Supporting Information

For

Closed-shell Phenalenyl-based Dinuclear Iron(III) Complex as a Robust Cathode for One-Compartment H_2O_2 Fuel Cell

Nisha Kamboj[a], Ayan Dey[b], Prem Lama[c], Moumita Majumder[b], Srijan Sen Gupta*[b], Ramesh K. Metre*[a]*

[a] Department of Chemistry, Indian Institute of Technology Jodhpur, Rajasthan- 342030, India

[b] Department of Metallurgical and Materials Engineering, Indian Institute of Technology Jodhpur, Rajasthan- 342030, India

[c] CSIR-Indian Institute of Petroleum, Haridwar Road, Mokhampur, Dehradun- 248005, India

Table of Contents

CORRESPONDING AUTHOR FOOTNOTE: * To whom correspondence should be addressed. E-mail: rkmetre@iitj.ac.in, srijansengupta@iitj.ac.in, mmajumder@iitj.ac.in Phone: (+91) 291-280-1309.

1. Materials and general methods

All the chemicals were obtained from commercial sources, and used without further purification. Carbon black, and N-methyl pyrrolidine (NMP) were procured from Alfa Aesar, and Nafion solution (5 wt. %) was procured from Sigma Aldrich. The commercially available H_2O_2, 30% w/v, procured from Alfa Aesar, was used to perform the experiments. The solvents required for synthesis, and conducting CV measurements were dried and distilled using standard techniques. *9-hydroxy-1H-phenalen-1-one* was prepared using the literature method.[1]

Crystals suitable for single crystal X-ray diffractions (SCXRD) were loaded on a Bruker Smart Apex CCD diffractometer at 100 K. All the structures were solved by direct methods using SHELXS-97 and refined by full-matrix least squares on F^2 using SHELXL-97 softwares.[2] The details of crystallographic refinement parameters is given in Table S1. Anisotropic displacement parameters are used to refine the non-hydrogen atoms. All the hydrogen atoms were included in idealized positions, and were refined isotropically by a riding model.

The cyclic voltammetric (CV) tests were performed using a three-electrode assembly; glassy carbon (GC) working electrode, Pt counter electrode, and Ag/AgCl (3.0 M KCl) reference electrode. The electrochemical studies of complex **1** with CV were conducted in 10 ml DMF solution of complex **1** (1 mM) and the supporting electrolyte, tetrabutylammonium hexafluorophosphate (0.1 M). The CV measurements were carried out under an oxygen-free atmosphere by purging nitrogen gas, and the scan rate was fixed at 50 mV s^{-1}. To test H_2O_2 fuel cell activity, the modified GC electrode and Ni foam anode were immersed in the supporting electrolyte for at least 5 min before adding H_2O_2 to the electrolytic solution. The performance tests are repeated at least 5 times to ensure the reproducibility.

2. Crystallographic data for the hmbh-PLYH_2 ligand and complex 1.

Table S1. Crystal data and structure refinement parameters for the ligand, hmbh-PLYH_2 and complex **1**.

Identification code	hmbh-PLYH_2	Complex **1**
Empirical formula	$C_{21}H_{16}N_2O_3$	$C_{65}H_{44}N_6O_9Cl_6Fe_2$
Formula weight	344.36	1377.46
Temperature/K	100	100
Crystal system	orthorhombic	monoclinic
Space group	*Aba2*	$P2_1/c$
a/Å	16.38(2)	23.2460(12)
b/Å	29.87(4)	13.2054(7)
c/Å	6.843(9)	19.6226(10)
α/°	90	90
β/°	90	101.358(2)
γ/°	90	90
Volume/Å^3	3348(7)	5905.6(5)
Z	8	4
ρ_{calc}g/cm^3	1.366	1.549
μ/mm^{-1}	0.093	0.829
F(000)	1440.0	2808.0
Crystal size/mm^3	0.21 × 0.19 × 0.16	0.2 × 0.19 × 0.16
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.996 to 49.998	4.234 to 50.698
Index ranges	$-14 \le h \le 19$, $-34 \le k \le 35$, $-8 \le l \le 8$	$-28 \le h \le 28$, $-15 \le k \le 15$, $-23 \le l \le 16$
Reflections collected	10271	52543
Independent reflections	2837 [R_{int} = 0.0935, R_{sigma} = 0.1068]	10810 [R_{int} = 0.0501, R_{sigma} = 0.0430]
Data/restraints/parameters	2837/7/231	10810/0/805
Goodness-of-fit on F^2	1.133	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0973, wR_2 = 0.1617	R_1 = 0.0797, wR_2 = 0.1928
Final R indexes [all data]	R_1 = 0.1336, wR_2 = 0.1759	R_1 = 0.0990, wR_2 = 0.2043
Largest diff. peak/hole / e Å^{-3}	0.25/-0.28	1.01/-1.18

3. Bond parameters of complex 1, and comparison with the iso-structural [$Fe_2^{III}(salhn)_3$] complex.

Table S2. Comparison of the bond distances of the reported $[Fe_2^{III}(salhn)_3]$ complex[3] with complex **1**.

$[Fe_2^{III}(salhn)_3]$		$[Fe^{III}_2(hmbh\text{-}PLY)_3]$, complex **1**	
Bond	**Bond Distance (Å)**	**Bond**	**Bond Distance (Å)**
Fel-O1	1.930(5)	Fe1-O1	1.935(4)
Fel-O3	1.925(3)	Fe1-O8	1.923(4)
Fel-O5	1.912(4)	Fe1-O5	1.906 (4)
Fe1-N1	2.164(5)	F1-N1	2.123(4)
Fe1-N3	2.197(6)	Fe1-N4	2.194(4)
Fe1-N5	2.178(4)	Fe1-N6	2.222(4)
Fe2-O2	1.910(5)	Fe2-O2	1.940(4)
Fe2-O4	1.927(3)	Fe2-O4	1.916(4)
Fe2-O6	1.919(5)	Fe2-O7	1.933(4)
Fe2-N2	2.167(4)	Fe2-N5	2.087(4)
Fe2-N4	2.183(5)	Fe2-N3	2.115(4)
Fe2-N6	2.182(5)	Fe2-N2	2.188(4)

Table S3. Comparison of the bond angles of the reported $[Fe_2^{III}(salhn)_3]$ complex with complex **1**.

$[Fe_2^{III}(salhn)_3]$		$[Fe^{III}_2(hmbh\text{-}PLY)_3]$, complex **1**	
Atoms	**Bond Angle (°)**	**Atoms**	**Bond Angle (°)**
O1-Fe1-N3	169.6(2)	O8-Fe1-N4	168.74(17)
O5-Fe1-N1	169.9(1)	O5-Fe1-N1	170.38(16)
O3-Fe1-N3	84.8(2)	O1-Fe1-N6	82.71(15)
O1-Fe1-N5	92.6(2)	O5-Fe1-O1	95.11(17)
O3-Fe1-O5	97.8(2)	O1-Fe1-N1	94.49(17)
O1-Fe1-N1	84.4(2)	O5-Fe1-N6	87.97(15)
N1-Fe1-N3	85.3(2)	N1-Fe1-N6	87.16(15)
O2-Fe2-N6	171.0(1)	O7-Fe2-N2	171.76(17)
O4-Fe2-N2	167.6(2)	O4-Fe2-N5	167.45(16)
O2-Fe2-N4	92.1(2)	O2-Fe2-N3	90.90(16)
O2-Fe2-O4	99.1(2)	O4-Fe2-O2	89.83(16)
N4-Fe2-N6	86.9(2	N5-Fe2-N3	96.14(17)
O2-Fe2-O6	84.4(2)	O2-Fe2-N5	84.09(16)
O6-Fe2-N6	170.7(2)	O4-Fe2-N3	165.94(16)

4. ^{1}H NMR and ^{13}C NMR Spectra

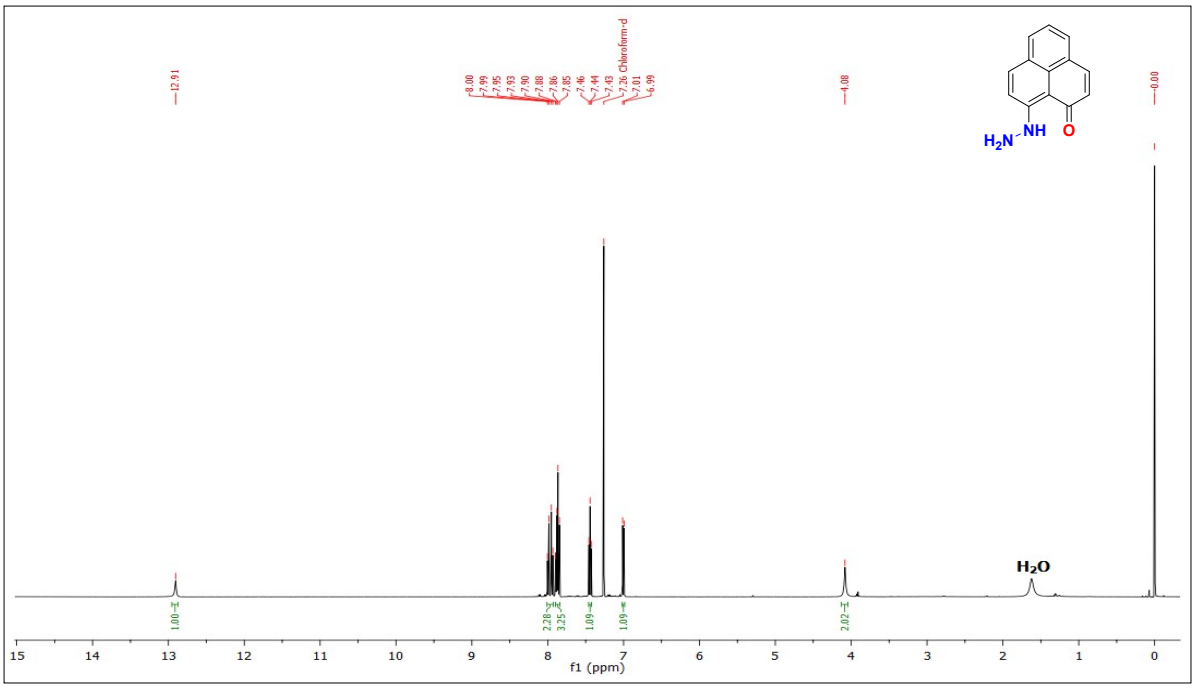


Figure S1. ^{1}H NMR spectrum of Hz-PLY in $CDCl_3$ solvent.

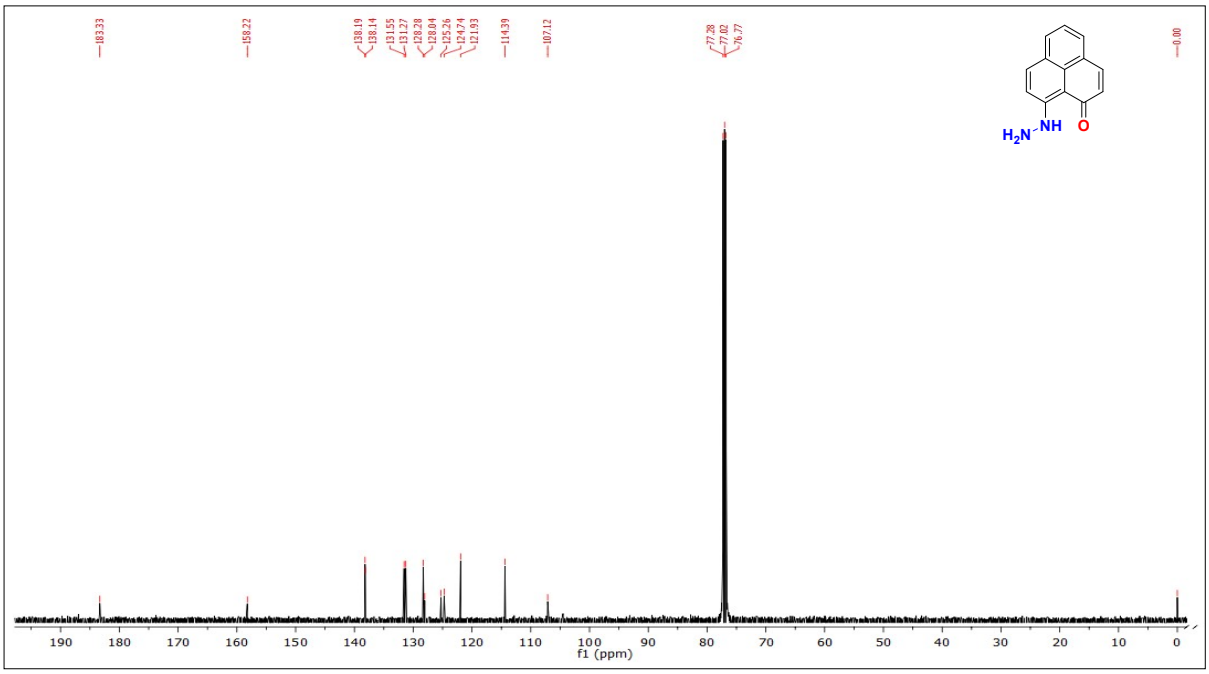


Figure S2. ^{13}C NMR spectrum of Hz-PLY in $CDCl_3$ solvent.

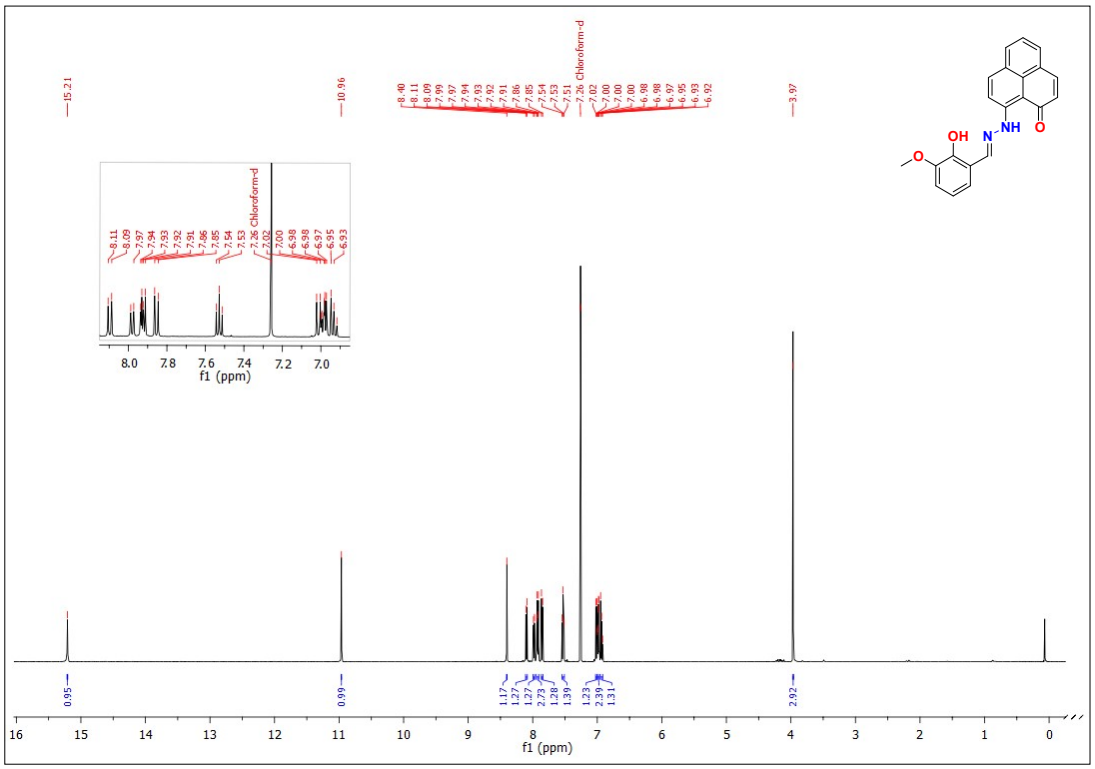


Figure S3. ^{1}H NMR spectrum of hmbh-PLYH_2 in $CDCl_3$ solvent.

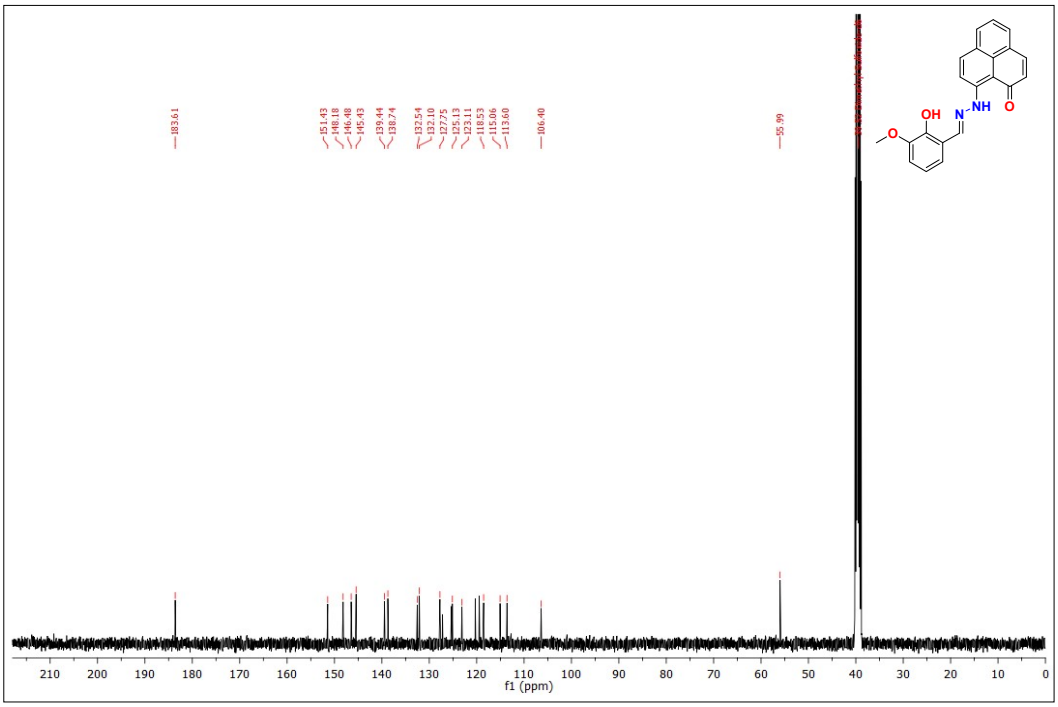


Figure S4. ^{13}C NMR spectrum of hmbh-PLYH_2 in DMSO-d6 solvent.

5. HRMS Spectra of Hz-PLY, hmbh-PLYH_2 and complex 1.

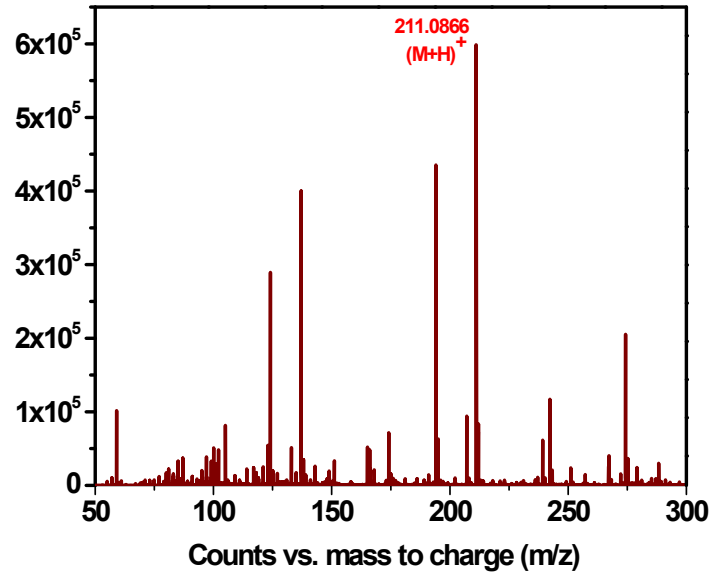


Figure S5. HRMS spectrum of Hz-PLY. HRMS (CH_3CN, positive ionization): calcd. for $C_{13}H_{10}N_2O$ m/z = 211.0867 $[M + H]^+$, found 211.0866 $[M + H]^+$.

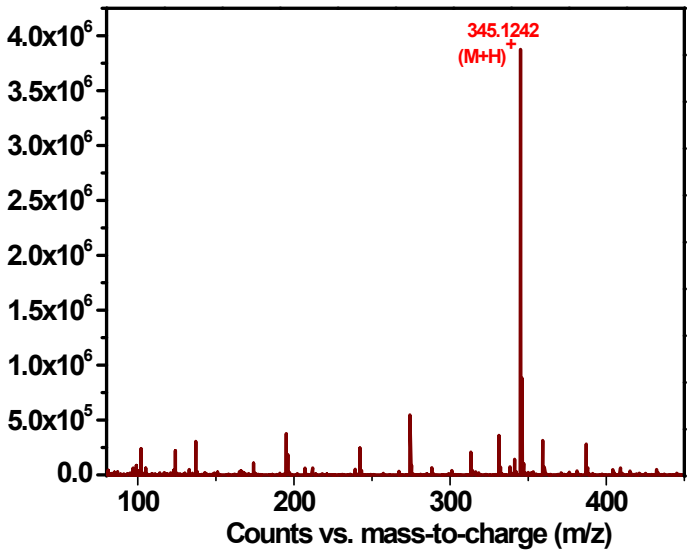


Figure S6. HRMS spectrum of hmbh-PLYH_2. HRMS (CH_3CN, positive ionization): calcd. for $C_{21}H_{16}N_2O_3$ m/z = 345.1234 $[M + H]^+$, found 345.1242 $[M + H]^+$.

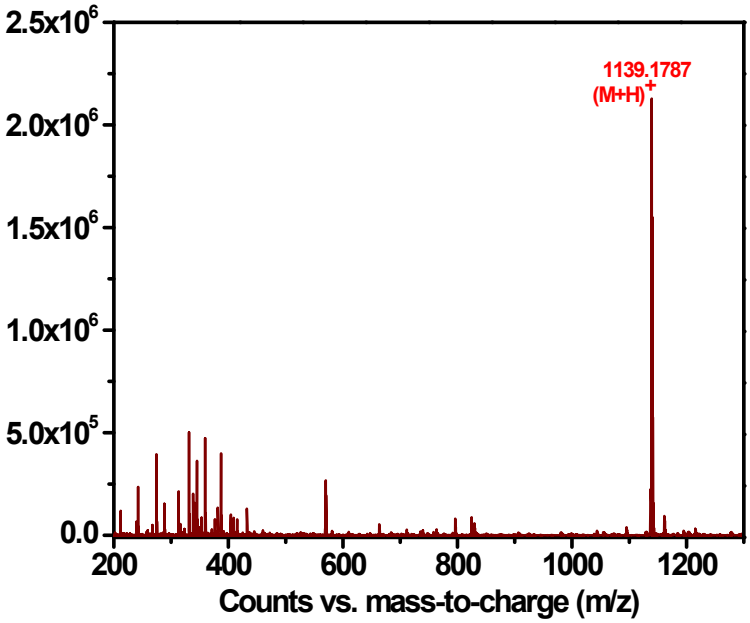


Figure S7. HRMS spectrum of complex **1**. HRMS (CH_3CN, positive ionization): calcd. for $C_{63}H_{42}Fe_2N_6O_9$ m/z = 1139.1785 $(M+H)^+$, found 1139.1787 $[M + H]^+$.

6. FT-IR Spectra of *9-hydrazineyl-1H-phenalen-1-one*, hmbh-PLYH_2 and complex 1.

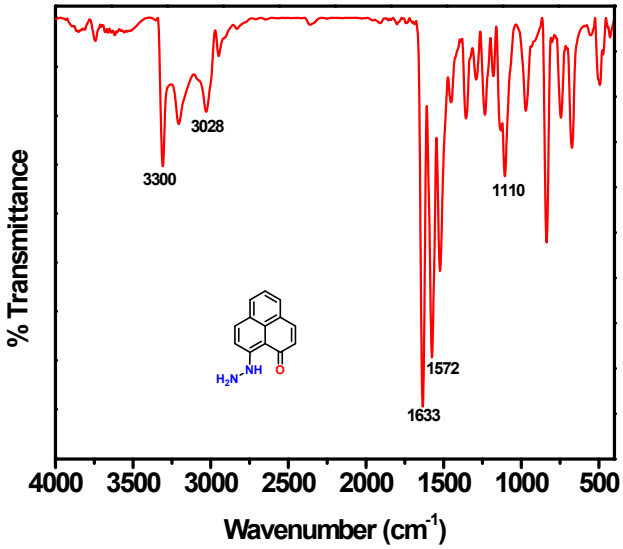


Figure S8. FT-IR spectrum of Hz-PLY.

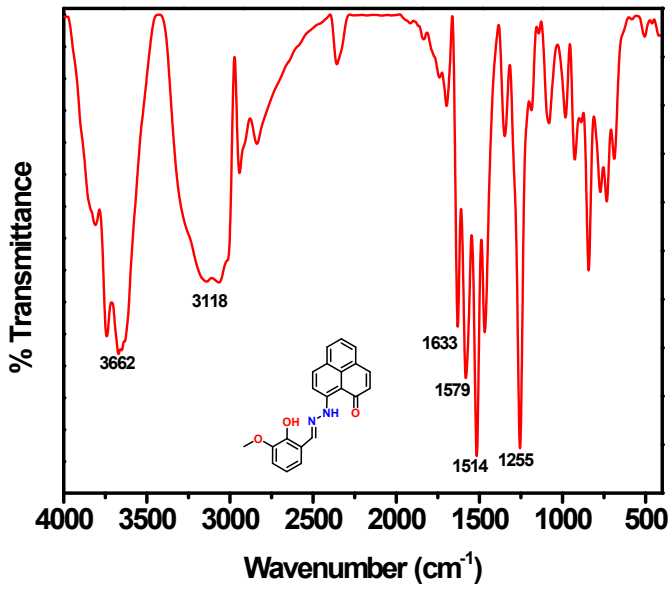


Figure S9. FT-IR spectrum of hmbh-PLYH_2.

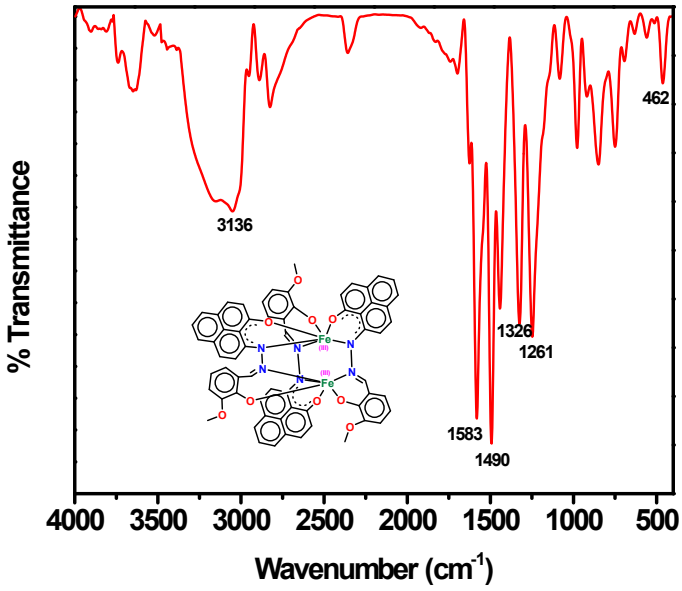


Figure S10. FT-IR spectrum of complex **1**.

7. Thermal stability, EPR, XPS and elemental analysis of the complex 1.

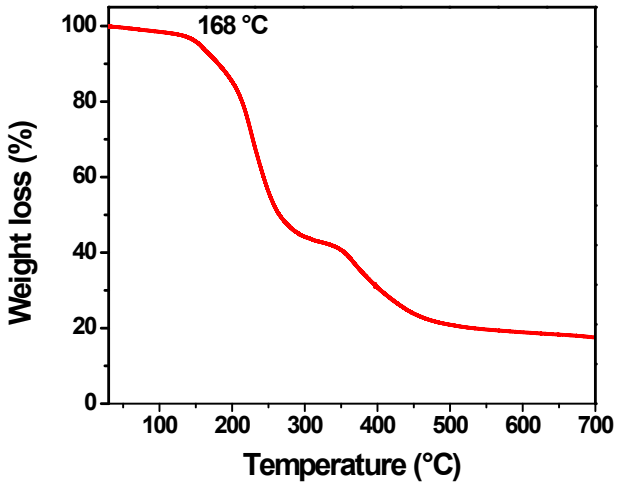


Figure S11. Thermogravimetric analysis (TGA) plot of the complex **1**.

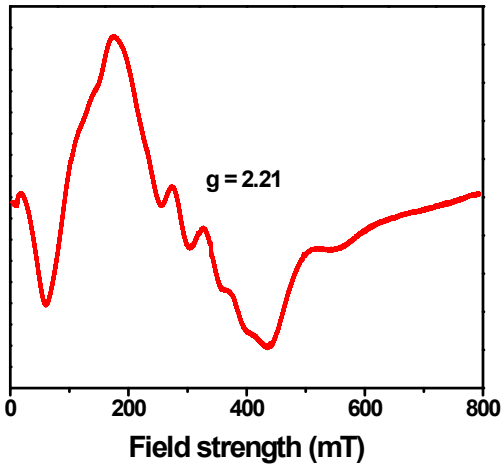


Figure S12. Solid state X-band EPR of complex **1** recorded at room temperature.

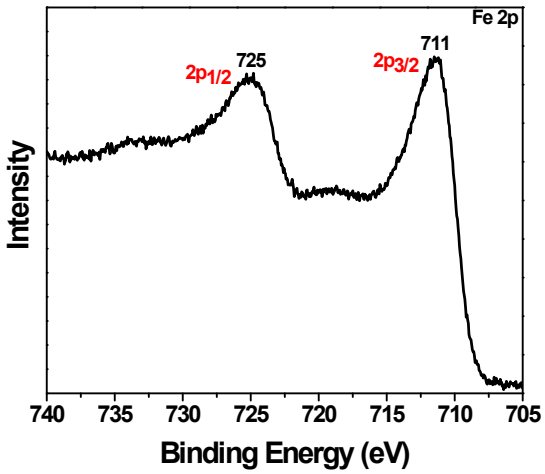
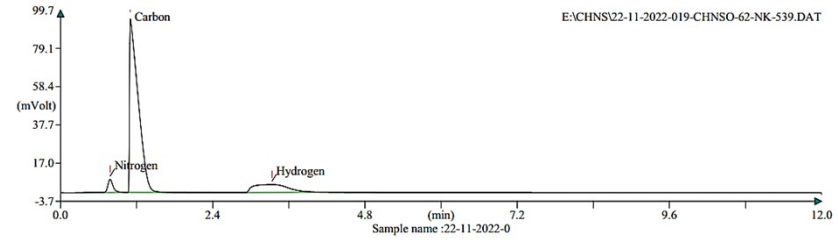


Figure S13. XPS analysis of the complex **1**.



Peak Number (#)	Retention Time (min)	Area (.1*uV*sec)	Element %	Component Name
1	0.783	425447	7.231	Nitrogen
2	1.100	8858511	66.291	Carbon
3	3.333	1688144	4.063	Hydrogen
		10972100	77.585	

Figure S14. Elemental analysis of complex **1**: calcd. for $C_{63}H_{42}Fe_2N_6O_9$: C, 66.45; H, 3.72; N, 7.38. Found: C, 66.29; H, 4.06; N, 7.23.

8. Electrocatalytic reduction of H_2O_2.

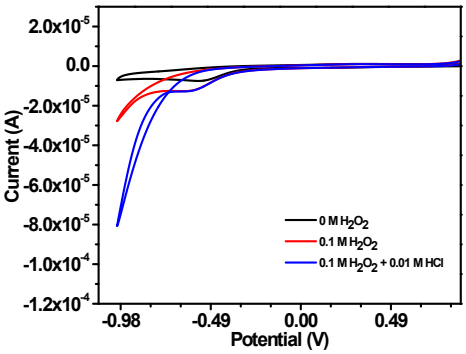


Figure S15. Electrocatalytic reduction of H_2O_2 with bare glassy carbon (GC) electrode in acetate buffer (pH 3), and acetate buffer (pH 3) containing 0.01 M HCl solution in the presence of H_2O_2 (0 M and 0.1 M, as mentioned in the graph). Ag/AgCl(3.0 M KCl) electrode is used as the reference, Pt-wire as the counter electrode, and a scan rate of 100 mV s^{-1} was maintained during the experiment.

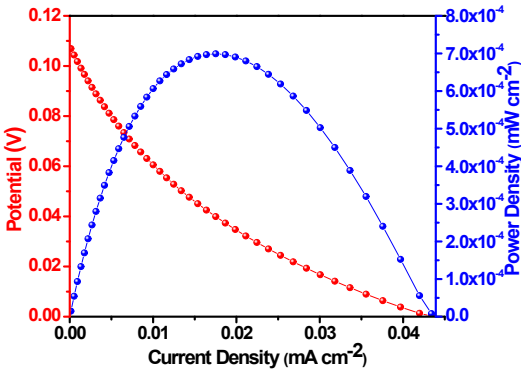


Figure S16. *I-V* (red) and *I-P* (blue) curves of one-compartment H2O2 fuel cell with **GC-1** cathode, and Ni foam anode at a scan rate 10 mV s^{-1}. The performance tests were conducted in an acetate buffer (pH 3) containing 0.3 M H_2O_2. Current density is normalized by the geometrical area of glassy carbon electrode.

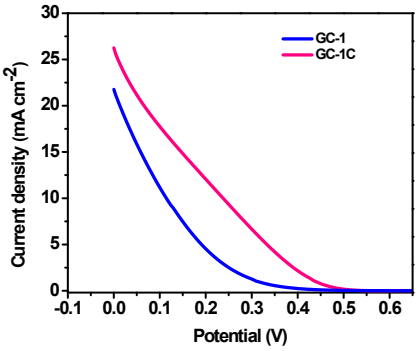


Figure S17. Polarization curves for **GC-1** (blue curve)/**GC-1C** (pink curve) as cathode in 0.1 M HCl containing 0.3 M H_2O_2, and Ni foam as the anode in one compartment H_2O_2 fuel cell at a scan rate 10 mV s^{-1}. Current density is normalized by the geometrical area of glassy carbon electrode.

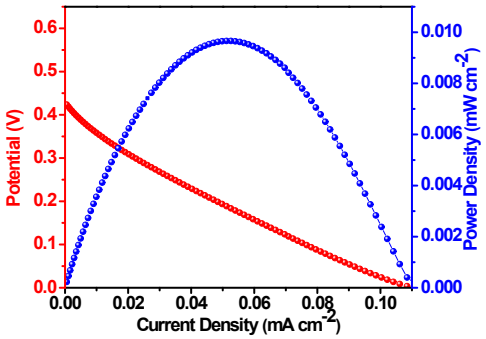


Figure S18. *I-V* (red) and *I-P* (blue) curves of a one-compartment H_2O_2 fuel cell with bare glassy carbon (GC) cathode and Ni foam as anode, at a scan rate 10 mV s^{-1}. The performance tests were conducted in 0.1 M HCl containing 0.3 M H_2O_2. Current density is normalized by the geometrical area of glassy carbon electrode.

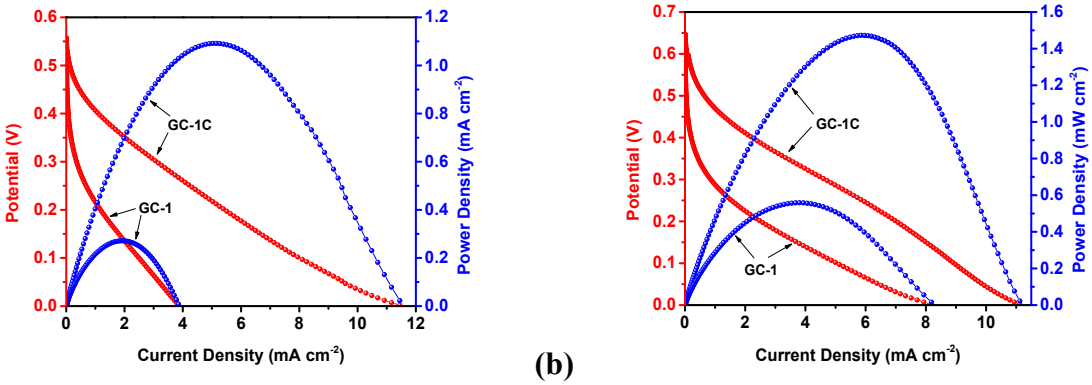


Figure S19. *I-V* (red) and *I-P* (blue) curves of a one-compartment H_2O_2 fuel cell with **GC-1/GC-1C** cathode and Ni foam anode, at a scan rate 10 mV s^{-1}. The performance tests were conducted in (a) 0.05 M and (b) 0.2 M HCl containing 0.3 M H_2O_2. Current density is normalized by the geometrical area of glassy carbon electrode.

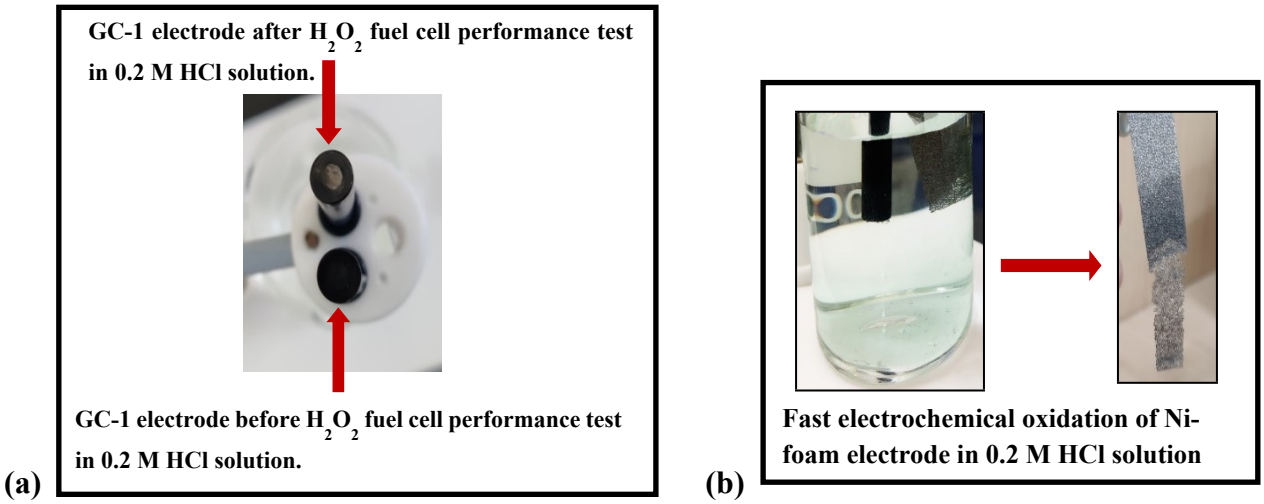


Figure S20. Image showing (a) **GC-1** electrode, before and after the fuel cell performance test in 0.2 M HCl as the electrolyte, and (b) the corrosion of Ni foam anode while running the performance tests in 0.2 M HCl as the electrolyte.

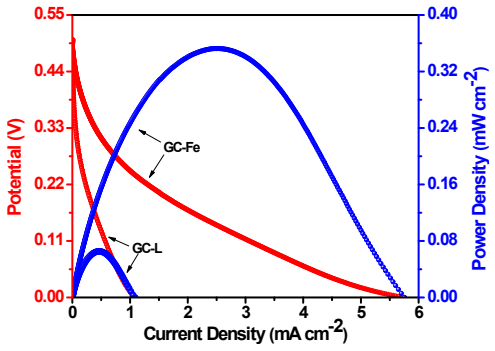


Figure S21. *I-V* (red) and *I-P* (blue) curves of a one-compartment H_2O_2 fuel cell with Ni-foam anode and $FeCl_3$ (**GC-Fe**) modified cathode; and Ni-foam anode and ligand, hmbh-PLYH_2 (**GC-L**) modified cathode at a scan rate 10 mV s^{-1}. The performance tests were

conducted in 0.1 M HCl containing 0.3 M H_2O_2. Current density is normalized by the geometrical area of glassy carbon electrode.

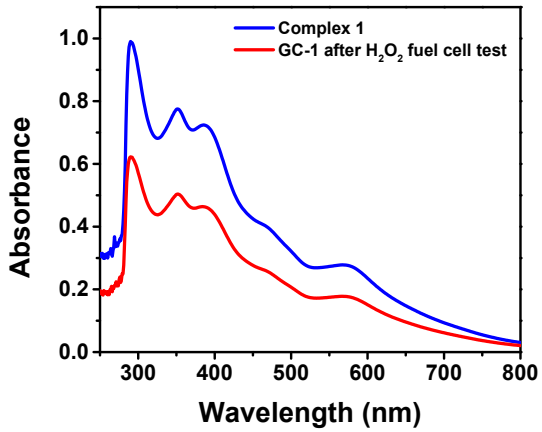


Figure S22. UV-vis spectra of complex **1** (blue line) and the recovered catalyst from **GC-1** electrode (red line) after running the H_2O_2 fuel cell test.

Anode: $H_2O_2 \rightarrow O_2 + 2H^+ + 2e^-$ ($E^\circ_{ox} = 0.68$ V vs. NHE) equation……S1

Cathode: $H_2O_2 + 2H^+ + 2e^- \rightarrow 2H_2O$ ($E^\circ_{red} = 1.78$ V vs. NHE) equation…...…..S2

Overall reaction: $2H_2O_2 \rightarrow O_2 + 2H_2O$ ($E^\circ_{cell} = 1.09$ V vs. NHE) equation…….S3

Scheme S1. Electrochemical equations for the one-compartment H_2O_2 fuel cell, and the potentials vs. Normal Hydrogen Electrode (NHE).

9. DFT calculations

The optimized geometry parameters around the metal centre of the distorted octahedral complex **1** in its high spin (S = 5) and broken symmetry spin states are presented in Table S4 along with respective experimental X-ray values for comparison. The DFT calculated bond distance and bond angle values obtained at method 1 (B3LYP/def2-SVP), method 2 (B3LYP+D3BJ/def2-SVP+def2-TZVP), method 3 (BP86+D3BJ/def2-SVP+def2-TZVP) are in good accord with the X-ray values with mean absolute deviation for bond distance values are estimated as 0.031, 0.028, 0.031 Å. The method 2 is selected for the present study. Note that, the metal ions are treated with def2-TZVP basis function during optimization.

Broken symmetry analysis is performed for **1** to **1**$^{-4}$ complexes. The magnetic coupling constant (J) is obtained using eq.

$$J = - \frac{(E_{HS} - E_{BS})}{\langle S_{max}^{2} \rangle - \langle S_{min}^{2} \rangle}$$

Where, $(E_{HS} - E_{BS})$ is the energy difference between is high spin (HS) and broken symmetry (BS) spin states and S_{max}^{2}, S_{min}^{2} are maximum and minimum magnetic spin moment values.

Table S4. Experimental (X-ray) and DFT optimized bond lengths around the transition metal (Fe) centers of the diiron(III) complex in its HS-HS (S = 5) and HS-BS (S = 0). M1 = B3LYP/def2-SVP, M2 = B3LYP+D3BJ/def2-SVP+def2-TZVP, and M3 = BP86+D3BJ/def2-SVP+def2-TZVP). Bond lengths are given in Å.

	X-ray	*Theoretical values*			
		HS-HS			**HS-BS**
		Method 1	Method 2	Method 3	Method 1
Fe1-O8	1.92284	1.93388	1.92668	1.93293	1.93476
Fe1-O1	1.93482	1.96268	1.95195	1.97649	1.96321
Fe1-O5	1.90552	1.93444	1.92497	1.93918	1.93568
Fe1-N1	2.12272	2.17895	2.17002	2.14833	2.17701
Fe1-N6	2.22154	2.21055	2.22931	2.21829	2.20973
Fe1-N4	2.19359	2.24161	2.23546	2.24145	2.24051
Fe2-O4	1.91546	1.96415	1.95795	1.95753	1.96518
Fe2-O2	1.94024	1.931	1.92471	1.93036	1.93279
Fe2-O7	1.93334	1.96135	1.94929	1.97399	1.96222
Fe2-N2	2.18752	2.24085	2.24258	2.24662	2.23982
Fe2-N5	2.08708	2.17166	2.16348	2.13945	2.1701
Fe2-N3	2.11589	2.18755	2.17127	2.1794	2.18635
N1-N2	1.4278	1.39802	1.39377	1.38572	1.39643
N6-N5	1.41773	1.3971	1.39418	1.38655	1.39531
N4-N3	1.43062	1.39811	1.39435	1.38692	1.39653
O1-Fe1-N6	170.3849	170.8865	169.0994	170.3281	170.9741
O5-Fe1-N1	168.7467	166.7828	166.6057	165.4511	166.8412
O8-Fe1-N4	165.9458	168.2884	165.2623	166.2056	168.3589
O4-Fe2-N5	171.7548	169.9623	169.1666	169.4211	169.9599
O2-Fe2-N3	167.4431	166.1594	165.4062	165.6744	166.1898
O7-Fe2-N2	172.2738	170.758	169.3859	169.9418	170.8186
Fe1-N4-N3-Fe2	64.9497	63.1119	69.0727	64.8317	62.9905
Fe1-N1-N2-Fe2	65.5179	64.2503	68.34	69.7711	64.1186
Fe1-N6-N5-Fe2	63.2717	67.0845	69.3545	72.003	66.9174
Average		-0.11038	0.0699	0.1511	-0.1154
Average(distance)		0.0237	0.0182	0.0191	0.0233
MAD (distance)		**0.031**	**0.028**	**0.031**	**0.031**

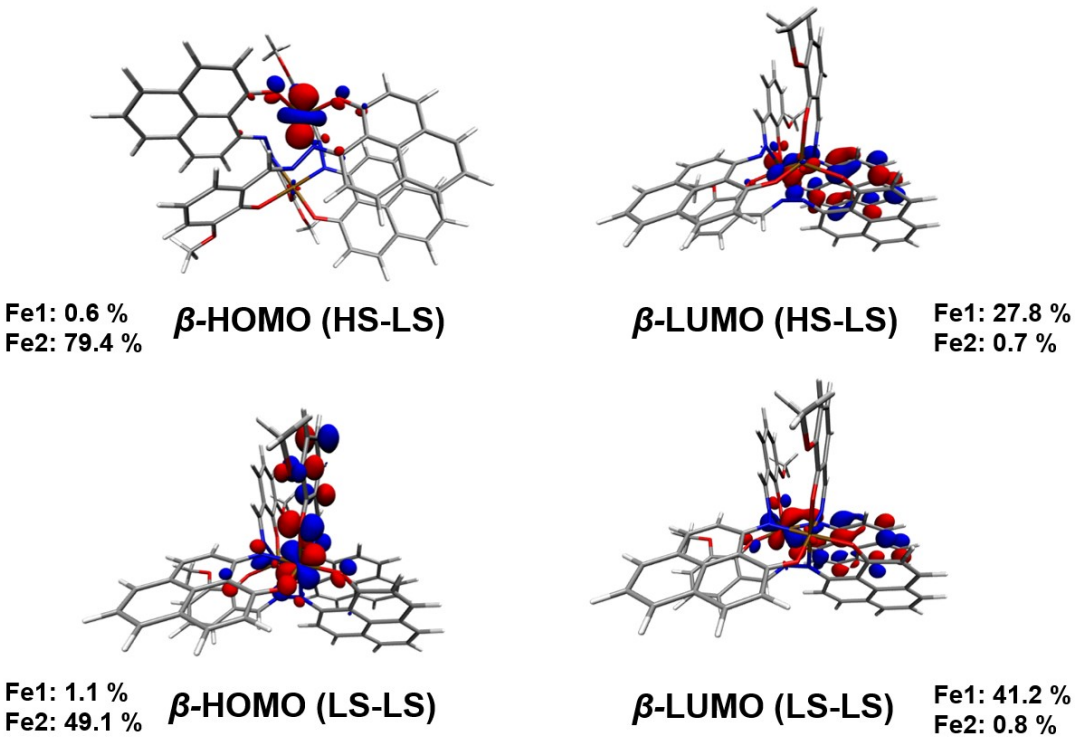


Figure S23. Molecular orbital plots of β-HOMO and β-LUMO orbitals of **1**$^{-1}$ complex in its LS-HS ($S = \frac{5}{2}$) and LS-LS ($S = \frac{1}{2}$) spin states . Molecular orbitals are generated at an isosurface value of 0.04 au. Compositions of metal ions are also given for each MO.

Theoretical computation of redox potential using DFT

The most popular method to compute the redox potential uses the Born-Haber cycle presented in Figure S24.

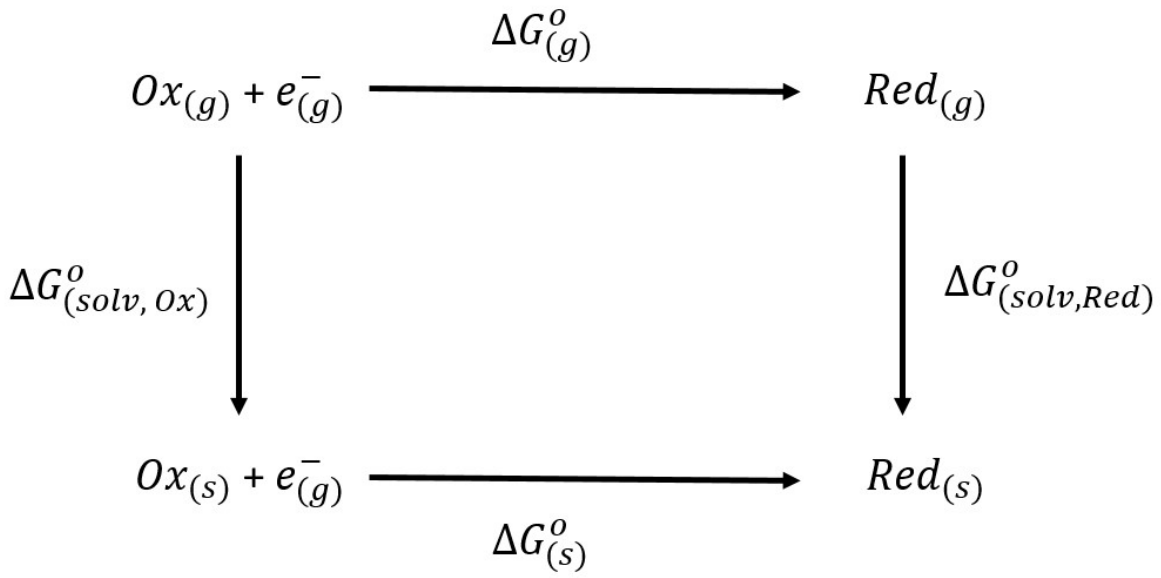


Figure S24. The Born-Haber cycle for redox potential calculation.

$\Delta G^{o}_{(g)}$ is the gas-phase Gibbs energy of the addition of one electron to the oxidant. It is a sum of the negative calculated electron affinity, and the thermal and entropic corrections. $\Delta G^{o}_{(solv,\,Ox)}$ and $\Delta G^{o}_{(solv,\,Red)}$ are solvation energy values of the oxidant and reductant molecule. This is achieved with the continuum solvation model CPCM. The entity $\Delta G^{o}_{(s)}$ is then calculated as:

$$\Delta G^{o}_{(s)} = \Delta G^{o}_{(g)} + \Delta G^{o}_{(solv,\,Red)} - \Delta G^{o}_{(solv,\,Ox)}$$

The absolute reduction potential E^{o}_{abs} of the Ox/Red couple in Solvent is defined as

$$E^{o\ (Solv)}_{abs} = - \frac{\Delta G^{o}_{(s)}}{nF} ,$$

where *n* is number of electrons involved in the half-reaction, present case *n* = 1. *F* is the Faraday constant (F = 96485 J. mol^{-1}.V^{-1} or 23.061 kcal/mol^{-1}.V^{-1}).

DFT optimized atomic Cartesian coordinates of metal complex 1

Fe	14.196272	6.363878	11.622023
Fe	15.348543	6.730234	15.274753
O	15.196000	5.265561	10.355397
O	15.529230	8.523003	15.951398
O	15.018141	10.490514	17.613761
O	17.100960	6.062971	15.838105
O	12.457178	5.588630	11.339114
O	10.046197	5.403265	10.329585
O	14.347902	5.922643	16.739755
O	14.058826	7.982809	10.586517
O	14.389046	9.562321	8.518990
N	16.200643	6.867802	12.283498
N	16.129361	7.691839	13.405315
N	15.398153	4.923480	14.071588
N	14.266346	4.845253	13.260970
N	13.358147	7.089710	14.506797
N	13.432479	7.684123	13.247877
C	16.418350	5.008527	10.063210
C	16.646157	4.105615	8.964571

H	15.756819	3.758128	8.435934
C	17.900758	3.691421	8.623778
H	18.045939	2.994411	7.793157
C	19.047174	4.146701	9.344265
C	20.344882	3.695270	9.023162
H	20.461990	2.990610	8.195068
C	21.455008	4.124674	9.739479
H	22.452624	3.760859	9.484167
C	21.282560	5.023577	10.797952
H	22.145114	5.360365	11.378710
C	20.013162	5.502398	11.142294
C	18.856861	5.070451	10.419650
C	17.546655	5.524004	10.779114
C	17.394921	6.446150	11.894351
C	18.599053	6.865389	12.592702
H	18.494010	7.527799	13.447694
C	19.827306	6.412465	12.236595
H	20.704782	6.725269	12.808295
C	16.285218	8.961232	13.195085
H	16.546642	9.276764	12.174662
C	16.077761	10.009234	14.156116
C	15.679022	9.722256	15.495355
C	15.410832	10.836763	16.366336
C	15.547591	12.140152	15.903147
H	15.338846	12.980042	16.566672

C	15.948572	12.400228	14.572953
H	16.038483	13.433164	14.230798
C	16.207525	11.351883	13.715528
H	16.488549	11.538808	12.676501
C	14.715084	11.508320	18.533585
H	15.588563	12.156789	18.734224
H	14.417895	11.011058	19.466744
H	13.880286	12.144857	18.183942
C	17.985422	5.261744	15.372273
C	19.314187	5.365080	15.920163
H	19.446885	6.086085	16.728655
C	20.351698	4.632126	15.423946
H	21.358073	4.748750	15.836729
C	20.154592	3.708633	14.350948
C	21.231210	2.987200	13.795751
H	22.231790	3.141749	14.209033
C	21.039794	2.105975	12.737799
H	21.886296	1.568091	12.306290
C	19.753135	1.919840	12.224783
H	19.587962	1.237051	11.387840
C	18.656382	2.612636	12.753442
C	18.834849	3.537920	13.827903
C	17.736476	4.306452	14.333047
C	16.425529	4.153783	13.726015
C	16.279285	3.157087	12.681018

H	15.303013	3.031599	12.221674
C	17.336123	2.439432	12.222361
H	17.194077	1.732353	11.401062
C	13.303955	4.080718	13.664034
H	13.474858	3.482325	14.570909
C	12.006948	3.971499	13.051294
C	11.656106	4.747164	11.907254
C	10.317457	4.619175	11.399961
C	9.406808	3.769863	12.017561
H	8.390214	3.685026	11.632054
C	9.772690	3.019393	13.156493
H	9.034776	2.373243	13.635669
C	11.051739	3.120201	13.663117
H	11.340801	2.562027	14.556919
C	8.763479	5.348638	9.760365
H	8.521021	4.336158	9.386352
H	8.762975	6.051012	8.915871
H	7.978378	5.651418	10.479310
C	13.140074	5.569002	16.979777
C	12.915137	4.794270	18.175513
H	13.795676	4.589061	18.786679
C	11.675595	4.337350	18.512251
H	11.532974	3.743435	19.419684
C	10.538850	4.617756	17.691201
C	9.255590	4.137817	18.025209

H	9.141275	3.542009	18.935016
C	8.152750	4.409004	17.222412
H	7.165266	4.029568	17.494111
C	8.320768	5.171602	16.062443
H	7.464853	5.387539	15.417404
C	9.579432	5.665428	15.695768
C	10.725119	5.398440	16.507075
C	12.023297	5.883406	16.137330
C	12.171146	6.655450	14.913227
C	10.979247	6.896143	14.119170
H	11.083369	7.426839	13.176788
C	9.762423	6.428450	14.495253
H	8.894145	6.607521	13.856246
C	13.208633	8.957577	13.183600
H	12.903828	9.467215	14.109217
C	13.365872	9.780331	12.014900
C	13.799218	9.235093	10.769170
C	13.971737	10.145428	9.666486
C	13.722148	11.502852	9.827815
H	13.856882	12.186029	8.988563
C	13.296997	12.020464	11.072338
H	13.115531	13.092290	11.174728
C	13.123586	11.172576	12.145731
H	12.815341	11.561916	13.118795
C	14.563871	10.363455	7.378510

H	13.623300	10.861917	7.077369
H	14.887606	9.694066	6.570033
H	15.337246	11.139757	7.532438

DFT optimized atomic Cartesian coordinates of metal complex 1^{-1}

Fe	14.228579	6.397862	11.685280
Fe	15.351556	6.740384	15.195331
O	15.195809	5.324699	10.343851
O	15.516799	8.609136	15.950178
O	14.919246	10.608209	17.547328
O	17.175785	6.050899	15.824916
O	12.483232	5.607626	11.343566
O	10.066207	5.426137	10.339519
O	14.346857	5.842825	16.740147
O	14.052589	8.014823	10.618250
O	14.364396	9.604344	8.551319
N	16.242459	6.913791	12.274152
N	16.192595	7.740065	13.396725
N	15.452201	4.883860	14.052483
N	14.318881	4.818375	13.246547
N	13.327516	7.093414	14.531388
N	13.403098	7.699204	13.280134
C	16.411352	5.039454	10.058417
C	16.624943	4.132202	8.957769

H	15.727943	3.806335	8.427600
C	17.869468	3.686143	8.620445
H	18.000672	2.984432	7.790630
C	19.024048	4.111076	9.345357
C	20.312097	3.626377	9.030504
H	20.413727	2.917188	8.203527
C	21.427402	4.024832	9.754207
H	22.416648	3.630570	9.509319
C	21.271798	4.927632	10.814186
H	22.137965	5.235060	11.405945
C	20.015743	5.440525	11.151366
C	18.850653	5.038933	10.421641
C	17.551678	5.524301	10.776473
C	17.419842	6.453101	11.892218
C	18.632889	6.838998	12.598807
H	18.530042	7.498699	13.456579
C	19.848818	6.354685	12.248767
H	20.731339	6.634663	12.829746
C	16.304778	9.013370	13.169983
H	16.526045	9.329489	12.139135
C	16.090519	10.061929	14.125868
C	15.662784	9.780903	15.469114
C	15.347616	10.931175	16.297283
C	15.479500	12.224221	15.817868
H	15.239299	13.074112	16.458953

C	15.917401	12.466658	14.490889
H	16.000777	13.493756	14.128209
C	16.209832	11.402289	13.668137
H	16.509921	11.571521	12.630386
C	14.555256	11.640442	18.416234
H	15.401421	12.321304	18.637209
H	14.226971	11.168061	19.353310
H	13.722841	12.251679	18.014080
C	18.033924	5.242309	15.363138
C	19.380920	5.335388	15.896968
H	19.519604	6.070422	16.692666
C	20.408862	4.583621	15.418920
H	21.417652	4.693567	15.830211
C	20.203418	3.644367	14.357931
C	21.273451	2.905057	13.819085
H	22.272800	3.054843	14.239054
C	21.082074	2.015303	12.766499
H	21.926598	1.464862	12.345227
C	19.798343	1.845955	12.242249
H	19.630880	1.166059	11.402730
C	18.705077	2.556236	12.755353
C	18.879681	3.486130	13.831422
C	17.784684	4.264662	14.327184
C	16.478788	4.120953	13.703799
C	16.340371	3.135386	12.643514

H	15.367407	3.029712	12.170210
C	17.391415	2.402169	12.200496
H	17.255146	1.700135	11.373265
C	13.341379	4.082041	13.663311
H	13.505721	3.491304	14.576308
C	12.036337	3.989678	13.057014
C	11.685541	4.768517	11.914122
C	10.342619	4.639765	11.414368
C	9.428946	3.795472	12.032413
H	8.409800	3.716786	11.651360
C	9.794953	3.048152	13.173164
H	9.055051	2.412018	13.663205
C	11.077539	3.148083	13.673188
H	11.366371	2.597146	14.571763
C	8.776345	5.390465	9.799002
H	8.508162	4.382978	9.424401
H	8.764650	6.096827	8.956723
H	8.006541	5.698181	10.533861
C	13.146802	5.509485	16.968846
C	12.905830	4.689776	18.144709
H	13.792117	4.450761	18.736276
C	11.666122	4.247781	18.488219
H	11.522560	3.631601	19.381775
C	10.521659	4.568199	17.688746
C	9.238190	4.096867	18.025708

H	9.128803	3.483991	18.925681
C	8.128183	4.391603	17.238630
H	7.139147	4.015721	17.512720
C	8.296037	5.168065	16.088420
H	7.439323	5.397186	15.447941
C	9.556063	5.656840	15.718519
C	10.710879	5.374391	16.518033
C	12.008196	5.858906	16.148204
C	12.147152	6.644785	14.930724
C	10.951120	6.883610	14.138226
H	11.057702	7.416929	13.196767
C	9.734475	6.422601	14.518343
H	8.862433	6.604044	13.884205
C	13.209328	8.976974	13.228108
H	12.924690	9.484964	14.160800
C	13.366274	9.805768	12.058588
C	13.789558	9.263308	10.808027
C	13.953994	10.182469	9.710877
C	13.708443	11.540152	9.875720
H	13.839284	12.225915	9.037389
C	13.297583	12.052869	11.126339
H	13.126051	13.125629	11.239967
C	13.134289	11.196689	12.196695
H	12.846925	11.582130	13.177829
C	14.553471	10.416150	7.427688

H	13.620507	10.929244	7.121863
H	14.879388	9.756854	6.610592
H	15.330716	11.187600	7.594806

DFT optimized atomic Cartesian coordinates of metal complex 1^{-2}

Fe	14.240533	6.266575	11.640320
Fe	15.311822	6.628729	15.170871
O	15.307183	5.219310	10.240663
O	15.489401	8.513336	15.956332
O	14.939356	10.511179	17.577677
O	17.143322	5.936322	15.821461
O	12.418317	5.401452	11.263778
O	9.950078	5.252349	10.375266
O	14.273746	5.764197	16.722467
O	14.003855	7.970253	10.491199
O	14.433868	9.641957	8.510249
N	16.263177	6.848521	12.229124
N	16.175308	7.656315	13.361702
N	15.435858	4.754877	14.017729
N	14.307877	4.659172	13.208618
N	13.274565	7.007073	14.473634
N	13.348813	7.597772	13.215146
C	16.528171	5.001580	9.982747
C	16.817872	4.112686	8.872125
H	15.943531	3.745793	8.329354

C	18.085173	3.742788	8.537489
H	18.264994	3.062913	7.697098
C	19.209847	4.219068	9.281309
C	20.522205	3.809875	8.969725
H	20.665770	3.125371	8.126975
C	21.612532	4.245000	9.714824
H	22.623389	3.906091	9.470959
C	21.397888	5.106679	10.796938
H	22.239060	5.438493	11.412609
C	20.113219	5.547533	11.133628
C	18.971274	5.115496	10.377740
C	17.648108	5.533899	10.724436
C	17.461099	6.430305	11.861589
C	18.649326	6.829388	12.605026
H	18.506152	7.452369	13.484709
C	19.891017	6.411340	12.260059
H	20.751824	6.704153	12.867939
C	16.259418	8.931519	13.154843
H	16.470595	9.266739	12.127451
C	16.038527	9.972924	14.126717
C	15.632310	9.683743	15.475716
C	15.343514	10.835719	16.312806
C	15.468982	12.132798	15.841015
H	15.243238	12.979417	16.492892
C	15.876877	12.380447	14.506992

H	15.948903	13.407990	14.141551
C	16.146579	11.313261	13.675617
H	16.417497	11.484832	12.630048
C	14.569708	11.539826	18.439857
H	15.407588	12.234931	18.657821
H	14.248744	11.070747	19.382411
H	13.729627	12.144649	18.040487
C	18.020003	5.161996	15.335132
C	19.364623	5.265692	15.874626
H	19.484792	5.981222	16.691522
C	20.412451	4.552968	15.376904
H	21.418871	4.674780	15.792834
C	20.231434	3.645314	14.286711
C	21.320326	2.950424	13.723259
H	22.316158	3.113506	14.148413
C	21.151669	2.097297	12.638922
H	22.010528	1.589712	12.192067
C	19.870534	1.916618	12.106748
H	19.720939	1.269474	11.238101
C	18.760215	2.578185	12.643281
C	18.910228	3.475971	13.752519
C	17.796630	4.211136	14.270522
C	16.489018	4.048842	13.643844
C	16.379734	3.095189	12.548795
H	15.407616	2.990000	12.073052

C	17.449453	2.409755	12.080145
H	17.335445	1.740081	11.222893
C	13.304993	3.998756	13.688608
H	13.445486	3.485625	14.653117
C	11.991113	3.906380	13.100744
C	11.632638	4.637971	11.915258
C	10.251829	4.514022	11.486716
C	9.336579	3.738512	12.179423
H	8.300253	3.675178	11.841221
C	9.720067	3.042203	13.350941
H	8.979103	2.463342	13.907225
C	11.023347	3.135059	13.793286
H	11.328483	2.632378	14.715744
C	8.635970	5.249815	9.916343
H	8.295077	4.239098	9.608257
H	8.598739	5.915288	9.040372
H	7.920863	5.624723	10.677556
C	13.059632	5.515216	16.981953
C	12.788467	4.778017	18.205605
H	13.670684	4.520827	18.796547
C	11.530966	4.431402	18.595065
H	11.367145	3.878367	19.526694
C	10.395193	4.770375	17.794153
C	9.090268	4.398049	18.177430
H	8.961745	3.851238	19.117517

C	7.988359	4.704472	17.386282
H	6.982402	4.405018	17.694518
C	8.185324	5.391197	16.181417
H	7.334516	5.621804	15.532777
C	9.463017	5.781230	15.765205
C	10.614965	5.490584	16.571169
C	11.929488	5.882348	16.159140
C	12.091670	6.602300	14.897372
C	10.898017	6.823625	14.090246
H	11.028611	7.272015	13.108217
C	9.667377	6.443841	14.506378
H	8.800806	6.603431	13.858522
C	13.162468	8.877304	13.161015
H	12.893176	9.392080	14.096922
C	13.325993	9.716442	12.001107
C	13.770873	9.194718	10.734362
C	13.985946	10.179475	9.684494
C	13.752737	11.529485	9.887464
H	13.920502	12.244502	9.079115
C	13.304433	12.005360	11.145368
H	13.143040	13.075913	11.295777
C	13.106398	11.107504	12.173331
H	12.801717	11.461550	13.162333
C	14.729920	10.503706	7.458057
H	13.840696	11.068945	7.107989

H	15.100592	9.883732	6.627537
H	15.512189	11.243835	7.725467

DFT optimized atomic Cartesian coordinates of transition state TS1

Fe	-0.48461655555535	-0.32077258237994	-1.43211093331095
Fe	0.48491928246371	0.37310699142011	2.02030346559354
O	0.50138817515903	-1.21835370334173	-2.95401906029831
O	0.65230495136602	2.33892670758948	2.57776479242973
O	0.24789330111341	4.46887294338122	4.06189074664703
O	2.33607258825462	-0.23376365491164	2.64593990421755
O	-2.39152057574865	-0.70906226085325	-1.69254652122479
O	-4.80596109601028	-0.88243109759236	-2.69257166447108
O	-0.47708391057206	-0.49193808260250	3.62696625250010
O	-1.26943936792481	1.94264706521954	-2.45566709206751
O	-1.15433149129926	3.77014335725025	-4.34249405546330
N	1.40339032521194	0.39443705284281	-0.97821648933310
N	1.29529187452809	1.28027146083343	0.09140757884903
N	0.59658303338371	-1.57784090199624	1.00216463757802
N	-0.52061767028610	-1.69508255307667	0.17694134735790
N	-1.58388109008104	0.71639043305056	1.45793014385310
N	-1.57345481307875	1.42893529357734	0.27997685484090
C	1.72484889707269	-1.59187303210914	-3.08206078174515
C	2.01600927985967	-2.61331152756961	-4.06114019775686
H	1.16300596290815	-2.99161674868474	-4.62918107859735
C	3.27621110821376	-3.09908124237933	-4.25332513898292

H	3.46376984817522	-3.88313995458575	-4.99441738727400
C	4.38254298224219	-2.60860703555150	-3.49331194254581
C	5.69118827774175	-3.10644561277773	-3.67920655793028
H	5.85422854523022	-3.88182084390639	-4.43459462383660
C	6.75688010220944	-2.63580653676642	-2.92271573181887
H	7.76356566357078	-3.03707946154855	-3.06899545630237
C	6.52736220292003	-1.65145464048285	-1.95421153969987
H	7.35127707403334	-1.28322222713427	-1.33662310408185
C	5.24778074190865	-1.12651705733004	-1.74449472907558
C	4.13419323010858	-1.59491397536069	-2.51373926295796
C	2.81365149191057	-1.08134926128747	-2.29660945652363
C	2.60989643893972	-0.07901613226786	-1.26163161105829
C	3.76938908557422	0.36459095150841	-0.50555753559316
H	3.61177532695222	1.07689605217862	0.29840031381432
C	5.00870294744214	-0.13143911725595	-0.73769185644266
H	5.84863785657642	0.20128766596765	-0.12264670170520
C	1.49237250162310	2.52485782764632	-0.20698802223192
H	1.76609857458245	2.75922657356189	-1.24825357532304
C	1.35586137279268	3.63825308256222	0.68273963937600
C	0.90908940901460	3.46230623985389	2.03807077924558
C	0.70885528092880	4.68282840854304	2.80043436998560
C	0.97535859112782	5.92978069433184	2.25755651405457
H	0.82827871965982	6.83095833122432	2.85481967070805
C	1.43914051896901	6.06130376893737	0.92365362500738
H	1.63950096042328	7.05354948155871	0.51315958820367

C	1.61718337463384	4.93123865736270	0.15810841316710
H	1.94489253552956	5.01106097302611	-0.88271149754083
C	0.01692993115111	5.57636030652130	4.88154056106582
H	0.93989788351740	6.16246531410701	5.06070207952538
H	-0.35184006731219	5.19056094670459	5.84243298019560
H	-0.74368238679036	6.26035047189392	4.45465146619473
C	3.18131442291311	-1.10314234850219	2.28221893767566
C	4.51944481179232	-0.98727772285296	2.83376548089691
H	4.65816319156723	-0.18004211602734	3.55630052126794
C	5.53800035693140	-1.80692938171158	2.45880623863148
H	6.53909206616402	-1.68168855169081	2.88440146051928
C	5.33320944674755	-2.83770045100124	1.48665474936262
C	6.39561615388298	-3.65219569028695	1.05162505257547
H	7.38632800426677	-3.49165129323958	1.48824826173251
C	6.20913855400957	-4.62899568648230	0.07828696061917
H	7.04851896326192	-5.24012594167949	-0.26221889868487
C	4.93812100665833	-4.80520440985635	-0.47405215645799
H	4.77567753718650	-5.55305995043097	-1.25520992781654
C	3.85163333512009	-4.02245148623361	-0.06148952553867
C	4.01940605945854	-3.00921667291627	0.93829210828600
C	2.93024845346179	-2.17028212058299	1.33890047635280
C	1.63226251226999	-2.35084710990503	0.70780293034276
C	1.50703641609775	-3.40073594524241	-0.29146929722331
H	0.54136811751064	-3.52802516393103	-0.77516617039598
C	2.55307023934211	-4.18594368591899	-0.64822921685196

H	2.42409397726545	-4.94777809988111	-1.42211590119659
C	-1.54137598377283	-2.34819093368325	0.61889877215795
H	-1.43929661757593	-2.88278694741214	1.57549779888377
C	-2.83230743522171	-2.41124245274116	-0.02734671822103
C	-3.17977386202751	-1.58272054335544	-1.14356182107619
C	-4.52175018739347	-1.70727591160985	-1.64448162813551
C	-5.43474567163788	-2.58316151708278	-1.06876387119222
H	-6.44851065096608	-2.65666006151204	-1.46251605487834
C	-5.07362637599718	-3.37020383544978	0.04515049716300
H	-5.81309606012984	-4.02602821281692	0.51114741044648
C	-3.79713296229874	-3.27327778918179	0.55442411801227
H	-3.51292918737407	-3.84929770222754	1.43933863713853
C	-6.08186108489654	-0.95256836412241	-3.26064801865575
H	-6.31309023848717	-1.96549427884290	-3.64489802774771
H	-6.09707617464434	-0.24387811968649	-4.10056069740909
H	-6.87595513565856	-0.67314621620236	-2.53973328636658
C	-1.63964693989873	-0.95076203571029	3.83397195582053
C	-1.80389029402275	-1.87258069588116	4.94495204872466
H	-0.89575059262874	-2.08750678751877	5.51214668879503
C	-3.00153734924938	-2.44074741212475	5.25467378016235
H	-3.08519146218125	-3.13977983856802	6.09309249635515
C	-4.17877454605457	-2.14383908092426	4.49480970439322
C	-5.42102058196827	-2.73234585319918	4.80203826277184
H	-5.47216798664147	-3.42878120632709	5.64448488009469
C	-6.56247312001262	-2.44579039543696	4.05827525749101

H	-7.51804433084676	-2.91370780414655	4.30871120650891
C	-6.47108843691782	-1.55594272934001	2.98344784407872
H	-7.35473708555627	-1.32949668283193	2.37972549373878
C	-5.25364481850936	-0.95476902574766	2.63968088122371
C	-4.06643241037749	-1.23325636677323	3.39278908555646
C	-2.80929020232088	-0.64469018218036	3.04304815382960
C	-2.73492280607370	0.21762808134288	1.87462450313282
C	-3.96573622731593	0.47603110748819	1.14263004239455
H	-3.90728029514959	1.08940535575474	0.24661009269323
C	-5.14807070870924	-0.07628906708550	1.50929064035813
H	-6.04526755254888	0.11028156787782	0.91245955333683
C	-1.68655767056190	2.70125595839977	0.38814421238189
H	-1.82889127629369	3.14722976577069	1.38466104715152
C	-1.60912369765009	3.63872576992142	-0.72982575438025
C	-1.43555534535271	3.24619681207662	-2.07155149278357
C	-1.33391108313170	4.23533698293727	-3.07878450765494
C	-1.43898683534631	5.59452965913976	-2.74958543973395
H	-1.37201084423541	6.35837721158557	-3.52340738673233
C	-1.62567139763724	5.97393617013124	-1.41564983228247
H	-1.69166965838724	7.03501642980521	-1.16069309672421
C	-1.71026931892073	5.01193207221956	-0.42117832533464
H	-1.81201990398420	5.30767784200776	0.62444202063810
C	-1.04897122938978	4.69792590971489	-5.39535062014704
H	-1.96447742196874	5.31035674866972	-5.49360849579463
H	-0.90664559576507	4.11380475762844	-6.31367081558909

H	-0.18634271082079	5.37608063388774	-5.25884174126472
H	-2.11132801387276	1.44251020564094	-2.50898437792624
H	-1.01661681631552	1.46879150249066	-4.56664278953885
H	-0.56102087064938	0.02889530636574	-4.36545899245076
O	-1.15396978492420	0.57191821833708	-4.91259749672777

DFT optimized atomic Cartesian coordinates of transition state TS2

Fe	-0.27017844274118	-0.28806700320260	-2.11615248868706
Fe	0.64624255226620	0.53828718073248	1.46752918829677
O	0.75013424355554	-1.44969448253170	-3.28569403707432
O	0.87447958701110	2.47953648327632	2.07156983397440
O	0.71734588670623	4.59993291182106	3.60822867096351
O	2.55298244412094	-0.03092904624140	1.99483046113882
O	-2.23178084832349	-0.48663656015053	-2.06283184789559
O	-4.71955228262820	-0.25871903712748	-2.77958333814257
O	-0.04813466114250	-0.38499986326340	3.15480899517698
O	-2.82179868762273	2.32375879277770	-2.19322467867817
O	-3.50724352369451	4.25806518699558	-3.97649031631556
N	1.53272329803460	0.46306131100034	-1.47284156978840
N	1.32896416754146	1.40279084788414	-0.45954347447774
N	0.74206403788503	-1.43619189455579	0.48722485978159
N	-0.37064035818431	-1.54499881815397	-0.34570333565227
N	-1.53855719564163	0.84401966979403	1.20262337576659
N	-1.86462637722133	1.71472092091558	0.17495902827754
C	1.96712163412629	-1.86486694727260	-3.21061584364670

C	2.29886595423604	-3.02537200640477	-3.99538333267755
H	1.49894257275094	-3.41896195487272	-4.62563217403841
C	3.52032116248868	-3.62652289531616	-3.91361710915137
H	3.73491913277063	-4.52941126682614	-4.49353991608104
C	4.53470353027887	-3.10666950320896	-3.05507223411870
C	5.77436938435955	-3.76347737381770	-2.90460631496502
H	5.94624281905580	-4.68636862553169	-3.46599394951816
C	6.74923993892912	-3.27236264329905	-2.04770613013360
H	7.69297522062335	-3.80687329724701	-1.91904754154416
C	6.50551914914825	-2.09188648705718	-1.33703193877604
H	7.25965544122916	-1.69749677232621	-0.65118829023708
C	5.29359719724900	-1.40478292244636	-1.46543475476972
C	4.26200577413951	-1.91013923790162	-2.31854548290844
C	2.98110380774154	-1.26824452497352	-2.39204085420433
C	2.73408663762965	-0.09181196793156	-1.56056789866756
C	3.83887061114319	0.43030336760351	-0.77760317475144
H	3.66196215561737	1.30877579964619	-0.16418573338160
C	5.03810381149430	-0.19912164103488	-0.72849103194786
H	5.83003366980973	0.19176832756543	-0.08471056966979
C	1.47467475415455	2.65196120545792	-0.78593739976436
H	1.69584441198915	2.87862104762445	-1.83625301130264
C	1.37641339739866	3.76963132766725	0.10840620754953
C	1.09817542495353	3.60009138263668	1.50857092553084
C	1.02255242101706	4.81605454816838	2.29998533674792
C	1.23630740941222	6.06265672228956	1.73450334201862

H	1.18046474351205	6.96196786947976	2.35024641565931
C	1.51813077617184	6.19328191826319	0.35077912171441
H	1.67006169354054	7.18613544383223	-0.07849030931048
C	1.57824917556239	5.06621201387578	-0.43794890092321
H	1.76729519865400	5.15053500167859	-1.51172287323554
C	0.60082773638863	5.70428262340794	4.45771481904244
H	1.54586412424291	6.27824305366972	4.53001102703896
H	0.34564937204406	5.31540910066822	5.45392465109435
H	-0.19694688330626	6.40047925107194	4.13053782886491
C	3.26163737717480	-1.07460929195633	1.91692510492872
C	4.53211167687258	-1.06110919655035	2.62190856207311
H	4.72976481569557	-0.16196306696731	3.20937382978829
C	5.42191137942776	-2.08729478659595	2.54767496629981
H	6.37174424016263	-2.04200344920046	3.09056055521726
C	5.14916659187444	-3.24083849097662	1.74508826378522
C	6.08616040901997	-4.28345373366100	1.62217265995658
H	7.02632240708486	-4.20539123282904	2.17677160582172
C	5.84336247005555	-5.38488824618387	0.80634756791068
H	6.58637424752819	-6.18086477890853	0.71316769259062
C	4.64426771422373	-5.45019064619840	0.09226622733883
H	4.44477398670553	-6.29540147878873	-0.57295781187318
C	3.67882032779737	-4.43935590058328	0.19617364295451
C	3.90142998721137	-3.30207666819022	1.03960031209996
C	2.93365590541403	-2.25183122740974	1.14353063799528
C	1.68688446768946	-2.35963510468502	0.39811889867866

C	1.52283087086712	-3.51401742986425	-0.47207540864811
H	0.62380105118982	-3.57027245545157	-1.08138875512009
C	2.46122735539635	-4.48958942542540	-0.56072385105683
H	2.30531837166457	-5.33187542004991	-1.24076321849637
C	-1.37894939515476	-2.22856061870338	0.09465453706618
H	-1.24464709393272	-2.79646239117502	1.02640604574846
C	-2.69691094469748	-2.24283718617943	-0.48915965654132
C	-3.05866473999499	-1.30738568720281	-1.50195411083268
C	-4.44426892839895	-1.23575277656938	-1.87641815402405
C	-5.37931153166624	-2.09794367353988	-1.32012629848473
H	-6.42681340933082	-2.03944414349805	-1.62069235834164
C	-4.99150128778185	-3.04144052270722	-0.34285299496310
H	-5.74238765564767	-3.69374516493279	0.10781641912207
C	-3.67729059821012	-3.09664056650018	0.07552559802909
H	-3.38154295820814	-3.77728112257194	0.87766439849613
C	-6.05604829521412	0.06443053667562	-3.04125472290292
H	-6.59066559111472	-0.74955383491500	-3.56996477206801
H	-6.04330753838132	0.95934453157688	-3.67927841116878
H	-6.61273819681869	0.29481457141369	-2.11221418905362
C	-1.10959051135103	-1.01547306940437	3.43268041934611
C	-1.02718705321966	-2.03433491006848	4.46498298275067
H	-0.03724419232959	-2.17670829911119	4.90352723652525
C	-2.10380087517447	-2.77092526295018	4.85164334213833
H	-2.00476641581842	-3.54014953689861	5.62432537749457
C	-3.39228169890038	-2.55466227530836	4.26435163812293

C	-4.51586952059977	-3.29996039222090	4.67094515642095
H	-4.38226869805637	-4.06208692297340	5.44478622441742
C	-5.77235664539458	-3.08002250185081	4.11249932551615
H	-6.63387177278366	-3.66813280371793	4.43891031875063
C	-5.91884212837974	-2.09509968942548	3.13139310719425
H	-6.89764461639405	-1.90756839221537	2.68043741333956
C	-4.82434284352024	-1.33865943927369	2.69209310910431
C	-3.52048946524030	-1.55366141839734	3.24442738326588
C	-2.38670356694343	-0.80184879805660	2.79254618335819
C	-2.55811674719094	0.16635740506999	1.71837070151006
C	-3.90823065351648	0.37016765146194	1.21376301419747
H	-4.04869791637055	1.09639189921179	0.41686125990512
C	-4.96716240965014	-0.34199766585873	1.67033031233671
H	-5.95753663200259	-0.18104436218384	1.23614901497980
C	-1.73633438126826	2.97406373533771	0.40983366897138
H	-1.41677478533931	3.31850890254336	1.40186500109410
C	-2.04631432708486	3.97419020594297	-0.60279322689961
C	-2.59088653257024	3.60462280600122	-1.85843446282984
C	-2.93107397404594	4.61353409457563	-2.78489942742944
C	-2.70447904406485	5.95390142007785	-2.47333255842425
H	-2.98180566297634	6.70523968985400	-3.21718373135000
C	-2.14860261976785	6.32101199100786	-1.24051579138645
H	-1.96340952222818	7.37262109189045	-1.01033282885632
C	-1.82520389570424	5.33433586752850	-0.31657115330771
H	-1.37243063237418	5.59649430873865	0.64172970953638

C	-2.59459935935451	4.07927883591636	-5.05054570656314
H	-2.21039823415810	5.05376820010306	-5.41228607006233
H	-3.14720008301955	3.59180077263396	-5.86768811625071
H	-1.73396017888053	3.45829722969734	-4.75452566983451
H	-2.56237880567163	1.73718149051250	-1.42265608119549
H	-1.62248193996655	1.42645208373203	-3.28919641510301
O	-0.71859428437063	1.07756487800009	-3.47946737506620
O	0.02219996190359	2.61610762785153	-3.54626294325252
H	0.65874126479812	2.32497198442248	-4.21961326699144

References

(1) B. Caes, D. J. Jensen, Synthesis and Characterization of 9-Hydroxyphenalenone Using 2D NMR Techniques, *J. Chem. Educ.* 2008, ***85*** (3), 413.

(2) G. M. Sheldrick, SHELXS-97 and SHELXL-97, Program for Crystal Structure Solution and Refinement, *University of Göttingen, Germany*, 1997.

(3) J. Saroja, V. Manivannan, P. Chakraborty, S. Pal, A Diiron(III) Complex Containing N-N Bridges. Synthesis, Structure, and Properties, *Inorg. Chem.* 1995, ***34*** (11), 3099–3101.