Supporting Information

Role of 2nd Sphere H-bonding Residues in Tuning the Kinetics of the CO_2 Reduction to CO by Iron Porphyrin Complexes

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Table S1. The calculated bonding parameters of CO_2 adduct of FePf'.

Parameters	FePf'-CO_2	FePf'-CO_2 +PhOH
d_{Fe-C} (Å)	2.13	1.95
d_{C-O} (Å)	1.23	1.25, 1.27
<O-C-O (°)	138.6	132.5

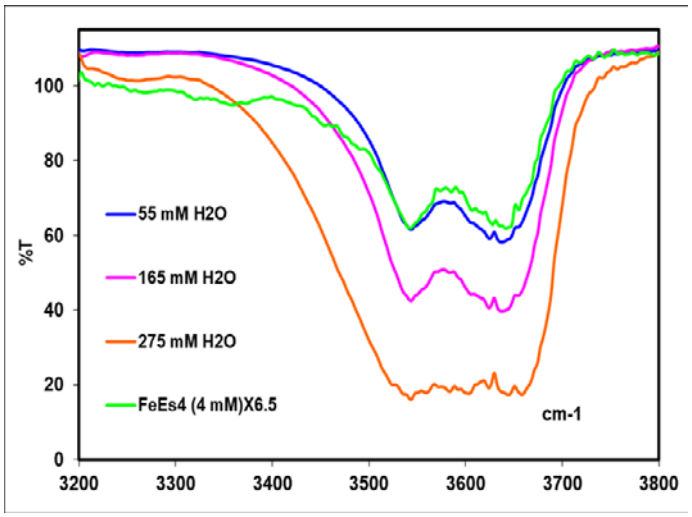

Figure. S1 FTIR data showing quantification of H_2O in $FeEs_4$. Using the O-H stretch of water at 3540 cm^{-1} and 3640 cm^{-1}, we have obtained the calibration curve of water in acetonitrile and compared it with the amount of water obtained from FTIR of re-crystallized $FeEs_4$ sample collected in dry acetonitrile (4 mM). The results indicate that there is approximately 2 water molecules (~8.34 mM) in these samples.

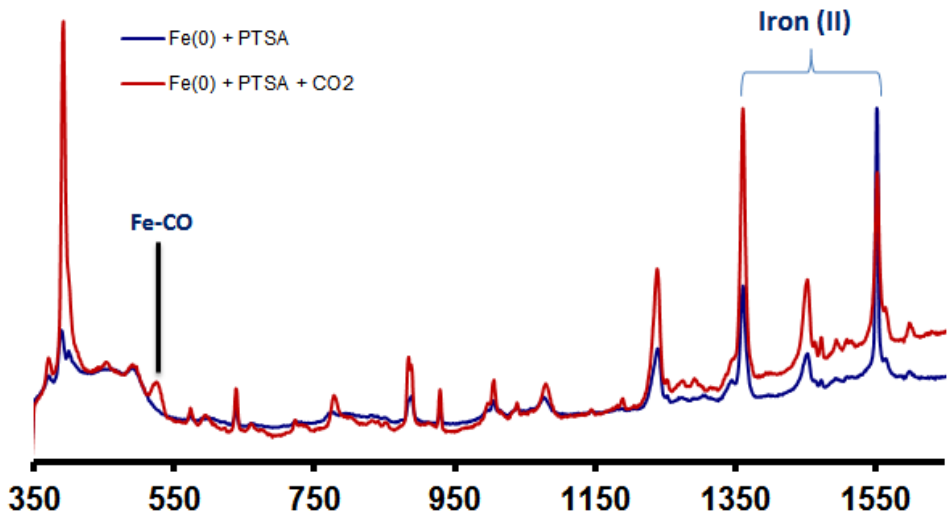

Figure. S2 Both CO_2 (weak acid) and H^+ (strong acid) can react with Fe(0) (base); Both CO_2 (weaker oxidant) and H^+ (stronger oxidant) can oxidize Fe(0) (reductant). Excitation wavelength = 413.1 nm.[3]

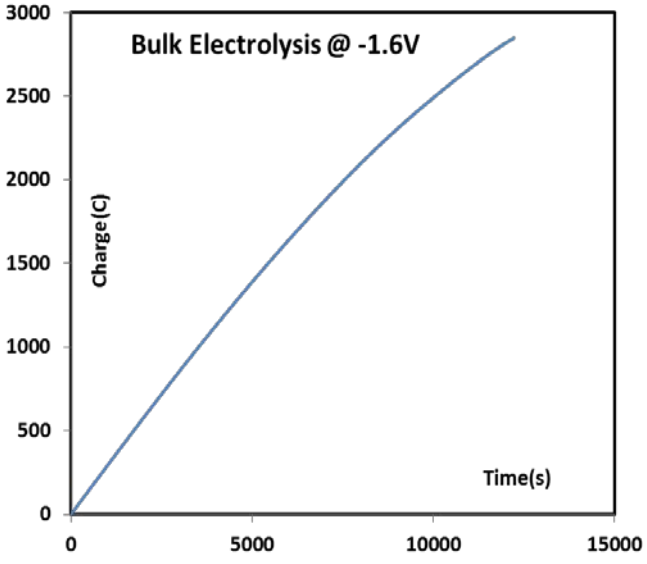

Figure. S3 Bulk electrolysis of FePf on Hg electrode (S=23cm^2). Faradaic yield for CO is 87%.

Table S2. The calculated bonding parameters of CO_2 adduct of various Fe porphyrins.						
Parameters	**Amide Dipole**		**Without distal superstructure**		**H-bond donor**	
	FePf-CO_2‡	**FePfCO_2+PhOH**	**FeTPP-CO_2**	**FeTPP-CO_2+PhOH**	**FeTriazole-$CO_2.H_2O$***	**FeTriazole-$CO_2.H_2O$. PhOH**
d_{Fe-C} (Å)	1.95	1.92	2.00	1.98	2.17	2.12
d_{C-O} (Å)	1.24, 1.25	1.25, 1.26	1.22, 1.25	1.25, 1.24	1.23, 1.23	1.24, 1.23
<O-C-O (°)	138.5	135.0	143.0	137.2	141.6	138.9

* with multiple water molecules (three) the parameters do not change significantly
‡ The binding of CO_2 to hindered side is favored by 3.7 kCal/mole for the FePf complex compared to the unhindered side.

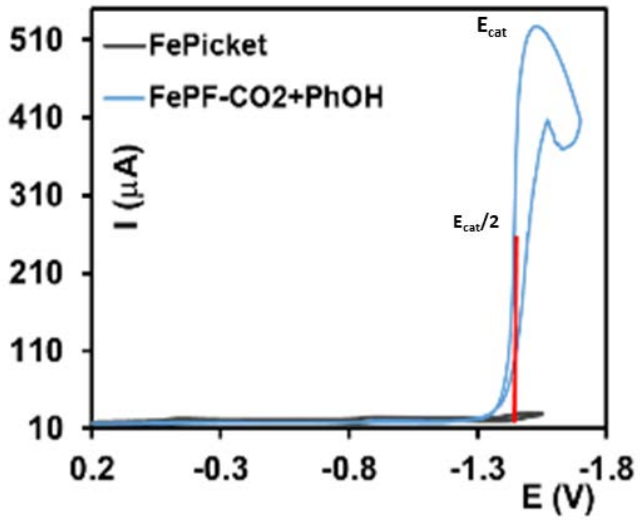

Figure. S4 showing $E^0_{Fe(I/0)} = E_{cat}/2$ for FePf.

Depending on the mechanism $E_{1/2}$ does not always equals to E^0. In fact, this is well documented in *ChemElectroChem,* **2014,** *1,* 1226 – 1236 that the well accepted mechanism for CO_2 reduction with Fe porphyrin is ECEC where,

$E_{1/2} = E^0_{Fe(I/0)} + 1/f \ln [1+ (\sqrt{k_1}C_A^0/ \sqrt{k_2}C_z^0)]$;

Now, $\sqrt{k_2}C_z^0 >> \sqrt{k_1}C_A^0$ ……(*)

Thus, $1/f \ln [1+ (\sqrt{k_1}C_A^0/ \sqrt{k_2}C_z^0)] << 1$

Hence, $E_{1/2} \sim E^0_{Fe(I/0)}$.

*except for CAT (where there is a pre-wave and the scan rate should be increased to get the r.d.s rate constant from the plateau: *J. Am. Chem. Soc.*, **2014**, *136,* 11821–11829; *PNAS,* **2014,** *111,* 14990-14994)

We also showed this for FePf (Fig. S4). The above discussion is further added for clarification.

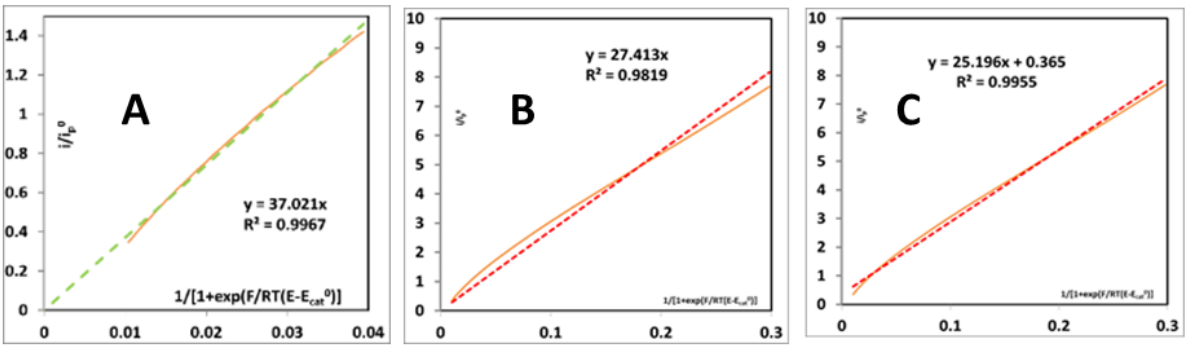

Figure. S5 : Foot-of the-wave analyses (FOWA) of Fe(tBu)4 at different axes ranges (A), (B), and (C), respectively

The Y-axis for plot A is truncated with i_{cat}/i_p up to 1.4 (still fit is taken up to i_{cat}/i_p>1 region).

However, it is not due to the fact that the curve deviates from linearity severely beyond this point. In fact, if plot B is considered, the plot is linear with R^2 = 0.98 from X-axis ranging from 0 to 0.3 with i_{cat}/i_p up to 8. But careful analysis suggests that a good R^2 does not represent a good fit here. Now if plot C is considered, it shows a good fit with an intercept along Y-axis of 0.365 (i_{cat}/i_p<1). Ideally the fit should pass through origin, but it is well accepted in literature that the fit could have a small intercept along Y-axis (*ACS Cent. Sci.*, **2016**, *2,* 850–856). Please note that if points only beyond 0.04 is considered, the fit would have large intercept along Y-axis which is not acceptable. Thus, to avoid confusion, the authors selected the initial range (foot of the wave) with i_{cat}/i_p up to 1.4 (>1) and the fit passing through origin. Also, considering slope of any of the regions would not change the conclusion significantly.

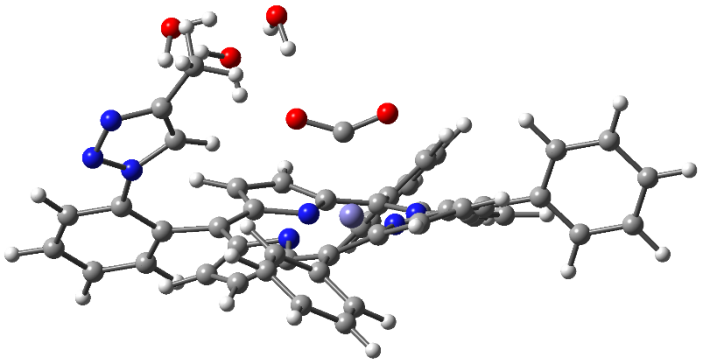

Figure. S6 Optimised structure of CO_2 adduct of Fe porphyrin with triazole and three water molecules (d_{Fe-C} = 2.16 Å; <O-C-O = 141.35°).

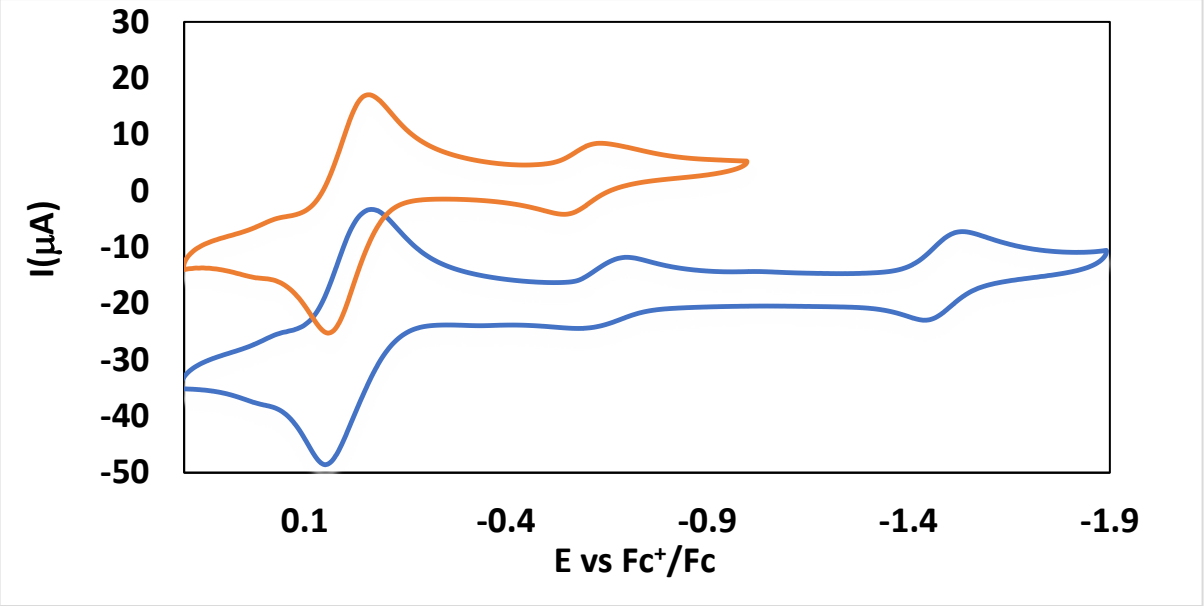

Fig. S7. The CV of 0.5 mM of FeFc4 in dry solvent (blue), in Ar in acetonitrile using glassy carbon as working electrode (GCE), Ag/AgCl as reference electrode and Pt wire as counter electrode. 100 mM TBAP was used as supporting electrolyte. Scan rate = 100 mV/s. Note that, the Fe(III/II) peak is broader due to ligand dissociation upon reduction. The CV Fe(III/II) process in the presence of >20 equivalents of imidazole results in a much more symmetric Fe(III/II) response (orange).[2]

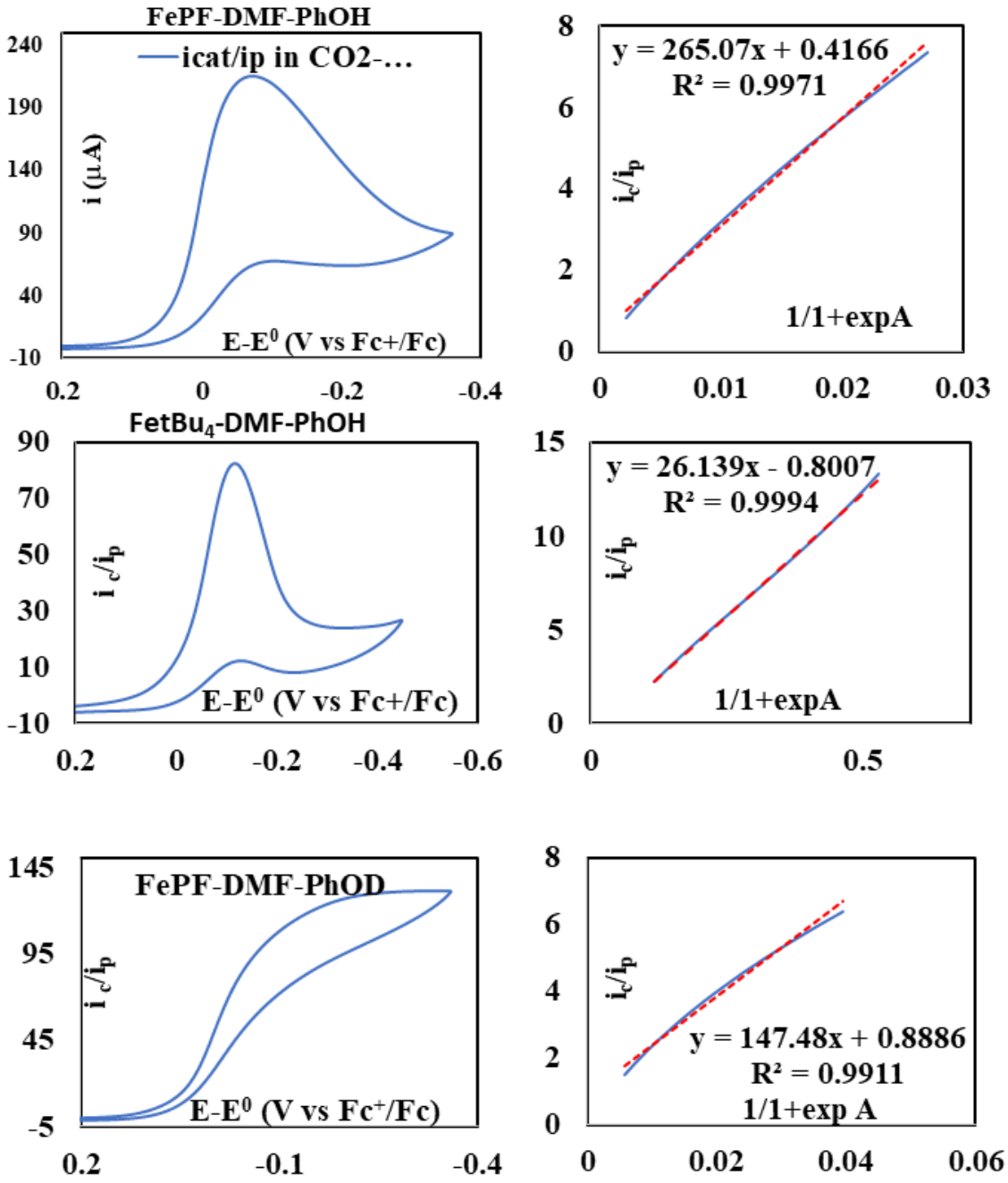

Fig. S8.. Cyclic voltammetry in DMF with 0.1 M n-Bu_4ClO_4 electrolyte at 0.1 V/s of 0.5 mM of the three iron porphyrins (FePF (A), $Fe(tBu)_4$ (B), $FeEs_4$ (C)) with 3 M PhOH in the presence of 0.28 M CO_2 . Foot-of the-wave analyses (FOWA) of the voltammograms in (A), (B), and (C), respectively. The potentials are reported vs Agwire/Ferrocene.

Table-S3: The comparison of experimental rates obtained in this work with those from other iron porphyrins reported in the literature.

Solvent	Catalyst E^0_{cat} ,V vs NHE	k_{cat}, s−1	logTOF, s^{-1}	Ref
DMF/10% H_2O	Fe_2DTPFPP, −1.25	1.6× 10^4	1.5− 3.9, 4.2	4
DMF/10% H_2O	Fe_2DTF_2PP, −1.34	3.7× 10^4	2.0− 4.3, 4.5	4
DMF/10% H_2O	Fe_2DTCl_2PP, −1.35	4.1× 10^3	1.8− 3.5, 3.6	4
DMF/10% H_2O	Fe_2DTPP, −1.40	2.0× 10^4	2.4− 4.2, 4.3	4
DMF/10% H_2O	Fe_2DTMP, −1.60	4.1× 10^3	2.3− 4.8, 5.8	4
DMF/10% H_2O	Fe_2TPFPP,−TMP −1.35	7.3× 10^5	2.8− 4.3, 4.7	4
DMF/10% H_2O	FeTPP, − 1.41	2.1× 10^3	1.4− 3.1, 3.3	4
DMF/5% H_2O /3M PhOH	CAT ,−1.35	>5.0× 10^6	1.8− 3.2, 3.8	5
DMF/5% H_2O /3M PhOH	FCAT ,−1.28	>5.0× 10^6	1.6− 3.8, 4.0	5
DMF/5% H2O /3M PhOH	FeTPP,−1.43	3.5× 10^4	2.5− 4.3, 4.5	5
DMF,100mMPhOH	Fe–ortho-1-amide ,-2.12	2.24 *10^4	4.35	6
DMF,100mMPhOH	Fe–ortho-2-amide,-1.466	5.50 *10^6	6.74	6
DMF,100mMPhOH	Fe–para-1-amide,-2.15	1.70 *10^2	2.23	6
DMF,100mMPhOH	Fe–para-2-amide ,-2.16	6.76 *10^3	3.84	6
DMF,3M PhOH	Fe-o-TMA	>10^6	6	7
MeCN,3MPhOH	FePF,-1.273	5.0*10^6	5.7	This work
MeCN,3MPhOH	$Fe(tBu)_4$,-1.193	1.0*10^3	3	This work
MeCN,3MPhOH	$FeEs_4$,-1.153	2.5*10^2	2.397	This work

Coordinates of optimized geometry[1]

$Fe(OH)_4$-CO_2

	X	Y	Z
Fe	3.56147600	37.71278000	8.30334500
N	1.75223500	37.54046900	7.52494300
N	4.36583300	37.44127800	6.52051900
N	5.35902200	37.49889900	9.09889300
N	2.74658800	37.64469900	10.10101600
C	1.40525900	37.42678800	10.45743700
C	1.22123400	37.68486100	11.85235000
H	0.26715100	37.61236900	12.37538600
C	2.44536100	38.09491800	12.36142600
H	2.68913300	38.38416400	13.38442400
C	3.38751100	38.02292300	11.28989000
C	4.78070700	38.18906600	11.43041100
C	5.69067100	37.78206300	10.42784500
C	7.07151800	37.50685200	10.66646700
H	7.56778200	37.61922500	11.63123800
C	7.59735600	37.00783000	9.48137400
H	8.60607900	36.63181400	9.30422600
C	6.55117700	37.06020900	8.50053900
C	6.72046200	36.81935000	7.11481200
C	5.68988700	37.11052300	6.18763900
C	5.88633800	37.23517300	4.77651700
H	6.83279800	37.05757800	4.26490300
C	4.68906500	37.67653100	4.23075500
H	4.46148500	37.89265200	3.18619100
C	3.74668900	37.75494300	5.30180800
C	2.36582100	37.99232600	5.14402700
C	1.43570000	37.72477500	6.17523200
C	0.04216700	37.50521500	5.95568500
H	-0.44780300	37.55790500	4.98263600
C	-0.50973200	37.14193600	7.17823600
H	-1.53628400	36.83411300	7.38251900
C	0.53813600	37.22353300	8.15521300
C	0.35622600	37.11877300	9.55644300
C	5.33591300	38.75603900	12.69493400
C	5.45073600	38.02954300	13.89653000
H	5.10981900	36.98719500	13.89814400
C	5.98907100	38.60315100	15.06322600

H	6.06974100	38.01185300	15.98398000
C	6.42924000	39.93757300	15.02990100
H	6.85592800	40.40136800	15.92955400
C	6.32401900	40.68990300	13.85098100
H	6.64968400	41.73586800	13.81039400
C	5.77572000	40.11356100	12.68393900
C	8.03752000	36.36473100	6.58129100
C	9.21736500	37.16005600	6.70488100
C	10.43699200	36.73653900	6.14045500
H	11.31282000	37.38580000	6.25616600
C	10.51186300	35.52591900	5.43508300
H	11.46866300	35.20928200	4.99956700
C	8.15219900	35.15283100	5.86163300
H	7.24777500	34.54305700	5.75307000
C	9.36308900	34.72804000	5.29143200
H	9.40940700	33.77813200	4.74425100
C	1.84055500	38.48394600	3.83621300
C	1.69344600	37.67208300	2.69402900
H	1.98627200	36.61829400	2.77471500
C	1.18201400	38.17678400	1.48419600
H	1.07496900	37.51969100	0.61199200
C	0.80172300	39.52790500	1.41203500
H	0.39604500	39.93880000	0.47762400
C	0.94084100	40.36429300	2.52930300
H	0.66267500	41.42382500	2.48723200
C	1.46318200	39.85695700	3.73943800
C	-0.98659000	36.80234400	10.12309600
C	-1.17403600	35.68396500	10.96875800
H	-0.30705800	35.03776600	11.14837600
C	-2.40738300	35.39560000	11.57464000
H	-2.50938400	34.51475600	12.22086500
C	-3.50720000	36.23940100	11.33861300
H	-4.48103900	36.02874900	11.79977200
C	-3.36019800	37.35976000	10.50718700
H	-4.19546300	38.04400200	10.31702400
C	-2.11766200	37.64847600	9.90861700
H	5.21502700	40.39872700	10.85126300
H	2.04066200	40.26009800	5.54425100
H	8.33173000	38.44797200	7.78995100
H	-1.16696200	38.76268400	8.68992100
C	3.62636700	39.88941900	8.21066300

O	4.24111200	40.33728700	9.17622600
O	3.03795100	40.28986600	7.20852900
O	1.59676300	40.72049300	4.77773900
O	5.67912300	40.89782400	11.58078300
O	-2.04554300	38.78495000	9.14971700
O	9.21351500	38.37065500	7.34248300

$Fe(OH)_4$-CO_2+PhOH

	X	Y	Z
Fe	3.66819200	37.69260800	8.05470900
N	1.78925500	37.47588100	7.27789600
N	4.48653900	37.27884100	6.17371000
N	5.54706400	37.49335200	8.82268600
N	2.84239700	37.29064500	9.93487400
C	1.49960000	37.16314400	10.27028200
C	1.35324100	37.19015800	11.71786900
H	0.41271600	37.06865800	12.25709000
C	2.59739500	37.43483700	12.24202400
H	2.87255600	37.56175800	13.29021600
C	3.52529000	37.49273200	11.12531700
C	4.90471800	37.73659600	11.23468700
C	5.85703800	37.60686600	10.17108700
C	7.26578400	37.43929700	10.37227000
H	7.76733300	37.45681400	11.34080100
C	7.82208400	37.17043700	9.12620900
H	8.85703100	36.90408500	8.90510900
C	6.75082000	37.22487200	8.16594600
C	6.89804700	37.05537500	6.74852000
C	5.82565100	37.14223300	5.83252900
C	5.97781100	37.27510700	4.39101400
H	6.92386600	37.21789000	3.85178900
C	4.73470500	37.55486300	3.88065200
H	4.46288100	37.74753100	2.84145100
C	3.80587700	37.55425100	4.99506500
C	2.42643400	37.81366700	4.88840800
C	1.47393000	37.69882900	5.94373800
C	0.04593800	37.71862500	5.76999000
H	-0.46721300	37.87375100	4.81973700
C	-0.51477300	37.47282700	7.01261200
H	-1.57262800	37.41233400	7.27048000
C	0.57307100	37.33397600	7.94462300

C	0.42998600	37.14796500	9.35355700
C	5.43402000	38.25467400	12.53388500
C	5.76149600	37.44639600	13.63856200
H	5.61684300	36.36327100	13.54330800
C	6.26508000	37.99445800	14.83277000
H	6.51362500	37.34222500	15.67914800
C	6.44934500	39.38478300	14.92268800
H	6.84280300	39.83077400	15.84589100
C	6.12634000	40.21628300	13.84059800
H	6.24786100	41.30379500	13.90011800
C	5.61426700	39.66604800	12.64486100
C	8.27032400	36.86229000	6.19134200
C	9.30722400	37.82751000	6.38069300
C	10.56861000	37.65544400	5.77637300
H	11.32650100	38.42986100	5.94188600
C	10.83183900	36.53256900	4.97784900
H	11.81948900	36.41559100	4.51315000
C	8.57871500	35.73579400	5.39301600
H	7.79008500	34.98821700	5.24920700
C	9.83275400	35.56317400	4.78530100
H	10.02785300	34.67507600	4.17147700
C	1.92553400	38.35921600	3.58612600
C	1.47409100	37.55551500	2.52324900
H	1.49056100	36.46743600	2.66081900
C	1.01399800	38.11266400	1.31597300
H	0.66822000	37.46323400	0.50227100
C	1.00361200	39.51069900	1.17062200
H	0.64773300	39.96585400	0.23654400
C	1.44794400	40.33683800	2.21194700
H	1.45138100	41.42832300	2.11283200
C	1.91229000	39.77683600	3.42443700
C	-0.96091400	36.97117300	9.88479300
C	-1.67735900	35.78318200	9.62322900
H	-1.17281600	35.00950200	9.03258700
C	-2.98433700	35.57409300	10.09159200
H	-3.50615500	34.63461300	9.87198700
C	-3.60812900	36.58160200	10.84811800
H	-4.62885900	36.44051500	11.22746000
C	-2.92977300	37.77597200	11.11895400
H	-3.39926000	38.58099400	11.69590900
C	-1.61633300	37.98701500	10.63996000

H	4.87653000	40.05108000	10.87668500
H	2.66466800	40.15699200	5.19543900
H	8.29456200	38.84621400	7.63944300
H	-0.14689700	39.29722600	10.54633500
O	1.25590300	40.59080300	10.19994100
H	2.18580000	40.37942800	9.84580900
C	1.04428000	41.93482800	10.21603600
C	-0.19557400	42.41049400	10.70197100
C	2.01971400	42.85721300	9.76970900
C	-0.44581800	43.78868700	10.74396300
H	-0.94177500	41.68060400	11.03267900
C	1.74934200	44.23156900	9.82105400
H	2.96893100	42.47098400	9.38233200
C	0.52089700	44.71281500	10.30815300
H	-1.41338800	44.14433900	11.12276000
H	2.51436200	44.93586100	9.46957300
H	0.31819100	45.79040000	10.34292800
C	3.61313400	39.63652200	8.05495000
O	3.46762200	40.17102700	6.94327700
O	3.71236100	40.13093200	9.23167100
O	2.33521800	40.63645600	4.38153500
O	5.30363600	40.52797800	11.64383900
O	9.12750500	38.96717200	7.11395200
O	-1.05190400	39.18449500	10.94938400

FePF-CO_2

	X	Y	Z
Fe	3.50807700	37.81877200	8.07533200
N	1.82853200	37.56917800	6.91239200
N	4.68208400	37.66670700	6.33036800
N	5.21558300	37.63637300	9.21532100
N	2.42843100	37.02177100	9.71793200
N	4.99838200	39.27329600	13.14635200
N	8.13995200	40.33081300	6.54795500
N	1.63759700	40.11766300	3.50936100
N	-1.44810200	39.05175600	10.10588200
C	1.04028600	36.90785400	9.77796600
C	0.62855200	36.62738100	11.13748300
H	-0.39900000	36.45570700	11.46240600
C	1.76583100	36.63470300	11.90994500
H	1.84102600	36.48827400	12.98784400

C	2.88176600	36.90400600	11.01962100
C	4.22039500	37.09817500	11.45048600
C	5.31135200	37.42047000	10.58480700
C	6.69196300	37.49590400	11.00333200
H	7.05030300	37.34515300	12.02285800
C	7.44586400	37.74341500	9.87124300
H	8.52933300	37.84428600	9.80198800
C	6.53164000	37.78995200	8.75888000
C	6.92546100	37.87403400	7.39590700
C	6.06534800	37.80334800	6.27658400
C	6.49450900	37.91902000	4.89760200
H	7.52950100	38.01206600	4.56343900
C	5.35721800	37.90288500	4.12255900
H	5.28764700	37.99749400	3.03843500
C	4.22964000	37.75584100	5.02833000
C	2.86511000	37.78833500	4.63485100
C	1.75207000	37.68171400	5.52889000
C	0.37301900	37.59837500	5.10443000
H	0.03011300	37.63110300	4.06903500
C	-0.39348600	37.42098300	6.24222400
H	-1.47508400	37.29757300	6.30447400
C	0.51659700	37.37208800	7.35641600
C	0.14865800	37.08720400	8.69893400
C	4.51273000	36.91030000	12.90696000
C	4.38741900	35.63744100	13.50411800
H	4.09323700	34.80254600	12.85814300
C	4.62883100	35.42586100	14.87051800
H	4.52470300	34.42055000	15.29778600
C	5.01483900	36.50894400	15.67603000
H	5.21286400	36.36263500	16.74561600
C	5.14970500	37.79224500	15.12534000
H	5.43508800	38.65209600	15.73354000
C	4.89900200	38.00021500	13.75122300
C	5.36353700	40.47781500	13.70127900
C	8.40229500	37.99274000	7.13107200
C	9.00154300	39.22656900	6.73636700
C	10.39920600	39.31053400	6.53842400
H	10.82367300	40.27339200	6.25045100
C	11.19976900	38.17468700	6.72239400
H	12.28299400	38.25498600	6.56453400
C	9.24096800	36.87426400	7.30264100

H	8.77449700	35.93144000	7.60886100
C	10.62863100	36.94977300	7.10182800
H	11.25478000	36.06009400	7.24225100
C	8.45144500	41.63043500	6.21391300
C	2.57638500	37.90884100	3.17051800
C	2.92808000	36.87002000	2.28207200
H	3.38762900	35.97182600	2.70975900
C	2.70554900	36.96239800	0.89922000
H	2.98980000	36.13243100	0.24011300
C	2.10830700	38.11953100	0.37467400
H	1.92324700	38.20871600	-0.70349400
C	1.74224100	39.17719600	1.22082300
H	1.29024600	40.09256900	0.83530300
C	1.97246600	39.08018200	2.61069500
C	1.06775500	41.34421200	3.25797300
C	-1.31704800	36.89898300	8.97360800
C	-1.95772700	35.72508600	8.52977200
H	-1.34659000	34.98353200	8.00339800
C	-3.32603900	35.49697600	8.74256900
H	-3.79350900	34.57028500	8.38744800
C	-4.07949000	36.46908500	9.41800700
H	-5.15144200	36.31408800	9.59661900
C	-3.47962600	37.65010700	9.87566400
H	-4.05163900	38.41454700	10.40229600
C	-2.09856400	37.87709300	9.66134300
C	-1.97224000	40.09971100	10.84271300
O	-3.16514000	40.16653500	11.18609800
O	9.61384100	42.04907000	6.06550600
O	5.63483800	40.63608500	14.90603000
O	0.78861800	41.76263600	2.11923500
H	4.79497000	39.25481200	12.14123300
H	1.82340600	39.87400800	4.48830900
H	7.14740100	40.08990200	6.64467600
H	-0.44234100	39.07465600	9.89674500
C	0.79442700	42.23558200	4.50813400
C	-0.95654200	41.21517500	11.22473700
C	7.24098000	42.59957700	6.05491400
C	5.42226500	41.69372900	12.72655400
C	3.03242700	39.62928100	8.62871600
O	3.68114900	40.08160800	7.65026000
O	2.34771300	40.05737900	9.56490400

C	6.81709200	42.33980400	12.91682900
H	6.87575100	43.28901500	12.35207600
H	7.00356500	42.54064100	13.98515900
H	7.61558400	41.67242700	12.54392800
C	5.21348000	41.34711400	11.23811400
H	5.95431200	40.60951800	10.87800700
H	4.20015500	40.96510900	11.01489600
H	5.34164100	42.26096000	10.62835900
C	-0.64938800	42.77426600	4.35986500
H	-1.38752800	41.95814600	4.46610000
H	-0.85742200	43.52483900	5.14513700
H	-0.78581600	43.23685300	3.36822900
C	0.93484900	41.51208000	5.86402700
H	0.27580100	40.62668600	5.92680300
H	1.96775900	41.19018900	6.09431000
H	0.63942500	42.19942200	6.67795800
C	1.79071900	43.42047200	4.43176800
H	1.58201300	44.14693000	5.23958900
H	2.83211300	43.07047500	4.55097300
H	1.70437400	43.93509800	3.45858300
C	0.20258000	40.62146700	12.06593500
H	0.83660400	39.92725600	11.48953600
H	0.85981700	41.44162800	12.41242200
H	-0.18338800	40.09501600	12.95815400
C	-1.71255700	42.26844200	12.06143000
H	-2.54857100	42.70840100	11.49086400
H	-2.13729300	41.82383200	12.97792000
H	-1.01523400	43.07666900	12.35059300
C	-0.39321000	41.88395300	9.94389000
H	-1.20957100	42.22013200	9.27769300
H	0.20426100	42.77143200	10.22602700
H	0.28320400	41.21398800	9.38711300
C	7.51706000	43.45757800	4.79708900
H	8.52530200	43.90058800	4.84799300
H	7.45580400	42.84422600	3.87915400
H	6.76627800	44.26564900	4.71629600
C	5.87324700	41.90019500	5.91143800
H	5.53463200	41.37651200	6.82373400
H	5.09762000	42.65771000	5.69266100
H	5.86761900	41.17395700	5.07827000
C	7.24016200	43.51392800	7.30757900

H	6.45408500	44.28667300	7.21372900
H	7.03532900	42.93169900	8.22387000
H	8.21801300	44.01425900	7.42267900
C	4.33093100	42.68917400	13.19468800
H	4.39911700	43.62961200	12.61601300
H	3.32027700	42.26905200	13.04113400
H	4.45484800	42.91855700	14.26736500

FePF-CO_2+PhOH

	X	Y	Z
Fe	3.45514900	37.88657800	7.98652900
N	1.71692300	37.45298500	6.95335600
N	4.50565500	37.53321500	6.17457100
N	5.28025000	37.84399000	8.95820500
N	2.52527000	37.22400300	9.74746300
N	4.88148900	39.98462600	12.81763300
N	8.94065500	39.72163400	7.24315200
N	1.14298200	39.85820700	3.46386500
N	-1.55537000	38.78182600	10.18132400
C	1.17682500	36.97110700	9.91980600
C	0.88307700	36.79879000	11.33505200
H	-0.09695800	36.55734800	11.75001500
C	2.05873000	37.01056300	12.01544800
H	2.22170400	36.98373000	13.09369200
C	3.07972100	37.28337200	11.01982000
C	4.42386100	37.59518300	11.30940700
C	5.45403900	37.81939700	10.34764100
C	6.85659300	37.84200500	10.66910900
H	7.27109100	37.80901200	11.67766300
C	7.54537000	37.80516300	9.46891000
H	8.62466700	37.74508100	9.32291100
C	6.55958600	37.79888600	8.41583200
C	6.85569600	37.67924500	7.01965500
C	5.87863800	37.59856000	5.99723400
C	6.19129400	37.66972800	4.57940300
H	7.19529900	37.75026100	4.16264900
C	4.99813100	37.69489800	3.90470200
H	4.84473000	37.78750700	2.82963100
C	3.94465000	37.60676500	4.89923000

C	2.56515800	37.61644700	4.60464300
C	1.52185700	37.50586600	5.57126500
C	0.13098300	37.30934300	5.26002700
H	-0.29252800	37.27266300	4.25502100
C	-0.52671900	37.11617600	6.46379000
H	-1.58780400	36.91923700	6.61999300
C	0.47011600	37.18032200	7.50333900
C	0.20691500	36.94387200	8.88955800
C	4.83345400	37.56448800	12.75626500
C	4.98952000	36.33120300	13.41857100
H	4.81705500	35.41750000	12.83919100
C	5.34947400	36.25861900	14.77415400
H	5.46247300	35.28296100	15.26250200
C	5.56454500	37.44638400	15.48965500
H	5.84709800	37.41057200	16.54954400
C	5.42053100	38.69416400	14.86580200
H	5.56999300	39.62924200	15.40727800
C	5.05713900	38.76017200	13.50154100
C	4.95853600	41.27007100	13.30637100
C	8.28236200	37.46969700	6.60476300
C	9.30764500	38.45966800	6.72287000
C	10.63112900	38.17285600	6.31659900
H	11.38296100	38.95572800	6.42441300
C	10.94861700	36.91600500	5.78376300
H	11.98149200	36.71232200	5.47362800
C	8.64680800	36.22029200	6.05384500
H	7.86159900	35.46173500	5.96331700
C	9.95623200	35.93347000	5.64276600
H	10.19812400	34.94763900	5.22647000
C	9.74580700	40.79142100	7.56427400
C	2.16634700	37.67177000	3.15943400
C	2.48248100	36.59615400	2.30290200
H	2.99577300	35.73350300	2.74154300
C	2.16700200	36.61382600	0.93556700
H	2.43149900	35.76052100	0.29897600
C	1.51139700	37.73201700	0.39920100
H	1.25866000	37.76823100	-0.66809200
C	1.16931800	38.81810900	1.21773700
H	0.67047400	39.70163600	0.81729900
C	1.48461800	38.79483000	2.59498700
C	0.55613200	41.06960300	3.16439100

C	-1.20205600	36.57535300	9.25967900
C	-1.70572500	35.29557300	8.95403900
H	-1.03349000	34.59155900	8.45086000
C	-3.01827200	34.91690600	9.27869500
H	-3.37806700	33.91021300	9.03263200
C	-3.85750300	35.83780000	9.92626400
H	-4.88527000	35.55835400	10.19146100
C	-3.39886500	37.12445600	10.24138300
H	-4.03546500	37.85724000	10.73970200
C	-2.07743600	37.49962200	9.90757800
C	-2.13224100	39.83986300	10.85152900
O	-3.29403400	39.82585100	11.29340000
O	10.97514400	40.82023600	7.36941900
O	5.22260500	41.54743300	14.49019600
O	0.29904500	41.44622600	2.00625900
H	4.65070700	39.86243200	11.82591600
H	1.32362800	39.65190500	4.45198100
H	7.93355900	39.81660900	7.40539900
H	-0.58394600	38.88752700	9.86634400
C	0.20193500	41.98651200	4.37317200
C	-1.18554000	41.05619100	11.07752500
C	9.04825400	42.01499600	8.23068000
C	4.69389400	42.41496300	12.28298500
O	6.08346400	40.98578300	5.51592800
H	5.21243100	40.65096100	5.90520700
C	5.88447100	41.49306600	4.27343900
C	6.97535700	42.11496200	3.62284800
C	4.63953700	41.41499800	3.60567200
C	6.81447800	42.65769800	2.34048100
H	7.94149900	42.15082100	4.13835800
C	4.49308100	41.96242500	2.32296400
H	3.80540200	40.90584100	4.09782700
C	5.57442900	42.59175500	1.68031900
H	7.67281400	43.13672800	1.85105200
H	3.52005900	41.88601400	1.82280400
H	5.45391700	43.01680200	0.67672200
C	3.36461200	39.77470400	7.64793000
O	3.74195100	40.52719200	6.72336600
O	2.71033100	39.92987200	8.71166000
C	5.95175100	43.31965300	12.30343300
H	5.77833000	44.22416100	11.69090500

H	6.18850600	43.62336200	13.33717300
H	6.82771900	42.78983400	11.88695300
C	4.41394500	41.94913300	10.84119500
H	5.26146100	41.38334200	10.41481000
H	3.50743000	41.32669300	10.74174300
H	4.26194800	42.82883400	10.18945100
C	-1.31338700	42.28951200	4.25411100
H	-1.91543200	41.37750500	4.42315800
H	-1.61017300	43.03790200	5.01266700
H	-1.54914200	42.68031800	3.24985300
C	0.50073600	41.38360500	5.76010400
H	-0.03677000	40.43126800	5.92719000
H	1.57959100	41.21648700	5.93433000
H	0.16268800	42.08704400	6.54345800
C	1.00199700	43.30002400	4.18636100
H	0.70725700	44.03613900	4.95784500
H	2.08800700	43.12196200	4.28095600
H	0.80631000	43.72912000	3.18864700
C	-0.26470400	40.70764200	12.27739600
H	0.35809300	39.81915700	12.07197800
H	0.41188300	41.55633700	12.49257600
H	-0.86244400	40.50674300	13.18554200
C	-2.05891400	42.27663600	11.43547200
H	-2.69345700	42.57595300	10.58160400
H	-2.72656800	42.04662300	12.28156900
H	-1.41291800	43.13306900	11.70375400
C	-0.32672700	41.38600800	9.83232700
H	-0.95734300	41.51969600	8.93459700
H	0.21729900	42.33343700	10.00417400
H	0.44710200	40.63217800	9.59986100
C	9.79609900	42.26192500	9.56537600
H	9.62596200	41.43019100	10.27345700
H	10.88097200	42.34881000	9.38648000
H	9.43027200	43.19290600	10.03769700
C	9.26578600	43.22676900	7.29137500
H	8.69717000	43.10575400	6.35184100
H	8.91751100	44.15597900	7.78078600
H	10.33627700	43.33233000	7.04460700
C	7.54411200	41.83005800	8.50787700
H	7.15307000	42.72465000	9.02687400
H	6.95898300	41.71061300	7.57792300

H	7.35674800	40.96057800	9.16565200
C	3.48436400	43.21829600	12.82262600
H	3.32119800	44.12137700	12.20520400
H	2.56007700	42.61286500	12.78993100
H	3.66221000	43.52397300	13.86775300

FeTPP-CO_2

	X	Y	Z
Fe	3.52018000	37.85359400	8.07581200
N	1.67408900	37.49842300	7.18965000
N	4.41246100	37.61368100	6.15048000
N	5.41493700	37.65437900	8.90479600
N	2.70087800	37.13435200	9.92840200
C	1.34521000	37.13537800	10.21997900
C	1.14878300	37.24552400	11.65245200
H	0.18458600	37.32082200	12.15697200
C	2.39760500	37.29792800	12.22497800
H	2.63780700	37.42502300	13.28132800
C	3.36149300	37.21954800	11.14442200
C	4.77070600	37.27290000	11.31161300
C	5.71275600	37.37252200	10.23926300
C	7.12314500	37.11861300	10.38274200
H	7.61804200	36.81300600	11.30555900
C	7.69250900	37.26220300	9.13184900
H	8.73449500	37.09826000	8.85367100
C	6.63140200	37.60840200	8.22283200
C	6.80936300	37.82151100	6.82045100
C	5.74890000	37.88485300	5.88056600
C	5.90042700	38.27309900	4.49339800
H	6.83208900	38.58870000	4.02235300
C	4.65209900	38.22084300	3.92144900
H	4.38008200	38.48623000	2.89916100
C	3.72852300	37.80046300	4.95485800
C	2.33212000	37.63435600	4.76833800
C	1.40171300	37.39035600	5.82586400
C	0.04718200	36.94503300	5.62798300
H	-0.40829100	36.71867700	4.66296400
C	-0.51943300	36.80314900	6.88034300
H	-1.51957500	36.43850400	7.11867700
C	0.48985900	37.15617800	7.84523500
C	0.29915000	37.08722700	9.26128900

C	5.31134600	37.20117500	12.69320900
C	4.89471900	36.19714200	13.61119600
H	4.16904700	35.45051600	13.27084400
C	5.39967900	36.13922800	14.91821300
H	5.05737400	35.34342500	15.59399800
C	6.35109000	37.07554200	15.36105000
H	6.74945000	37.02817400	16.38283600
C	6.78563100	38.07364900	14.46643100
H	7.51959100	38.82230000	14.79418800
C	6.27678100	38.13361400	13.16237300
C	8.19950600	37.97377500	6.31968400
C	9.11197700	38.87904900	6.92704100
C	10.42348700	39.02820700	6.45701300
H	11.09300300	39.74945700	6.94496000
C	10.88106700	38.27626100	5.35691200
H	11.90843900	38.39301300	4.98828700
C	8.68639800	37.21924400	5.21659900
H	8.01281300	36.49666600	4.74330300
C	9.99735300	37.37141600	4.74203500
H	10.33722500	36.76468800	3.89147100
C	1.79611000	37.70710800	3.38493100
C	2.36474000	36.95686500	2.31857400
H	3.21088000	36.29746800	2.54044100
C	1.86023500	37.03558500	1.01234600
H	2.32357500	36.43459800	0.21782800
C	0.75920300	37.85964800	0.71813500
H	0.36185700	37.91887900	-0.30343300
C	0.17412000	38.60563700	1.76037800
H	-0.67900000	39.26510300	1.55097000
C	0.68182600	38.52970000	3.06404200
C	-1.09313200	36.93629900	9.75693100
C	-1.45085300	35.92888000	10.69515200
H	-0.67213500	35.23970300	11.03930300
C	-2.76483400	35.79643900	11.16730900
H	-3.00233200	35.00045400	11.88640700
C	-3.77917900	36.65871600	10.71386300
H	-4.80853500	36.55284400	11.08023500
C	-3.44983100	37.65898100	9.77778500
H	-4.22395800	38.35078000	9.41904000
C	-2.13586300	37.79316000	9.31012800
C	3.53672200	39.84486500	7.85935500

O	3.91326000	40.59567300	6.97308700
O	3.01463100	39.82194500	8.99553600
H	-1.88504400	38.58075400	8.59153200
H	8.75964900	39.47692000	7.77428700
H	6.61109300	38.92033300	12.47751800
H	0.22955500	39.12298900	3.86592200

FeTPP-CO_2+PhOH

	X	Y	Z
Fe	3.48368300	37.76329700	8.08249200
N	1.64939800	37.40850800	7.18604500
N	4.39245300	37.61203000	6.16381600
N	5.35767100	37.62149700	8.92419800
N	2.65227200	37.07668800	9.90712500
C	1.29019000	37.01207500	10.18263900
C	1.07263800	37.10753500	11.61296800
H	0.09925000	37.13330100	12.10391200
C	2.30856700	37.21747100	12.19988500
H	2.52954600	37.35668800	13.25864700
C	3.29206700	37.18456200	11.13459100
C	4.69051600	37.27876600	11.32551400
C	5.64613900	37.38034800	10.26462500
C	7.05966800	37.16848700	10.43274500
H	7.54935800	36.90319400	11.37043800
C	7.64303700	37.30295000	9.18672000
H	8.69312700	37.16701900	8.92582100
C	6.58665400	37.60052500	8.25797700
C	6.77817400	37.81081900	6.85840200
C	5.73124300	37.88125600	5.90975400
C	5.89691200	38.29817900	4.53010400
H	6.83494300	38.61569400	4.07348300
C	4.65283300	38.26830100	3.95127300
H	4.38700900	38.56387600	2.93575800
C	3.71862300	37.82779200	4.97043300
C	2.32486200	37.67744200	4.77644900
C	1.39001700	37.37690600	5.81930200
C	0.04552400	36.91999800	5.58344100
H	-0.39743700	36.74557100	4.60216600
C	-0.52973900	36.69240000	6.81981700
H	-1.52674700	36.30277800	7.02855900
C	0.46399800	37.01235900	7.80869100

C	0.26138200	36.90967000	9.21911500
C	5.21433600	37.24684100	12.71638200
C	4.84417700	36.22613700	13.63317000
H	4.16675800	35.43688900	13.28916500
C	5.33615200	36.20591600	14.94674600
H	5.03188900	35.39762600	15.62548200
C	6.22606800	37.19915300	15.39125400
H	6.61351100	37.18254100	16.41804000
C	6.61290600	38.21563800	14.49626600
H	7.29662100	39.00808000	14.82820100
C	6.11734400	38.23769600	13.18573200
C	8.17420200	37.97267000	6.36887700
C	9.06270900	38.91013500	6.95777800
C	10.37545600	39.06729500	6.49219600
H	11.02991400	39.81285800	6.96265400
C	10.85142600	38.29019000	5.41854700
H	11.87941200	38.41318500	5.05415100
C	8.67698200	37.19422500	5.29252700
H	8.01603700	36.45031200	4.83456400
C	9.98939500	37.35373500	4.82257500
H	10.34558200	36.73066700	3.99117800
C	1.78724100	37.82058000	3.39822100
C	2.33624000	37.10597500	2.29909500
H	3.16769200	36.41807900	2.48771500
C	1.82895600	37.25446500	0.99963600
H	2.27616300	36.68097700	0.17638100
C	0.74530500	38.11441000	0.74947200
H	0.34589100	38.22856600	-0.26644300
C	0.17940000	38.82520900	1.82593600
H	-0.65997000	39.51093300	1.64983900
C	0.68974400	38.67986100	3.12267500
C	-1.12843100	36.68684400	9.70303400
C	-1.44221000	35.62579900	10.59313000
H	-0.63549600	34.95540300	10.90903500
C	-2.75038200	35.42109700	11.05744800
H	-2.95726300	34.58686900	11.74122200
C	-3.79479300	36.26446800	10.64132900
H	-4.81898300	36.10340100	11.00153200
C	-3.50646500	37.31903600	9.75379100
H	-4.30670600	37.99640600	9.42774800
C	-2.19853800	37.52434200	9.29325400

O	2.94637400	42.62250700	10.42155300
H	3.04820700	41.70632000	9.97953000
C	2.91756100	43.61989500	9.51325500
C	2.79192800	44.94564000	10.00286700
C	3.00431500	43.41353000	8.11232500
C	2.75569600	46.03196600	9.11908100
H	2.72512500	45.09077900	11.08750300
C	2.96677400	44.51435300	7.24480100
H	3.09660300	42.39134300	7.71681600
C	2.84332800	45.82974300	7.72975100
H	2.65816000	47.04970100	9.52209200
H	3.03548200	44.33337700	6.16429000
H	2.81547300	46.68096100	7.03801400
C	3.26059100	39.71526400	8.38645300
O	3.20976100	40.21828400	7.25229500
O	3.22440900	40.11568200	9.57140700
H	-1.97766800	38.35345900	8.61267600
H	8.69383600	39.52615300	7.78466300
H	6.40872400	39.03995700	12.49961200
H	0.25449800	39.24631200	3.95277500

CO_2 adduct of Fe-porphyrin having triazole and water

	X	Y	Z
Fe	3.13554000	37.96897000	8.24594100
N	1.45828400	37.71505300	7.23640300
N	4.17238100	37.46343000	6.61821700
N	4.80662300	38.07348800	9.27796000
N	2.11566600	37.90251000	9.95234400
N	-1.51182600	40.22364000	10.88328700
N	-2.05760800	40.88325300	11.97240100
N	-1.23346500	41.86012000	12.29254600
C	0.72109800	37.84373100	10.08669000
C	0.36403900	37.50248100	11.42446000
H	-0.65656100	37.35328500	11.77928500
C	1.54322700	37.37877000	12.14222600
H	1.65940800	37.11341300	13.19287400
C	2.61556600	37.68797200	11.24761000
C	3.96917500	37.85956600	11.62821000
C	4.96610600	38.16232300	10.67113000
C	6.29809800	38.57696900	10.98457800
H	6.67083900	38.76585300	11.99148600

C	6.98886800	38.68553600	9.78930900
H	8.04215200	38.92870400	9.64834900
C	6.07978800	38.33438300	8.74257700
C	6.46674800	38.04280800	7.41649900
C	5.56821300	37.49441300	6.47181100
C	5.93906200	36.98130100	5.18895600
H	6.95876600	36.90336000	4.81251500
C	4.77085800	36.63604100	4.53244400
H	4.66988300	36.19624600	3.54044900
C	3.68239000	37.01372000	5.38214700
C	2.32690300	37.06759300	4.97737700
C	1.31657500	37.54295600	5.84866800
C	-0.00141700	37.91172800	5.43994100
H	-0.35206700	37.92658900	4.40773200
C	-0.70439000	38.26415100	6.58284100
H	-1.73627500	38.60919000	6.65312400
C	0.17567900	38.07524600	7.69191700
C	-0.21107600	38.09829100	9.05115600
C	4.35270300	37.76559400	13.05792300
C	5.44070700	36.94995700	13.47503900
H	5.98422500	36.38016100	12.71328400
C	5.81362100	36.85335600	14.82250800
H	6.65258300	36.20307900	15.10511100
C	5.11201800	37.56715400	15.81244000
H	5.40176700	37.49033800	16.86820900
C	4.03402900	38.38360100	15.42251300
H	3.48370300	38.96318300	16.17555200
C	3.66391000	38.48328800	14.07413400
C	7.88345900	38.28101100	7.03077800
C	8.43085800	39.58878100	7.08683100
C	9.76550900	39.83816200	6.73582700
H	10.15411500	40.86409500	6.78113100
C	10.59981600	38.78793200	6.30959600
H	11.64271100	38.98337400	6.02894400
C	8.74465800	37.23421200	6.61294700
H	8.35342400	36.21094000	6.59183100
C	10.07749900	37.48386100	6.25131200
H	10.71846500	36.64933500	5.93656000
C	1.94449900	36.69464900	3.59325500
C	0.87587400	35.78725000	3.35212100
H	0.35255300	35.36187400	4.21555400

C	0.49635200	35.42374400	2.05314300
H	-0.32616100	34.70984500	1.91073600
C	1.17066300	35.95245400	0.93574700
H	0.87632900	35.66644400	-0.08212300
C	2.22534600	36.85934300	1.14924500
H	2.75025500	37.30169700	0.29175800
C	2.60152400	37.22619500	2.44911600
C	-1.65589500	38.20267000	9.38468200
C	-2.54627900	37.25041200	8.81364100
H	-2.10530000	36.50694200	8.14181800
C	-3.91284600	37.20839100	9.09995100
H	-4.54333200	36.43289200	8.64663000
C	-4.46210800	38.15026200	9.99305300
H	-5.53172000	38.13950700	10.23667100
C	-3.63143800	39.11822900	10.56259300
H	-4.02813900	39.87480500	11.24401200
C	-2.24855000	39.15962600	10.27184400
C	-0.32116000	40.80831400	10.53033200
H	0.31486100	40.44279600	9.72483800
C	-0.15499500	41.85087500	11.43605700
C	0.97068300	42.83807200	11.54763800
H	1.86871600	42.37865300	12.00186900
H	1.25654900	43.21612600	10.54826000
H	0.65864800	43.68291300	12.18649600
H	2.83789000	39.13988000	13.78137800
H	3.40436700	37.95527200	2.60065100
H	7.77633700	40.40973700	7.39933200
C	3.10388900	40.11619900	7.91233400
O	4.08413000	40.43479300	7.25896900
O	2.09662300	40.60370600	8.44286400
H	0.19298200	42.85697100	8.51205400
O	1.05393300	43.21448900	8.21204800
H	1.59970000	42.38349100	8.18571200

CO_2 adduct of Fe-porphyrin having triazole, water and phenol

	X	Y	Z
Fe	3.18795400	37.88470800	8.48264600
N	1.48876000	37.72490200	7.51750300
N	4.19580500	37.56959700	6.80416300
N	4.88766100	37.90562500	9.46720300
N	2.20345400	37.57863900	10.19850600

N	-1.56172600	40.61031400	9.52485600
N	-2.22885100	41.65044800	8.92062100
N	-1.39707700	42.67515200	8.90581600
C	0.81461400	37.60819600	10.38887800
C	0.49019800	37.27461000	11.74044100
H	-0.52027700	37.22121900	12.14758300
C	1.68658500	37.02429700	12.39459100
H	1.82662500	36.71920600	13.43126600
C	2.74059900	37.29157700	11.46403200
C	4.11161500	37.38669500	11.80016100
C	5.08472000	37.79320100	10.85472700
C	6.42500800	38.15686800	11.18686300
H	6.82897300	38.18983900	12.19878100
C	7.08043700	38.45424600	10.00229000
H	8.12854200	38.72250200	9.87033500
C	6.14418000	38.26019100	8.94145400
C	6.49602100	38.18191600	7.57263700
C	5.57930700	37.71844800	6.59946100
C	5.91063500	37.39200300	5.24800500
H	6.90925100	37.44399700	4.81584500
C	4.73623200	37.02803700	4.61157500
H	4.61318000	36.70143800	3.57940700
C	3.67221600	37.21912500	5.54660100
C	2.29971200	37.19781900	5.20914300
C	1.29720700	37.56299400	6.13466700
C	-0.06321300	37.83456600	5.79238600
H	-0.46524600	37.81711400	4.77943000
C	-0.73564300	38.13057600	6.96737800
H	-1.79352700	38.36457900	7.09223500
C	0.21049200	38.01845300	8.03075200
C	-0.12584900	37.96905900	9.39753500
C	4.55105600	37.12833600	13.19528000
C	5.59551400	36.20428600	13.47049900
H	6.06002400	35.68094500	12.62736400
C	6.02589600	35.94857200	14.77971600
H	6.82809600	35.21853600	14.95221500
C	5.42743300	36.60725000	15.87051000
H	5.76156000	36.40597500	16.89631400
C	4.39784100	37.53319700	15.62135100
H	3.93318100	38.07456900	16.45635300
C	3.97177100	37.79205700	14.31054300

C	7.89162500	38.51323800	7.18594200
C	8.43217600	39.79575800	7.46735100
C	9.75067200	40.12810900	7.12596500
H	10.12934400	41.13399200	7.34989500
C	10.58038300	39.19013600	6.48351800
H	11.61029200	39.45148000	6.20928800
C	8.75151200	37.57708600	6.55285900
H	8.37462400	36.56695400	6.35855000
C	10.06792100	37.91155100	6.20138800
H	10.70544800	37.15937600	5.71747100
C	1.88099800	36.86213200	3.82171600
C	0.93984400	35.82582400	3.58405400
H	0.54096800	35.27924200	4.44592700
C	0.52774000	35.49148800	2.28619200
H	-0.19405300	34.67682100	2.14013900
C	1.04287600	36.18349900	1.17451200
H	0.72287700	35.92232600	0.15773800
C	1.96758100	37.22160200	1.38801100
H	2.36201200	37.78917400	0.53484200
C	2.37532400	37.55816800	2.68748600
C	-1.55845700	38.13105500	9.77851300
C	-2.32521100	36.98967100	10.11828000
H	-1.81004500	36.02306100	10.11713500
C	-3.69450200	37.06133000	10.40949300
H	-4.25156000	36.14750000	10.65131000
C	-4.35185000	38.30362400	10.36035000
H	-5.42537300	38.37780400	10.57280700
C	-3.62429300	39.45917800	10.05342800
H	-4.10006100	40.44347600	10.02671700
C	-2.24338500	39.37853200	9.77759700
C	-0.29658500	40.99434900	9.88777700
H	0.42061500	40.31467200	10.34041900
C	-0.20098300	42.32174500	9.49605900
C	0.93703600	43.28780700	9.63689000
H	0.88249500	43.83909800	10.59625600
H	1.89754700	42.74825300	9.60046100
H	0.89627900	44.02052100	8.81358300
H	3.18970800	38.53605200	14.12583600
H	3.07295800	38.38731100	2.84568800
H	7.78657200	40.53578600	7.95307800
C	3.03645800	40.00109600	8.33710200

O	3.14113000	40.39399000	7.16142600
O	2.85161900	40.46007900	9.46099400
H	-0.92944100	43.91292900	7.38386400
O	-0.38538800	44.34079300	6.67521800
H	0.32963100	43.67838500	6.53161100
O	2.18422800	42.82388400	6.50870300
C	3.19234300	43.64816700	6.11584700
C	2.87041500	45.00185500	5.85944200
C	4.52434600	43.20190300	5.95167500
C	3.87041800	45.88580300	5.43395400
H	1.83618700	45.32921400	6.01596700
C	5.51073400	44.10449100	5.52717800
H	4.76665900	42.15434900	6.16067700
C	5.19696600	45.44906700	5.26143000
H	3.60815400	46.93408800	5.23840700
H	6.53990300	43.74465000	5.40267800
H	5.97502500	46.14680900	4.92820300
H	2.54211400	41.90753100	6.76088700

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