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Supporting Information

For

O_2 Reduction by Iron Porphyrins with Electron Withdrawing Groups: To Scale or not to Scale

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Experimental details:

Materials: All reagents were of the highest grade commercially available. Iodine, trifluoroacetic acid (TFA), 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), ethanol, aqueous ammonia solution, ceric ammonium nitrate (CAN), sarcosine, potassium *tert*-butoxide, benzaldehyde, magnesium sulphate, *p*-toluenesulphonic acid (PTSA), *p*-toluenesulfonylmethyl isocyanide (TosMIC), phosphorus oxychloride ($POCl_3$), dichloroethane (DCE), propionic acid were purchased from Spectrochem Ltd. Diethyl ether, Tetrahydrofuran (THF), Acetonitrile, Dichloromethane, and Toluene were purchased from RANKEM Ltd., paraformaldehyde, anhydrous Ferrous bromide ($FeBr_2$), 2,4,6-Collidine, Tetrabutylammonium hexafluophosphate ($TBAPF_6$), Trifluoromethane sulphonic acid, silver triflate were purchased from Sigma-Aldrich chemical company. Na_2SO_4, Zinc acetate were purchased from MERCK and used without any further purification. N,N-dimethylformamide (DMF) were purchased from FINAR Ltd. Unless otherwise mentioned all reactions were performed at room temperature. The column chromatography was performed with silica gel (mesh size: 60-100, 100-200 and 230-400) and neutral Alumina, preparative TLC was performed with Silica gel GF-254 (~13% $CaSO_4$, 0.5 H_2O binders with fluorescent indicator). These were purchased

from SRL Pvt. Ltd. $^{57}FeCl_2$ was provided by Prof. Nicolai Lehnart's group from the University of Michigan, USA. THF was dried using K-metal in the presence of benzophenone until the colour of benzophenone turned intense bluish-green. Toluene was dried using Na-metal in the presence of benzophenone until the colour of benzophenone turned intense blue. MeOH was first dried like toluene using sodium after that it was distilled from Mg-cake. DCM and chloroform were distilled with both anhydrous $CaCl_2$ followed by CaH_2. Ultra-high purity N_2 cylinders and O_2 cylinders were purchased from Indian Refrigeration Stores. DMF was distilled and kept over activated 4Å molecular sieves before use. The solvents were kept over activated 4Å molecular sieves for one week prior to use for any electrochemical analyses. N,N′-dimethylformamidium triflate ([DMF-H]OTf) were synthesized using previously reported methods.[1]

Instrumental Details

All electrochemical experiments were performed using CH Instruments (model CHI700E and CHI710D electrochemical analyzer). Glassy carbon, Platinum, and reference electrodes (standard double-junction silver/silver chloride filled with 4 M KNO_3 solution) were purchased from Pine Instruments.

UV−Vis absorption data were recorded in an Agilent technologies spectrophotometer model 8453 fitted with a diode-array detector. The cuvettes were purchased from Starna Scientific.

X-ray single-crystal data were collected on a Bruker D8VENTURE Microfocus diffractometer equipped with PHOTON II Detector, with Mo Kα radiation (λ = 0.710 73 Å), controlled by the APEX3 software package.[2] Raw data were integrated and corrected for Lorentz and polarization effects using the Bruker APEX III program suite. Absorption corrections were performed using SADABS. Space groups were assigned by analysis of metric symmetry and systematic absences (determined by XPREP) and were further checked by PLATON[3,4] for additional symmetry. The structures were solved by direct methods and refined against all data in the reported 2θ ranges by full-matrix least-squares on F^2 with the SHELXL[5] program suite using the OLEX 2[6] interface. Hydrogen atoms at idealized positions were included during the final refinements of each structure. The OLEX 2 interface was used for structure visualization, analysis of bond distances, angles, and drawing ORTEP plots.

Mössbauer spectra were recorded using an alternating constant WissEl Mössbauer spectrometer, consisting of an MR 360 drive unit, an MVT 1000 velocity transducer, and an LND-45431 proportional counter mounted on an MB-600 Mössbauer bench with cryostat stand. The system was operated in a horizontal transmission geometry with source (^{57}Co in Rh-

matrix), absorber and detector in a linear arrangement. The temperature was controlled and maintained using MBBC-N20106 Mössbauer cryostat for liquid nitrogen connected with Lake Shore-325 temperature controller unit. Measurements were performed at 100K. Data acquisition was performed using a 512 channel analyzer. Isomer shifts were referenced versus α-iron metal foil at the same temperature. The simulation of experimental data was performed using the Normos-A Mössbauer Fit programmes Site and Dist.

Synthesis of Fe(P)-OTf:

The porphyrins were metalated using $FeBr_2$ under inert atmosphere inside a glove box, and purifications were performed outside the glove box. In presence of O_2, the complexes form the corresponding μ-oxo dimer (as evident from the crystal structure of FeDEsP and FeTEsP, resulting a mixture of Fe^{III}(P)Cl and the $[Fe(P)]_2O$. To avoid that, the complexes were treated with a solution of sodium hydroxide to make the dimer and then the oxo-bridges were broken with a strong acid (trifluoromethane sulfonic acid). The solution was kept under activated 4Å molecular sieves and extracted with dry THF and evacuated under vacuum.

$$Fe^{III} - O - Fe^{III} + 2\,HOTf \rightarrow 2\,Fe^{III} - OTf + 2\,H_2O$$

FeTPPCl was not found to form the dimer, hence, it was treated with one equivalent silver triflate in dry THF to form FeTPP-OTf and AgCl. FeTPP-OTf was remain in the solution and silver chloride was precipitated out. It was then filtered and evacuated under vacuum to obtain FeTPP-OTf as a amorphous solid.

$$Fe^{III}TPPCl + AgOTf \rightarrow Fe^{III}TPP - OTf + AgCl\downarrow$$

Cyclic voltammetry:

Homogeneous condition: All anaerobic electrochemical investigations were performed under an inert atmosphere in a N_2 Glove Box from MBRAUN. All other CV data were collected in a custom-made electrochemical cell by purging O_2 gas. 4 ml of 0.5 mM compound solution in DMF was taken in the presence of 100 mM $TBAPF_6$ as the supporting electrolyte. The glassy carbon electrode was taken as the working electrode, standard double-junction silver/silver chloride as the reference electrode, and a Pt was taken as the counter electrode. Ferrocene (Fc) was used as an internal reference, and the potential scale is normalized with respect to the potential of the $Fc^{+/0}$ couple. All the electrochemical experiments were performed at room temperature.

Heterogeneous condition: A very dilute solution (~1 mM) of the Fe-porphyrins in $CHCl_3$ is physiadsorbed on an edge-plane graphite (EPG) electrode. The resultant EPG bearing physiadsorbed complexes are cleaned with deionized water and used as the working electrode. A Pt wire is used as a counter electrode, and a Ag/AgCl (saturated KCl) standard electrode is used as the reference electrode. Phosphate buffer solutions (100mM in phosphate) are used to maintain the pH of an electrolyte solution containing 100 mM $KPF_{6.}$

Rotating Disk Electrochemistry (RDE): The RDE measurements were performed using a CHI 710D bipotentiostat along with a Pine Instruments modulated speed rotor fitted with an E6 series change-disc tip. The complex is physiadsorbed on an edge plane graphite electrode as described above. The RDE experiment was performed by measuring linear sweep voltammetry (LSV) at a scan rate of 10−100 mV/s at different rotation rates using Ag/AgCl (saturated KCl) reference and Pt counter electrodes.

Mössbauer: ^{57}Fe enriched Fe-porphyrins were synthesized using the same protocol as with the natural abundant isotope. THF solutions of the complex (150 μL; 10 mM) were prepared inside the glove box, and the resting state data was collected. Then the sample was reduced using half equivalent of Na_2S inside a glove box, then taken outside, and purged with O_2 for 5 minutes. The sample vial was appropriately sealed and reinserted in the glove box. With this sample, the data for the intermediates were collected. In every case, 150 μL sample was taken in a custom-made Nylon capsule, frozen with liquid N_2 in situ, attached to the sample holder (immersed into liquid N_2) using a screw joint, and inserted into the cryostat maintained at 100K for data collection.

Computational details. All calculations were performed at the IACS computer cluster using Gaussian 03 software.[7] BP86 functional reproduced better agreement with the experimental frequencies, and hence further calculations were performed with that functional. A mixed basis set with 6-311g* on Fe and 6-31g* on C, O, N, and H atoms were used for optimization.[8,9] For the final energy and ground-state calculations, a 6-311+g* basis set was used on all atoms. The solvent effect was corrected using the Polarizability Continuum Model (PCM).[10] For all complexes, spin-unrestricted schemes have been adopted which distinguish between α and β spin orbitals. Frequency calculations were performed using the basis set used for optimization, and no negative frequencies were found for the structures reported.

Table S1. Crystal data and structural refinement details		
Description	**Experimental data**	
	FeDEsP	FeTEsP
Chemical formula moiety	$C_{76}\ H_{56}\ Fe_2\ N_8\ O_9$	$C_{88}\ H_{72}\ Fe_2\ N_8\ O_{17}$
Chemical formula sum	$C_{76}\ H_{56}\ Fe_2\ N_8\ O_9$	$C_{88}\ H_{76}\ C_{l2}\ Fe_2\ N_{12}\ O_{13}$
CCDC number	1854376	2116511
Chemical formula weight	1336.98	1692.20
Cell length a (Å)	15.7335(16)	8.0718(9)
Cell length b (Å)	15.6057(16)	26.641(3)
Cell length c (Å)	26.314(3)	36.191(4)
Cell angle α (°)	90	90
Cell angle β (°)	100.540(3)	95.657(4)
Cell angle γ (°)	90	90
Cell volume ($Å^3$)	6351.9(12)	7744.7(15)
Cell formula units_Z	2	4
Space group (crystal system)	Monoclinic	Monoclinic
Space group (name)	P 21/c	P 21/c
Crystal density ($g.cm^{-3}$)	1.398	1.451
F000	2768	3512
Radiation wavelength, λ (Å)	0.71073	0.71073
Temperature (K)	293(2)	110.17
R1[a]	0.0836	0.0680
wR2[b]	0.1587	0.1423
Goodness of fit[c]	0.956	1.081

a. $R1 = \Sigma \| F_o \| - \| F_c \| / \Sigma | F_o |$;

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

c. $GOF = [\ \Sigma \{ w (F_o^2 - F_c^2)^2 \} / (M-N)]^{1/2}$, where M is the number of reflections, and N is the parameters refined

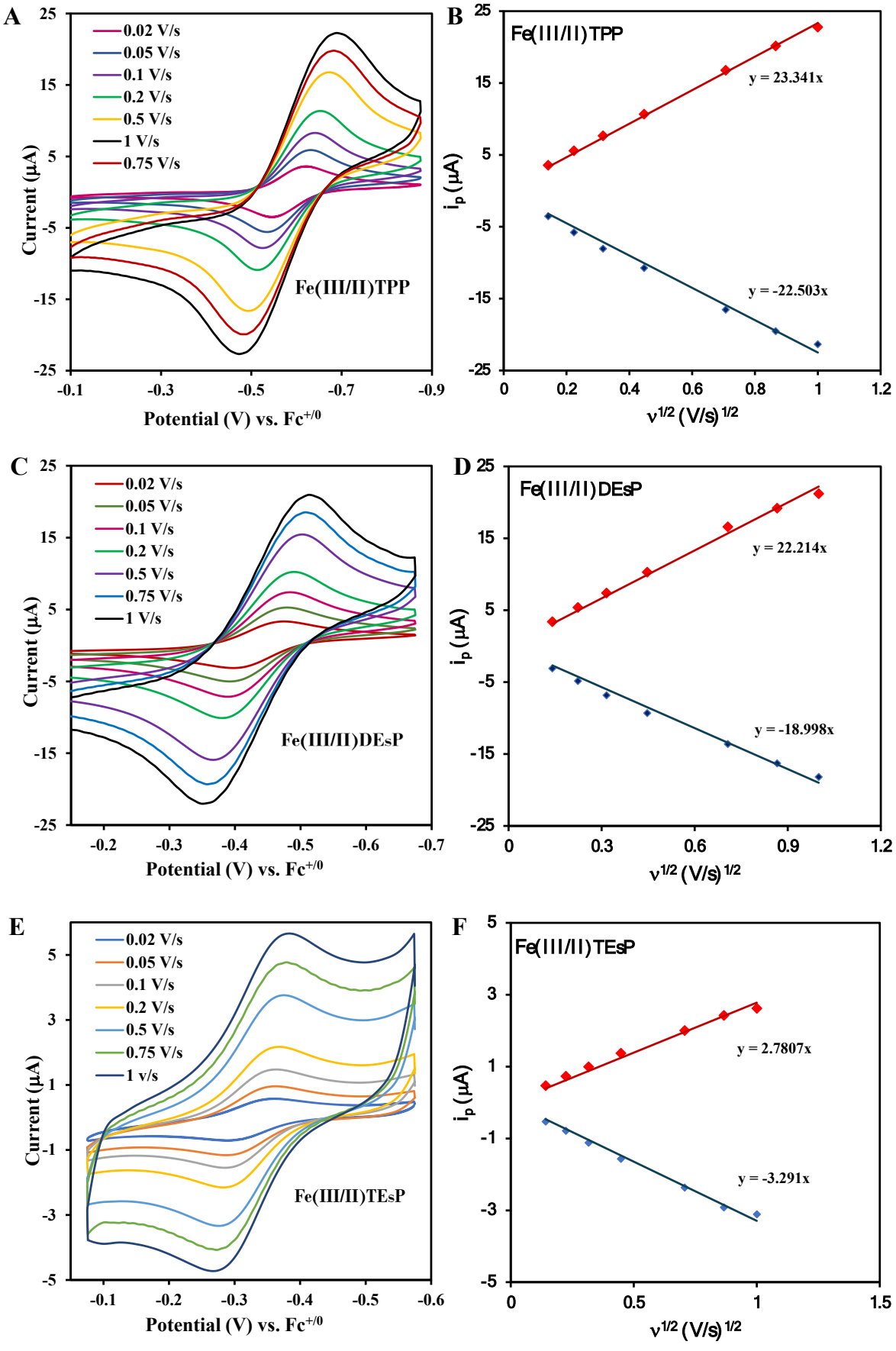
A
0.02 V/s
0.05 V/s
0.1 V/s
0.2 V/s
0.5 V/s
1 V/s
0.75 V/s
Current (μA)
Fe(III/II)TPP
Potential (V) vs. Fc+/0
B
Fe(III/II)TPP
y = 23.341x
y = -22.503x
ip (μA)
ν1/2 (V/s)1/2
C
0.02 V/s
0.05 V/s
0.1 V/s
0.2 V/s
0.5 V/s
0.75 V/s
1 V/s
Current (μA)
Fe(III/II)DEsP
Potential (V) vs. Fc+/0
D
Fe(III/II)DEsP
y = 22.214x
y = -18.998x
ip (μA)
ν1/2 (V/s)1/2
E
0.02 V/s
0.05 V/s
0.1 V/s
0.2 V/s
0.5 V/s
0.75 V/s
1 v/s
Current (μA)
Fe(III/II)TEsP
Potential (V) vs. Fc+/0
F
Fe(III/II)TEsP
y = 2.7807x
y = -3.291x
ip (μA)
ν1/2 (V/s)1/2

Figure S1. Cyclic voltammograms of A) FeTPP-Im_2, B) FeDEsP-Im_2, and C) FeTEsP-Im_2 complexes recorded at different scan rates: 0.02, 0.05, 0.1, 0.2, 0.5, 0.75 and 1 V/s (Left). Figures on the right show the linear dependence of the peak current (anodic peak: blue diamonds, cathodic peak: red diamonds) of the Fe(III/II) process on the square root of the scan rates.

Calculation of diffusion constants from cyclic voltammograms of S1 (A, B & C)

The peak current is given by the Randles-Sevcik equation

$$i_p = 0.4463\ (F/RT)^{1/2} n_p^{3/2} FAD^{1/2}[C_0]\nu^{1/2} \qquad (1)$$

In equation (1), i_p is peak current, *F* is Faraday's constant (F = 96500 C mol^{-1}), R is the universal gas constant (R = 8.314 J K^{-1} mol^{-1}), T is temperature (T = 298 K) n_p is the number of electrons transferred (n_p = 1 for $Fe^{II/I}$), A is the active surface area of the electrode (A = 0.07 cm^2), *D* is the diffusion coefficient for the complex, $[C_0]$ is the concentration of the catalyst, and ν is the scan rate. The diffusion coefficients (*D*) were calculated from the slopes of i_p *vs.* $\nu^{1/2}$ plots (Figure S1 (right)).

Diffusion coefficient of FeTPP-Im_2= 6.16×10^{-6} cm^2s^{-1}

Diffusion coefficient of FeDEsP-Im_2= 5.58×10^{-6} cm^2s^{-1}

Diffusion coefficient of FeTEsP-Im_2= 1.22×10^{-7} cm^2s^{-1}

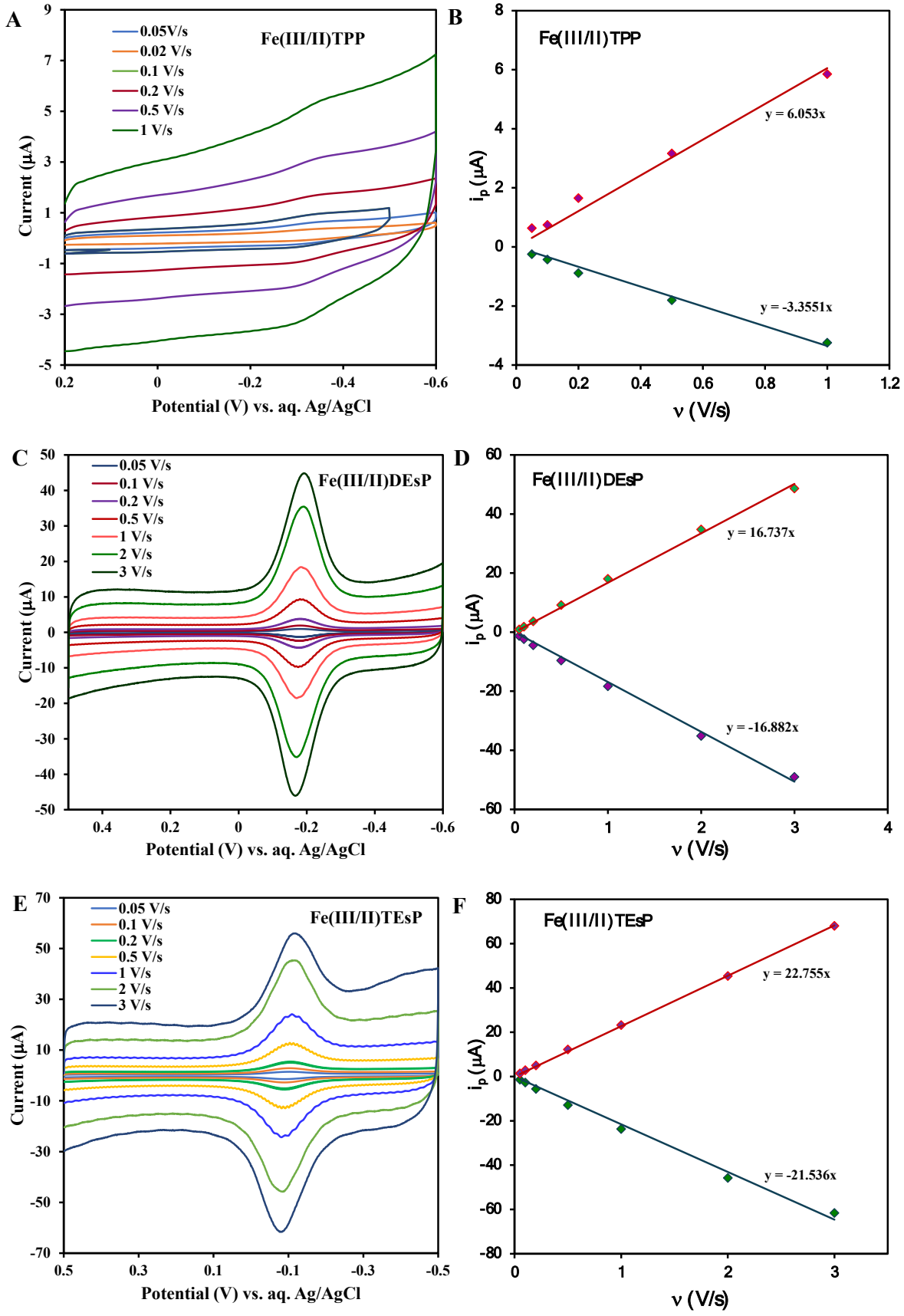
A
0.05V/s
0.02 V/s
0.1 V/s
0.2 V/s
0.5 V/s
1 V/s
Fe(III/II)TPP
Current (µA)
Potential (V) vs. aq. Ag/AgCl
B
Fe(III/II)TPP
y = 6.053x
y = -3.3551x
i_p (µA)
ν (V/s)
C
0.05 V/s
0.1 V/s
0.2 V/s
0.5 V/s
1 V/s
2 V/s
3 V/s
Fe(III/II)DEsP
Current (µA)
Potential (V) vs. aq. Ag/AgCl
D
Fe(III/II)DEsP
y = 16.737x
y = -16.882x
i_p (µA)
ν (V/s)
E
0.05 V/s
0.1 V/s
0.2 V/s
0.5 V/s
1 V/s
2 V/s
3 V/s
Fe(III/II)TEsP
Current (µA)
Potential (V) vs. aq. Ag/AgCl
F
Fe(III/II)TEsP
y = 22.755x
y = -21.536x
i_p (µA)
ν (V/s)

Figure S2. Cyclic voltammograms of A) FeTPP-OTf, B) FeDEsP-OTf, and C) FeTEsP-OTf complexes recorded at different scan rates: 0.05, 0.1, 0.2, 0.5, 1, 2 and 3 V/s (Left). Figures on the right show the linear dependence of the peak current (anodic peak: green diamonds, cathodic peak: red diamonds) of the Fe(III/II) process on the scan rates.

In case of heterogeneous cyclic voltammograms, if the electrode surface has $A\Gamma_O^*$ moles of adsorbed molecules, the peak current is given by the equation,

$$i_p = \frac{n^2F^2}{4RT} v A \Gamma_O^* \qquad (2)$$

The peak current, and indeed the current at each point on the wave, is proportional to *v,* in contrast to the $v^{1/2}$ dependence observed for Nernstian waves of diffusing species, i.e., for homogeneous cyclic voltammograms.

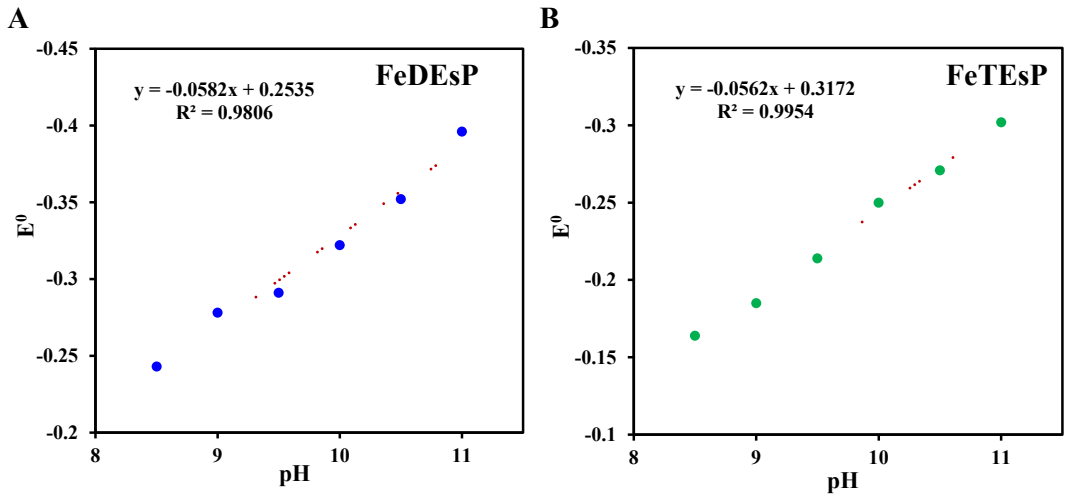

Figure S3. E° versus pH plot

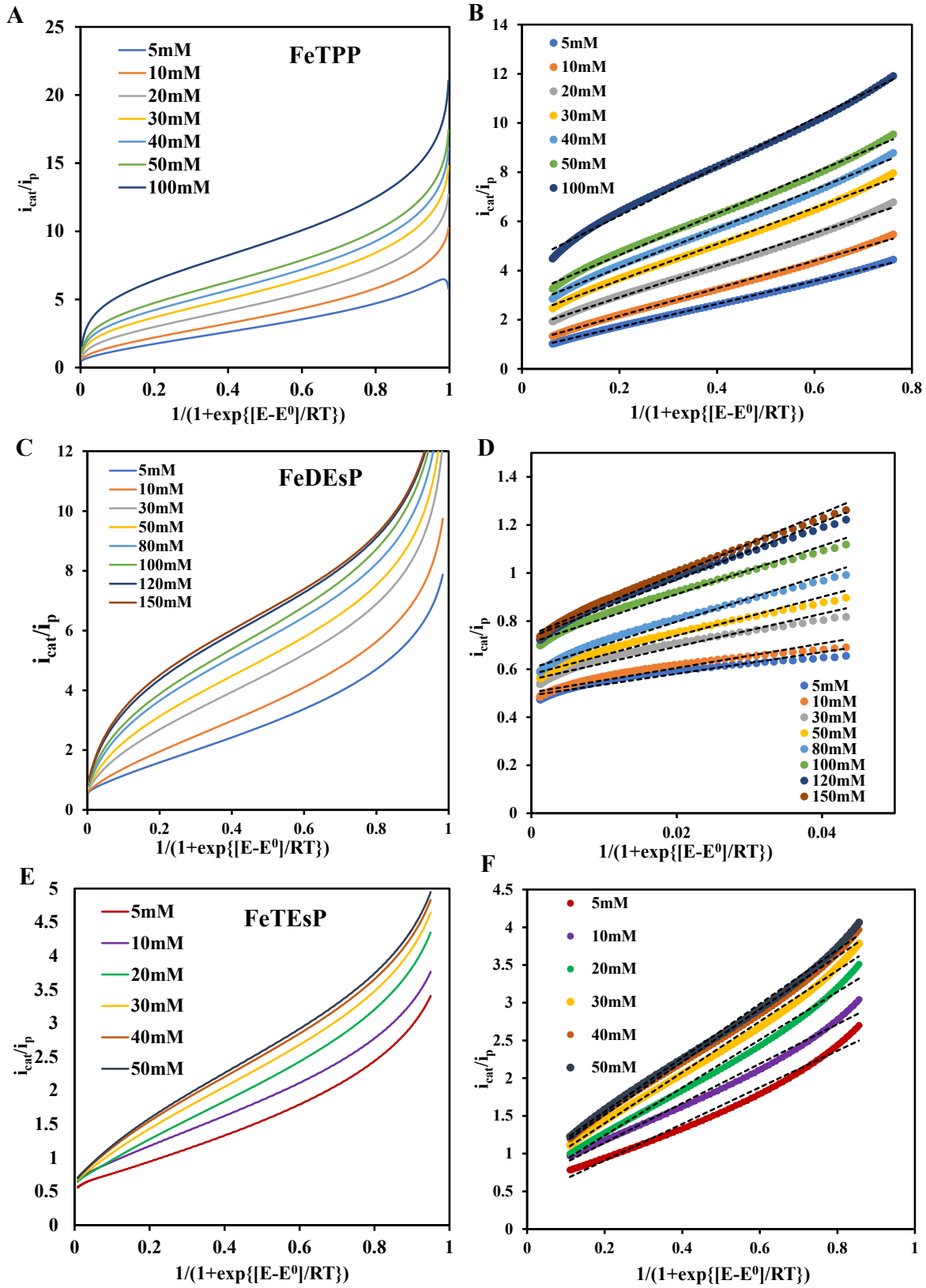

Figure S4. Determination of TOF at different acid concentration by the foot-of-the-wave analysis (FOWA)

Calculation of rate from foot-of-the-wave analysis:

The addition of an acid source results in a considerable increase in the catalytic current with the current–potential responses to be peak shaped rather than the typical sigmoidal one. For such a rapid catalytic process, the catalytic rate can be derived by the foot-of-the-wave analysis (FOWA) at the foot of the catalytic wave where the secondary phenomena (any catalyst decomposition, inhibition by-products, or extensive substrate consumption) are less. To analyze the catalytic rate from FOWA, the slope of the linear fit of the plot of the catalytic enhancement (i_{cat}/i_p) as a function of $[1 + \exp(F/RT)(E - E°)]^{-1}$ (where $E° = E_{1/2}\ Fe^{(III/II)}$) at initial points at the $i_{cat}/i_p > 1$ region is treated as per the following equation:

$$\frac{i_{cat}}{i_p} = 2.24\ [\left(\frac{RT}{Fv}\right) \times \frac{2kC_A^{0\frac{1}{2}}}{\left(1 + \exp\left(\frac{F}{RT}\right)(E - E^0)\right]}] \qquad (3)$$

where, R = universal gas constant, T = temperature in absolute scale, F = Faraday constant, ν = scan rate, k = apparent catalytic rate constant, C_A^0 = initial concentration of the substrate (here,O_2), E = applied potential from the electrode, and $E° = E^{1/2}$ for the Fe(III/II) process.

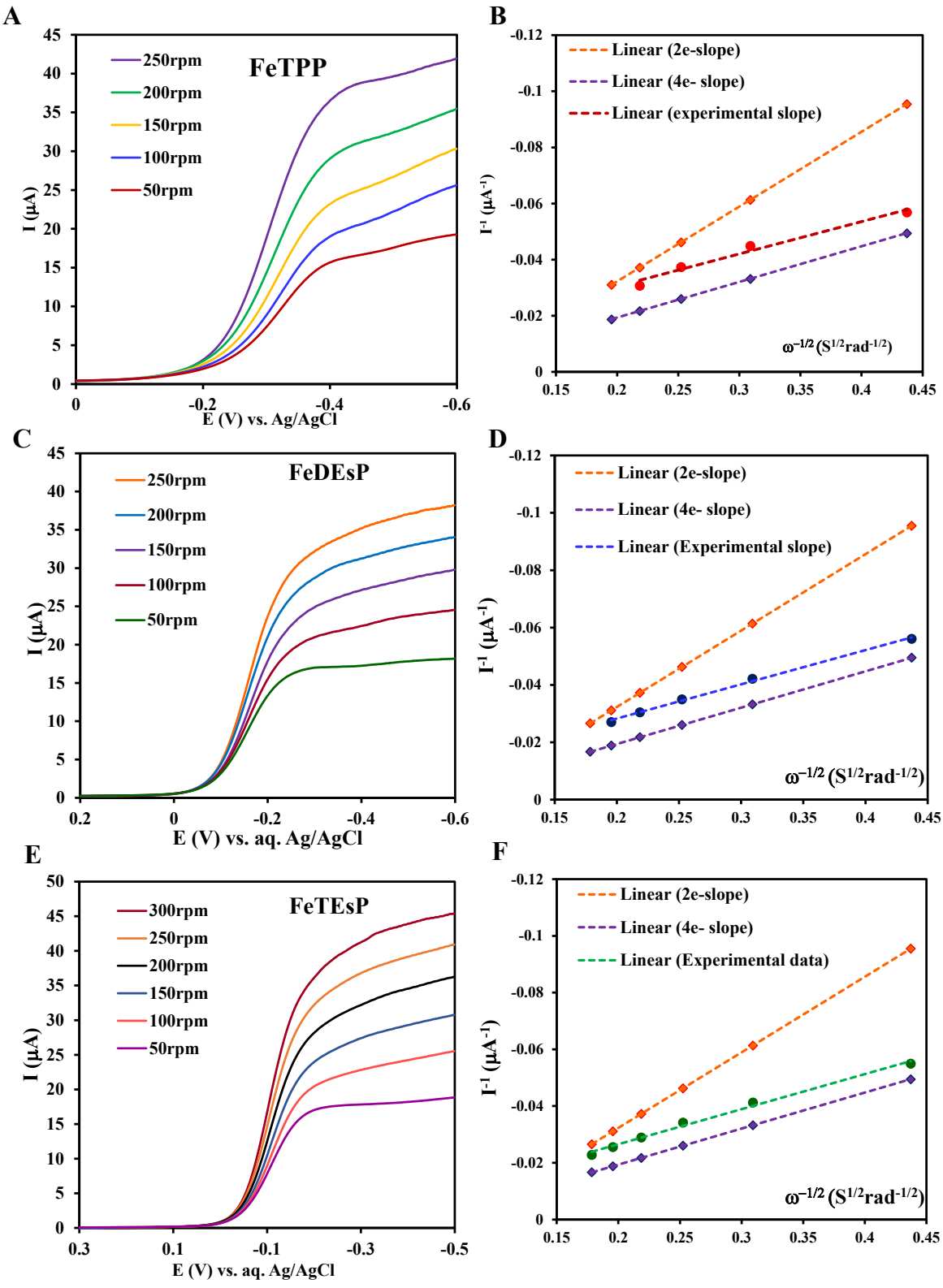

Figure S5. Determination of the 2nd order rate constant (k_{cat}) from the LSV at different rotation speed by the Kautecky-Levich analysis (K-L)

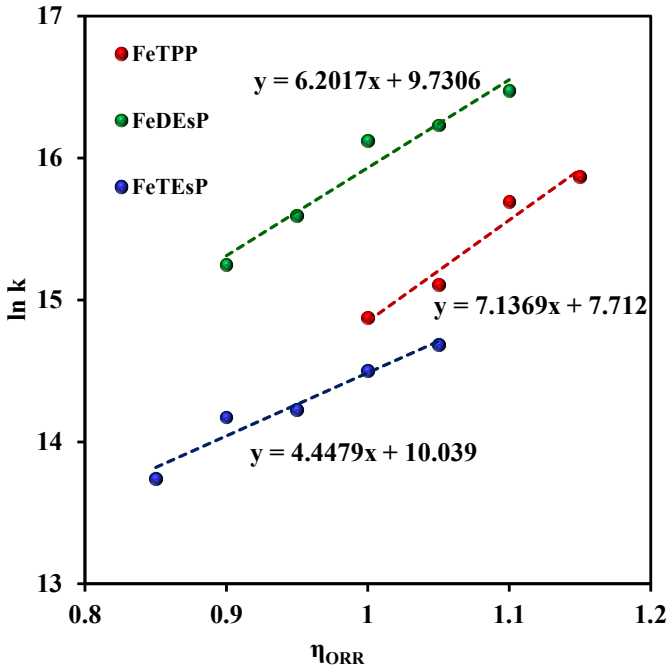

Figure S6. Correlation between the logarithm of the 2nd order rate constant (k_{cat}) and the overpotential of ORR at pH 7

DFT optimized coordinates

Fe^{III}TPP-oxy

C	5.67352800	3.89622300	14.46923700
C	6.62425100	3.16646600	15.19925900
H	6.72620800	3.33527000	16.27732600
C	7.43610700	2.21901900	14.55415400
H	8.17881200	1.64989000	15.12447100
C	7.29053900	2.00531200	13.17356400
H	7.92442800	1.27308100	12.66044400
C	6.33812400	2.73274300	12.44360100
H	6.23254400	2.57164900	11.36495500
C	5.51482700	3.68940300	13.07990200
C	4.49828800	4.46657300	12.30324400
C	3.45790400	3.76618800	11.66588100
C	3.25187600	2.34379700	11.78965100
H	3.84591200	1.68191200	12.41840400

C	2.17725200	2.02206100	11.00170600
H	1.71925100	1.04508900	10.85430600
C	1.71943900	3.24757500	10.39595700
C	0.64650600	3.32006800	9.49038700
C	-0.00196800	2.04603400	9.04492600
C	0.72522100	1.08040700	8.31292000
H	1.77432600	1.27734600	8.06505300
C	0.11649100	-0.11302200	7.89505600
H	0.69568700	-0.84644600	7.32243800
C	-1.23045000	-0.36410500	8.20396500
H	-1.70573700	-1.29637500	7.87877800
C	-1.96383000	0.58574100	8.93409800
H	-3.01272300	0.39425500	9.18764500
C	-1.35610600	1.78001700	9.35073900
H	-1.92414500	2.51477500	9.93153900
C	0.14199500	4.53865900	9.00513500
C	-0.91758600	4.63530000	8.02803500
H	-1.37987200	3.78727000	7.52495600
C	-1.19350600	5.96729900	7.87112200
H	-1.92821700	6.42984800	7.21335200
C	-0.30109900	6.69053300	8.74791600
C	-0.32391200	8.08820500	8.90296900
C	-1.39446000	8.86521100	8.20057600
C	-1.06895700	9.80187700	7.19358600
H	-0.01742100	9.95157600	6.92441500
C	-2.07452300	10.52602200	6.53481900
H	-1.80254200	11.24335500	5.75204000
C	-3.42366700	10.32805700	6.87176700
H	-4.20870200	10.89412500	6.35786600
C	-3.76065300	9.40094700	7.87172200

H	-4.81016700	9.24511000	8.14627500
C	-2.75578700	8.67501700	8.52957600
H	-3.01785000	7.95983600	9.31700100
C	0.61965200	8.78469200	9.67886100
C	0.59340800	10.21696300	9.87821800
H	-0.18583200	10.88321900	9.51080000
C	1.70398600	10.53644000	10.61101800
H	2.02073400	11.51687000	10.96351800
C	2.40741100	9.29885100	10.86499700
C	3.62684800	9.22700500	11.56072500
C	4.29157100	10.50397000	11.97310700
C	4.75025800	11.42327800	11.00283200
H	4.62318400	11.18429700	9.94119400
C	5.37273600	12.62089500	11.38706500
H	5.72843800	13.31814600	10.61986500
C	5.54528300	12.92220200	12.74812100
H	6.03012800	13.85800400	13.04820000
C	5.09229200	12.01750500	13.72245000
H	5.21643000	12.24764400	14.78679300
C	4.47222200	10.81826300	13.33896300
H	4.10967800	10.11746700	14.09901100
C	4.24348600	8.00816100	11.88855600
C	5.53320500	7.91536700	12.53991100
H	6.17237300	8.76413000	12.77852700
C	5.76946400	6.58690100	12.75911000
H	6.64348300	6.12264400	13.21381300
C	4.62696200	5.86560800	12.23741100
Fe	2.05011700	6.27122200	10.64944700
N	2.50030700	4.32506100	10.81942800
N	0.55462600	5.81008900	9.40760300

N	1.71953900	8.22293400	10.31685400
N	3.71077600	6.74340400	11.67191200
O	3.30549000	6.20680900	8.85708500
H	2.59690300	6.15296700	8.17707200
H	3.59184700	5.27190700	8.97334500
H	5.03274500	4.62702200	14.97459700
O	1.06923300	6.30496100	12.11513200
O	0.16127800	5.40965100	12.30091700

Fe^{III}TPP-peroxy

C	5.69087100	3.96691300	14.49808100
C	6.63911700	3.24918600	15.24308800
H	6.77736900	3.47662900	16.30729800
C	7.40107800	2.23731800	14.63476500
H	8.14122700	1.67519000	15.21702300
C	7.20530400	1.95315800	13.27281300
H	7.79924600	1.17121900	12.78349300
C	6.25803200	2.67344700	12.52882900
H	6.11465700	2.45644300	11.46455200
C	5.47984100	3.69359600	13.12560000
C	4.47065200	4.46375300	12.33649000
C	3.42123000	3.76360100	11.71328800
C	3.20944200	2.34017000	11.83326800
H	3.78874800	1.67322700	12.47130700
C	2.15457500	2.02280400	11.01646200
H	1.69905500	1.04577100	10.85668400
C	1.71040300	3.25321400	10.40729700
C	0.66189200	3.33550600	9.47465900
C	0.03534000	2.06347800	8.99732200
C	0.79097700	1.09218200	8.30043300

H	1.85166100	1.28823500	8.10747000
C	0.20308700	-0.10223800	7.85516200
H	0.81017400	-0.83707400	7.31205000
C	-1.15793000	-0.35331700	8.09616600
H	-1.61863400	-1.28594200	7.74855900
C	-1.92269200	0.60045300	8.78900900
H	-2.98399800	0.41151000	8.99201400
C	-1.33275600	1.79326600	9.23499400
H	-1.92491100	2.53160600	9.78611400
C	0.15557300	4.55422600	8.98834900
C	-0.88404000	4.65460400	7.99043100
H	-1.32372700	3.81130000	7.45818600
C	-1.18101400	5.98642100	7.85675800
H	-1.90820300	6.44940400	7.18992500
C	-0.31451200	6.70410000	8.76369900
C	-0.34791100	8.09947000	8.94199400
C	-1.42404100	8.87374000	8.24973100
C	-1.11442400	9.86175300	7.28561200
H	-0.06224900	10.05400100	7.04830500
C	-2.12756200	10.58227500	6.63415800
H	-1.86037600	11.33952600	5.88663400
C	-3.47791200	10.32966900	6.92890000
H	-4.27029100	10.89165600	6.41979900
C	-3.80312700	9.35032800	7.88262100
H	-4.85335000	9.14840000	8.12686600
C	-2.78874500	8.63243100	8.53485900
H	-3.04220700	7.87559400	9.28518100
C	0.59769300	8.79496100	9.71841800
C	0.57480200	10.22758600	9.92206200
H	-0.20876700	10.89803900	9.57009100

C	1.70018200	10.54335000	10.63557800
H	2.02194400	11.52372100	10.98623700
C	2.40398900	9.30263700	10.87538000
C	3.63898900	9.22073100	11.54189900
C	4.32092300	10.49343200	11.93470300
C	4.72943800	11.43131000	10.95817000
H	4.54410600	11.20534800	9.90239200
C	5.36744500	12.62678700	11.32427100
H	5.68017800	13.33544900	10.54742500
C	5.61286500	12.91249700	12.67784100
H	6.11123100	13.84641700	12.96482800
C	5.21344200	11.99108800	13.66047200
H	5.39303400	12.20613100	14.72107000
C	4.57507300	10.79627000	13.29256700
H	4.25548500	10.08182000	14.05895800
C	4.26258900	8.00169700	11.85650800
C	5.56651500	7.90246300	12.47506700
H	6.22556200	8.74497100	12.68371400
C	5.78998700	6.57282900	12.71356200
H	6.67110300	6.10584700	13.15317900
C	4.62517600	5.85988500	12.23292800
Fe	2.04697900	6.28376500	10.65955900
N	2.47167800	4.33443400	10.86337700
N	0.54830700	5.82599000	9.42358300
N	1.70156700	8.22263600	10.34550200
N	3.70758500	6.73768100	11.66108000
O	3.29848500	6.09314000	8.76730400
H	2.48161400	5.98529900	8.22980200
H	3.49481200	5.17237100	9.05791800
H	5.08995600	4.74854200	14.97533500

O	1.02958800	6.34323500	12.17178600
O	0.14740000	5.39918300	12.36433500

Fe^{III}TPP-hydroperoxy

C	5.04556600	3.99521200	14.89275400
C	5.84521800	3.30508900	15.81632700
H	5.76073600	3.53445600	16.88466200
C	6.74610000	2.32178000	15.37519900
H	7.37136900	1.78342800	16.09630900
C	6.84355900	2.03482400	14.00366500
H	7.55178200	1.27706600	13.64933300
C	6.04232000	2.72302500	13.07939200
H	6.13174600	2.50871800	12.00857800
C	5.12815600	3.71091200	13.51062700
C	4.26821700	4.46286700	12.54278400
C	3.32756100	3.75691000	11.76909200
C	3.18571700	2.32089000	11.75708400
H	3.71436000	1.63678100	12.41964900
C	2.28523500	2.00948100	10.76887500
H	1.92732800	1.02445000	10.47198700
C	1.83106000	3.25652500	10.20225800
C	0.81872800	3.36329900	9.22766500
C	0.32156700	2.10202300	8.59034400
C	1.17773300	1.32928400	7.77379600
H	2.20493500	1.67138800	7.60377400
C	0.72468800	0.14298900	7.17640100
H	1.40260500	-0.43819800	6.54088600
C	-0.59267800	-0.29538100	7.38816600
H	-0.94668900	-1.22193900	6.92250200
C	-1.45231300	0.45908400	8.20361400

H	-2.47860200	0.11928600	8.38352700
C	-0.99968400	1.64593200	8.80030100
H	-1.66711900	2.22568000	9.44731700
C	0.20941600	4.58916700	8.89380900
C	-0.93010100	4.71639300	8.01319100
H	-1.36568500	3.90420600	7.43294700
C	-1.33635300	6.02386200	8.07552500
H	-2.16466900	6.49620000	7.54876800
C	-0.41794700	6.71292600	8.95279800
C	-0.46172400	8.10017800	9.19571500
C	-1.65766600	8.85878700	8.70983600
C	-1.55346500	9.82406100	7.68306200
H	-0.57550900	10.01585200	7.22766400
C	-2.68731300	10.52034100	7.23633900
H	-2.58818100	11.26119900	6.43468100
C	-3.94456300	10.26393100	7.80776000
H	-4.82925100	10.80882900	7.45950100
C	-4.06174900	9.30368100	8.82624600
H	-5.03818400	9.09949300	9.28014300
C	-2.92930400	8.60490100	9.27183600
H	-3.01731600	7.86199600	10.07209200
C	0.59186200	8.79701800	9.81432300
C	0.65874600	10.23987500	9.92848600
H	-0.14033400	10.92604300	9.65112800
C	1.89538200	10.54096800	10.43049100
H	2.31178900	11.52196800	10.65534000
C	2.56753900	9.28047800	10.67326100
C	3.83072400	9.17741800	11.28637100
C	4.61660600	10.43349900	11.50083100
C	5.08879600	11.17419700	10.39377500

H	4.88182000	10.80883100	9.38178500
C	5.82475700	12.35423100	10.58145600
H	6.18939000	12.91078200	9.71047900
C	6.09748700	12.81789500	11.87894200
H	6.67140900	13.73985900	12.02543300
C	5.62711000	12.09500400	12.98767000
H	5.82556500	12.45519100	14.00359500
C	4.89284600	10.91371900	12.80099300
H	4.51300600	10.35880900	13.66580400
C	4.34198600	7.95720100	11.76411100
C	5.57038000	7.83112600	12.52202000
H	6.27741300	8.63911700	12.70413200
C	5.64087500	6.53217000	12.94593100
H	6.42207600	6.05730800	13.53823100
C	4.48285900	5.84909600	12.40471500
Fe	2.05295300	6.28734500	10.64292400
N	2.46603000	4.33341900	10.83210800
N	0.54835900	5.83368300	9.42698100
N	1.75610000	8.22009400	10.30231900
N	3.70744200	6.72664900	11.66273700
O	3.27538100	6.22113400	8.88161100
H	2.57209400	6.12115800	8.20049000
H	3.64305400	5.31437900	8.98577300
H	4.33785000	4.75748400	15.23649900
O	1.07206000	6.38745300	12.09229400
O	0.09764700	5.31193100	12.29630900
H	0.64432600	4.52758100	12.04222300

Fe^{III}DEsP-oxy

C	4.40650400	-2.37620600	0.07343800

C	5.20505200	-1.26659500	-0.00617300
C	4.35890500	-0.16959500	-0.41570800
C	3.07682800	-1.96640400	-0.33300500
C	1.97294500	-2.83142700	-0.43835400
C	4.80190800	1.14676100	-0.49812100
C	3.98478000	2.26028300	-0.71375600
C	4.43660000	3.63644400	-0.66117300
C	3.30927100	4.42885500	-0.85631200
C	2.19934700	3.52132600	-1.05511400
C	0.89377500	3.91946400	-1.34421700
C	-0.14059000	3.04406300	-1.64989600
C	-1.43193800	3.48523200	-2.12342300
C	-2.14492100	2.35850100	-2.42987000
C	-1.30264000	1.22358200	-2.10012800
C	-1.70833600	-0.11804100	-2.21562000
C	-0.90631400	-1.19517000	-1.79867400
C	-1.36567100	-2.56886300	-1.77830000
C	-0.35986300	-3.31707400	-1.23320300
C	0.72659700	-2.40648300	-0.93458700
H	6.26868000	-1.17640000	0.22152200
H	4.68033700	-3.38692900	0.37293000
H	-0.33343600	-4.39239000	-1.06282000
H	-2.34240000	-2.90185500	-2.12653600
H	-3.15287000	2.28491300	-2.83604800
H	-1.72504200	4.53066400	-2.23109200
N	2.62235600	2.20365200	-0.97611300
N	3.05593600	-0.60984200	-0.63112500
N	0.38099000	-1.10644700	-1.28517500
N	-0.06817600	1.65429500	-1.63933200
H	0.70593400	4.99372000	-1.40977900

H	5.85562900	1.33654300	-0.28461400
Fe	1.45425000	0.55795000	-1.02473400
C	-3.06719000	-0.41638600	-2.77400500
C	-3.19745400	-1.05075300	-4.02930100
C	-4.23881600	-0.07740800	-2.06152900
C	-4.46546800	-1.33554400	-4.55947400
H	-2.29340500	-1.31126900	-4.59088500
C	-5.50649200	-0.36367700	-2.59225400
H	-4.14722400	0.40292100	-1.08101000
C	-5.62364200	-0.99279800	-3.84265200
H	-4.54789200	-1.82311400	-5.53755600
H	-6.40498000	-0.09897400	-2.02326500
H	-6.61357200	-1.21572900	-4.25628600
C	2.13515700	-4.26844600	-0.04641500
C	2.97436600	-5.13794400	-0.77817600
C	1.43925900	-4.78221600	1.07069800
C	3.11633500	-6.48255200	-0.40106500
H	3.50734000	-4.75420600	-1.65546200
C	1.58274900	-6.12637000	1.44778200
H	0.79070900	-4.11347100	1.64726300
C	2.42193600	-6.98057800	0.71361700
H	3.76710300	-7.14398700	-0.98434500
H	1.03960900	-6.50554600	2.32084700
H	2.53334800	-8.03017400	1.00793700
C	5.84532000	4.11671800	-0.57816400
C	3.19252000	5.90785100	-0.83683000
O	6.32110800	4.99547000	-1.28638000
O	6.56312800	3.44511000	0.37430000
C	7.95480800	3.86393900	0.49300600
H	8.45452400	3.72044100	-0.48158500

H	7.97569000	4.94443500	0.71878000
C	8.58847500	3.03330400	1.59920900
H	8.56773900	1.95744900	1.35408100
H	9.64211300	3.33501700	1.73374400
H	8.06049200	3.18106500	2.55647000
O	2.33455800	6.55824600	-1.43421800
O	4.14266200	6.47109400	-0.04449600
C	4.15816600	7.92662500	-0.03717100
H	3.20768300	8.28791700	0.39497200
H	4.20813700	8.28454600	-1.08029000
C	5.36756800	8.35767400	0.77932500
H	6.29627900	7.96600700	0.33136300
H	5.42821800	9.45993400	0.80506400
H	5.29679400	7.99049300	1.81760700
O	1.04898200	0.64944700	0.65675500
O	0.70046600	1.75845200	1.20475700
O	2.09284900	0.38049500	-3.07146200
H	2.84607400	-0.24324200	-2.96546100
H	2.51080200	1.25572600	-3.23069600

Fe^{III}DEsP-peroxy

C	4.37618000	-2.44769800	0.18327200
C	5.09397200	-1.30651700	0.41524100
C	4.26398000	-0.19761800	-0.00237100
C	3.09788500	-2.03309600	-0.36641100
C	2.04547200	-2.91634200	-0.65564000
C	4.69357500	1.12182300	0.05292600
C	3.97815500	2.21920100	-0.43863700
C	4.47989600	3.57540600	-0.52250000
C	3.49632600	4.31025700	-1.20698400

C	2.42451000	3.39046800	-1.49129200
C	1.21265700	3.75463300	-2.09088200
C	0.12296900	2.91408000	-2.24968700
C	-1.14381500	3.35650200	-2.78595500
C	-1.99287700	2.28452000	-2.73363600
C	-1.23908700	1.17286400	-2.18280300
C	-1.74520500	-0.13069100	-2.04634600
C	-0.94141000	-1.22691500	-1.67101600
C	-1.41072700	-2.59501100	-1.65099400
C	-0.33773300	-3.37744600	-1.31444900
C	0.77408600	-2.48421200	-1.07866500
H	6.10011000	-1.20328800	0.82771900
H	4.66313700	-3.48028700	0.38116900
H	-0.29925500	-4.46267500	-1.22483900
H	-2.42781500	-2.91211800	-1.87901400
H	-3.03284000	2.22968500	-3.05534300
H	-1.34092400	4.36935200	-3.14351600
N	2.72117500	2.11228200	-1.02874400
N	3.03663200	-0.64812600	-0.48179600
N	0.40226500	-1.16128500	-1.31094700
N	0.06765000	1.55914600	-1.89783700
H	1.12247100	4.78880200	-2.43268600
H	5.67731200	1.31516700	0.48416500
Fe	1.52157200	0.47877300	-1.08488300
C	-3.19039600	-0.36056400	-2.36163800
C	-3.59247400	-1.15830300	-3.45793400
C	-4.19928500	0.23609100	-1.57019500
C	-4.95126300	-1.35881900	-3.74797100
H	-2.82182800	-1.61638000	-4.08789000
C	-5.55838600	0.04078000	-1.86178500

H	-3.89981900	0.85293000	-0.71576100
C	-5.94118900	-0.75953800	-2.95113300
H	-5.23737200	-1.97911900	-4.60633400
H	-6.32186000	0.51106400	-1.23003600
H	-7.00288100	-0.91425800	-3.17830500
C	2.28063300	-4.38367300	-0.46940400
C	3.20327000	-5.07899400	-1.28400500
C	1.59621700	-5.11236900	0.53049500
C	3.43345100	-6.45264400	-1.10681300
H	3.73657500	-4.52619500	-2.06539200
C	1.82168300	-6.48669900	0.70602500
H	0.88737700	-4.58244100	1.17618600
C	2.74200300	-7.16357000	-0.11181300
H	4.15168300	-6.97073700	-1.75416600
H	1.28140800	-7.02917700	1.49154900
H	2.91988300	-8.23692200	0.02612200
C	5.82291000	4.06534000	-0.16534300
C	3.44681800	5.75228000	-1.49901400
O	6.46625300	4.92619500	-0.76603700
O	6.33223200	3.43886900	0.96069100
C	7.66459600	3.86182200	1.32694100
H	8.35333400	3.68851200	0.47905800
H	7.65811200	4.95059000	1.51931900
C	8.06969800	3.07027300	2.56471700
H	8.09006100	1.98692600	2.35423000
H	9.07734400	3.37783200	2.89874400
H	7.35972600	3.24450100	3.39143200
O	2.86972200	6.28345900	-2.45332400
O	4.10695000	6.48685900	-0.54673100
C	4.23687800	7.89483400	-0.83851800

H	3.24627500	8.38067800	-0.74949400
H	4.56990100	8.02048700	-1.88445000
C	5.24449500	8.46199800	0.15432100
H	6.20843100	7.93520900	0.05509100
H	5.40340700	9.53956800	-0.03355500
H	4.88837400	8.33822300	1.19204300
O	0.91580900	0.67555400	0.61525000
O	0.62506200	1.87434600	1.03428500
O	2.26061000	0.30994700	-3.20415000
H	2.93337300	1.01390500	-3.06572500
H	1.48341700	0.80404100	-3.55012700

Fe^{III}DEsP-hydroperoxy

C	4.35247000	-2.43970200	0.20237900
C	5.07663500	-1.29778900	0.41475000
C	4.25996300	-0.19288300	-0.03235600
C	3.08630900	-2.03090100	-0.37438500
C	2.03611400	-2.91449600	-0.68419100
C	4.68254700	1.13118400	0.01325100
C	3.94616800	2.23404500	-0.42956500
C	4.45476200	3.58589900	-0.51186400
C	3.44802200	4.35590100	-1.09071800
C	2.33801900	3.46147600	-1.33734700
C	1.09982500	3.84345900	-1.85789700
C	0.01851700	2.98549900	-2.02882200
C	-1.27003800	3.43332600	-2.50827600
C	-2.08575700	2.33632000	-2.52358700
C	-1.28855500	1.21280800	-2.06474800
C	-1.76226300	-0.11036400	-2.01469200
C	-0.94290300	-1.20629200	-1.69342500

C	-1.39978600	-2.58159400	-1.73140900
C	-0.33010700	-3.36511800	-1.40434100
C	0.77544300	-2.46980100	-1.12269900
H	6.07611100	-1.19572800	0.84133900
H	4.62992800	-3.46912200	0.42493700
H	-0.28146100	-4.45140800	-1.34706300
H	-2.41091200	-2.89343000	-1.98898500
H	-3.12857400	2.27079600	-2.83115100
H	-1.49920700	4.46177900	-2.79162200
N	2.64953400	2.16612300	-0.93157400
N	3.04106200	-0.65135300	-0.52561200
N	0.39355000	-1.14842700	-1.32395200
N	0.00112700	1.61896500	-1.76968700
H	0.98517200	4.89193800	-2.14311500
H	5.67476000	1.32857700	0.42464400
Fe	1.46896300	0.50416400	-1.04980400
C	-3.20219600	-0.35833600	-2.35244200
C	-3.56675900	-1.00699500	-3.55300400
C	-4.22322500	0.06602700	-1.47374000
C	-4.91738900	-1.22858700	-3.86465700
H	-2.78152800	-1.32824100	-4.24648300
C	-5.57341800	-0.15717600	-1.78624200
H	-3.94805700	0.56548400	-0.53819200
C	-5.92453600	-0.80519800	-2.98194700
H	-5.18273500	-1.72888100	-4.80301000
H	-6.35274200	0.17368500	-1.09035500
H	-6.97877100	-0.97847500	-3.22554300
C	2.26237200	-4.38329500	-0.49191600
C	3.19086600	-5.08110800	-1.29598900
C	1.56114500	-5.09857000	0.50478500

C	3.40891200	-6.45548600	-1.11226000
H	3.73578200	-4.53834000	-2.07665800
C	1.77968100	-6.47268200	0.68798100
H	0.84979900	-4.56359500	1.14356300
C	2.70345600	-7.15583300	-0.12007800
H	4.12855400	-6.98082900	-1.75046600
H	1.23019800	-7.00925700	1.46977100
H	2.87362500	-8.22872600	0.02344800
C	5.84556700	4.02904000	-0.20608000
C	3.42291100	5.81249200	-1.36705800
O	6.53320600	4.72730500	-0.94019700
O	6.27817100	3.54120400	0.99700600
C	7.63966600	3.92280000	1.35427200
H	8.32938700	3.54767000	0.57718100
H	7.70589400	5.02479900	1.35044900
C	7.93329300	3.33275500	2.72563900
H	7.86559000	2.23140700	2.71037700
H	8.95474700	3.61086700	3.03963000
H	7.22332400	3.71275300	3.47965900
O	2.72235000	6.35688400	-2.22112900
O	4.25542700	6.49326400	-0.53522400
C	4.36197000	7.92094900	-0.79877300
H	3.37683900	8.38808400	-0.61947500
H	4.61047900	8.06532900	-1.86466300
C	5.44038700	8.46778600	0.12480100
H	6.40353300	7.96517300	-0.06540800
H	5.56871300	9.55057200	-0.04949600
H	5.16947700	8.31759900	1.18404700
O	0.92550300	0.57777800	0.61719000
O	0.56370200	1.89700800	1.12510300

H	1.31681300	2.43503300	0.77485500
O	2.22327400	0.28960200	-3.01849200
H	3.00841200	-0.27367200	-2.83029600
H	2.59495900	1.17454200	-3.22977100

Fe^{III}TEsP-oxy

O	7.22284200	3.69527900	8.72692800
O	8.60322000	2.76357000	10.30073400
N	11.40048500	8.14743100	9.23697600
O	7.85723100	9.16817400	11.84512400
N	11.20536100	5.68736500	7.98316400
N	13.35672000	8.95851200	7.28247900
O	9.33098700	1.37928000	7.82088300
O	9.20302600	7.89357300	13.18790300
N	13.14817900	6.53279100	6.06135100
O	11.47006700	1.48685200	7.04018000
C	11.45606600	4.45292900	7.42116500
C	9.57967800	4.17642500	8.68206900
C	10.27248300	7.71688300	9.93421800
C	13.90453300	7.13288400	5.06418100
C	9.55843700	6.53107600	9.64754400
C	14.28434200	8.48769100	5.03399800
C	13.13982400	5.18185300	5.75899600
C	10.06726700	5.54363400	8.77362400
C	12.40203500	4.20694900	6.42064500
H	12.49173000	3.17832300	6.06886800
C	10.47973300	3.48271600	7.88538000
C	10.00600100	8.62291800	11.04009200
C	11.00383900	9.59002200	11.01741600
C	8.32748800	3.55028700	9.22849900

C	15.01425200	9.00481600	3.83621200
C	8.21571700	6.30555800	10.28073200
C	8.99131400	8.49429400	12.14224100
C	14.04680900	9.33225800	6.13339400
C	11.83242300	9.30208500	9.86164200
C	13.46557000	10.03796400	8.14882600
C	13.92521700	4.92339100	4.57110300
H	14.08226600	3.93490900	4.13600900
C	14.37546100	6.13535700	4.12132100
H	14.99992000	6.34930900	3.25478200
C	12.82474700	10.16238500	9.37808300
H	13.02929700	11.04809300	9.98425400
C	10.34140400	2.03858800	7.58733500
C	16.35605300	9.44039800	3.91801900
H	16.87866000	9.38820100	4.87975900
O	10.23382300	10.81401600	12.88378100
C	14.25223700	11.09067400	7.54686500
H	14.47882000	12.04408800	8.02702900
C	14.57365400	10.67390500	6.28141300
H	15.13093400	11.21050400	5.51465600
O	12.19030200	11.48294700	11.93089200
C	8.06433400	5.60542900	11.49433100
H	8.95087000	5.24970900	12.02667700
C	14.36227400	9.05116900	2.58318200
H	13.31968400	8.72226300	2.51451100
C	16.36454200	9.96301000	1.54067900
H	16.88701800	10.33497500	0.65224000
C	17.02478300	9.91594400	2.77946500
H	18.06748800	10.24367600	2.86004500
C	11.22682100	10.71413100	11.95401500

C	7.06686400	6.78136500	9.61252800
H	7.18367500	7.31849500	8.66542700
C	15.03203200	9.52853300	1.44624400
H	14.50837200	9.56502400	0.48428000
C	7.47267400	1.97613300	10.77361100
H	7.09612400	1.37636500	9.92728100
H	6.67229700	2.66927400	11.08806300
C	11.36630100	0.06435700	6.74413900
H	11.11810800	-0.47062900	7.67760400
H	10.52905200	-0.09220100	6.04112800
C	6.78307500	5.37933400	12.02562200
H	6.67893900	4.84295600	12.97561900
C	6.84029900	9.15574300	12.89180100
H	7.27594400	9.60208900	13.80317700
H	6.58216600	8.10688600	13.11398900
C	5.64437000	5.84257400	11.34633200
H	4.64534800	5.65403200	11.75604900
C	12.70059800	-0.38065000	6.16367000
H	13.52358500	-0.19696100	6.87530200
H	12.66792700	-1.46226200	5.94404400
H	12.92587900	0.15291000	5.22407600
C	5.78950800	6.54845400	10.14009700
H	4.90531800	6.90449500	9.59981900
C	7.97261200	1.10906400	11.91969500
H	8.35970400	1.72749800	12.74799000
H	7.14528200	0.48910500	12.30815100
H	8.77977200	0.43722300	11.58145100
C	5.64922100	9.94592700	12.37205200
H	4.85537400	9.97319400	13.13939500
H	5.93487900	10.98418100	12.13062300

H	5.23741500	9.47694800	11.46270600
C	10.42919300	11.86485200	13.87249500
H	10.47524400	12.83694800	13.35022300
H	11.40470300	11.70728400	14.36536600
C	9.27092600	11.79147400	14.85597300
H	9.39691400	12.56223300	15.63668600
H	8.30728200	11.97040400	14.34887900
H	9.23297300	10.80338200	15.34520400
Fe	12.20044200	7.37317400	7.55779300
O	10.89244900	7.98595600	6.60520400
O	11.09006400	8.51571400	5.45129600
O	13.75724800	6.66975100	8.85639600
H	13.41214800	6.86534500	9.75568200
H	14.46211200	7.33724600	8.70224000

Fe^{III}TEsP-peroxy

O	7.19752300	3.74549700	8.69868100
O	8.57065100	2.79911500	10.26488800
N	11.33544900	8.24873000	9.15046300
O	7.87355300	9.15275500	11.95915100
N	11.21460700	5.73043600	7.98505300
N	13.23914900	9.05212100	7.19399900
O	9.34209500	1.40400800	7.82715100
O	9.28629800	7.82151600	13.16292800
N	13.16992800	6.55280100	6.08072700
O	11.51409100	1.50040700	7.14055100
C	11.47963900	4.47714400	7.45208300
C	9.56473500	4.22867600	8.66739700
C	10.24874000	7.77548700	9.89608100
C	13.95778300	7.12913000	5.08650200

C	9.54468100	6.58020200	9.62275200
C	14.30337400	8.49111000	5.02663000
C	13.19940600	5.18521300	5.81550000
C	10.05126300	5.58796200	8.75565000
C	12.45620300	4.21581000	6.48543400
H	12.56788900	3.18133200	6.15847100
C	10.49161000	3.51341900	7.90831200
C	9.98239000	8.66539600	11.00853200
C	10.92467800	9.69166600	10.93743200
C	8.30815600	3.60622900	9.19122000
C	15.08569400	8.97186500	3.84707200
C	8.19841900	6.36180900	10.25114000
C	9.03754900	8.47246000	12.15423300
C	13.99146600	9.38040700	6.06900300
C	11.72123600	9.43120100	9.75025400
C	13.30215600	10.17627200	8.00690800
C	14.03501000	4.90255100	4.67138100
H	14.22255500	3.90316900	4.27265600
C	14.48548900	6.11126200	4.20301400
H	15.14190500	6.30609800	3.35469600
C	12.65419100	10.32913000	9.22633700
H	12.81951500	11.24776300	9.79329800
C	10.35730100	2.07705100	7.63248400
C	16.41175200	9.44550400	3.97340000
H	16.87702600	9.45736600	4.96534300
O	10.22084600	10.80728300	12.90223300
C	14.09002800	11.21889100	7.38781600
H	14.27643000	12.19856200	7.83262300
C	14.48795900	10.74029500	6.16790700
H	15.07475300	11.24623100	5.40144400

O	11.98004200	11.70358400	11.76718600
C	8.02464100	5.62925900	11.44299700
H	8.90330600	5.24340900	11.96696500
C	14.50659200	8.94491300	2.55736900
H	13.47675000	8.58662200	2.45314700
C	16.54250400	9.85393400	1.57613200
H	17.10487500	10.19576400	0.69885300
C	17.13190500	9.88420600	2.85095900
H	18.16103900	10.24386900	2.97272500
C	11.12245000	10.81872600	11.85589600
C	7.05801100	6.87994500	9.59929700
H	7.19238400	7.44379100	8.67020000
C	15.22686700	9.38113300	1.43448800
H	14.75494800	9.35744000	0.44465700
C	7.43709200	2.00985300	10.70128300
H	7.07063600	1.42212500	9.84123800
H	6.62809000	2.69303000	11.01831800
C	11.40085300	0.08773200	6.85261600
H	11.12087000	-0.44877600	7.77778800
H	10.58391300	-0.07312500	6.12538600
C	6.73760300	5.41185700	11.96504000
H	6.62037800	4.84816200	12.89847900
C	6.92763500	9.06380700	13.05582000
H	7.39493100	9.49145000	13.96180700
H	6.71332900	7.99995400	13.25525300
C	5.60926900	5.91728900	11.29856600
H	4.60487300	5.73616000	11.70050400
C	12.74744000	-0.37646900	6.31133500
H	13.55117700	-0.19526600	7.04580300
H	12.71376600	-1.45895200	6.09206600

H	13.00542000	0.15721000	5.38021800
C	5.77384300	6.65733200	10.11535500
H	4.89840000	7.04860600	9.58372300
C	7.91798000	1.12002800	11.84028100
H	8.29559000	1.72494100	12.68322800
H	7.08626300	0.49226300	12.20854000
H	8.73148900	0.45624400	11.50025300
C	5.67974100	9.82877000	12.63635500
H	4.92868700	9.80170700	13.44673000
H	5.91698000	10.88400000	12.41502500
H	5.23632000	9.37547600	11.73375000
C	10.41730400	11.86510800	13.86649400
H	10.30138200	12.84363000	13.36451200
H	11.45348500	11.81923500	14.24909000
C	9.39444500	11.67009300	14.97841300
H	9.52699500	12.44582000	15.75439200
H	8.36544600	11.74594800	14.58620200
H	9.51329600	10.67906200	15.44891000
Fe	12.16852000	7.43962400	7.53970700
O	10.76249600	7.97185500	6.50484600
O	10.99381300	8.45697100	5.31735400
O	13.78755100	6.61692500	8.83121800
H	14.29515800	6.26060100	8.06773100
H	13.26276100	5.84636300	9.14340500

Fe^{III}TEsP-hydroperoxy

O	7.07418700	4.00062100	8.66198400
O	8.35223100	2.57886100	9.92392500
N	11.06789600	8.31619400	8.99752300
O	7.83831400	9.32510500	12.09255300

N	11.12287100	5.71592800	7.98472700
N	13.01991400	9.12416200	7.00787600
O	9.07546700	1.55102500	7.33119700
O	9.26399200	7.81771600	13.06070300
N	13.14464300	6.53475700	6.07588500
O	11.33228500	1.50311900	7.00747600
C	11.36737300	4.49030900	7.40303300
C	9.46920000	4.20172400	8.62418900
C	10.10608900	7.77848500	9.85376100
C	14.09452000	7.06393600	5.20155000
C	9.50986400	6.50687800	9.70140300
C	14.37920900	8.43325300	5.04675100
C	13.22407100	5.15760400	5.90103700
C	9.98969000	5.55206800	8.77841700
C	12.39528400	4.21654600	6.49569200
H	12.52412000	3.17412900	6.19999800
C	10.35809800	3.52541600	7.80225400
C	9.78154400	8.74142400	10.89676500
C	10.51801300	9.88618500	10.62835800
C	8.16102800	3.61939200	9.07167800
C	15.31727900	8.85773400	3.96231500
C	8.33545500	6.15704400	10.55992300
C	8.94946200	8.54504600	12.12857900
C	13.82942900	9.39987300	5.90993100
C	11.27964600	9.61462300	9.42413300
C	12.80455900	10.35422800	7.61631500
C	14.24013100	4.82142100	4.93015500
H	14.49563200	3.80369400	4.63018000
C	14.77553300	6.00099900	4.48855100
H	15.57113300	6.15582700	3.76091700

C	12.06069300	10.57005700	8.76968300
H	12.03364800	11.57961800	9.18734700
C	10.16183100	2.12190000	7.36291700
C	16.54096700	9.49743200	4.26505700
H	16.80602400	9.67475800	5.31332000
O	10.21760200	10.96262800	12.70629800
C	13.47866300	11.40759300	6.89508300
H	13.45452700	12.46171200	7.17618900
C	14.09657100	10.82137100	5.82278300
H	14.68693600	11.29526400	5.03981900
O	10.98842300	12.22904600	10.97553500
C	8.44837800	5.19659100	11.58733100
H	9.41641300	4.72256900	11.77619200
C	14.99990800	8.61806800	2.60593200
H	14.04893200	8.13389100	2.35791900
C	17.08912900	9.64694000	1.89827400
H	17.77404100	9.95351400	1.09986400
C	17.41842900	9.88825700	3.24224800
H	18.36555200	10.37707500	3.49733500
C	10.59820400	11.14380000	11.40823600
C	7.09073300	6.78474700	10.33964200
H	6.99762300	7.52147300	9.53535400
C	15.87714900	9.01061000	1.58362600
H	15.60874200	8.82421500	0.53765900
C	7.14392200	1.83439600	10.24869700
H	6.67114200	1.51555100	9.30406300
H	6.44601400	2.51182300	10.77205800
C	11.17776100	0.12358100	6.56521300
H	10.71427800	-0.45641900	7.38250300
H	10.48177200	0.10052400	5.70803300

C	7.33792200	4.87133300	12.37937800
H	7.44419000	4.13964400	13.18808100
C	7.00379300	9.25174600	13.28367400
H	7.61874400	9.52502900	14.15961000
H	6.67493900	8.20626600	13.41422600
C	6.09686100	5.48523500	12.14081000
H	5.22584800	5.21989600	12.75120300
C	12.56051900	-0.39832300	6.20315300
H	13.24240500	-0.35046800	7.06931900
H	12.48716300	-1.45109400	5.87831400
H	13.00378300	0.18473800	5.37745900
C	5.97569600	6.44123500	11.11825600
H	5.00752400	6.91335500	10.91729100
C	7.56143900	0.65268600	11.11172300
H	8.04603900	0.99148400	12.04379000
H	6.67405500	0.05298800	11.38111200
H	8.26800900	0.00274700	10.56826300
C	5.83450600	10.20297200	13.07659200
H	5.17352000	10.18258000	13.96108400
H	6.18518300	11.23870800	12.92874400
H	5.24041100	9.91070300	12.19404100
C	10.28919800	12.15586200	13.53824600
H	9.53030600	12.87765500	13.18580500
H	11.27940000	12.62275200	13.39764300
C	10.05325900	11.72780300	14.97902100
H	10.11511600	12.60831900	15.64261400
H	9.05628600	11.27199700	15.10390300
H	10.81100800	10.99418900	15.30201000
Fe	12.01566900	7.45196100	7.45388900
O	10.66242000	7.84646700	6.40805800

O	10.96685000	8.13937100	5.01355100
H	11.64000300	7.43615800	4.83013000
O	13.55355800	7.06936800	8.83983100
H	14.17078100	7.80788800	8.63462200
H	13.15602600	7.30441600	9.70801900

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