Supporting Information

A dinuclear iron complex as an efficient electrocatalyst for homogeneous water oxidation reaction

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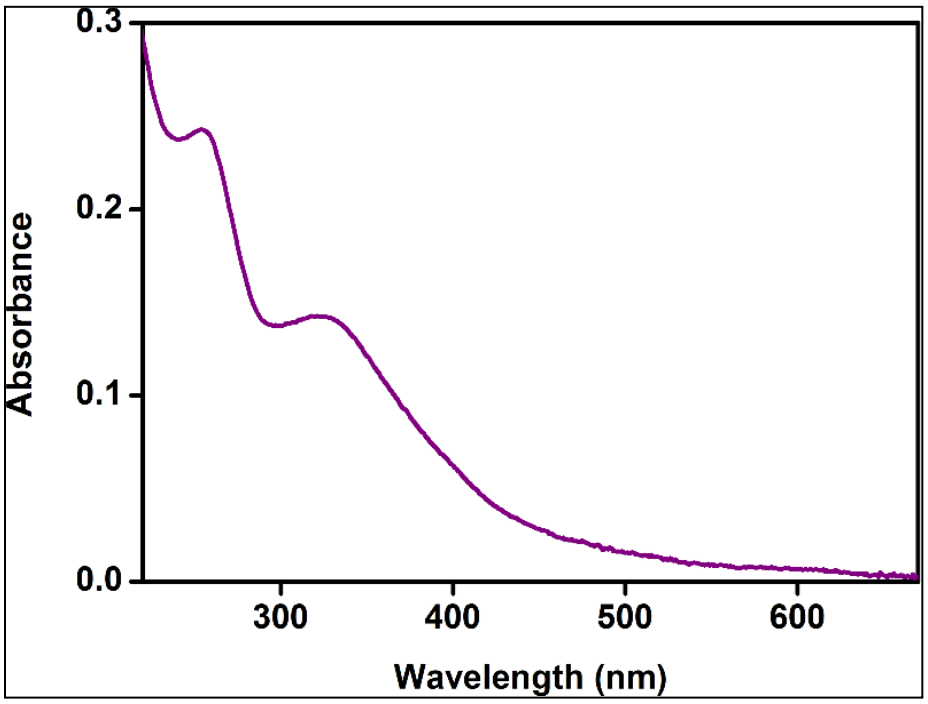

Fig. S1 UV-visible spectrum of the **complex 1** in ACN.

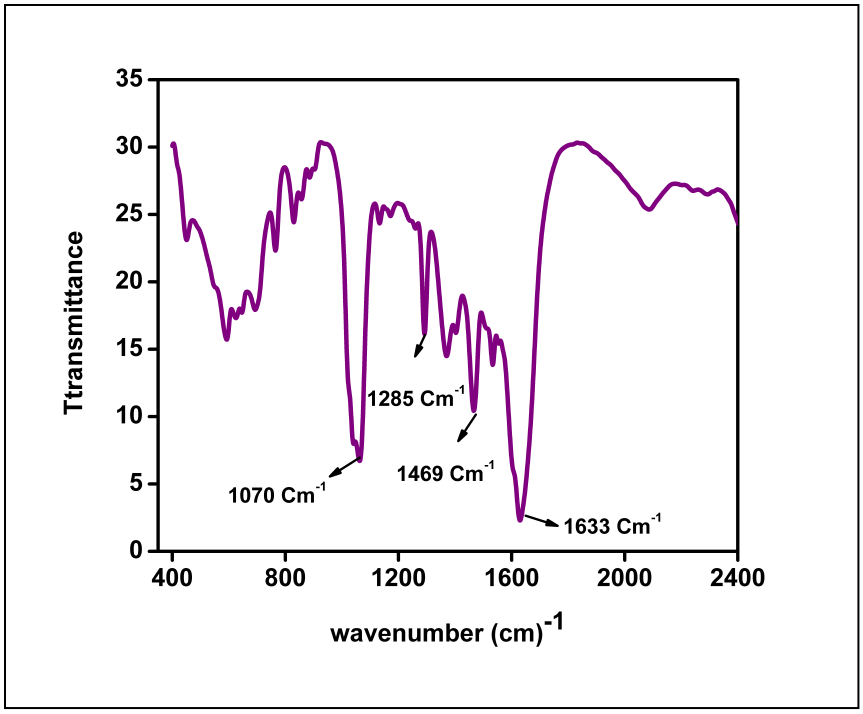

Fig. S2 FT-IR spectrum of the **complex 1**.

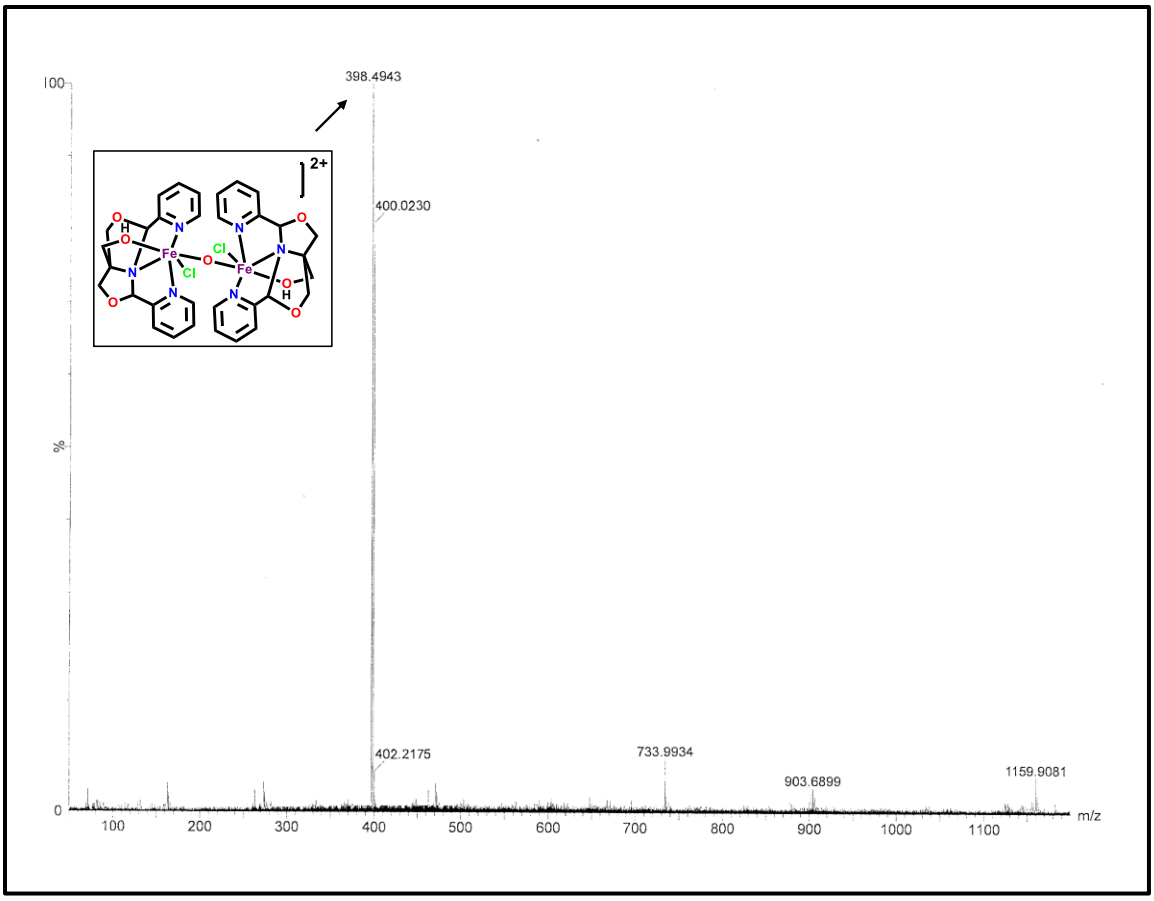

Fig. S3 ESI-MS spectrum of the **complex 1** in ACN medium.

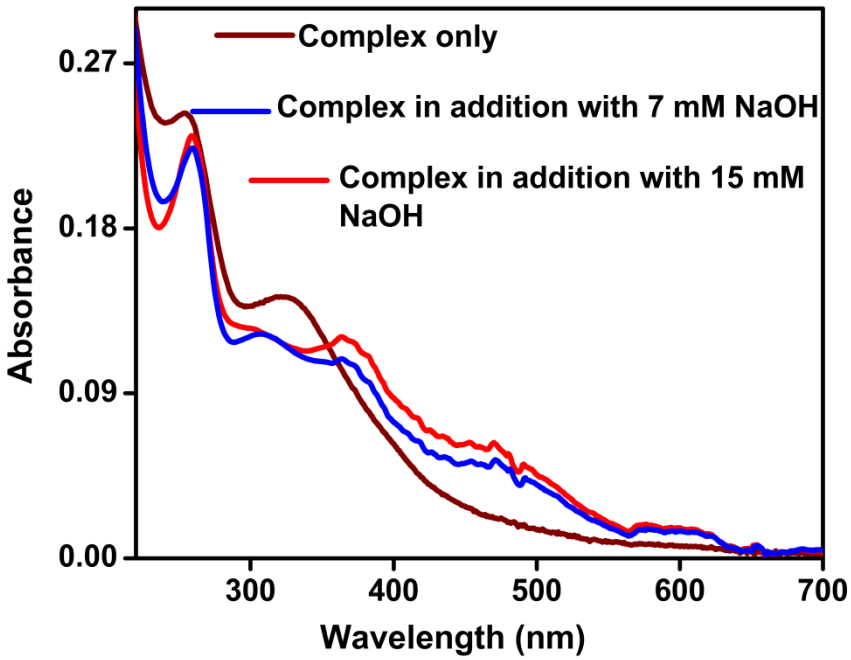

Fig. S4 UV-visible spectra of the **complex 1** (brown) and of the **complex 1** under basic conditions, when the Cl ligands at the metal centres of the complex were found replaced by OH anions.The peak intensity increases with increasing the basic concentration. The transformation resulted in 43 nm red-shifting of UV-Vis band from 326 nm $[(FeLCl)_2O]^{2+}$ to 369 nm $[(FeLOH)_2O]^{2+}$, which was also confirmed by DFT calculation.

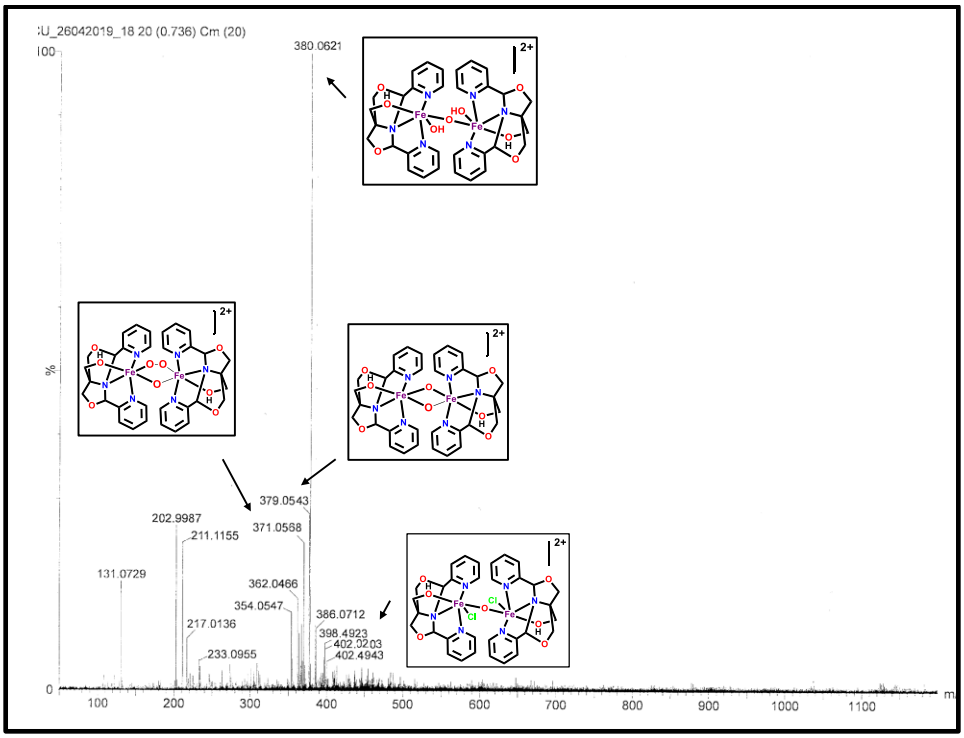

Fig. S5 ESI-MS spectrum of the **complex 1** under basic conditions, when the Cl ligands at the metal centres of the complex were found replaced by OH. ESI-MS analysis revealed an intense peak at m/z =379.0111 amu, which corresponds to A $[(FeLOH)_2O]^{2+}$. The corresponding intermediates have been characterized.

X-ray Crystal Structure Determination

Table S1. Crystallographic Data and Details of Refinement for complexes $[(FeLCl)_2O](FeCl_4)_2$ **1** and $[(FeLCl)_2O]Cl_2$ **2**.

	1	2
formula	$C_{36}H_{46}Cl_{10}Fe_4N_6O_9$	$C_{32}H_{40}Cl_4Fe_2N_6O_{10}$
fw	1284.69	922.20
crystal system	Monoclinic	Monoclinic
space group	*P* 2_1/n	*P* 2_1/c
***a* (Å)**	13.612(3)	11.8719(6)
***b* (Å)**	13.537(2)	16.9617(8)
***c* (Å)**	14.409(3)	9.4064(5)
***β* (deg)**	109.931(6)	102.136(2)
***V* (Å)**	2496.0(8)	1851.81(16)
Z	2	2
ρcalcd (g cm^{-3})	1.709	1.654
μ (mm^{-1})	1.730	1.137
F(000)	1300	948
θ range data collection (deg)	2.13 - 26.73	2.52 - 26.39
reflections collected	18516	20605
unique reflections	5264	3781
***R*(int)**	0.1046	0.0804
reflections $I > 2\sigma(I)$	4383	3083
no. of parameters	300	259
Goodness of fit [b]	1.116	1.040
***R*1**[a]	0.0867	0.0487
***wR*2**[a] **[$I>2\sigma(I)$]**	0.2206	0.1100
residual density (eÅ^{-3})	1.740, -0.746	0.838, -0.713

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$
[b] GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (°) for complexes $[(FeLCl)_2O](FeCl_4)_2$ (**1**) and $[(FeLCl)_2O]Cl_2$ (**2**).

1		2	
Fe(1)-N(1)	2.119(6)	Fe-N(1)	2.143(3)
Fe(1)-N(2)	2.125(6)	Fe-N(2)	2.147(3)
Fe(1)-N(3)	2.180(6)	Fe-N(3)	2.214(3)
Fe(1)-O(3)	2.212(5)	Fe-O(3)	2.158(3)
Fe(1)-O(4)	1.8041(10)	Fe-O(4)	1.7825(5)
Fe(1)-Cl(1)	2.276(2)	Fe-Cl(1)	2.2802(10)
Fe(2)-Cl(2)	2.195(2)		-
Fe(2)-Cl(3)	2.196(2)		-
Fe(2)-Cl(4)	2.199(2)		-
Fe(2)-Cl(5)	2.200(2)		-
O(4)-Fe(1)-N(1)	90.38(16)	O(4)-Fe-N(1)	88.61(8)
O(4)-Fe(1)-N(2)	91.97(17)	O(4)-Fe-N(2)	92.78(8)
N(1)-Fe(1)-N(2)	155.1(2)	N(1)-Fe-N(2)	152.86(11)
O(4)-Fe(1)-N(3)	91.03(16)	O(4)-Fe-N(3)	95.31(8)
N(1)-Fe(1)-N(3)	78.3(2)	N(1)-Fe-N(3)	77.12(11)
N(2)-Fe(1)-N(3)	76.9(2)	N(2)-Fe-N(3)	75.77(11)
O(4)-Fe(1)-O(3)	165.14(15)	O(4)-Fe-O(3)	170.07(7)
N(1)-Fe(1)-O(3)	86.0(2)	N(1)-Fe-O(3)	87.39(11)
N(2)-Fe(1)-O(3)	85.4(2)	N(2)-Fe-O(3)	86.69(11)
N(3)-Fe(1)-O(3)	74.1(2)	O(3)-Fe-N(3)	74.94(10)
O(4)-Fe(1)-Cl(1)	104.88(7)	O(4)-Fe-Cl(1)	101.66(3)
N(1)-Fe(1)-Cl(1)	101.70(17)	N(1)-Fe-Cl(1)	104.09(8)
N(2)-Fe(1)-Cl(1)	101.60(18)	N(2)-Fe-Cl(1)	102.16(9)
N(3)-Fe(1)-Cl(1)	164.08(17)	N(3)-Fe-Cl(1)	163.00(8)
O(3)-Fe(1)-Cl(1)	89.97(14)	O(3)-Fe-Cl(1)	88.13(7)
Fe(1)-O(4)-Fe(1)#1	180.0	Fe-O(4)-Fe#2	180.0

Symmetry code: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z+1.

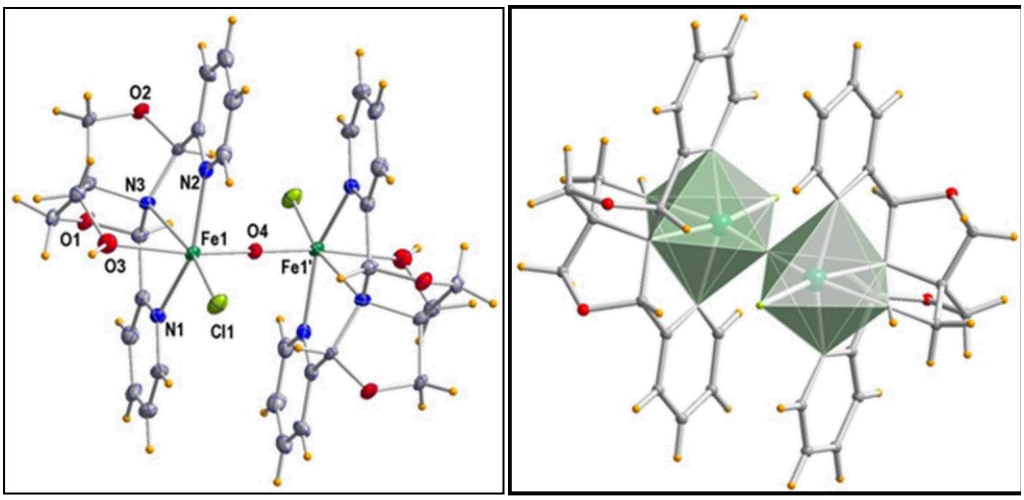

Fig. S6 ORTEP view (ellipsoids at 50% probability) of thecentrosymmetric **Complex 1** cation $[(FeLCl)_2O]^{2+}$ (C atoms not labelled for sake of clarity) and molecular structure with polyhedra around Fe ions.

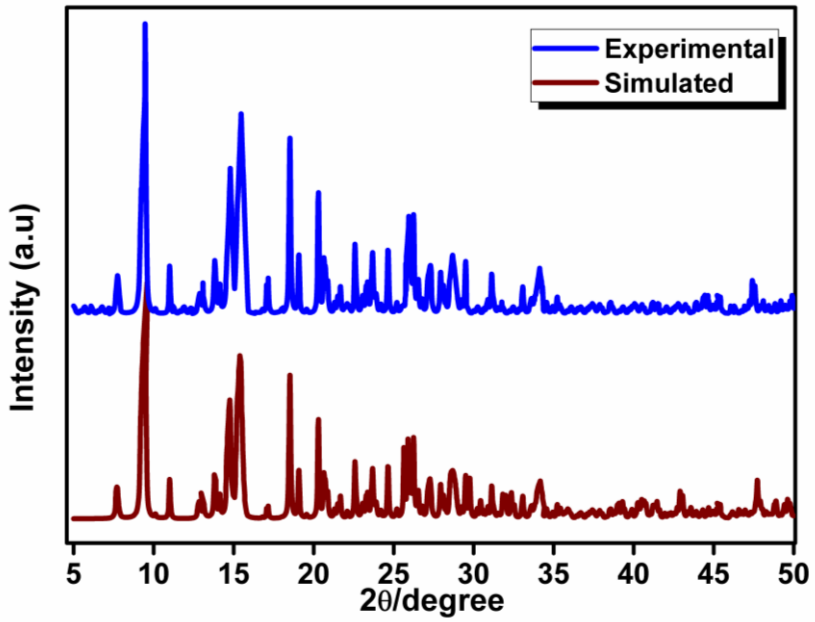

Fig. S7 PXRD pattern of the **Complex 1** (bulk) and the simulated one. It indicates that the bulk materials are same as the simulated one which comes from the single crystal. So, the materials are pure.

Electrochemical Measurements

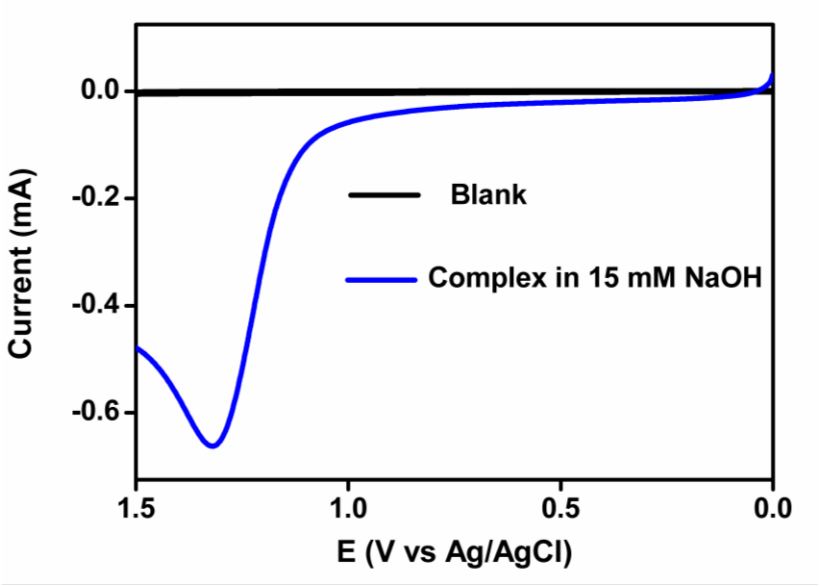

Fig. S8 The Fig. is the overlay of LSVs of acetonitrile in presence (blue) and in absence (black) of 0.4 mM **complex 1** containing 15 mM aqueous NaOH and 100 mM tetrabutylammonium perchlorate as supporting electrolyte (GC working electrode, Pt counter electrode).

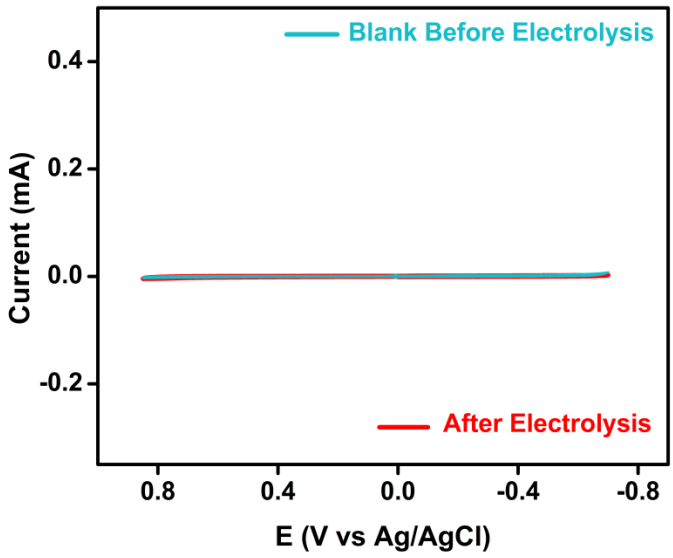

Fig. S9 Cyclic Voltammetry (CV) of the blank (without **complex 1** cyan color) and after bulk

electrolysis just rinsing the electrode without polishing (red) (0.4 mM in ACN, scan rate: 0.1 V/s, GC working electrode, 0.1 M nBu_4NClO_4 as a supporting electrolyte). This experiment further proved that there is no deposition of any particle on the working electrode surface.

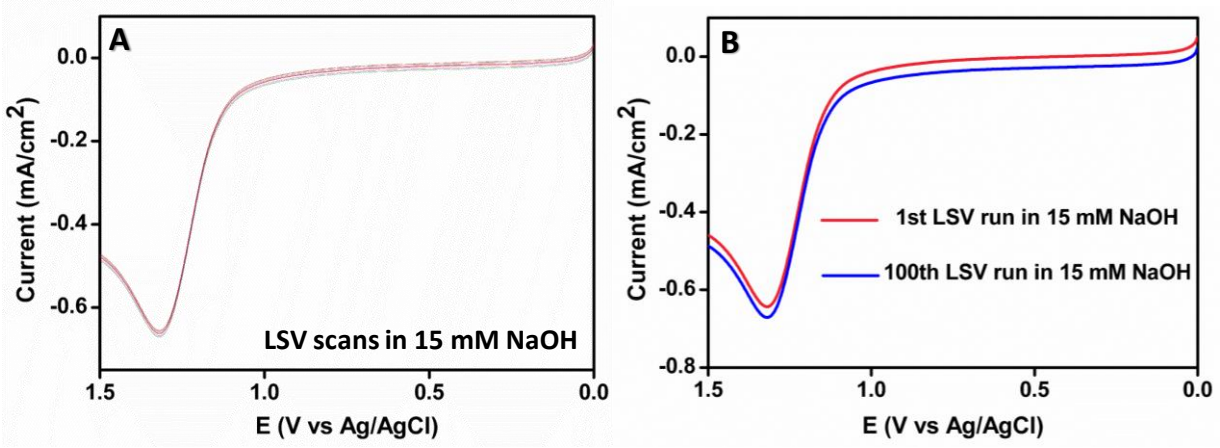

Fig. S10(A) Continuous 1-15, 20, 25, 30, 35 upto 100 LSV scans of the catalyst (0.4mM solution of **complex 1** in ACN with 15mMconcentration of NaOH) (scan rate: 0.1 V/s, GC working electrode) and **(B)** a clear picture of 1st LSV scan with 100th LSV scan of the complex in the same electrolytic condition.

Overpotential Calculation

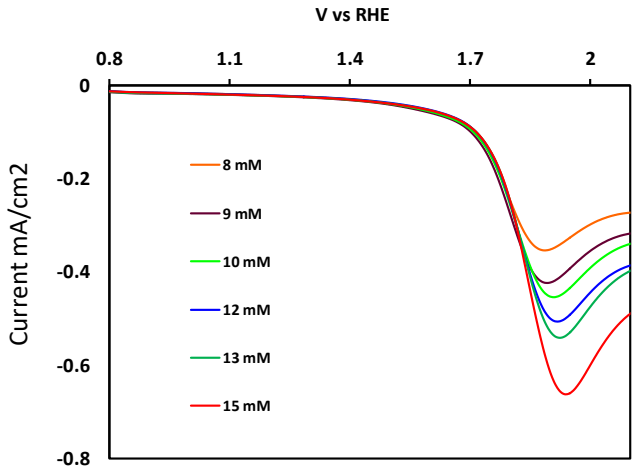

Fig. S10 (C) Linear Sweep Voltammetry (LSV) of 0.4 mM solution of complex with increasing concentration of NaOH.

The thermodynamic potential for H_2O/O_2 couple at a particular pH could be determined from Nernst equationand the equation could be represented as $E = E_{RHE} - 1.23$ V as the standards potential $E^0_{H2O/O2} = 1.23$ V.

Onset potential for OER is 1.82 V vs RHE (considering mid wave potential).

So, overpotential for OER of the complex at pH 7.18 is (1.82-1.23) V = 0.59 V.

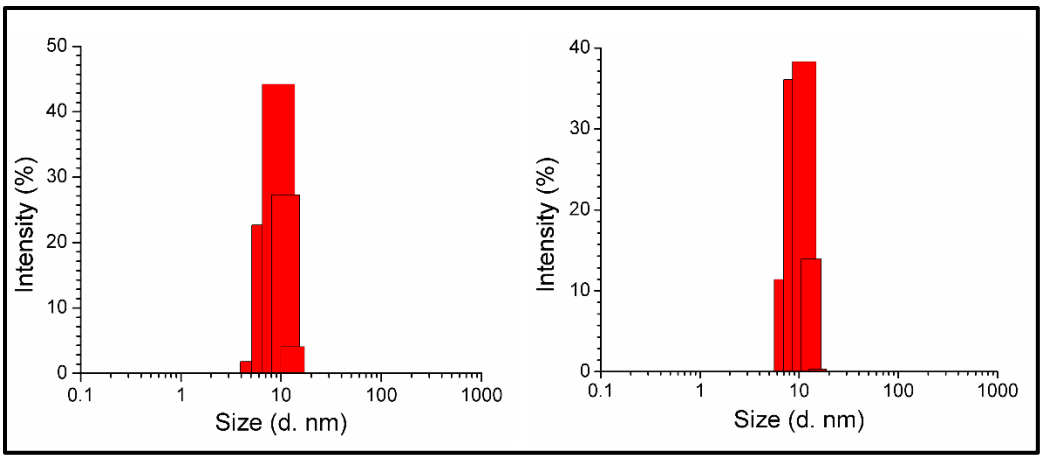

Fig. S11 Dynamic Light Scattering (DLS) experiment of the electrolytic solution before (left) and after (right) electrolysis of the catalyst solution.

Bulk Electrolysis (BE) and Gas Collection

The BE experiment was done in a four neck, two compartment, three electrode electrochemical cell brought from PINE with 1.77cm^2Hg-pool working electrode connected to an inverted burette for product analysis. The gas evolved during BE was collected into the burette by vertical displacement of water. The amount of gas evolved during the experiments was measured from the volume of water displaced. To check the stability of the catalyst BE was performed on a 1.77 cm^2Hg-pool electrode in the custom made 4 neck two compartment electrochemical cell with 6mL 0.4mMcatalyst in ACN solution containing 15 mM NaOH. Same reaction was performed by using acetonitrile medium varying the base concentration.

Calculation of Diffusion Constants from Cyclic Voltammograms of Complex

According to the Randles-Sevcik equation peak current of a redox event is given by

$$i_p = 0.4463(F/RT)^{1/2} n_p^{3/2} F A D^{1/2} [C_0] \upsilon^{1/2}$$

where, $i_p$is thepeak current, F Faraday's constant (F = 96500 C mol^{-1}), R the universal gas constant (R = 8.314 J K^{-1} mol^{-1}), T temperature (T = 300 K), n_p is the number of electrons transferred (n_p = 1 for $Fe^{3+/2+}$ in **complex1**), A is the active surface area of the electrode (here aGC electrode,A = 0.068 cm^2), D is the diffusion coefficient for the complex, $[C_0]$ is the concentration of the catalyst ($[C_0]$ = 0.4 mM), and υ is the scan rate. The diffusion coefficient D(= 2.21 x10^{-6} cm^2s^{-1})was calculated from the slope of $i_p vs \upsilon^{1/2}$ plot (Fig. S12). Therefore, $0.4463(F/RT)^{1/2} n_p^{3/2} F A D^{1/2} [C_0]$ = 10.83.

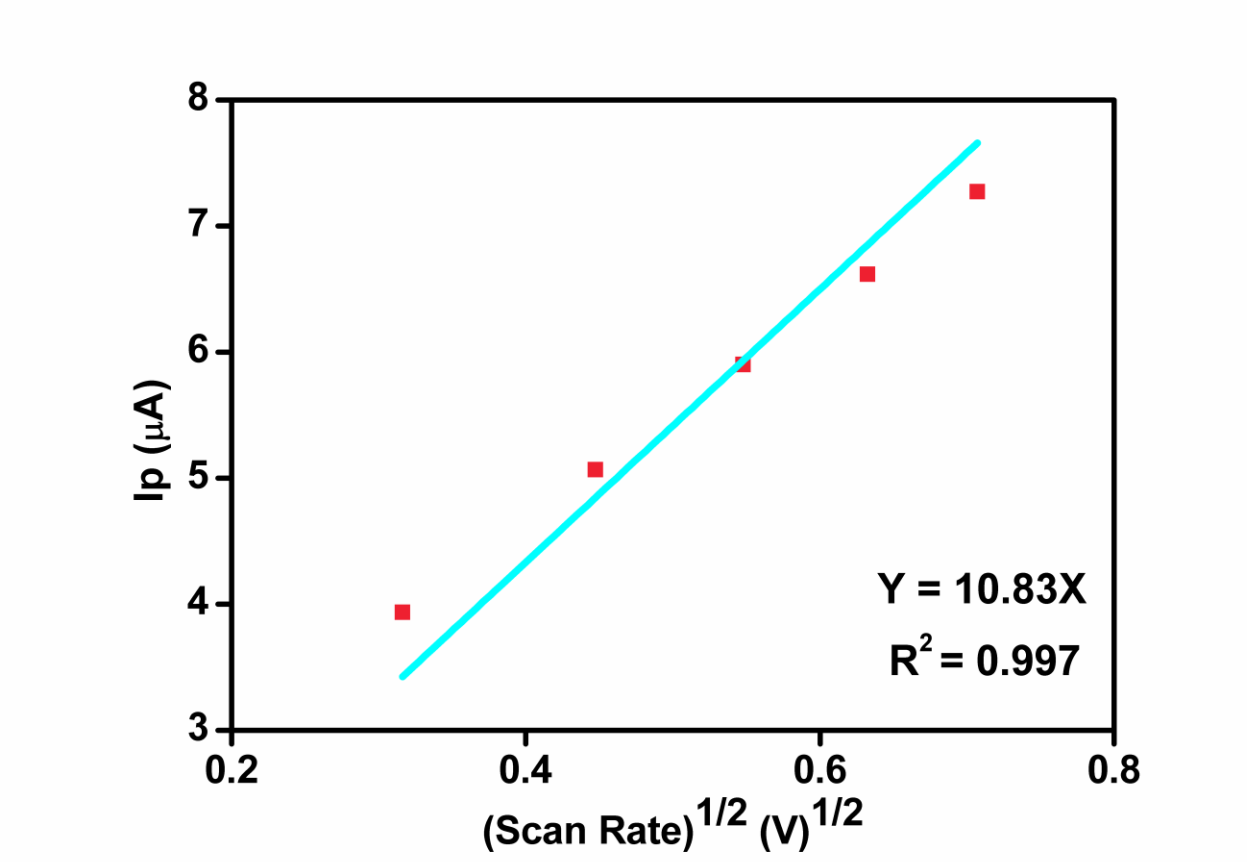

Fig. S12 Plot of the peak current of the $Fe^{3+/2+}$ process *vs* square root of the scan rates.

Calculation of Faradic Efficiency (FE) from Total Charge Accumulated During Control Potential Electrolysis (CPE)

The Faradic efficiency (FE (%)) was calculated based on following equation:

$$FE(\%) = \frac{4 \times amount\ of\ O_2\left(moles\right) \times 100}{n\left(moles\ of\ \ electrons\right)}$$

$$\text{Where, } n = \frac{Q\left(columb\right)}{F\left(Faraday\ const.\right)}$$

During the Constant Potential Electrolysis (CPE) at 1.0 V vs Ag/AgCl total charge consumed was 21.8 C in 17.3 min and 0.97 mL O_2 gas was collected in an inverted burette set up connected to electrolyser cell through a channel. Total moles of O_2 produced during bulk electrolysis = (0.97/22400)mol = 43.3 x 10^{-6}, and Faradaic Yield (FY) = 78.6%.

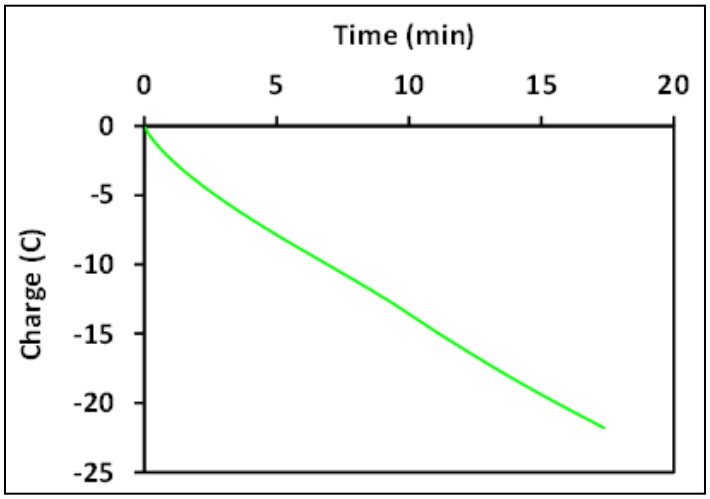

Fig. S13 Total accumulated charge during bulk electrolysis at 1.0 V vs Ag/AgCl on a 1.77 cm^2 Hg-pool electrode in ACN solution containing 15 mM of NaOH (0.4mM**complex1**).

TON Calculation

At 1.0 V vs Ag/AgClTON= (Total no. of moles of O_2 produced/ total no. of moles of catalyst used).

During bulk electrolysis (BE) at 1.0 V *vs* Ag/AgCl potential using Hg-pool electrode amount of O_2 collected is 3.8 mL,*i.e.*(3.8/22400) moles.

During BE, 4 mL 0.4mM solution was used and after 1 hr of electrolysis decay of the catalyst was 26%. (Fig. S16)

TON= (3.8/22400) x (10^3/0.4x10^{-3} x4) x (100/26) =~408

TOF after 1 hr is 0.11 s^{-1}

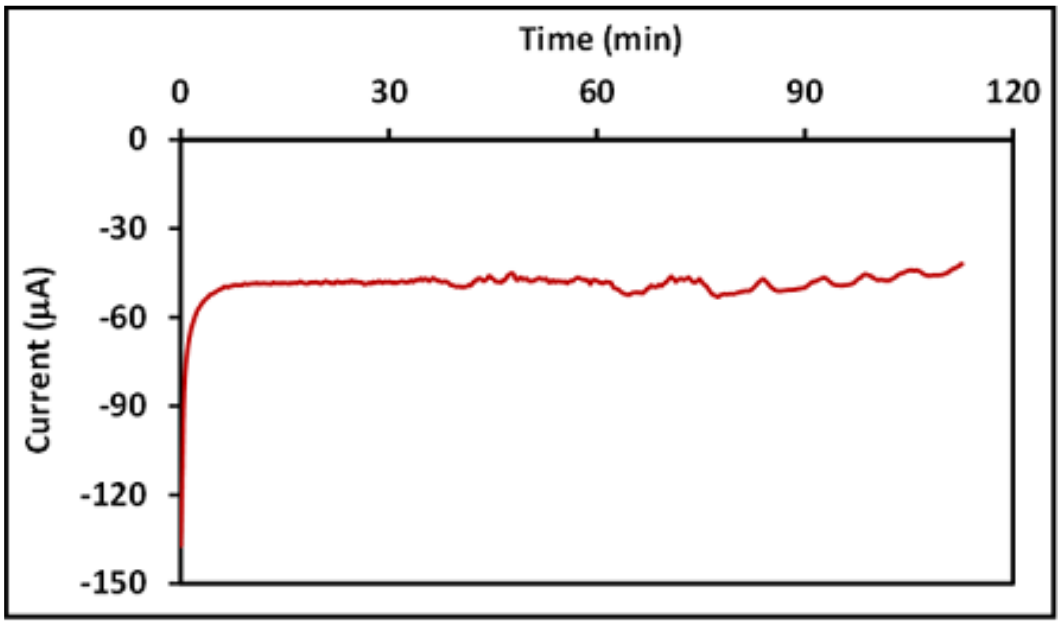

Fig. S14 Total current generated during bulk electrolysisat 1.0 V vs Ag/AgCl on a Glassy Carbon (GC) electrode in ACN solution containing 15 mM of NaOH (0.4mM **complex 1**).

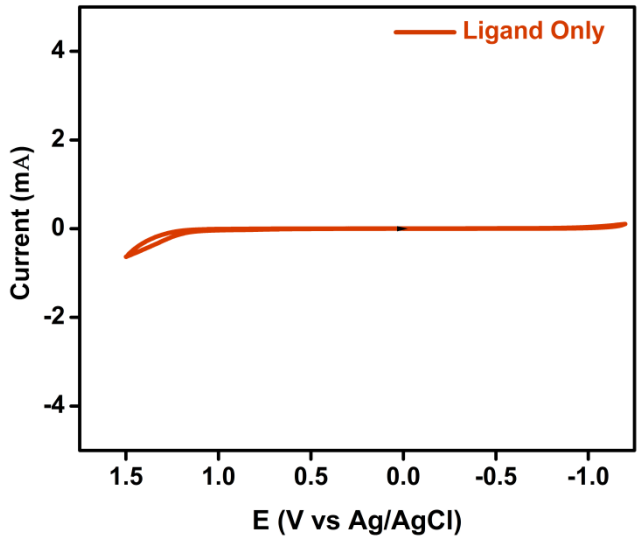

Fig. S15 Cyclic Voltammetry (CV) of the ligand (0.4 mM in ACN, scan rate: 0.1 V/s, GC working electrode, 0.1 M nBu4NClO4 as a supporting electrolyte). The result suggests that the ligand system is redox inactive, and it does not take part in electrolysis process.

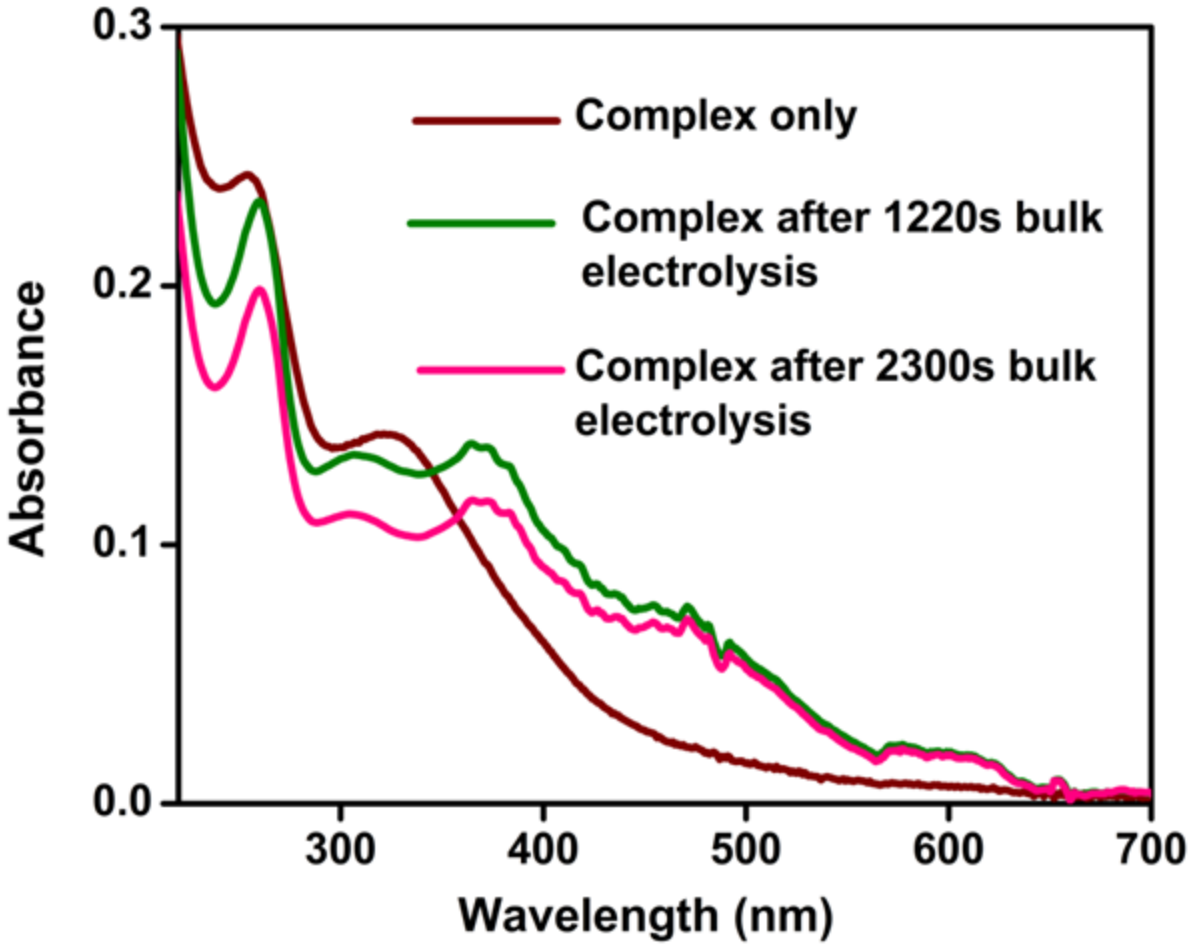

Fig. S16 UV-visible spectra of the **complex 1** in ACN medium (brown), bulkelectrolysis of the **complex** after 1220s (green) maintaining the electrolytic condition and bulk electrolysis of the **complex** after 2300s (red).

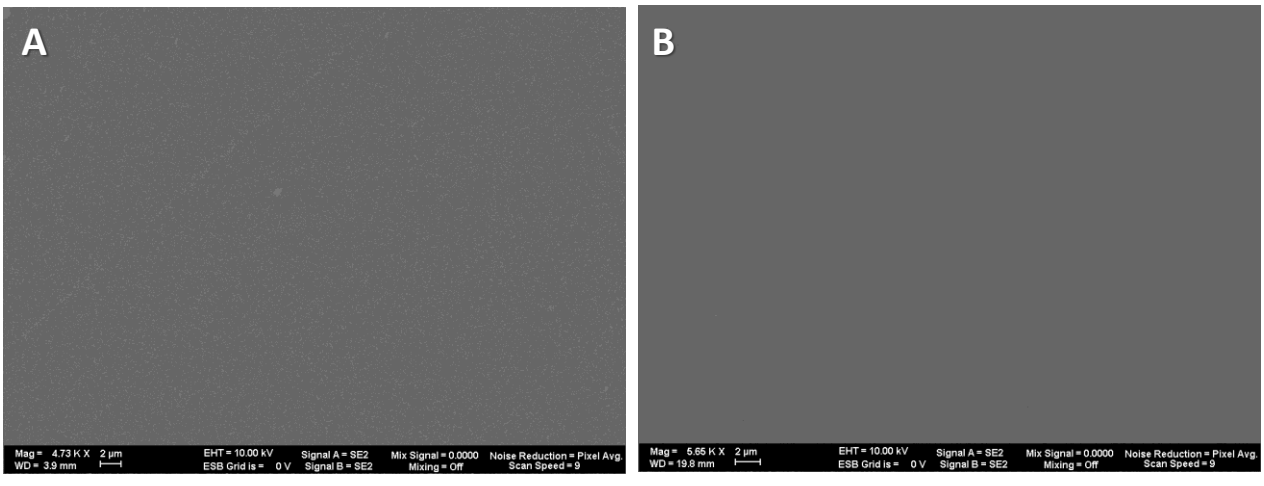

Fig. S17 SEM images of the electrode (A) before bulk electrolysis and (B) after electrolysis.

Synthesis procedure of complex 2

Complex 2 $[(FeLCl)_2O]Cl_2$was synthesized by adding an acetonitrile solution of tris(hydroxymethyl)aminomethane (2-amino-2-(hydroxymethyl) propane-1,3-diol) (0.121 g, 1.0 equiv.) drop wise to a solution of pyridine-2- carbaldehyde (0.107 g, 1.0 equiv.) under stirring condition, and the resulting mixture was refluxed in an water bath maintaining the temperature at 100°C for 3h. Then, a 1:1 acetonitrile–water solution of anhydrous iron(III) chloride (0.162 g, 1 mM) was added to it drop wise to avoid precipitation under reflux for further 4h. Then the solution was filtered washed several times with ether and kept in a $CaCl_2$ desiccator. After a few days, square shaped brownish black colored crystals suitable for X-ray diffraction were obtained.

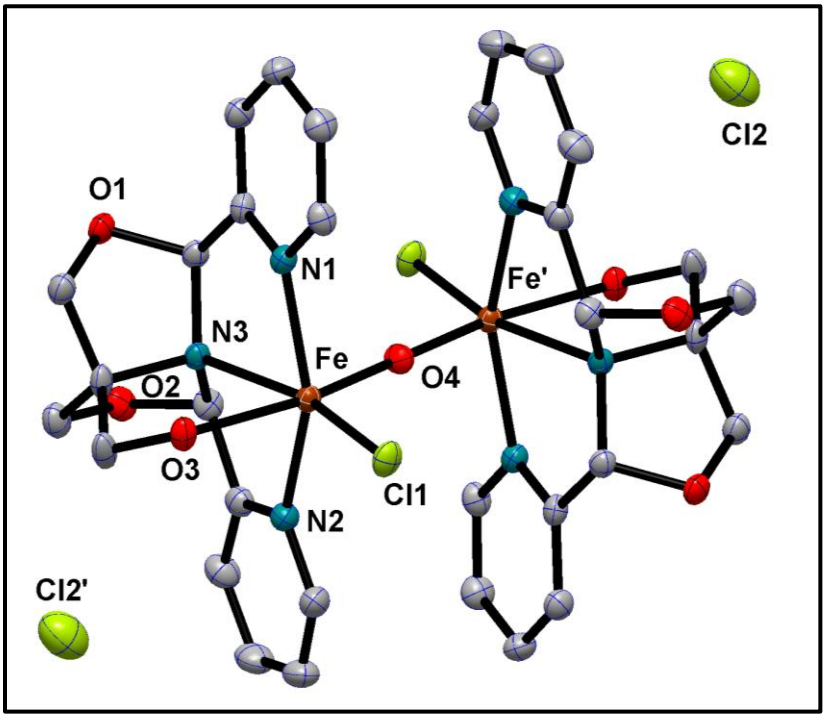

Fig. S18 ORTEP view (ellipsoids at 50% probability) of centrosymmetric complex **2** $[(FeLCl)_2O]Cl_2$ (Fe' at -x+1, -y+1, -z+1; lattice water molecules not shown).

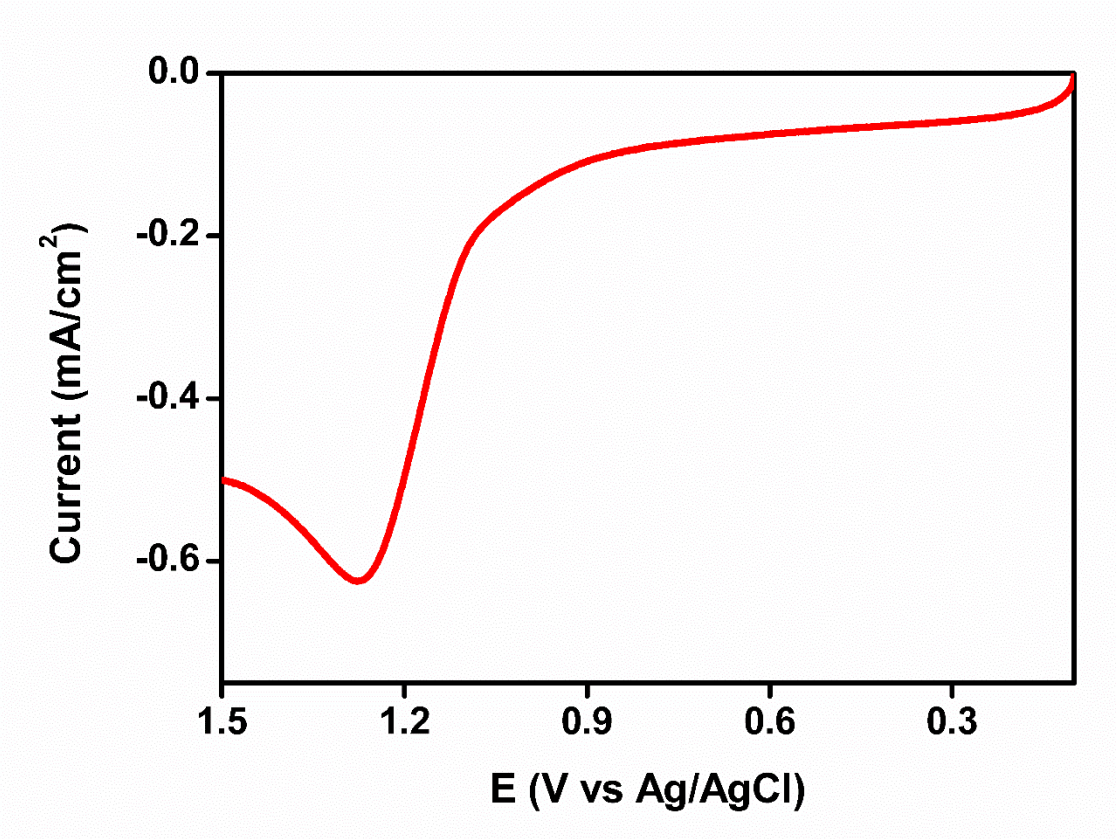

Fig. S18 (A) LSVs of newly synthesized **complex 2** (replacing the anionic part). We maintain the electrocatalytic condition as those applied for **complex 1** (0.4 mM complex containing 15 mM aqueous NaOH and 100 mM tetrabutylammonium perchlorate as supporting electrolyte GC working electrode, Pt counter electrode). We found the same result as for complex **1**. Herein, we assure that the cationic part of our synthesized **complex 1** is mainly responsible for the electrocatalytic process.

Tafel Plot and Electron Count Analysis

As Oxygen Evolving Reaction (OER) consists of large number of intermediate, so Tafel slop generally cannot be used for predicting the mechanism of OER reaction but it is important to determine the number of electrons transferred during the OER reaction. The Tafel plot of an electrocatalytic process (OER) is acquired by plotting the linear sweep voltammogram (LSV, maintaining the catalytic condition) as a plot of log(j) versus η.

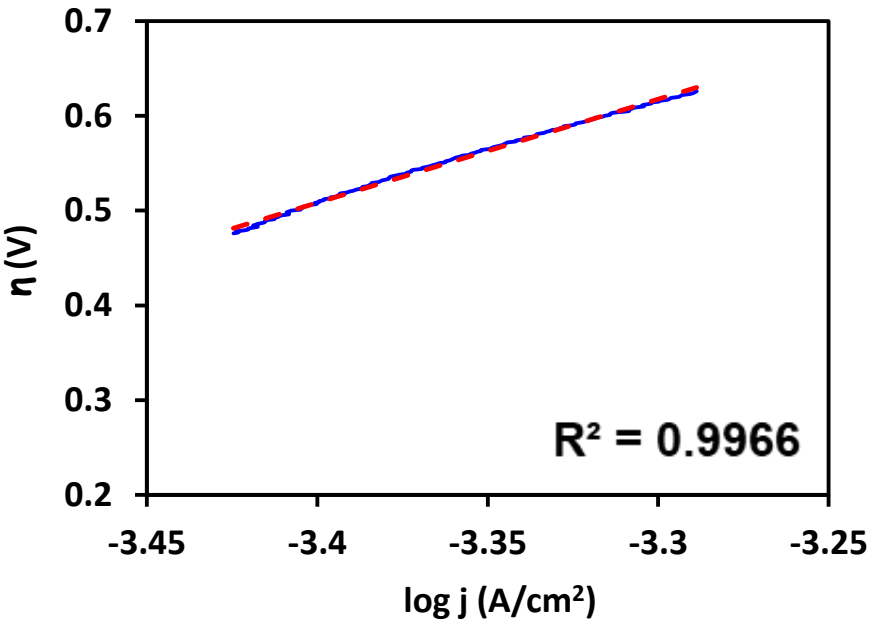

Fig. S19 Tafel plot of the complex maintaining the catalytic condition followed by voltammetry methodology. From the graph the calculated value of the Tafel slope is 110 mV dec^{-1}, which is in agreement with literature value for one electron transfer process.

XPS Spectra analysis for complex 1

The metal electron binding energy (BE) values in the complex is important to analyze the coordination model. Dinuclear iron (III) complexes have been characterized by X-ray photoelectron spectra (XPS). C1s, N1s, O1s, Cl2s, Cl2p and Fe2p bands of the complex are approximately the same as those reported in the literature.

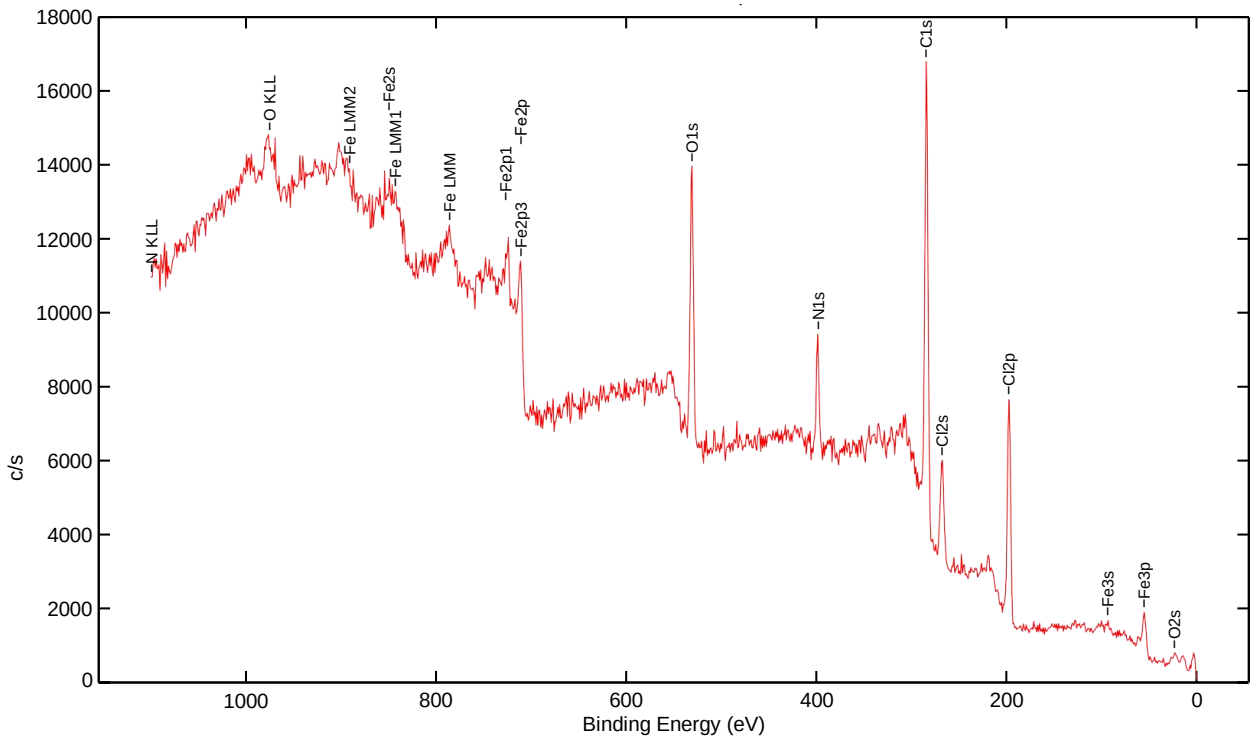

Fig. S20 X-ray photoelectron spectra (XPS) of the catalytic complex **1**.

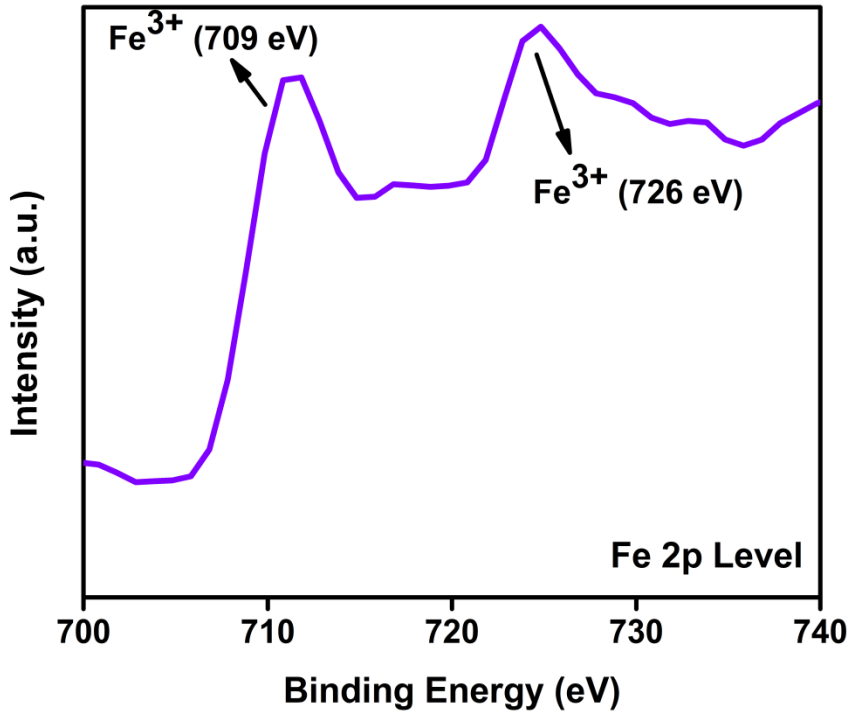

Fig. S20A XPS spectra of Fe2p level in the purple ruby of complex **1**.

The electrochemical impedance study

To explore the electron transfer kinetics, electrochemical impedance spectroscopy (EIS) measurements have been performed with complex 1 maintaining the same catalytic medium. It should be noted that all EIS measurement has been performed at the over potential and the results are displayed in Fig. S21 as Nyquist plots. The semicircular region i.e. the kinetically controlled region of the impedance spectra of the complex have been fitted using the Randles equivalent circuits to calculate charge transfer resistance. The charge transfer resistance for the water splitting reaction using complex 1 as electrocatalyst has been found to be 1690 Ω cm2 which is also consistent with the OER activity of these types of homogeneous catalysts.

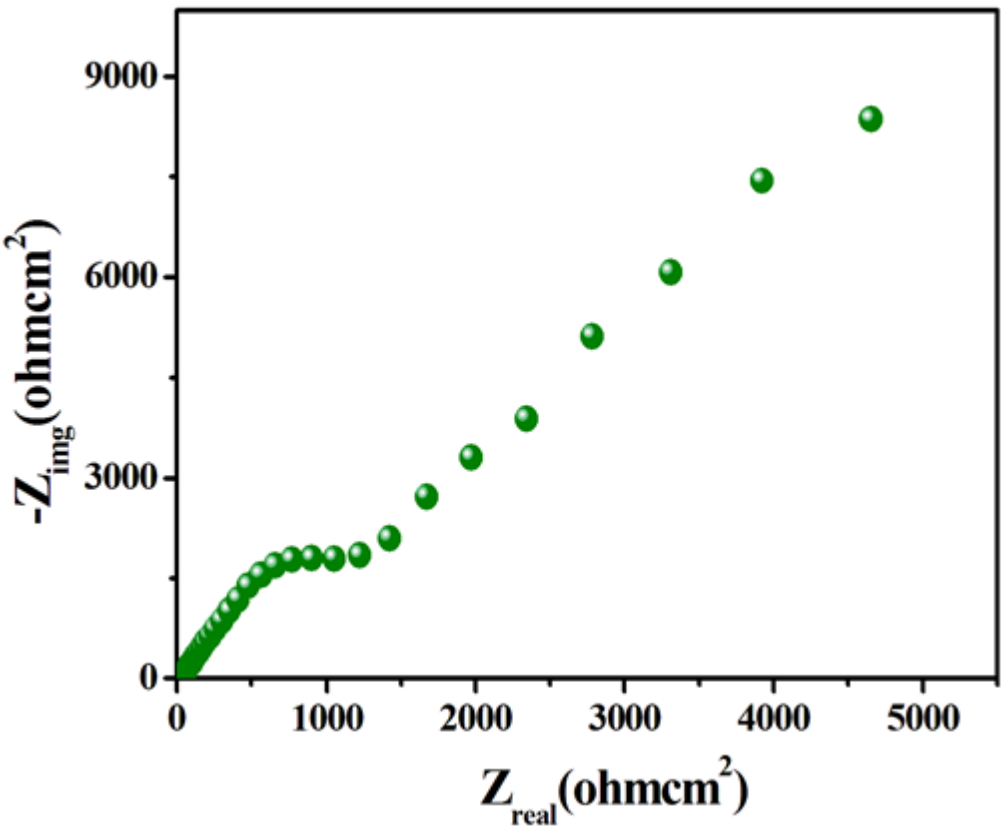

Fig. S21 Impedance spectra of **complex 1** (green), electrical equivalent electrical circuit models used to explain the EIS response of the water oxidation reaction.

Computational Results

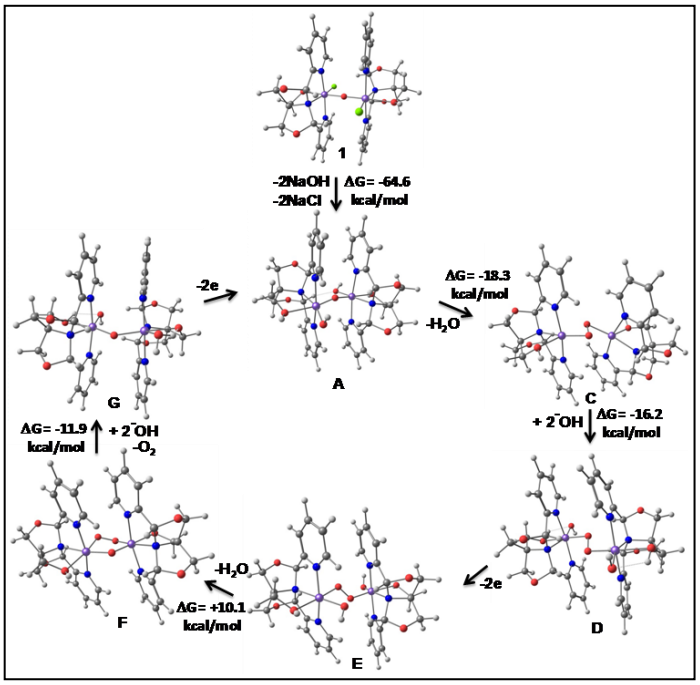

Fig. S22M06-2X/6-31G(d) optimized geometries for the intermediates of electrocatalytic water oxidation of**complex 1 cation**.

Coordinates of optimized geometries

Complex 1

Charge 2, Multiplicity 1

Fe	0.445000	-1.513400	0.724700
O	0.000000	0.000000	0.000000
Fe	-0.445000	1.513400	-0.724700
C	2.312800	-2.033100	-1.597300
H	1.485800	-2.615000	-1.991500
C	3.503200	-1.870000	-2.293400
H	3.619900	-2.324000	-3.270300
C	4.523800	-1.121000	-1.714800
H	5.465700	-0.977800	-2.233500
C	4.321200	-0.554800	-0.461200
H	5.090800	0.027400	0.032900
C	3.097300	-0.752600	0.165300
C	2.858400	-0.164800	1.551100
H	2.767800	0.924900	1.511100
C	3.617000	-1.858600	2.785100
H	4.250900	-2.131600	3.627400
H	3.785900	-2.552400	1.950300
C	2.130800	-1.783100	3.149400
C	1.366000	-3.093800	2.995500

H	1.963400	-3.935100	3.357500
H	0.416800	-3.065000	3.538300
C	1.902300	-1.076500	4.515900
H	1.126700	-1.588300	5.097200
H	2.814500	-1.007400	5.107500
C	0.815200	0.164500	2.986100
H	0.769800	1.152600	2.516400
C	-0.574200	-0.440900	3.141000
C	-1.351400	-0.172200	4.257200
H	-0.960000	0.466900	5.040800
C	-2.618100	-0.745600	4.334100
H	-3.252300	-0.557000	5.193700
C	-3.060900	-1.552300	3.291300
H	-4.045300	-2.005000	3.305900
C	-2.214300	-1.784700	2.212500
H	-2.498500	-2.416500	1.377600
N	2.121900	-1.484800	-0.391000
N	1.618500	-0.764400	2.149000
N	-0.989600	-1.249500	2.150600
O	3.906200	-0.518600	2.407900
O	1.124000	-3.239300	1.591500
O	1.493400	0.251200	4.197600
H	0.559900	-4.011600	1.405400
Cl	-0.833900	-2.877700	-0.657300
C	-2.312800	2.033100	1.597300
H	-1.485800	2.615000	1.991500
C	-3.503200	1.870000	2.293400
H	-3.619900	2.324000	3.270300
C	-4.523800	1.121000	1.714800
H	-5.465700	0.977800	2.233500
C	-4.321200	0.554800	0.461200
H	-5.090800	-0.027400	-0.032900
C	-3.097300	0.752600	-0.165300
C	-2.858400	0.164800	-1.551100
H	-2.767800	-0.924900	-1.511100
C	-3.617000	1.858600	-2.785100
H	-4.250900	2.131600	-3.627400
H	-3.785900	2.552400	-1.950300
C	-2.130800	1.783100	-3.149400
C	-1.366000	3.093800	-2.995500
H	-1.963400	3.935100	-3.357500
H	-0.416800	3.065000	-3.538300
C	-1.902300	1.076500	-4.515900
H	-1.126700	1.588300	-5.097200
H	-2.814500	1.007400	-5.107500
C	-0.815200	-0.164500	-2.986100

H	-0.769800	-1.152600	-2.516400
C	0.574200	0.440900	-3.141000
C	1.351400	0.172200	-4.257200
H	0.960000	-0.466900	-5.040800
C	2.618100	0.745600	-4.334100
H	3.252300	0.557000	-5.193700
C	3.060900	1.552300	-3.291300
H	4.045300	2.005000	-3.305900
C	2.214300	1.784700	-2.212500
H	2.498500	2.416500	-1.377600
N	-2.121900	1.484800	0.391000
N	-1.618500	0.764400	-2.149000
N	0.989600	1.249500	-2.150600
O	-3.906200	0.518600	-2.407900
O	-1.124000	3.239300	-1.591500
O	-1.493400	-0.251200	-4.197600
H	-0.559900	4.011600	-1.405400
Cl	0.833900	2.877700	0.657300

Intermediate A

Charge 2, Multiplicity 1

Fe	-1.320900	-0.209700	-1.117600
C	-0.165000	-2.833900	-2.155200
H	0.062800	-2.249300	-3.041200
C	0.238800	-4.155100	-2.012800
H	0.785800	-4.643800	-2.810300
C	-0.062700	-4.818000	-0.825700
H	0.250100	-5.845900	-0.673700
C	-0.773500	-4.148100	0.165100
H	-1.044300	-4.635400	1.095500
C	-1.152500	-2.829300	-0.063500
C	-2.020300	-2.103100	0.968000
H	-1.484000	-1.961800	1.910600
C	-4.036600	-2.554800	0.122500
H	-5.040400	-2.908100	0.356000
H	-3.685900	-3.020900	-0.809000
C	-3.932800	-1.028000	0.047900
C	-4.223400	-0.424300	-1.328300
H	-5.095900	-0.908900	-1.777700
H	-4.421100	0.648700	-1.241500
C	-4.721300	-0.336200	1.200400
H	-5.300400	0.516100	0.825700
H	-5.386700	-1.024900	1.721600
C	-2.569700	0.317200	1.397600
H	-1.701300	0.313500	2.067600
C	-2.634100	1.623500	0.601100
C	-3.333900	2.729300	1.064600

H	-3.848000	2.680000	2.018100
C	-3.370200	3.870200	0.264300
H	-3.918400	4.747900	0.589800
C	-2.696400	3.872200	-0.953300
H	-2.695100	4.745900	-1.594600
C	-2.018600	2.721500	-1.345000
H	-1.477800	2.635000	-2.283400
N	-0.841200	-2.190600	-1.198200
N	-2.500300	-0.797100	0.432100
N	-2.006500	1.623900	-0.585500
O	-3.176300	-2.867500	1.210600
O	-3.070900	-0.637700	-2.154600
O	-3.737900	0.102600	2.136000
H	-3.186200	-0.167100	-2.996700
O	0.114600	-0.166400	0.205100
Fe	1.264900	0.489700	1.147900
C	0.129900	3.208500	1.391100
H	-0.239900	2.825500	2.336100
C	-0.057100	4.520200	0.978600
H	-0.614300	5.206200	1.605500
C	0.483100	4.924900	-0.240500
H	0.358100	5.946000	-0.584500
C	1.183300	4.007200	-1.015200
H	1.628900	4.280100	-1.965000
C	1.320200	2.707600	-0.542100
C	2.073900	1.660600	-1.348000
H	1.424500	1.253100	-2.138800
C	4.167600	2.195400	-0.781200
H	5.174600	2.358900	-1.163300
H	3.913600	2.978100	-0.052900
C	3.973700	0.798700	-0.172600
C	4.237300	0.723300	1.327200
H	5.122100	1.305300	1.600100
H	4.369200	-0.312100	1.654700
C	4.664000	-0.316200	-1.007100
H	5.113700	-1.073100	-0.353200
H	5.421500	0.076200	-1.684800
C	2.463100	-0.800300	-1.045500
H	1.585800	-0.858800	-1.701400
C	2.435200	-1.835200	0.078900
C	2.893200	-3.125900	-0.137600
H	3.269200	-3.402000	-1.116700
C	2.863800	-4.031600	0.920400
H	3.210200	-5.049500	0.777900
C	2.391800	-3.612900	2.159000
H	2.355100	-4.282800	3.009200

C	1.966900	-2.296700	2.299900
H	1.609600	-1.927500	3.255300
N	0.807500	2.336000	0.637400
N	2.507700	0.550700	-0.428500
N	1.991600	-1.430800	1.284100
O	3.256600	2.194900	-1.870800
O	3.071000	1.286800	1.930700
O	3.630900	-0.892700	-1.801300
H	3.093600	1.208600	2.900100
O	0.608200	0.730700	2.788600
H	0.622000	-0.097100	3.294600
O	-0.232300	0.374900	-2.624800
H	-0.506700	-0.068400	-3.439700

Intermediate B

Charge 1, Multiplicity 2

O	-0.153400	-2.908400	0.164500
Fe	-0.089900	-1.301600	0.015700
C	-3.013800	-1.841600	-0.056700
H	-2.652000	-2.825100	0.222400
C	-4.358600	-1.542700	-0.216500
H	-5.104600	-2.312100	-0.059300
C	-4.718300	-0.246100	-0.576300
H	-5.762000	0.019600	-0.705000
C	-3.724400	0.706800	-0.772000
H	-3.960100	1.728200	-1.048600
C	-2.398000	0.329200	-0.603000
C	-1.280700	1.343600	-0.834000
H	-1.192000	1.574900	-1.898700
C	-1.095800	2.286000	1.180400
H	-1.027100	3.235400	1.710500
H	-1.776600	1.607700	1.712800
C	0.264700	1.621100	0.954200
C	0.702600	0.718400	2.102000
H	0.591200	1.248500	3.053700
H	1.749700	0.418000	1.984900
C	1.361500	2.632000	0.516200
H	2.304300	2.438300	1.041900
H	1.063500	3.668400	0.676000
C	1.191500	1.111900	-1.140000
H	0.948700	1.002800	-2.200600
C	2.311600	0.150200	-0.752100
C	3.646500	0.490000	-0.912900
H	3.908000	1.470900	-1.293700
C	4.614300	-0.449600	-0.566500
H	5.667400	-0.213200	-0.675000
C	4.216900	-1.692200	-0.081900

H	4.941700	-2.448600	0.194000
C	2.859300	-1.953500	0.055200
H	2.474200	-2.896300	0.428700
N	-2.061400	-0.917000	-0.242500
N	0.013100	0.819400	-0.300700
N	1.934200	-1.042500	-0.265500
O	-1.546300	2.533300	-0.143800
O	-0.149700	-0.422900	2.060300
O	1.525200	2.442800	-0.886800
H	0.079900	-1.036200	2.777300

Intermediate C

Charge 2, Multiplicity 1

Fe	-1.702000	0.320200	0.431600
C	-1.515000	3.304900	0.312300
H	-0.632600	3.118900	0.917700
C	-1.874400	4.567000	-0.141000
H	-1.276400	5.430400	0.126700
C	-3.008000	4.689600	-0.942500
H	-3.318500	5.661000	-1.312000
C	-3.736100	3.551100	-1.272600
H	-4.620600	3.602700	-1.897900
C	-3.304700	2.322700	-0.781200
C	-4.070300	1.044300	-1.129700
H	-4.003000	0.828000	-2.198700
C	-5.463500	0.927500	0.606500
H	-6.499500	0.776800	0.908600
H	-5.024400	1.756700	1.178700
C	-4.609000	-0.336200	0.728000
C	-3.965700	-0.528500	2.099100
H	-4.683500	-0.292400	2.890900
H	-3.619200	-1.558800	2.229700
C	-5.354200	-1.598900	0.208400
H	-5.232600	-2.440600	0.900600
H	-6.416000	-1.416700	0.041900
C	-3.463200	-1.408600	-1.007300
H	-3.086500	-1.290300	-2.026800
C	-2.548900	-2.313100	-0.170900
C	-2.736900	-3.688400	-0.123200
H	-3.524900	-4.145300	-0.711400
C	-1.915000	-4.439700	0.714300
H	-2.041900	-5.515000	0.780600
C	-0.938900	-3.797300	1.471600
H	-0.287700	-4.349800	2.138700
C	-0.807900	-2.418600	1.354900
H	-0.062100	-1.854500	1.907500
N	-2.229000	2.217900	0.005000

N	-3.552600	-0.103500	-0.323900
N	-1.597100	-1.699600	0.550100
O	-5.425000	1.189100	-0.788900
O	-2.857300	0.373300	2.158300
O	-4.768400	-1.906200	-1.055500
H	-2.392200	0.271700	3.004600
Fe	1.717100	0.193000	-0.490100
C	0.603400	-2.436100	-1.407800
H	-0.098800	-1.798900	-1.937300
C	0.603500	-3.818300	-1.536000
H	-0.111100	-4.302400	-2.191300
C	1.531800	-4.553500	-0.801200
H	1.553200	-5.636100	-0.868400
C	2.445100	-3.885100	0.007300
H	3.206800	-4.417700	0.565300
C	2.392300	-2.495700	0.061300
C	3.456200	-1.715300	0.842600
H	3.280200	-1.760200	1.920100
C	5.050400	-1.722600	-0.710700
H	6.112700	-1.880200	-0.893600
H	4.462100	-2.206900	-1.502500
C	4.671900	-0.241900	-0.574800
C	4.267100	0.422000	-1.889000
H	4.935300	0.105700	-2.696200
H	4.302800	1.511700	-1.802400
C	5.733600	0.564900	0.226700
H	5.893600	1.553800	-0.220000
H	6.687800	0.043900	0.304100
C	3.814900	0.727000	1.382600
H	3.342300	0.489600	2.339400
C	3.334400	2.086900	0.865900
C	3.860600	3.271000	1.366700
H	4.647700	3.238300	2.112100
C	3.353400	4.475000	0.884800
H	3.741500	5.417500	1.255700
C	2.342200	4.455700	-0.072300
H	1.918300	5.372900	-0.464000
C	1.880000	3.226400	-0.528500
H	1.085800	3.134600	-1.262800
N	1.473600	-1.798200	-0.617100
N	3.496200	-0.298500	0.370200
N	2.378200	2.074000	-0.072900
O	4.721900	-2.254200	0.565800
O	2.929100	-0.002100	-2.169500
O	5.203300	0.694000	1.541800
H	2.610700	0.433600	-2.976800

O	0.188400	0.740400	0.671600
O	-0.142000	0.740800	-0.759400

Intermediate D

Charge 0, Multiplicity 1

Fe	-1.831600	-0.534200	-1.238700
C	-0.130400	-2.946900	-2.020600
H	-0.214800	-2.545000	-3.026400
C	0.665200	-4.049200	-1.743900
H	1.218700	-4.535500	-2.539000
C	0.732100	-4.499900	-0.426000
H	1.346300	-5.356200	-0.165800
C	0.002400	-3.837400	0.550800
H	0.019800	-4.162200	1.586100
C	-0.771200	-2.735000	0.186700
C	-1.645600	-2.063900	1.243500
H	-1.027900	-1.682600	2.054400
C	-3.658200	-3.001000	0.879900
H	-4.510800	-3.483300	1.359900
H	-3.412900	-3.525800	-0.055000
C	-3.877700	-1.510500	0.609400
C	-4.556300	-1.245400	-0.744300
H	-5.451800	-1.874300	-0.824300
H	-4.865000	-0.199400	-0.822800
C	-4.552500	-0.767400	1.798800
H	-5.355900	-0.109100	1.441500
H	-4.956400	-1.452200	2.546600
C	-2.568900	0.252100	1.410600
H	-1.588900	0.481500	1.836000
C	-3.033300	1.379700	0.489800
C	-3.652700	2.515900	0.997300
H	-3.827600	2.600900	2.064500
C	-4.034700	3.518200	0.109500
H	-4.514900	4.419900	0.476300
C	-3.790600	3.350800	-1.250600
H	-4.069600	4.111200	-1.971200
C	-3.181800	2.174500	-1.678000
H	-2.968100	1.954200	-2.719900
N	-0.836400	-2.310200	-1.080800
N	-2.473900	-0.988500	0.642400
N	-2.821300	1.214900	-0.823700
O	-2.560400	-3.008700	1.774900
O	-3.626200	-1.580800	-1.764500
O	-3.522000	-0.003200	2.420000
H	-3.580400	-0.960300	-2.514400
Fe	1.808600	0.626400	1.245600
C	0.134900	3.105400	1.819100

H	0.173100	2.760200	2.848500
C	-0.668700	4.172400	1.441200
H	-1.279300	4.682400	2.177500
C	-0.667300	4.558200	0.101900
H	-1.280900	5.388600	-0.232900
C	0.129100	3.863600	-0.798800
H	0.160700	4.132800	-1.849500
C	0.879400	2.781400	-0.341200
C	1.747200	2.008500	-1.331600
H	1.127100	1.604500	-2.129700
C	3.802200	2.855300	-0.992800
H	4.687700	3.257900	-1.486900
H	3.574200	3.450700	-0.096700
C	3.933100	1.375800	-0.624600
C	4.578700	1.169900	0.756100
H	5.497800	1.765900	0.812300
H	4.843400	0.120200	0.909400
C	4.574900	0.517200	-1.753600
H	5.334800	-0.160900	-1.343000
H	5.024100	1.125700	-2.540500
C	2.533600	-0.362300	-1.322100
H	1.544000	-0.567300	-1.739100
C	2.940800	-1.442200	-0.320300
C	3.557300	-2.617100	-0.734400
H	3.749400	-2.779400	-1.789500
C	3.917600	-3.555400	0.229400
H	4.397900	-4.483600	-0.064200
C	3.654100	-3.289400	1.569600
H	3.916000	-3.997400	2.347500
C	3.054400	-2.078200	1.902200
H	2.835400	-1.778300	2.923100
N	0.890800	2.427800	0.950900
N	2.503200	0.932900	-0.644700
N	2.718200	-1.179700	0.975100
O	2.718600	2.867600	-1.904100
O	3.648000	1.611100	1.736200
O	3.507400	-0.228500	-2.336700
H	3.567200	1.044700	2.522100
O	0.167700	-0.231200	0.644300
O	-0.200300	0.336000	-0.644700
O	-1.988600	-0.135300	-3.207400
H	-1.611200	-0.846900	-3.742200
O	1.904900	0.349900	3.237700
H	1.560000	1.120000	3.709900

Intermediate E

Charge 2, Multiplicity 1

Fe	2.134500	-0.176900	1.236300
O	-0.463000	-0.183200	0.605900
O	0.616600	0.440500	0.524900
O	1.970500	0.307500	3.016600
H	1.844000	-0.459700	3.591900
C	0.731700	-2.667600	2.235000
H	0.691000	-2.142800	3.182800
C	0.138400	-3.911100	2.073700
H	-0.367100	-4.379900	2.909100
C	0.209900	-4.527800	0.827500
H	-0.242200	-5.500900	0.667500
C	0.862100	-3.876300	-0.212800
H	0.940000	-4.316600	-1.201100
C	1.416500	-2.623400	0.023200
C	2.087000	-1.876300	-1.128000
H	1.333300	-1.562600	-1.859800
C	4.196800	-2.567800	-0.890100
H	5.068500	-2.956900	-1.415600
H	4.052300	-3.119900	0.049400
C	4.273100	-1.058600	-0.631200
C	4.937400	-0.678400	0.689600
H	5.835800	-1.278700	0.859900
H	5.206400	0.381400	0.702700
C	4.822700	-0.268900	-1.853300
H	5.520100	0.514200	-1.531800
H	5.314300	-0.915300	-2.580700
C	2.739700	0.519800	-1.480100
H	1.729800	0.580200	-1.907900
C	3.062100	1.746100	-0.627400
C	3.511400	2.930800	-1.193800
H	3.677900	2.985200	-2.264000
C	3.740300	4.020000	-0.355500
H	4.091700	4.960000	-0.767700
C	3.511900	3.893000	1.012200
H	3.673400	4.722300	1.690200
C	3.075000	2.669800	1.506800
H	2.878900	2.483700	2.558000
N	1.363600	-2.044300	1.233300
N	2.813500	-0.676400	-0.608800
N	2.867300	1.627200	0.697300
O	3.060600	-2.684900	-1.733700
O	3.970100	-0.949500	1.710200
O	3.683800	0.306700	-2.486300
H	4.224700	-0.538500	2.556200
Fe	-1.689100	0.286300	-0.839000
C	-0.308300	2.947900	-1.045900

H	0.231700	2.447100	-1.843300
C	-0.002100	4.233200	-0.621600
H	0.802300	4.782900	-1.096300
C	-0.750300	4.788300	0.414900
H	-0.539200	5.791400	0.769700
C	-1.771600	4.041900	0.993100
H	-2.378100	4.438200	1.800100
C	-2.006400	2.755600	0.518000
C	-3.112800	1.902900	1.143000
H	-2.891300	1.697200	2.193300
C	-4.817000	2.312100	-0.240200
H	-5.871900	2.579500	-0.293200
H	-4.249700	2.881300	-0.990000
C	-4.566000	0.809300	-0.393300
C	-4.397700	0.352800	-1.840400
H	-5.161000	0.817000	-2.472400
H	-4.484700	-0.734600	-1.920500
C	-5.586100	-0.053900	0.404000
H	-5.942900	-0.897300	-0.199300
H	-6.438900	0.526600	0.756400
C	-3.536300	-0.580800	1.190700
H	-2.926700	-0.572500	2.098400
C	-3.212600	-1.811700	0.337500
C	-3.791300	-3.045500	0.598600
H	-4.501200	-3.148000	1.411700
C	-3.443200	-4.123000	-0.214500
H	-3.879500	-5.100600	-0.039300
C	-2.536300	-3.932500	-1.252600
H	-2.242100	-4.750000	-1.900400
C	-2.004500	-2.662600	-1.450500
H	-1.288200	-2.428700	-2.233100
N	-1.291600	2.233700	-0.486600
N	-3.286000	0.628300	0.381100
N	-2.345300	-1.632400	-0.672600
O	-4.342300	2.575800	1.072300
O	-3.094600	0.770500	-2.265000
O	-4.884100	-0.526800	1.551200
H	-2.915700	0.423100	-3.154900
O	-0.230300	-0.093400	-2.066500
H	-0.366400	0.347700	-2.917600

Intermediate F

Charge 2, Multiplicity 1

Fe	-1.528400	0.083800	-0.644700
Fe	1.382100	0.190600	0.324800
O	0.956300	0.000100	-1.558700
O	-0.230300	0.462700	-1.889000

O	-0.416600	-0.000300	0.752800
C	-0.562100	-2.621700	-1.647300
H	0.031400	-2.031700	-2.336600
C	-0.510500	-4.009600	-1.633500
H	0.134700	-4.532300	-2.329700
C	-1.299400	-4.698800	-0.716400
H	-1.283800	-5.782900	-0.680500
C	-2.111500	-3.980100	0.154500
H	-2.755800	-4.475200	0.872300
C	-2.098800	-2.591100	0.082300
C	-3.013500	-1.776500	0.997800
H	-2.657800	-1.786900	2.030400
C	-4.851400	-1.810400	-0.258300
H	-5.928400	-1.973400	-0.258200
H	-4.399100	-2.306700	-1.128300
C	-4.463500	-0.328000	-0.207600
C	-4.324600	0.340300	-1.576100
H	-5.122300	0.002800	-2.245000
H	-4.375900	1.429500	-1.484400
C	-5.353500	0.467300	0.793300
H	-5.644200	1.439000	0.375900
H	-6.247100	-0.084000	1.085500
C	-3.231400	0.679900	1.518700
H	-2.555700	0.475000	2.351000
C	-2.909600	2.020000	0.849200
C	-3.448400	3.209100	1.320600
H	-4.080200	3.201100	2.201400
C	-3.176900	4.383700	0.621300
H	-3.584900	5.328100	0.964800
C	-2.394100	4.329800	-0.528200
H	-2.171700	5.220200	-1.104200
C	-1.884100	3.099900	-0.929000
H	-1.252300	2.991200	-1.806300
N	-1.339400	-1.934000	-0.802000
N	-3.130100	-0.378300	0.491700
N	-2.131900	1.980100	-0.245100
O	-4.309800	-2.312900	0.956200
O	-3.051200	-0.047000	-2.104300
O	-4.556200	0.645400	1.961700
H	-2.911100	0.362200	-2.974200
C	0.813700	3.144300	0.480500
H	-0.025700	2.823600	1.088800
C	1.064000	4.483600	0.206800
H	0.401700	5.246500	0.599000
C	2.170600	4.808800	-0.571500
H	2.391600	5.843400	-0.810600

C	3.010300	3.791800	-1.015600
H	3.909500	4.006300	-1.581800
C	2.695600	2.478400	-0.689000
C	3.679000	1.355800	-1.025600
H	3.706700	1.142300	-2.095800
C	4.946600	1.508400	0.801800
H	5.969300	1.538500	1.175600
H	4.340800	2.267200	1.316800
C	4.302900	0.120600	0.912000
C	3.566700	-0.137300	2.228900
H	4.144700	0.260600	3.068700
H	3.410200	-1.209100	2.382300
C	5.298500	-1.013300	0.527700
H	5.198800	-1.870500	1.204800
H	6.335000	-0.676900	0.520400
C	3.584600	-1.157500	-0.924500
H	3.319000	-1.098400	-1.982400
C	2.771700	-2.231200	-0.198700
C	3.159700	-3.564400	-0.199100
H	4.037200	-3.868700	-0.758600
C	2.415600	-4.469300	0.554100
H	2.695700	-5.516800	0.579800
C	1.321100	-4.013200	1.284400
H	0.727900	-4.685600	1.892800
C	0.990300	-2.665100	1.219800
H	0.147500	-2.232200	1.749400
N	1.599400	2.167700	0.018100
N	3.336600	0.131900	-0.243600
N	1.702700	-1.803700	0.488300
O	4.963900	1.734100	-0.601600
O	2.300800	0.533000	2.153100
O	4.957400	-1.389600	-0.803700
H	1.776600	0.343300	2.948700

Intermediate G

Charge 0, Multiplicity 1

Fe	1.282100	-0.025000	-0.846000
C	1.036500	2.924300	-1.746800
H	0.476200	2.532000	-2.591500
C	1.232800	4.291200	-1.590800
H	0.818500	4.985300	-2.313000
C	1.954400	4.732200	-0.486300
H	2.119900	5.791400	-0.319200
C	2.482200	3.789900	0.390200
H	3.088200	4.086000	1.239500
C	2.249100	2.438000	0.149100
C	2.956600	1.399300	1.023700

H	2.571700	1.413300	2.043400
C	4.842100	1.168000	-0.158000
H	5.930400	1.129500	-0.100400
H	4.538100	1.778200	-1.020700
C	4.185700	-0.216200	-0.213500
C	4.016400	-0.774700	-1.638700
H	4.977600	-0.696500	-2.163000
H	3.743900	-1.833200	-1.594200
C	4.863100	-1.223900	0.761600
H	4.983000	-2.206600	0.285800
H	5.834800	-0.878100	1.117900
C	2.700100	-1.051000	1.392700
H	2.035900	-0.750300	2.199600
C	2.144700	-2.266200	0.651900
C	2.394400	-3.558800	1.099200
H	2.967500	-3.712300	2.007000
C	1.918400	-4.627600	0.343800
H	2.099500	-5.648500	0.664800
C	1.217600	-4.369700	-0.830700
H	0.832000	-5.174900	-1.445900
C	1.013300	-3.045700	-1.207700
H	0.484600	-2.757600	-2.112500
N	1.514000	2.019500	-0.889100
N	2.866500	0.047600	0.438500
N	1.471000	-2.026100	-0.479800
O	4.338200	1.714700	1.053700
O	3.029000	-0.022100	-2.326300
O	3.995600	-1.318900	1.886200
H	2.319500	-0.562900	-2.754900
O	0.222100	0.135100	0.768900
Fe	-1.627700	-0.161000	1.185400
C	-1.381400	-3.192400	1.345600
H	-0.995500	-2.987800	2.340400
C	-1.603200	-4.487700	0.893900
H	-1.373800	-5.332600	1.533400
C	-2.120800	-4.664400	-0.387300
H	-2.313000	-5.660600	-0.773300
C	-2.382200	-3.545100	-1.167600
H	-2.792900	-3.631600	-2.167400
C	-2.129700	-2.281100	-0.636700
C	-2.422200	-1.033900	-1.469900
H	-1.614000	-0.878000	-2.197200
C	-4.609700	-0.893000	-1.084900
H	-5.587400	-0.732300	-1.541300
H	-4.665900	-1.718800	-0.361600
C	-4.039000	0.355900	-0.410100

C	-4.377700	0.450100	1.101800
H	-5.462200	0.235900	1.197800
H	-4.254400	1.512400	1.396800
C	-4.307500	1.631700	-1.252200
H	-4.544400	2.482800	-0.598700
H	-5.108800	1.504700	-1.982100
C	-2.075500	1.415200	-1.132700
H	-1.162400	1.247400	-1.708900
C	-1.846400	2.405200	0.010200
C	-1.798300	3.770700	-0.252100
H	-1.920200	4.123600	-1.270600
C	-1.594200	4.651700	0.804900
H	-1.535700	5.720600	0.626900
C	-1.472900	4.138000	2.092200
H	-1.317800	4.784100	2.948600
C	-1.564000	2.761300	2.265500
H	-1.488700	2.317200	3.253600
N	-1.650400	-2.116400	0.600900
N	-2.555700	0.149100	-0.586700
N	-1.740000	1.913500	1.251300
O	-3.668900	-1.186600	-2.113800
O	-3.598500	-0.415400	1.829700
O	-3.103000	1.888800	-1.975700
H	-2.492700	-0.442600	3.205200
O	-1.531900	-0.615700	3.394800
H	-1.214000	0.132200	3.920500
O	0.385900	-0.447300	-2.633800
H	0.224700	0.344900	-3.166600

Intermediate H

Charge 0, Multiplicity 2

Fe	0.019500	-1.430000	-0.228500
O	-0.017800	-1.447600	-2.083100
C	3.005800	-1.929900	0.031700
H	2.694400	-2.946800	0.251000
C	4.341300	-1.554100	0.086400
H	5.098400	-2.282100	0.352600
C	4.668400	-0.233300	-0.202800
H	5.700000	0.100600	-0.165600
C	3.654800	0.656600	-0.542700
H	3.861600	1.695100	-0.772500
C	2.340700	0.200800	-0.577200
C	1.212500	1.148400	-1.009300
H	1.073100	1.062100	-2.090100
C	1.175900	2.616000	0.676100
H	1.094300	3.679200	0.904400
H	1.924500	2.147000	1.326900

C	-0.157800	1.864100	0.788200
C	-0.364600	1.217500	2.159800
H	-0.471200	2.020700	2.903200
H	-1.319700	0.668200	2.134800
C	-1.376600	2.719800	0.358800
H	-2.247300	2.491100	0.990200
H	-1.182500	3.792700	0.394800
C	-1.266000	1.017000	-1.107000
H	-1.064100	0.784300	-2.154000
C	-2.372900	0.091700	-0.588500
C	-3.698300	0.508800	-0.559000
H	-3.947300	1.512800	-0.883000
C	-4.669000	-0.377900	-0.101100
H	-5.710900	-0.077400	-0.065300
C	-4.285000	-1.648700	0.313700
H	-5.007600	-2.366900	0.682400
C	-2.938000	-1.987000	0.254600
H	-2.575500	-2.957500	0.576900
N	2.030400	-1.073400	-0.290800
N	-0.047300	0.845400	-0.302200
N	-2.008300	-1.137900	-0.191100
O	1.541500	2.477100	-0.694200
O	0.696600	0.385200	2.518100
O	-1.639300	2.365800	-0.992900
H	0.446300	-0.545500	2.211800
O	0.020900	-1.967700	1.637800
H	0.861500	-2.396400	1.857800

Intermediate I

Charge 1, Multiplicity 1

Fe	0.063700	-1.147000	-0.114800
O	0.082400	-1.337100	-1.705900
O	-0.069600	-2.717300	0.718900
H	0.799000	-3.092100	0.926800
C	3.026400	-1.788300	0.078300
H	2.709900	-2.790400	0.345000
C	4.373800	-1.475000	-0.032600
H	5.120200	-2.236400	0.157200
C	4.730300	-0.178200	-0.388100
H	5.774000	0.102300	-0.478000
C	3.728900	0.755700	-0.631700
H	3.958000	1.778700	-0.907700
C	2.403700	0.357800	-0.512400
C	1.291800	1.361700	-0.807400
H	1.210300	1.543500	-1.881900
C	1.106400	2.359000	1.177700
H	1.038200	3.321100	1.683900

H	1.798700	1.699300	1.718300
C	-0.254700	1.682400	0.982900
C	-0.661800	0.762000	2.127500
H	-0.458300	1.239500	3.091400
H	-1.726200	0.512100	2.072900
C	-1.358800	2.683500	0.542400
H	-2.300700	2.480800	1.065200
H	-1.070500	3.722200	0.702600
C	-1.204700	1.160600	-1.111900
H	-0.960500	1.031800	-2.168500
C	-2.320800	0.210200	-0.687100
C	-3.659500	0.539600	-0.824300
H	-3.939000	1.503100	-1.235600
C	-4.611500	-0.391100	-0.411200
H	-5.668300	-0.165200	-0.503400
C	-4.195900	-1.606000	0.124300
H	-4.910200	-2.348900	0.458100
C	-2.832900	-1.857700	0.238400
H	-2.427800	-2.774700	0.653000
N	2.065500	-0.887800	-0.149300
N	-0.015700	0.863600	-0.266300
N	-1.930200	-0.959900	-0.159500
O	1.540500	2.574400	-0.158700
O	0.136900	-0.403300	1.962300
O	-1.514600	2.492800	-0.861800
H	-0.209200	-1.147600	2.484700