	0.917680	0.011532
C	-4.776753	5.173956	-1.302560	C	0.910430	-4.148888	0.032050
C	-0.014191	0.007985	1.857413	C	4.245766	-0.450311	0.056379
O	-0.025169	0.012580	3.003843	H	-4.980689	-1.639178	0.209897
F	6.270892	6.530322	-0.066504	H	1.060516	5.111879	-0.185899
F	4.923273	5.950680	2.211550	H	-5.131070	1.068931	0.241728
F	3.057416	4.020247	2.218810	H	-1.625462	4.963260	-0.096399

H	-1.059686	-5.120350	-0.007620	F	6.049874	6.725385	-0.328241
H	4.989351	1.635832	0.012057	F	4.653553	6.295340	1.954597
H	1.626692	-4.970273	0.047599	F	-4.285131	2.793551	-2.144374
H	5.141287	-1.071112	0.087735	F	-3.175580	3.907117	2.296260
C	-2.280280	-2.560327	0.026088	F	-5.185839	5.682023	2.345175
C	2.282824	2.554735	-0.084103	F	-6.297029	4.566054	-2.077368
C	2.553764	-2.289877	0.059415	F	-6.757802	6.018462	0.162756
C	-2.550049	2.286916	0.049468	H	-0.005190	-0.013535	-1.551770
C	3.657114	-3.281755	0.084959				
C	4.409397	-3.501917	1.241549		83		
C	4.003082	-4.019333	-1.049812		[FeCO ₂ (H ₂ O)] ⁻¹		
C	5.458652	-4.417523	1.274554	Fe	0.107483	0.013013	-0.024249
C	5.044884	-4.944552	-1.038134	N	-0.004210	-1.947326	-0.159452
C	5.776838	-5.140831	0.128818	N	2.118439	-0.113596	-0.267791
C	3.267940	3.661990	-0.149620	N	-1.843761	0.156995	-0.447536
C	4.006475	3.909552	-1.310047	N	0.234723	1.984396	-0.050430
C	3.513067	4.489410	0.949188	C	-1.157100	-2.710097	-0.160433
C	4.945268	4.936330	-1.380460	C	3.014678	0.920487	-0.220732
C	4.443170	5.525693	0.899288	C	1.031642	-2.857307	-0.159091
C	5.163727	5.746732	-0.270208	C	2.877580	-1.243011	-0.364693
C	-3.651822	3.279941	0.073791	C	-2.737361	-0.877046	-0.584882
C	-4.481774	3.477170	-1.033322	C	1.382881	2.737626	0.098237
C	-3.917639	4.044369	1.212737	C	-2.594591	1.298312	-0.539341
C	-5.529956	4.394502	-1.013301	C	-0.798038	2.893930	-0.030882
C	-4.957132	4.971221	1.253027	C	-0.833248	-4.111718	-0.075013
C	-5.767803	5.143519	0.135441	C	4.350254	0.442854	-0.360535
C	-3.268900	-3.666197	0.012542	C	0.516491	-4.204866	-0.089432
C	-3.491174	-4.466879	1.135691	C	4.265737	-0.921127	-0.449097
C	-4.039370	-3.934029	-1.122433	C	-4.041172	-0.381731	-0.855725
C	-4.429677	-5.496749	1.133267	C	1.049353	4.125721	0.299588
C	-4.986931	-4.954766	-1.145404	C	-3.952314	0.986693	-0.836854
C	-5.182129	-5.738425	-0.011768	C	-0.298366	4.224094	0.222182
F	-6.076417	-6.711335	-0.024244	H	-1.562335	-4.921624	-0.057638
F	-5.697874	-5.191461	-2.235518	H	5.247949	1.061127	-0.379746
F	-3.880947	-3.218229	-2.218989	H	1.124689	-5.109131	-0.082295
F	-4.618067	-6.240583	2.211171	H	5.081223	-1.638052	-0.542709
F	-2.803373	-4.266274	2.245260	H	-4.932323	-0.990411	-1.001856
F	4.136811	-2.838851	2.349673	H	1.770178	4.925563	0.469244
F	6.151328	-4.610981	2.384959	H	-4.748452	1.712817	-1.001989
F	6.768258	-6.014276	0.150981	H	-0.913161	5.119279	0.313599
F	5.349466	-5.632020	-2.126613	C	-2.436552	-2.234511	-0.359440
F	3.336423	-3.859729	-2.177950	C	2.679240	2.267847	0.007579
F	2.855001	4.309661	2.079796	C	-2.127341	2.601938	-0.279417
F	3.824582	3.168685	-2.386462	C	2.376484	-2.558714	-0.283671
F	5.625775	5.153488	-2.493985	C	-0.488970	-0.146062	1.928834

C	-3.124253	3.697932	-0.251944		F	3.800054	-3.338972	-2.610139
C	-3.166805	4.684782	-1.240704		F	5.587121	-5.338744	-2.668677
C	-4.081125	3.774775	0.765759		F	4.825297	-6.171027	1.887828
C	-4.109833	5.710235	-1.218615		F	6.108532	-6.764187	-0.423502
C	-5.037178	4.786738	0.803189					
C	-5.049351	5.758571	-0.193589	83				
C	3.796844	3.234872	0.149333		[FeCO ₂ (H ₂ O)] ²⁻			
C	4.600727	3.244923	1.292574		Fe	0.097676	0.013093	-0.042978
C	4.106209	4.152131	-0.857803		N	0.015550	-1.961121	-0.162298
C	5.667387	4.129798	1.432781		N	2.115798	-0.081470	-0.285210
C	5.165980	5.048706	-0.736273		N	-1.854059	0.125058	-0.469025
C	5.949941	5.034129	0.413130		N	0.201101	1.999724	-0.062016
C	3.352434	-3.674629	-0.320138		C	-1.125644	-2.742463	-0.152396
C	3.645136	-4.428945	0.819427		C	2.997349	0.966571	-0.218996
C	4.031266	-4.007797	-1.495446		C	1.069498	-2.859707	-0.165435
C	4.567461	-5.473042	0.794755		C	2.891625	-1.207395	-0.409007
C	4.962122	-5.042824	-1.541204		C	-2.736489	-0.926574	-0.593209
C	5.230131	-5.778050	-0.390220		C	1.334861	2.770150	0.113672
C	-3.571853	-3.181893	-0.255259		C	-2.626799	1.263796	-0.551030
C	-4.350990	-3.542635	-1.354555		C	-0.851751	2.896298	-0.033041
C	-3.932100	-3.706810	0.989815		C	-0.787065	-4.123054	-0.081405
C	-5.456670	-4.380058	-1.228939		C	4.339849	0.504515	-0.390127
C	-5.032444	-4.546773	1.136926		C	0.582504	-4.196924	-0.101415
C	-5.798474	-4.879869	0.023643		C	4.274523	-0.857356	-0.503902
O	-1.592839	-0.319196	2.334584		C	-4.050896	-0.442896	-0.864299
O	0.685196	0.000571	2.140212		C	0.982184	4.130171	0.344330
O	-4.461327	-0.904628	2.125159		C	-3.980883	0.925292	-0.849428
H	-4.486478	-0.131155	1.547879		C	-0.385392	4.209989	0.249627
H	-3.520809	-0.936991	2.355185		H	-1.502632	-4.946402	-0.076628
F	-6.841941	-5.680592	0.153250		H	5.229519	1.135590	-0.415694
F	-5.355231	-5.036213	2.321065		H	1.200507	-5.095708	-0.111533
F	-3.212033	-3.441116	2.059521		H	5.102203	-1.558868	-0.616466
F	-6.178024	-4.709773	-2.289018		H	-4.935345	-1.062190	-1.012215
F	-4.054815	-3.088697	-2.561632		H	1.685319	4.939521	0.545584
F	-2.301326	4.668382	-2.238180		H	-4.788796	1.638409	-1.019615
F	-4.126383	6.631089	-2.167888		H	-1.014194	5.094614	0.359260
F	-5.949316	6.724933	-0.165142		C	-2.427574	-2.268918	-0.347769
F	-5.926660	4.839318	1.779317		C	2.655212	2.303617	0.021820
F	-4.098303	2.876923	1.733032		C	-2.186911	2.566218	-0.297658
F	3.390608	4.192435	-1.966571		C	2.420470	-2.522394	-0.316865
F	4.362786	2.406833	2.281538		C	-0.406929	-0.144755	1.935924
F	6.410414	4.122794	2.526339		C	-3.193374	3.647383	-0.284292
F	6.957907	5.878471	0.537542		C	-3.206533	4.666562	-1.244870
F	5.437655	5.907179	-1.704894		C	-4.190037	3.704080	0.699879
F	3.041135	-4.169315	1.963396		C	-4.151876	5.689773	-1.229492

C	-5.151516	4.712049	0.725370	H	-4.426689	-0.229159	1.459083
C	-5.130260	5.712195	-0.241158	H	-3.398622	-0.863377	2.333250
C	3.753777	3.278656	0.179872	F	-6.755528	-5.822081	0.246587
C	4.620338	3.230372	1.280896	F	-5.213594	-5.176004	2.378096
C	3.996545	4.292092	-0.757011	F	-3.129778	-3.520243	2.086310
C	5.672245	4.129696	1.439830	F	-6.188669	-4.788775	-2.200167
C	5.034719	5.209330	-0.609470	F	-4.111018	-3.129593	-2.514487
C	5.879486	5.126748	0.492622	F	-2.321292	4.678398	-2.225598
C	3.408494	-3.620142	-0.369040	F	-4.143109	6.635075	-2.162817
C	3.693585	-4.412444	0.750354	F	-6.039092	6.679938	-0.222400
C	4.110493	-3.923985	-1.541905	F	-6.078163	4.742026	1.674945
C	4.621697	-5.450606	0.708280	F	-4.242825	2.795777	1.655709
C	5.051579	-4.949542	-1.601757	F	3.249253	4.398326	-1.841509
C	5.306901	-5.719346	-0.472239	F	4.455996	2.324614	2.225909
C	-3.544406	-3.226633	-0.220302	F	6.469889	4.060011	2.499555
C	-4.354997	-3.594361	-1.297563	F	6.876802	5.991750	0.637760
C	-3.859295	-3.787792	1.025529	F	5.244068	6.150036	-1.524255
C	-5.439536	-4.456987	-1.152577	F	3.092189	-4.187484	1.903133
C	-4.932704	-4.659138	1.188629	F	3.890073	-3.242762	-2.653109
C	-5.729288	-4.991705	0.096903	F	5.695362	-5.214089	-2.733232
O	-1.515613	-0.336816	2.341687	F	4.876225	-6.176934	1.790277
O	0.754167	0.014556	2.213219	F	6.198517	-6.702143	-0.519455
O	-4.357806	-0.869409	2.179552				