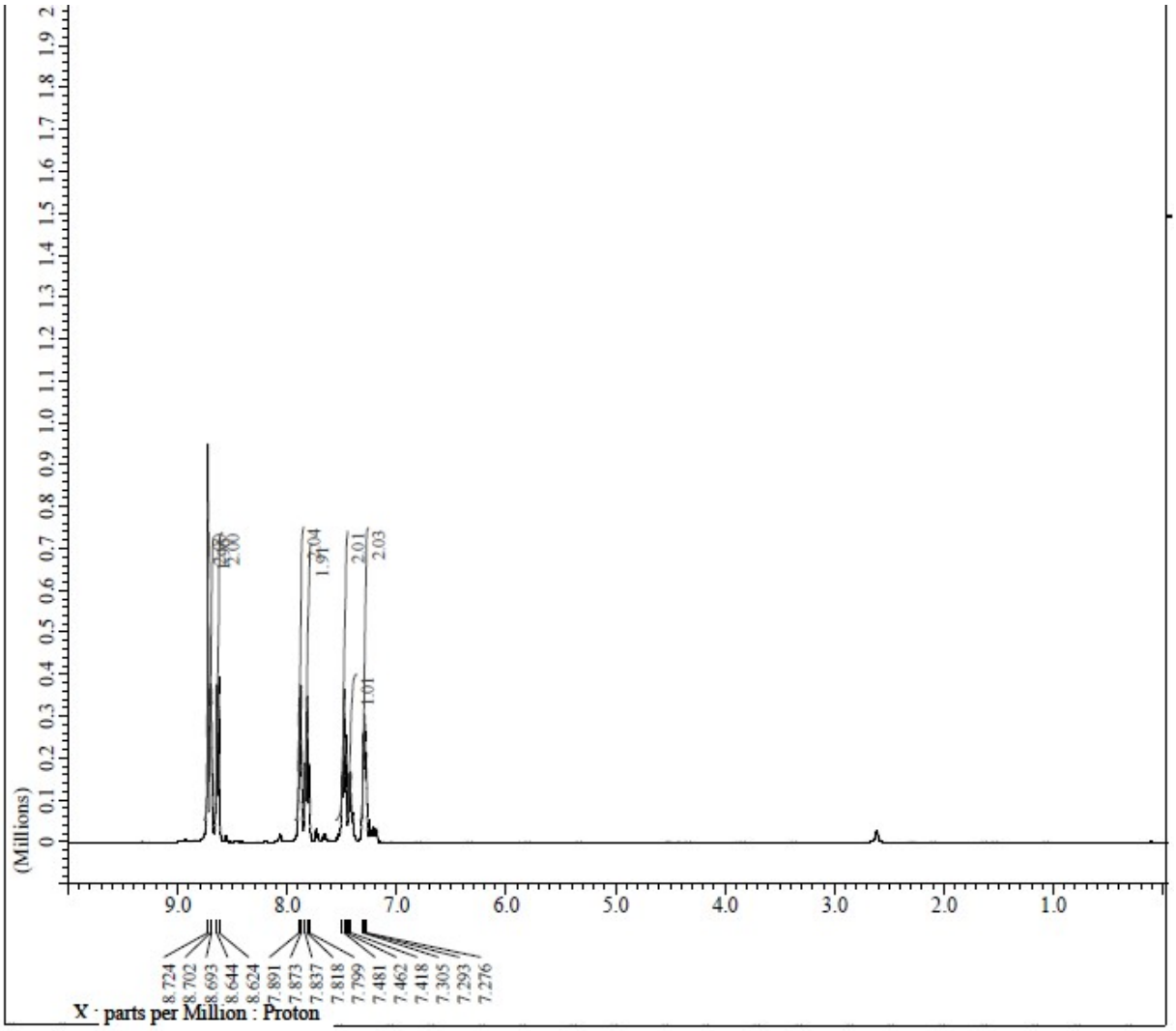
Supporting Information

Electro catalytic water oxidation by molecular Cobalt-terpyridine complexes in alkaline medium: Experimental and theoretical study

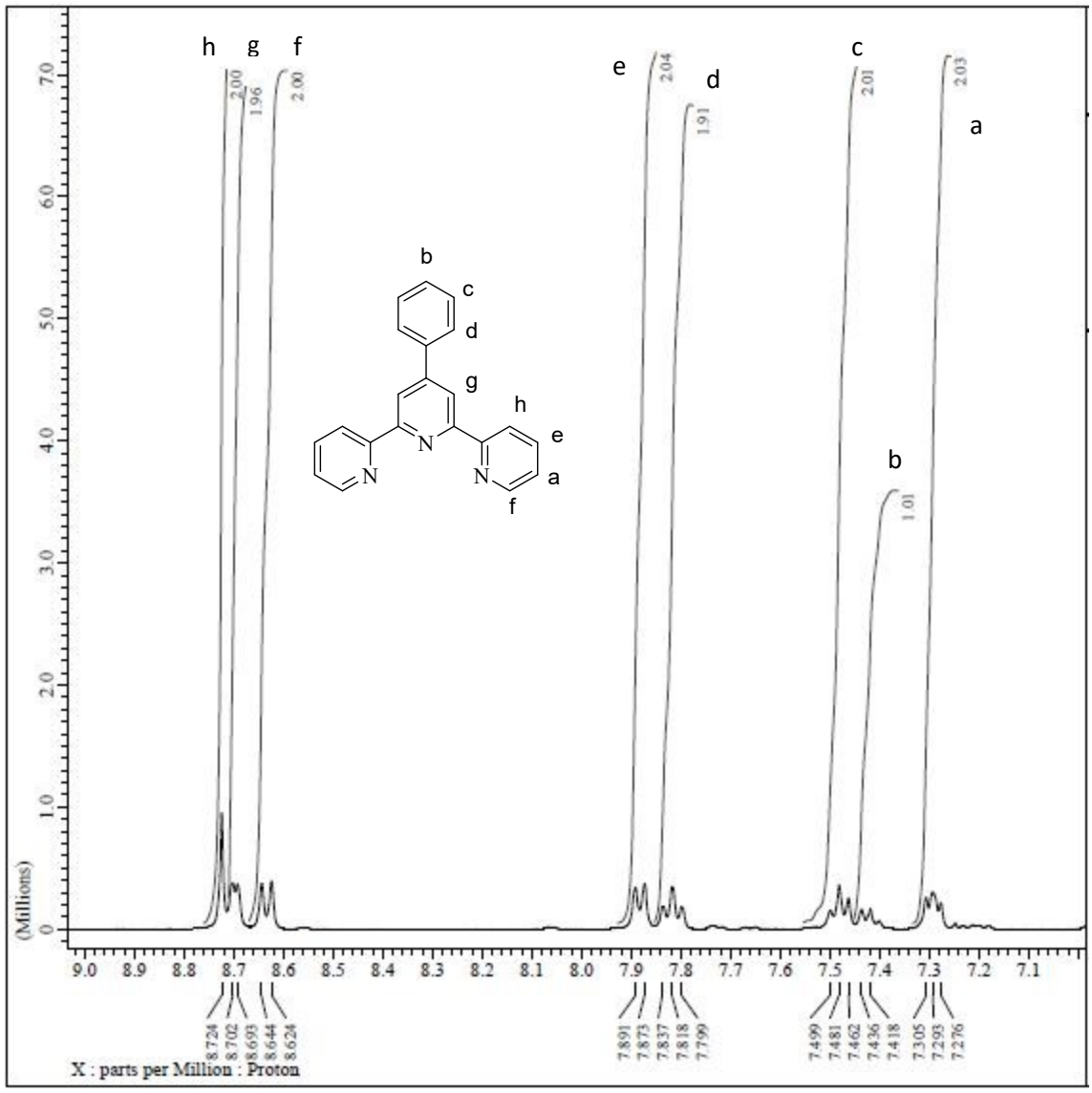
Md. Adnan Khan,[a] Sahanwaj Khan,[a] Swaraj Sengupta,[b*] Subhendu Naskar[a*]

[a] Department of Chemistry, Birla Institute of Technology-Mesra, Ranchi, India

[b] Department of Chemical Engineering, Birla Institute of Technology-Mesra, Ranchi, India

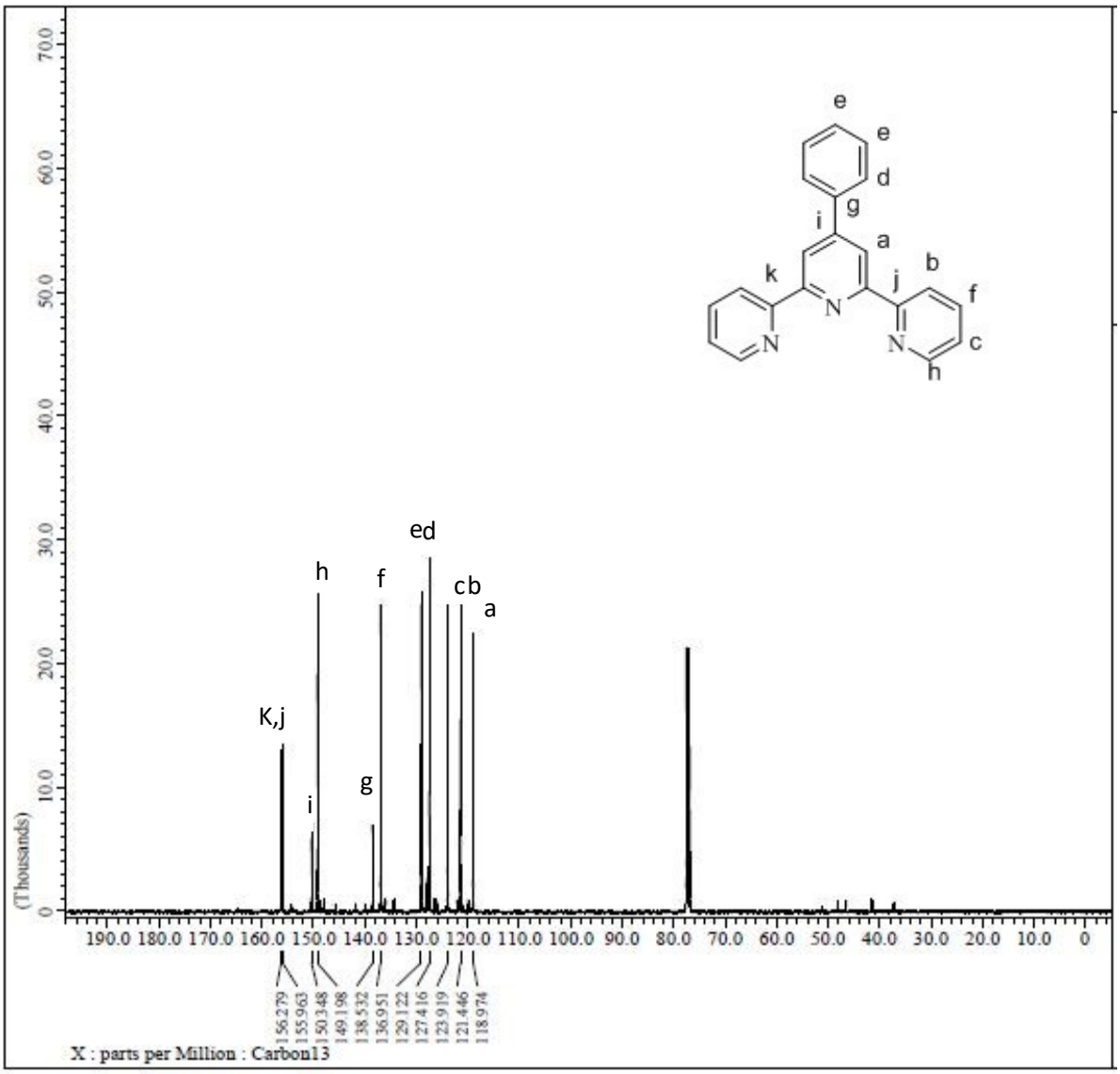


(a)


h
g
f
e
d
c
b
a
2.00
1.96
2.00
2.04
1.91
2.01
1.01
2.03
(Millions)
X : parts per Million : Proton
8.724
8.702
8.693
8.644
8.624
7.891
7.873
7.837
7.818
7.799
7.499
7.481
7.462
7.436
7.418
7.305
7.293
7.276

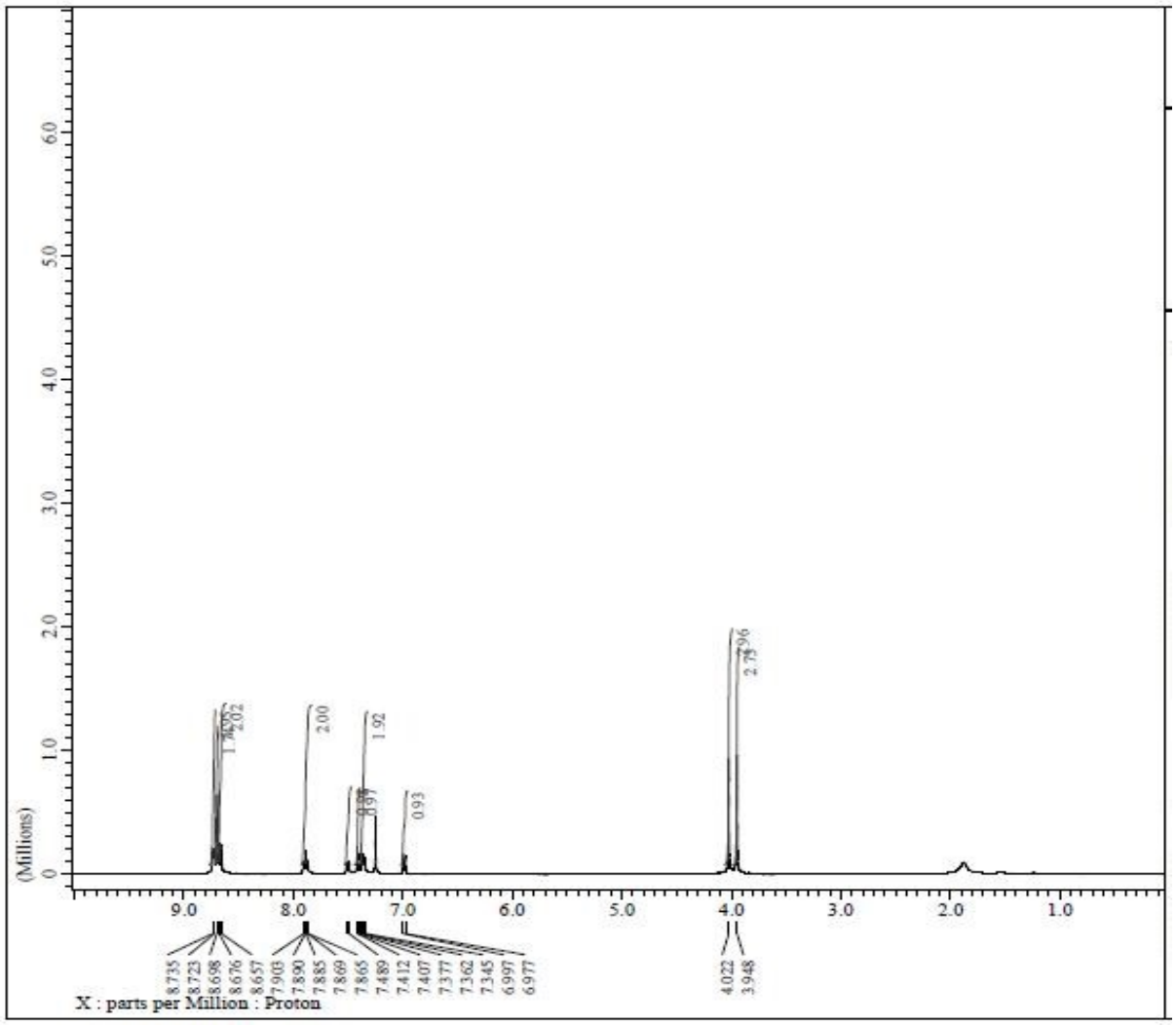
(b)

.



(c)

Fig S1- NMR spectra of ligand L1 (a) ^{1}H Full scale (b) magnified ^{1}H (c) ^{13}C NMR spectra.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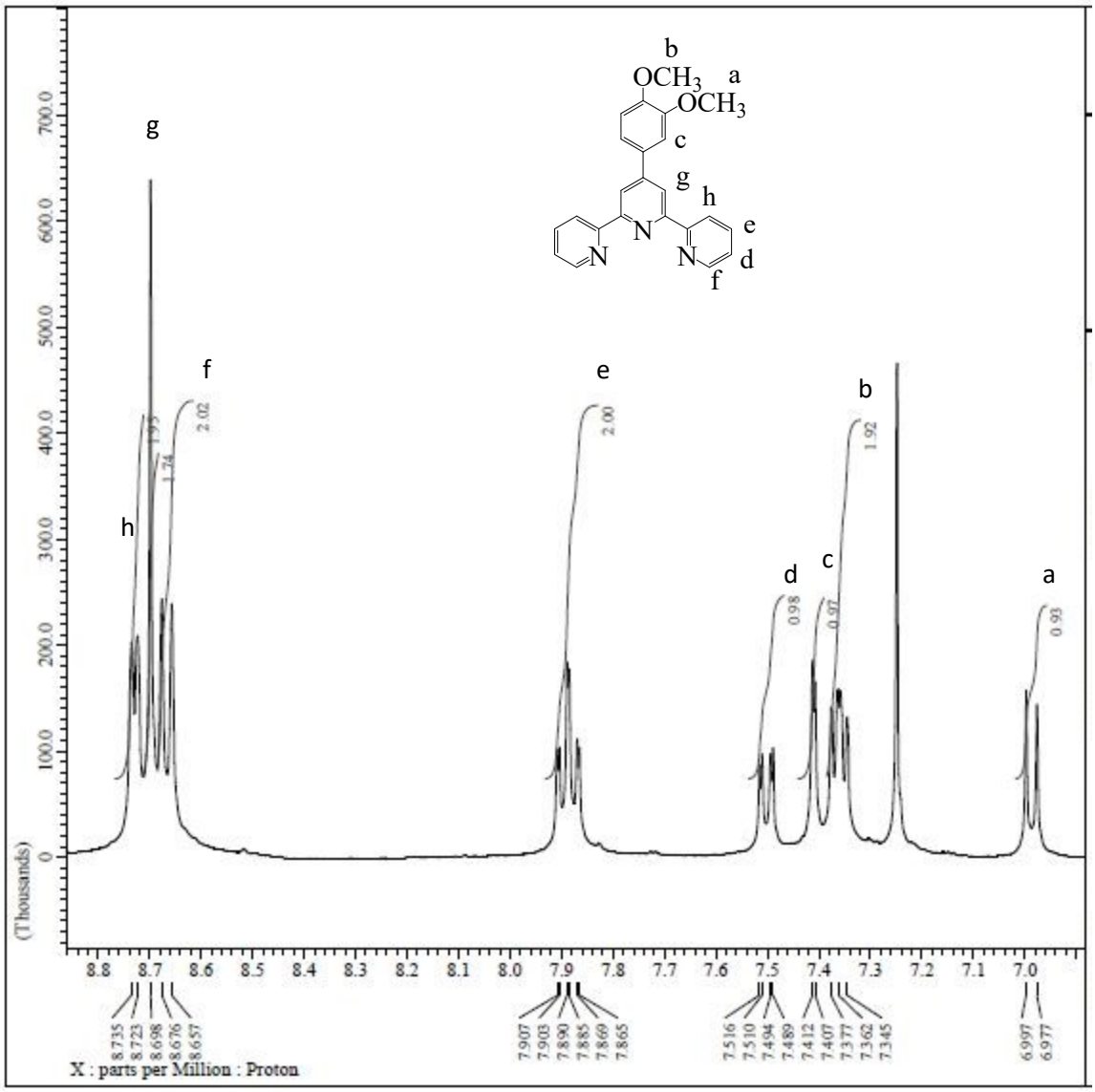
4.0
3.0
2.0
1.0
0
2.02
2.00
1.92
0.93
2.96
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.735
8.723
8.698
8.676
8.657
7.903
7.890
7.885
7.869
7.865
7.489
7.412
7.407
7.377
7.362
7.345
6.997
6.977
4.022
3.948
X : parts per Million : Proton

(a)


b
OCH3
a
OCH3
c
g
h
N
N
N
e
d
f
g
f
e
b
h
d
c
a
1.95
1.74
2.02
2.00
1.92
0.98
0.97
0.93
(Thousands)
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
8.735
8.723
8.698
8.676
8.657
7.907
7.903
7.890
7.885
7.869
7.865
7.516
7.510
7.494
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7.407
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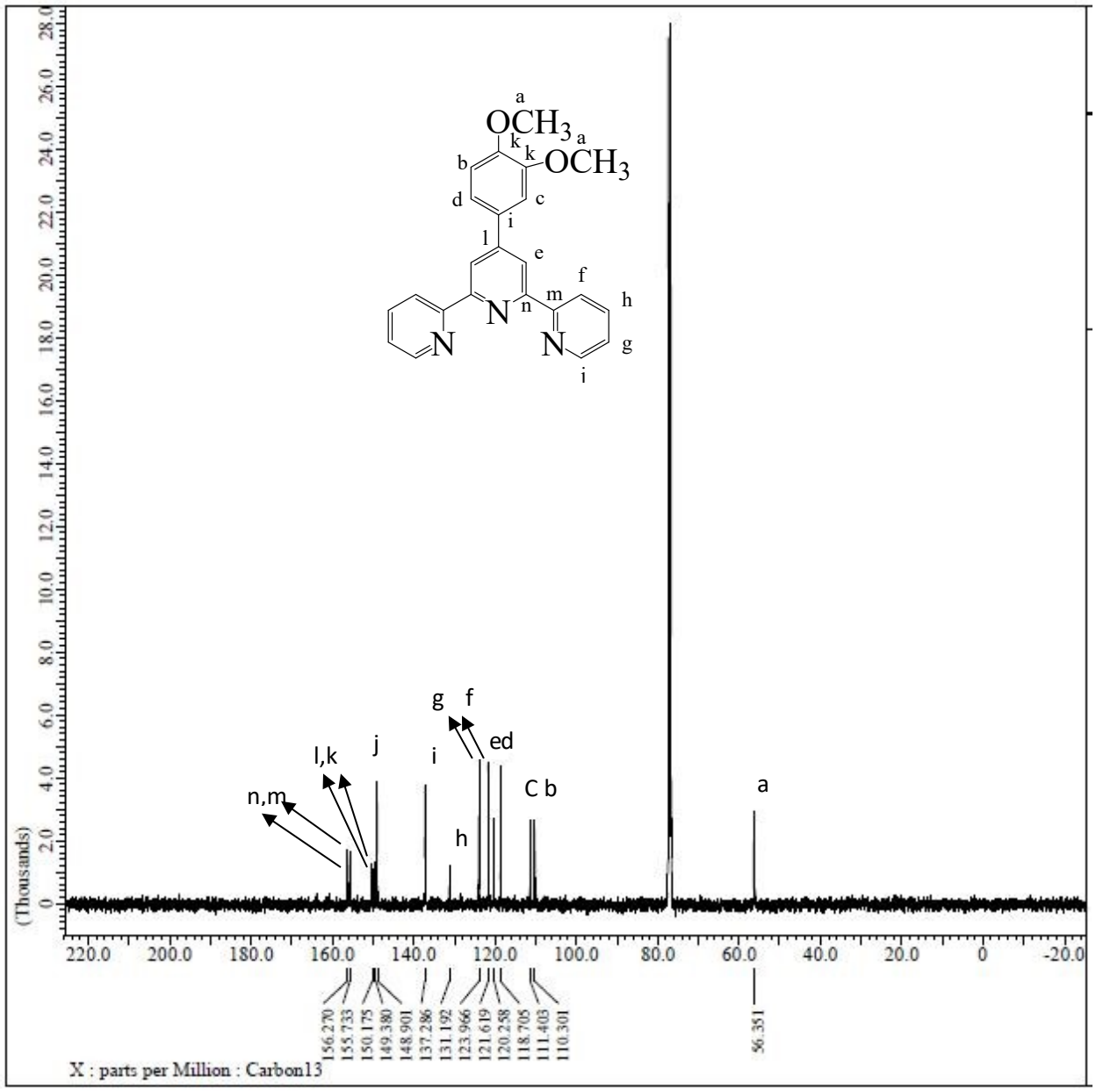
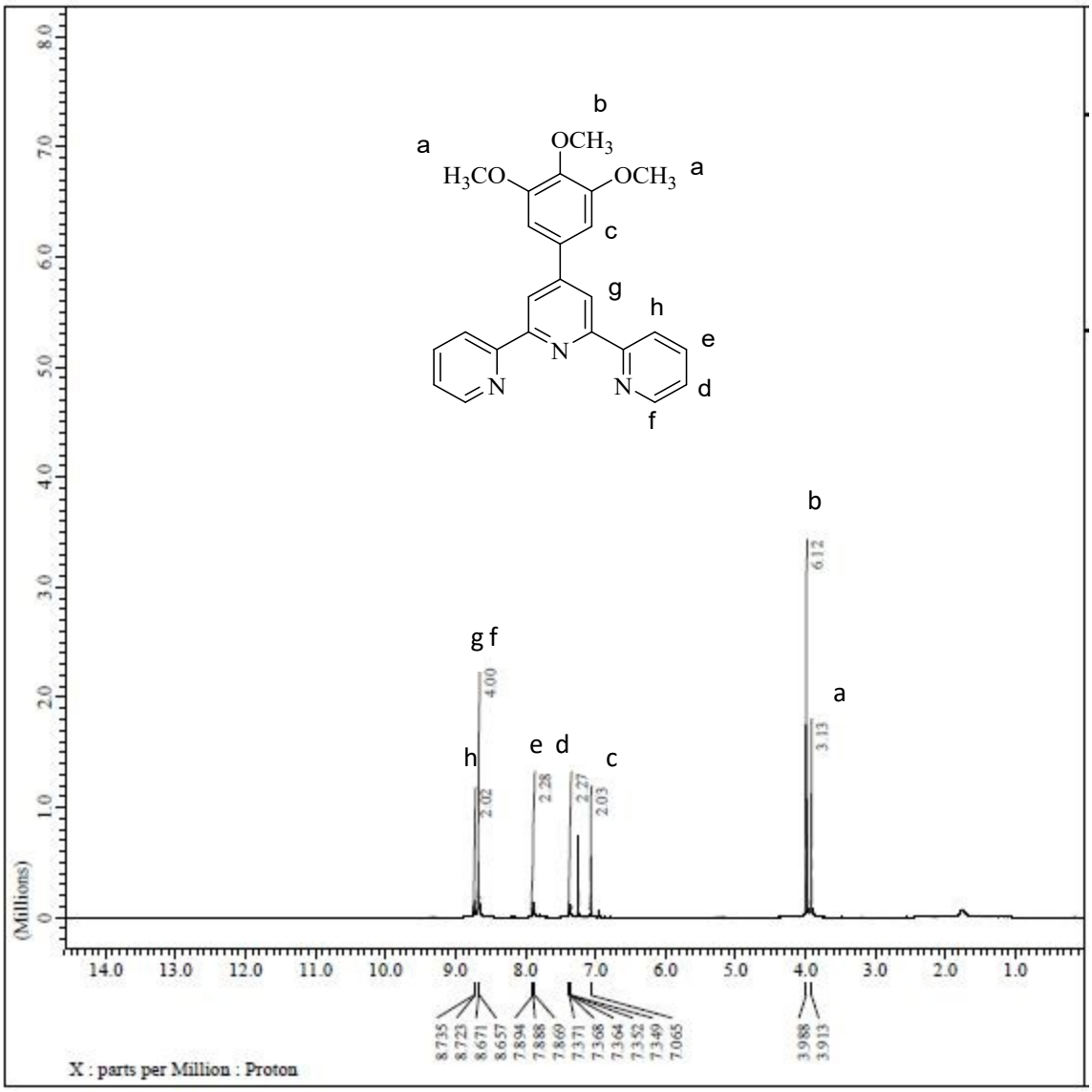
7.362
7.345
6.997
6.977
X : parts per Million : Proton

(b)



(c)

Fig S2- NMR spectra of ligand L2 (a) ^{1}H Full scale (b) magnidfied (c) ^{13}C NMR spectra


b
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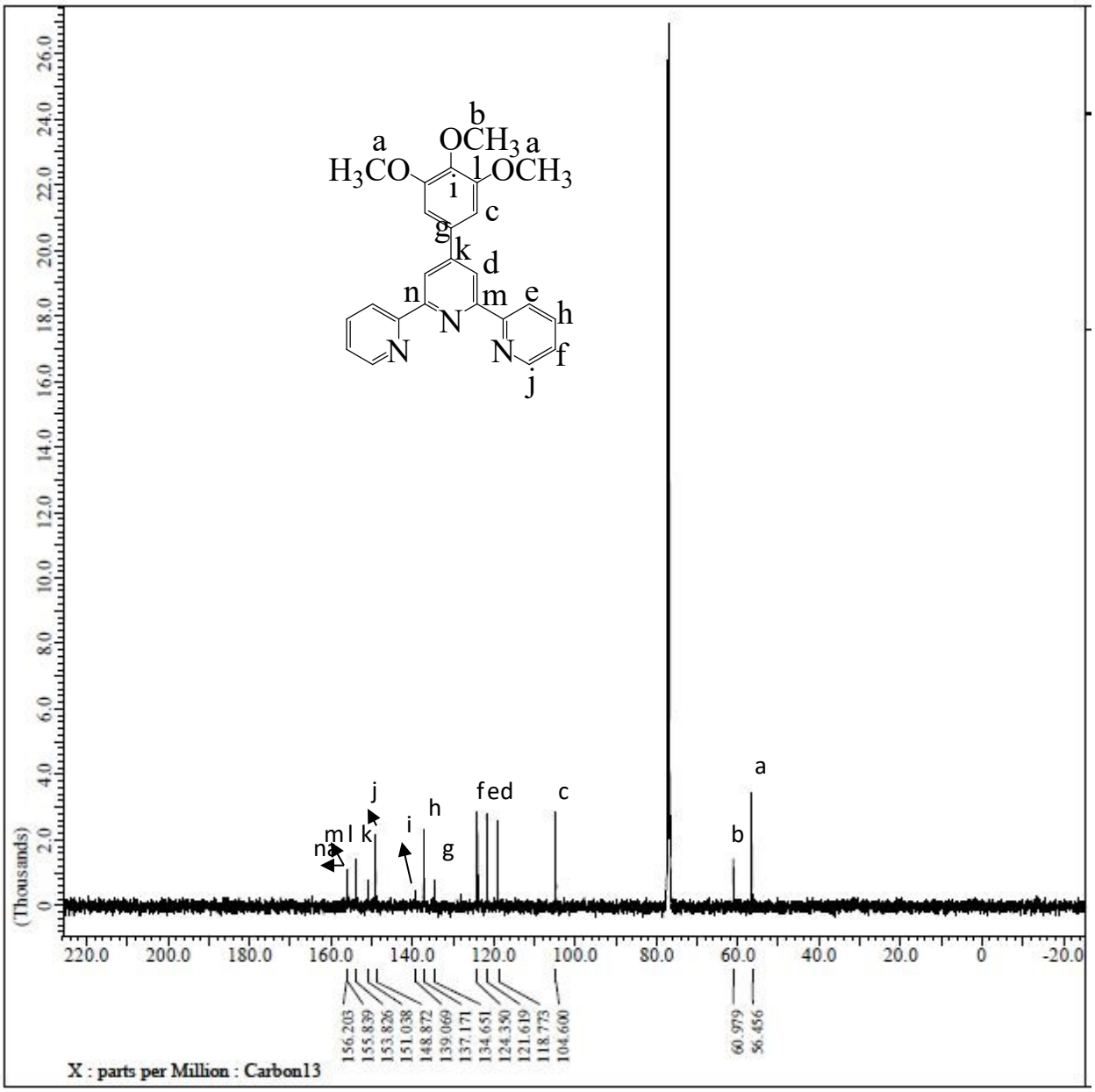
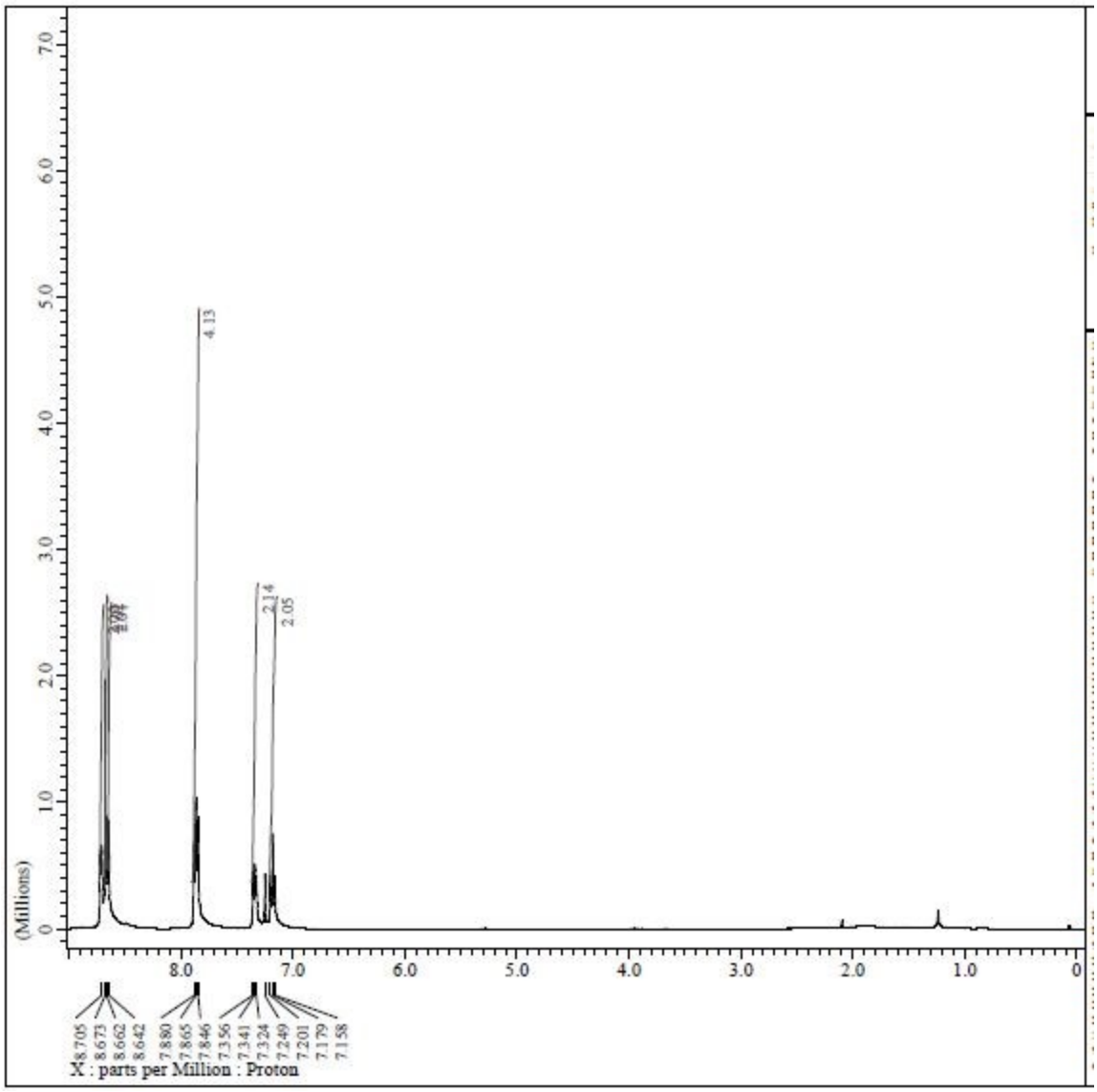
H3CO
OCH3
a
c
g
h
e
N
N
N
d
f
b
6.12
g f
4.00
a
3.13
h
e d
c
2.28
2.27
2.03
2.02
(Millions)
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.735
8.723
8.671
8.657
7.894
7.888
7.869
7.371
7.368
7.364
7.352
7.349
7.065
3.988
3.913
X : parts per Million : Proton

(a)



(b)

Fig S3- NMR spectra of ligand L3 (a) ^{1}H Full scale (b) ^{13}C NMR spectra


(Millions)
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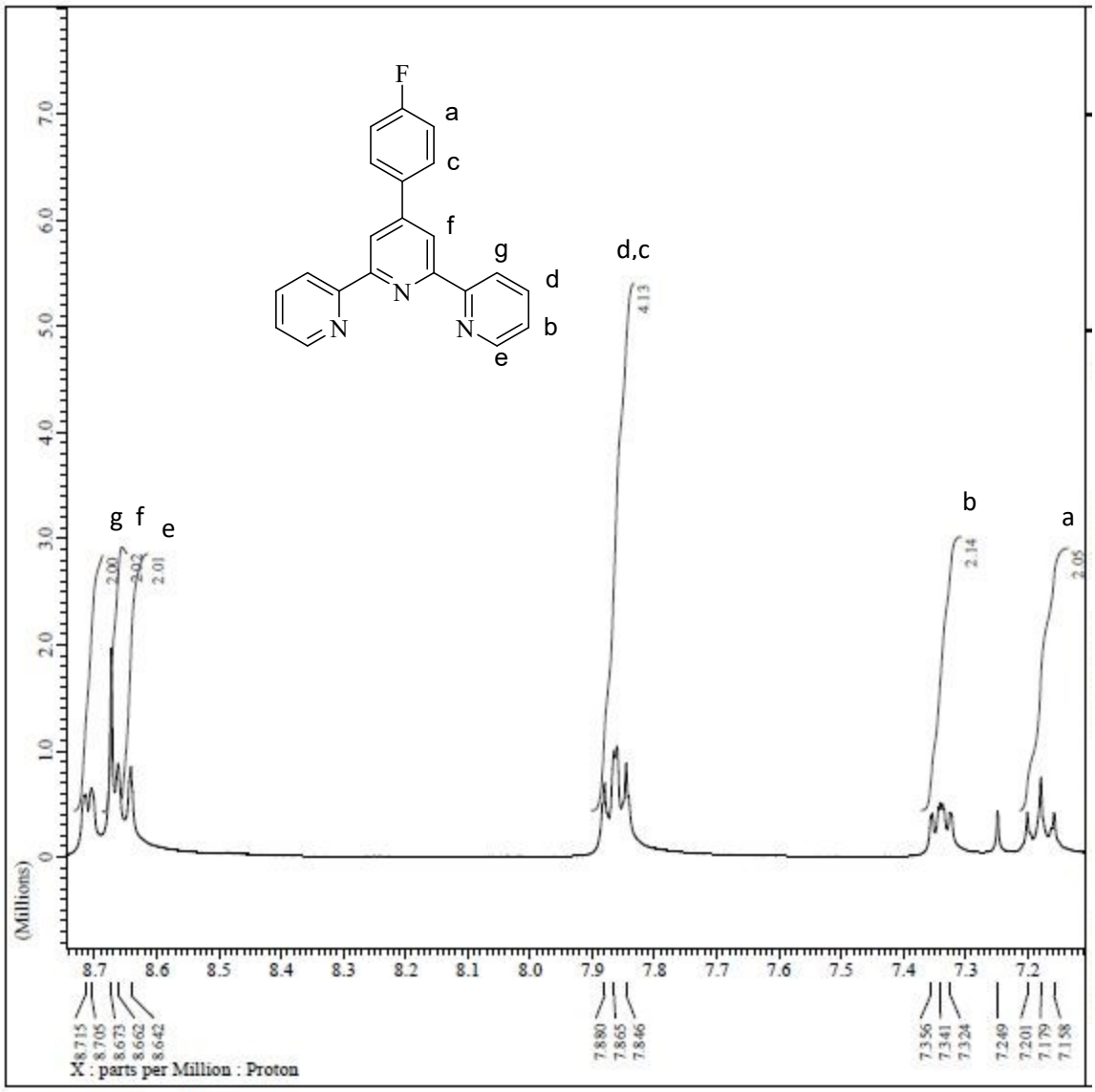
6.0
5.0
4.0
3.0
2.0
1.0
0
4.13
2.14
2.05
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.705
8.673
8.662
8.642
7.880
7.865
7.846
7.356
7.341
7.324
7.249
7.201
7.179
7.158
X : parts per Million : Proton

(a)


F
a
c
f
g
d
b
e
N
N
N
d,c
4.13
g f e
2.00
2.02
2.01
b
2.14
a
2.05
(Millions)
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
8.715
8.705
8.673
8.662
8.642
7.880
7.865
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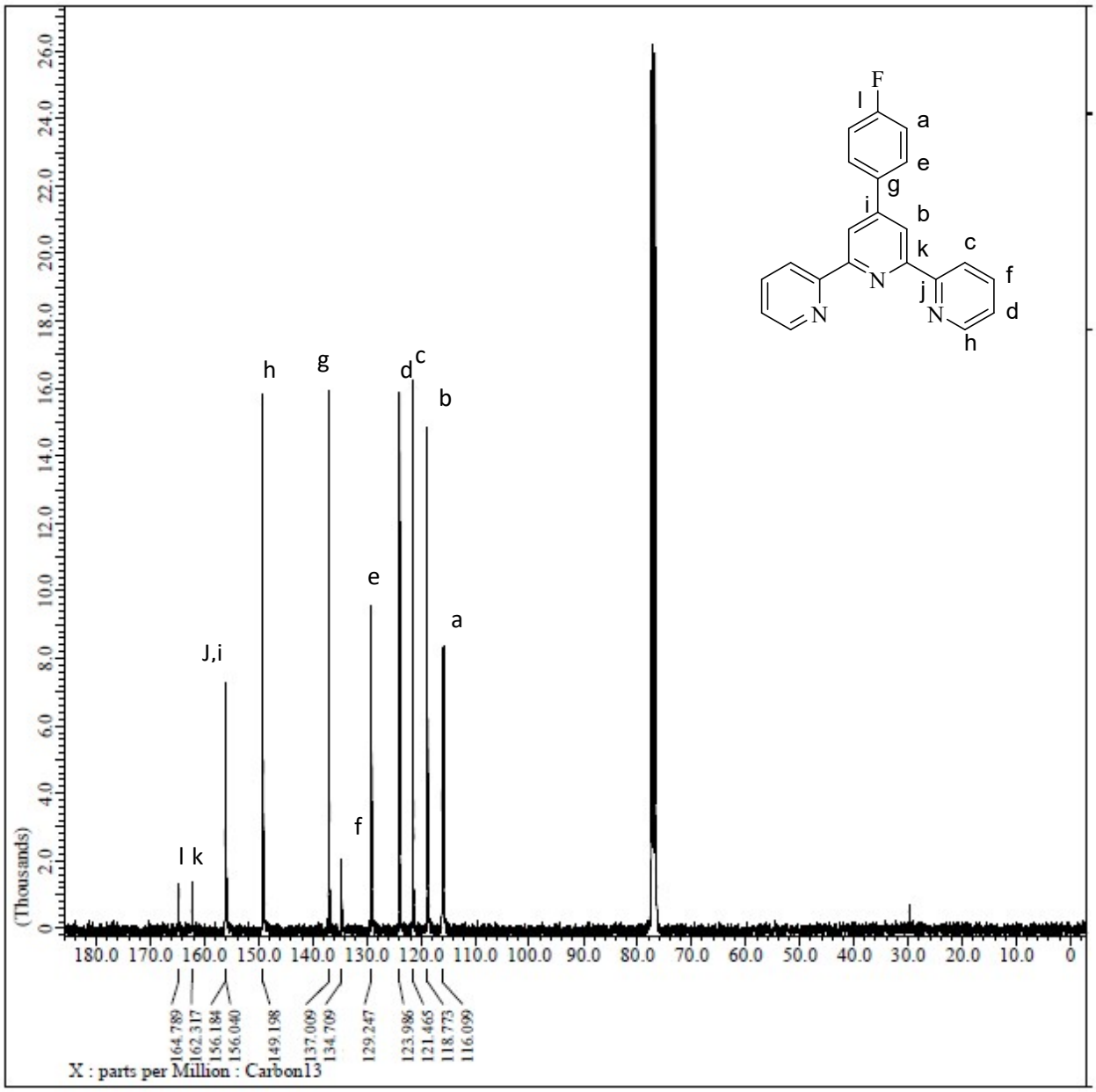
7.201
7.179
7.158
X : parts per Million : Proton

(b)



(c)

Fig S4- NMR spectra of ligand L4 (a) ^{1}H Full scale (b) magnidfied (c) ^{13}C NMR spectra.

The mass spectra of the Ligand and the complexes are recorded in methanol. Mass spectra were recorded using 0.01 mg of compound in 1 ml of mass grade methanol and sonicating 25 minutes at 40^0C.

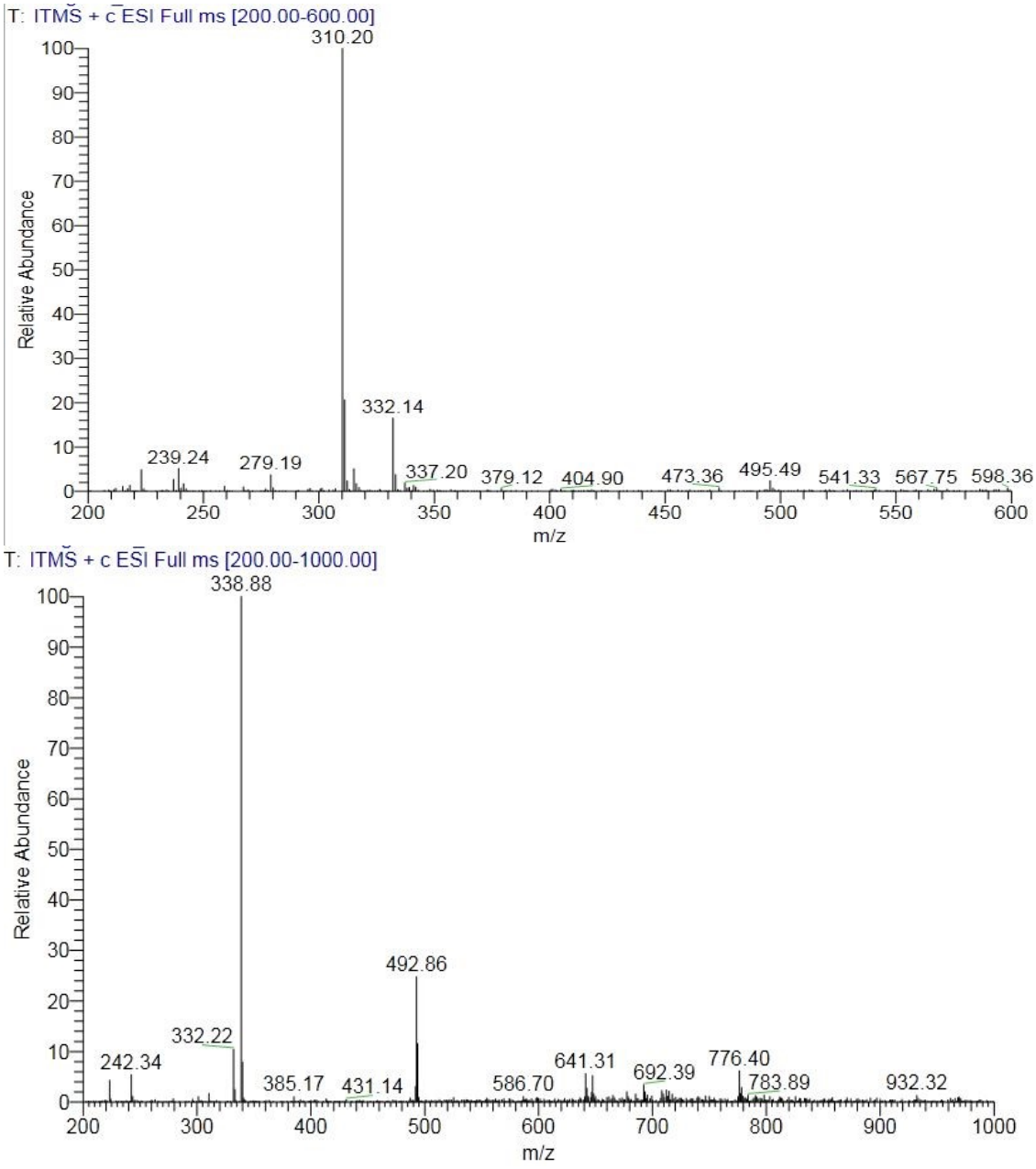


Fig S5 – Ligand L1 AND Complex 1 (Half mass) MASS SPECTRA

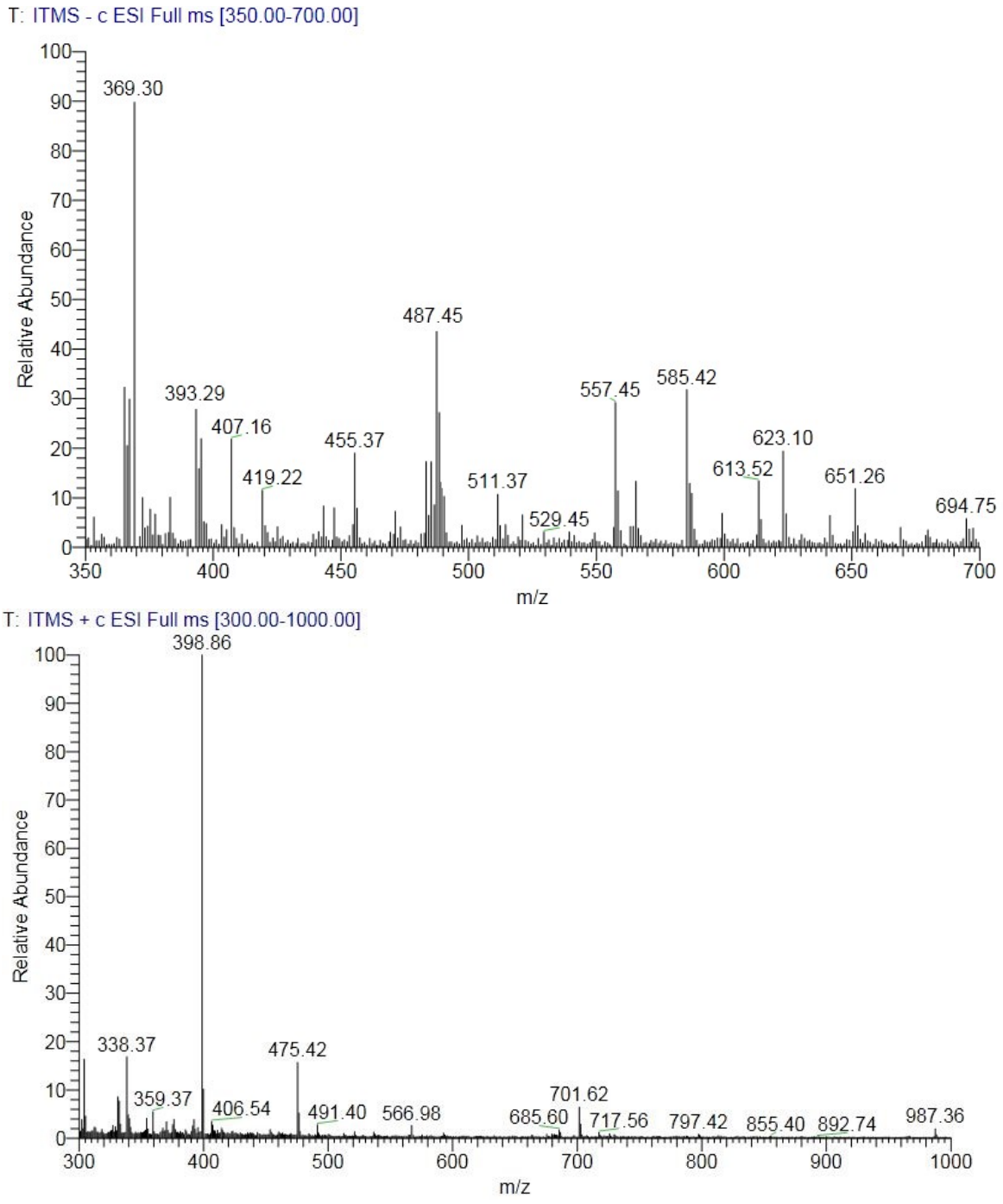


Fig S6 – Ligand L2 AND Complex 2 (Half mass) MASS SPECTRA

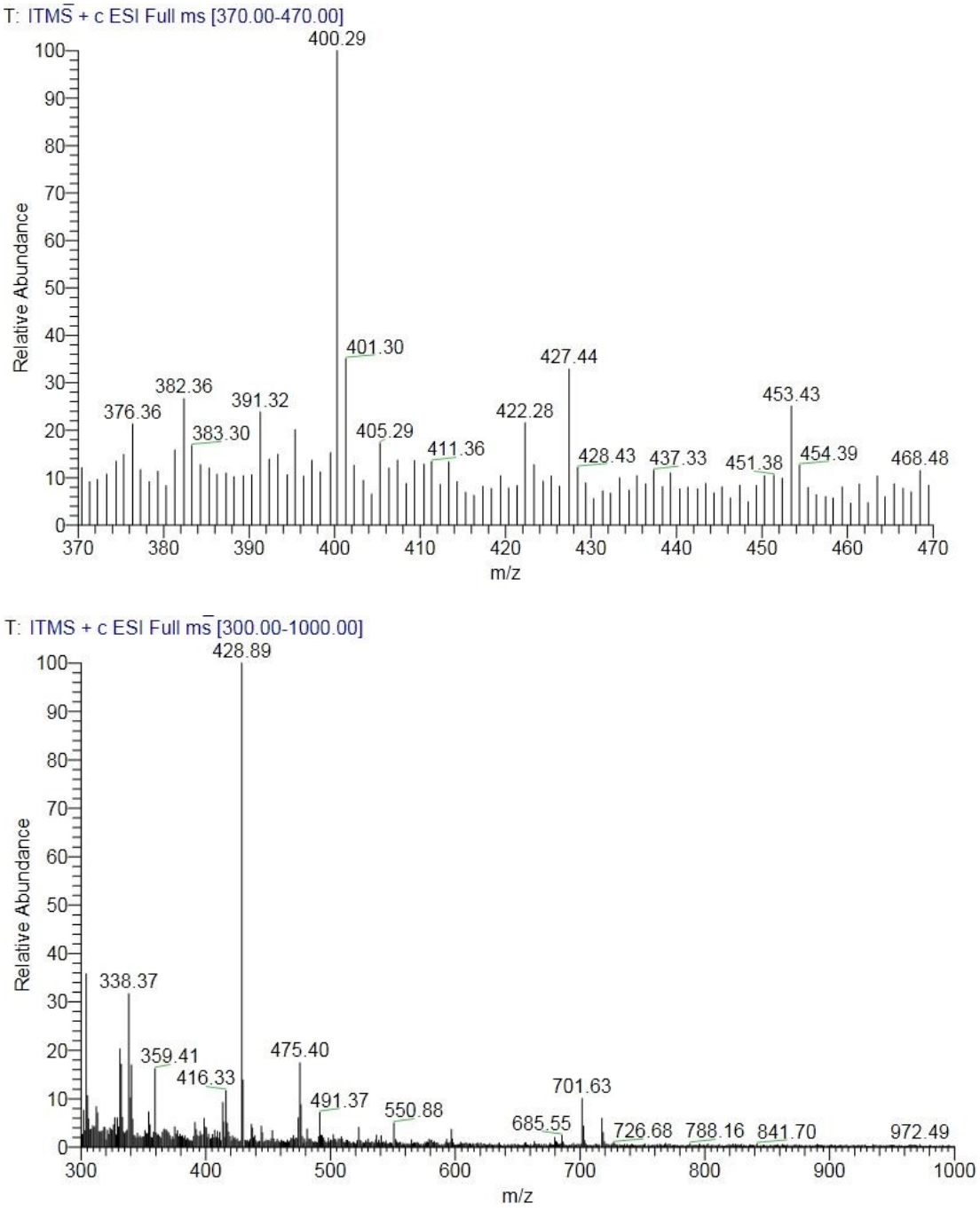


Fig S7 – Ligand L3 AND Complex 3 (Half mass) MASS SPECTRA

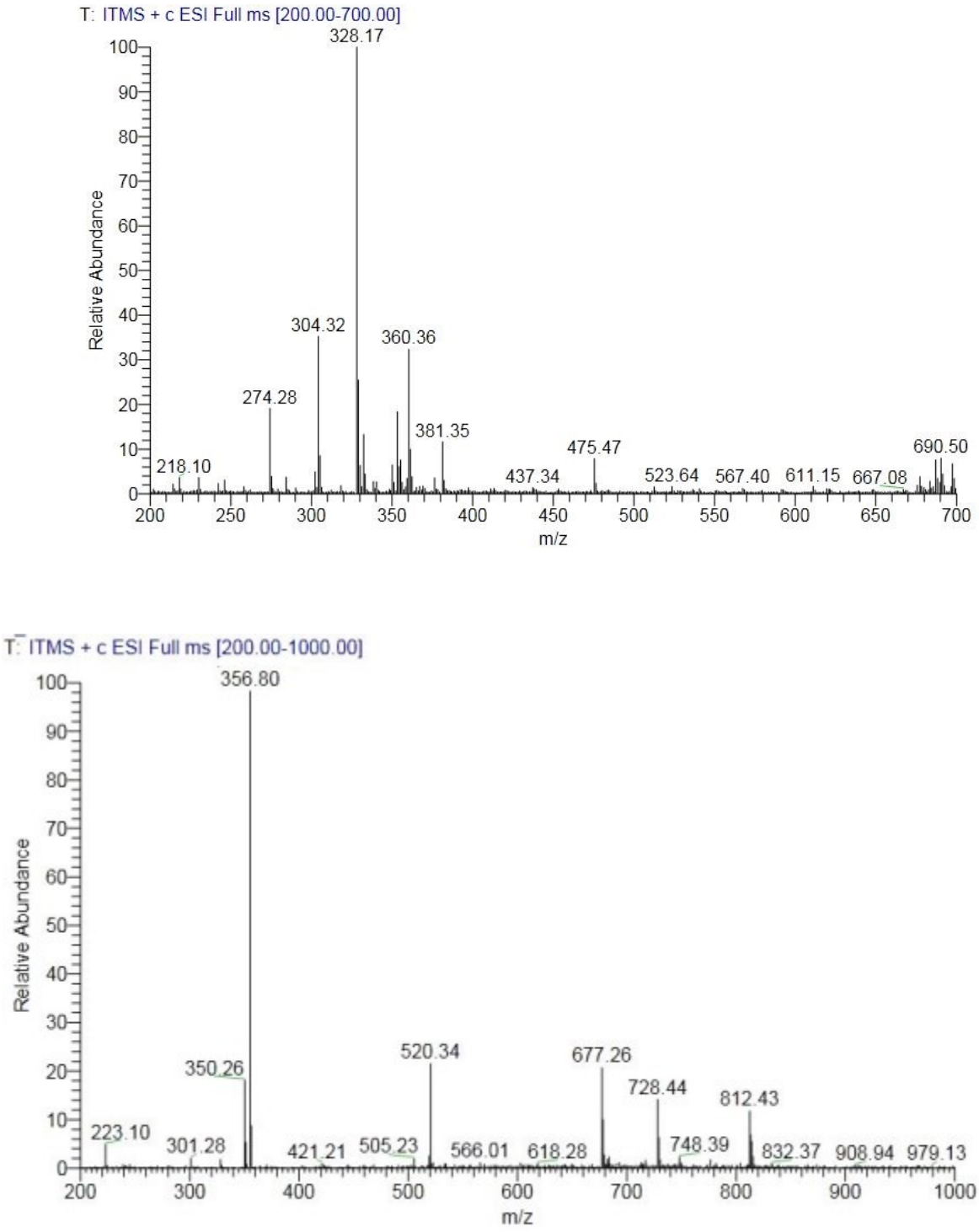


Fig S8 – Ligand L4 AND Complex 4 (Half mass) MASS SPECTRA

Table S1- Crystal data and structure refinement for Complex **2**.

Identification code	34_diome_sn
Empirical formula	$C_{47.5}H_{52.12}Cl_2CoN_6O_{9.56}$
Formula weight	989.89
Temperature/K	298.15
Crystal system	triclinic
Space group	P-1
a/Å	10.5223(8)
b/Å	10.9270(10)
c/Å	19.7925(12)
α/°	84.750(6)
β/°	89.913(6)
γ/°	83.450(7)
Volume/Å^3	2251.3(3)
Z	2
ρ_{calc}g/cm^3	1.460
μ/mm^{-1}	0.566
F(000)	1033.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.76 to 49.998
Index ranges	$-11 \leq h \leq 12$, $-12 \leq k \leq 12$, $-23 \leq l \leq 18$
Reflections collected	15464
Independent reflections	7897 [R_{int} = 0.0311, R_{sigma} =

	0.0534]
Data/restraints/parameters	7897/1/576
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	$R_1 = 0.0572$, $wR_2 = 0.1313$
Final R indexes [all data]	$R_1 = 0.0844$, $wR_2 = 0.1490$
Largest diff. peak/hole / e $Å^{-3}$	0.50/-0.41

Table S2- Crystal data and structure refinement for Complex **3** and **4** .

Identification code	njsk-4n_autored	4fc0
Empirical formula	$C_{48.5}H_{43.5}Cl_3CoN_6O_{14.25}$	$C_{42}H_{30}Cl_2CoF_2N_6O_5$
Formula weight	1103.67	866.55
Temperature/K	100.15	298.15
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	9.3891(2)	8.9320(7)
b/Å	12.8470(3)	10.3376(8)
c/Å	20.7104(5)	21.3919(16)
α/°	91.549(2)	85.981(6)
β/°	100.772(2)	78.249(6)
γ/°	105.942(2)	74.246(7)
Volume/$Å^3$	2351.58(10)	1861.0(3)
Z	2	2
$\rho_{calc}g/cm^3$	1.559	1.546
μ/mm^{-1}	0.613	0.672

F(000)	1137.0	886.0
Crystal size/mm^3	0.2 × 0.2 × 0.1	0.3 × 0.25 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.808 to 49.998	6.76 to 50
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 15, -24 ≤ l ≤ 24	-9 ≤ h ≤ 10, -12 ≤ k ≤ 11, -25 ≤ l ≤ 25
Reflections collected	45916	13213
Independent reflections	8255 [R_{int} = 0.0494, R_{sigma} = 0.0321]	6549 [R_{int} = 0.0349, R_{sigma} = 0.0576]
Data/restraints/parameters	8255/170/691	6549/187/598
Goodness-of-fit on F^2	1.041	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0332, wR_2 = 0.0867	R_1 = 0.0494, wR_2 = 0.1010
Final R indexes [all data]	R_1 = 0.0375, wR_2 = 0.0895	R_1 = 0.0722, wR_2 = 0.1130
Largest diff. peak/hole / e Å^{-3}	0.73/-0.35	0.34/-0.28

Table S3- Significant bond distances and bond angles of **2, 3** and **4.**

Complex **2**

Atom	Atom	Length/Å	Atom	Atom	Atom	Angle/°
Co1	N5	1.949(3)	N5	Co1	N3	89.57(12)
Co1	N1	1.859(3)	N5	Co1	N2	164.11(12)
Co1	N4	1.854(3)	N5	Co1	N6	91.13(12)
Co1	N3	1.963(3)	N1	Co1	N5	82.31(12)
Co1	N2	1.957(3)	N1	Co1	N3	97.30(12)
Co1	N6	1.951(3)	N1	Co1	N2	81.80(12)
			N1	Co1	N6	98.75(12)
			N4	Co1	N5	97.87(12)
			N4	Co1	N1	179.36(12)
			N4	Co1	N3	82.09(11)
			N4	Co1	N2	98.01(12)
			N4	Co1	N6	81.87(11)
			N2	Co1	N3	92.18(12)
			N6	Co1	N3	163.89(12)
			N6	Co1	N2	91.53(12)

Complex **3**

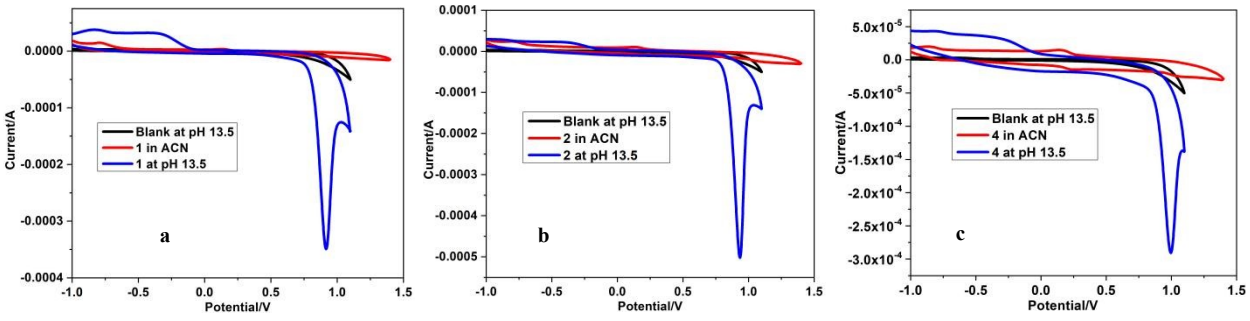
Atom	Atom	Length/Å	Atom	Atom	Atom	Angle/°
Co1	N1	1.9254(15)	N1	Co1	N2	101.59(6)
Co1	N2	1.9913(16)	N1	Co1	N4	96.15(6)

Co1	N3	1.8662(15)	N1	Co1	N5	78.77(6)
Co1	N4	2.0036(16)	N1	Co1	N6	78.70(6)
Co1	N5	2.1592(15)	N2	Co1	N4	162.21(6)
Co1	N6	2.1390(15)	N2	Co1	N5	88.13(6)
			N2	Co1	N6	93.48(6)
			N3	Co1	N1	177.26(6)
			N3	Co1	N2	81.07(6)
			N3	Co1	N4	81.18(6)
			N3	Co1	N5	102.05(6)
			N3	Co1	N6	100.59(6)
			N4	Co1	N5	96.74(6)
			N4	Co1	N6	88.60(6)
			N6	Co1	N5	157.28(6)

Complex **4**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Atom**	**Angle/°**
Co1	N5	2.078(2)	N5	Co1	N1	158.91(9)
Co1	N2	1.900(2)	N5	Co1	N3	92.94(9)
Co1	N4	1.897(2)	N2	Co1	N5	79.58(9)
Co1	N6	2.056(3)	N2	Co1	N6	99.94(10)

Co1	N1	2.080(2)	N2	Co1	N1	79.57(9)
Co1	N3	2.084(3)	N2	Co1	N3	100.80(10)
			N4	Co1	N5	100.75(9)
			N4	Co1	N2	179.60(10)
			N4	Co1	N6	79.82(10)
			N4	Co1	N1	100.09(10)
			N4	Co1	N3	79.43(10)
			N6	Co1	N5	91.58(9)
			N6	Co1	N1	88.90(9)
			N6	Co1	N3	159.24(9)
			N1	Co1	N3	94.04(9)



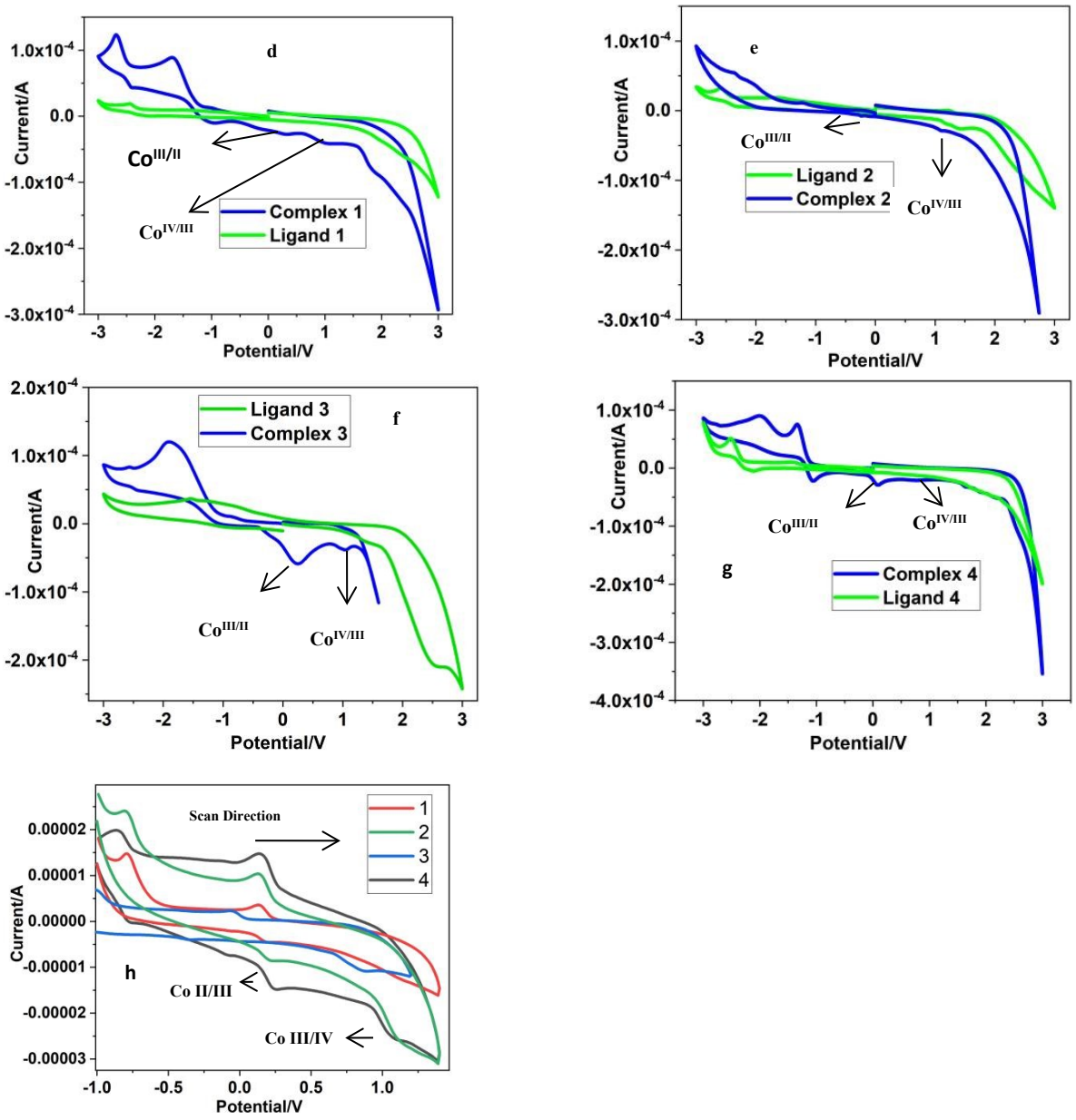


Figure S9 - CV of blank solution , 0.5 mM complexes in ACN and at pH 13.5 buffer solution (a) Complex 1 (b) Complex 2 (c) Complex 4. (d) Complex 1 and ligand 1 in ACN (e) Complex 2 and ligand 2 in ACN (f) Complex 3 and ligand 3 in ACN . (g) Complex 4 and ligand 4 in ACN (h) CV of complex 1-4 in ACN (CoIII/II and CoIV/III redox couple). The concentration and the scan rate for the CV of the respective ligands are 0.5 mM and 100mV/s.

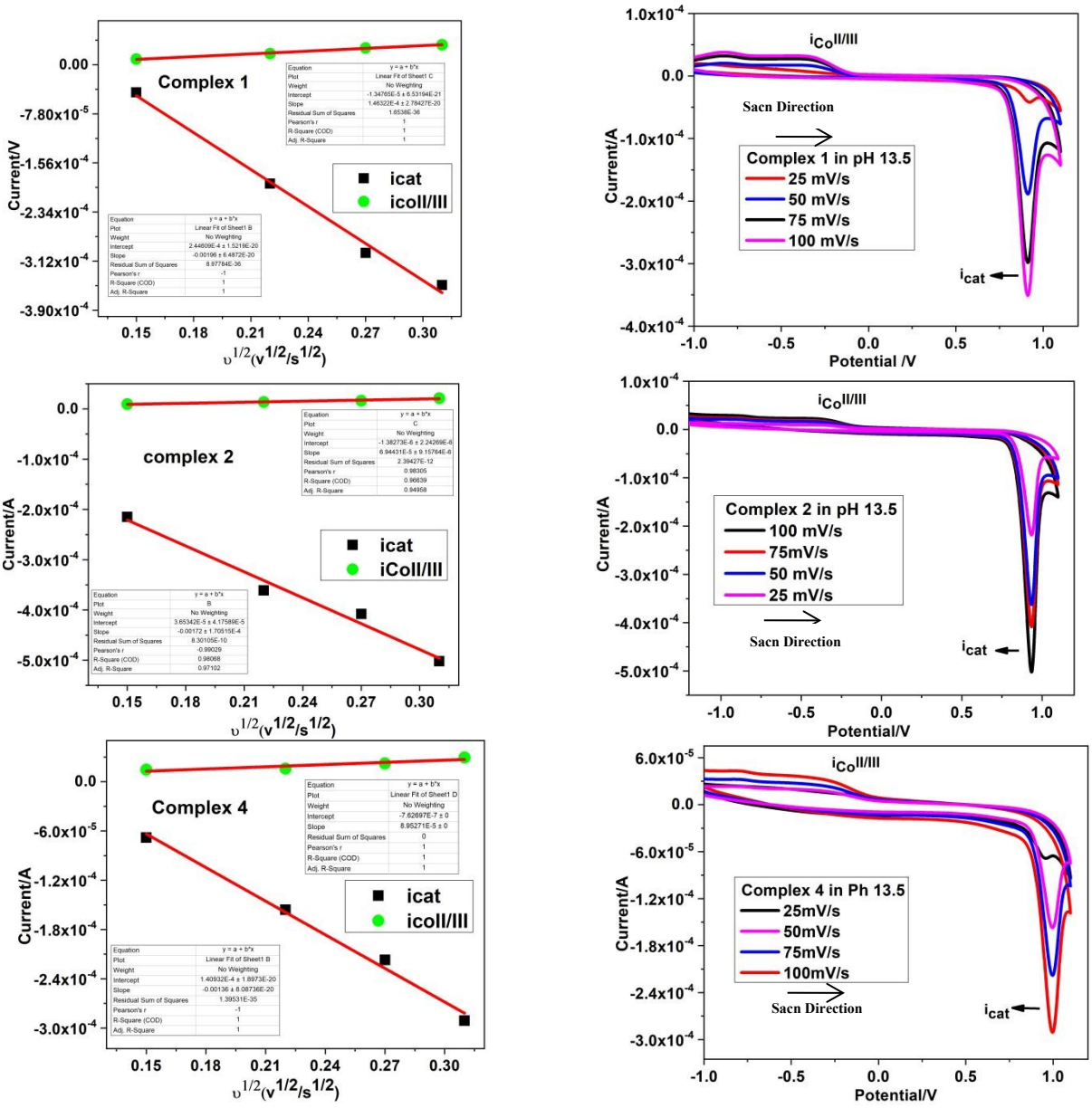


Figure S10- Linear Regression of i_{cat} and $i_{CoII/III}$ vs the square root of the scan rate for complexes **1**,**2** and **4**.

$$i_p = 0.446nFA[Ru]\left(\frac{vnFD_{Co}}{RT}\right)^{1/2} \quad (1)$$

$$i_{cat} = n_{cat}FA[Ru](k_{cat}D_{Co})^{1/2} \quad (2)$$

For all complexes the peak currents (i_p) of the redox couple Co^{II}/Co^{III} show constant redox currents (Figure S 10) and a linear relationship with the square root of scan rates, $v^{1/2}$ confirmed. Therefore, these redox currents of Co^{II}/Co^{III} can be used to calculate the diffusion coefficient.Thus, a diffusion coefficient of 2.75 x 10^{-8}, 5.95 x 10^{-9}, 1.43 x 10^{-7} and 1.27 x 10^{-8} was calculated for complexes **1-4** respectively.

The the dependence of the i_p on $v^{1/2}$ by using the Randles-Sevcik relation in Equation 1 and the dependence of the catalytic current (i_{cat}) on complex concentration could be observed in

Equation 2 . Thus using the eq. 1 and 2 we can evaluate the k_{cat} for the catalytic process (Figure S12).

$$\frac{i_{cat}}{i_p} = 1.38\, k_{cat}^{1/2} \nu^{-1/2} \quad (3)$$

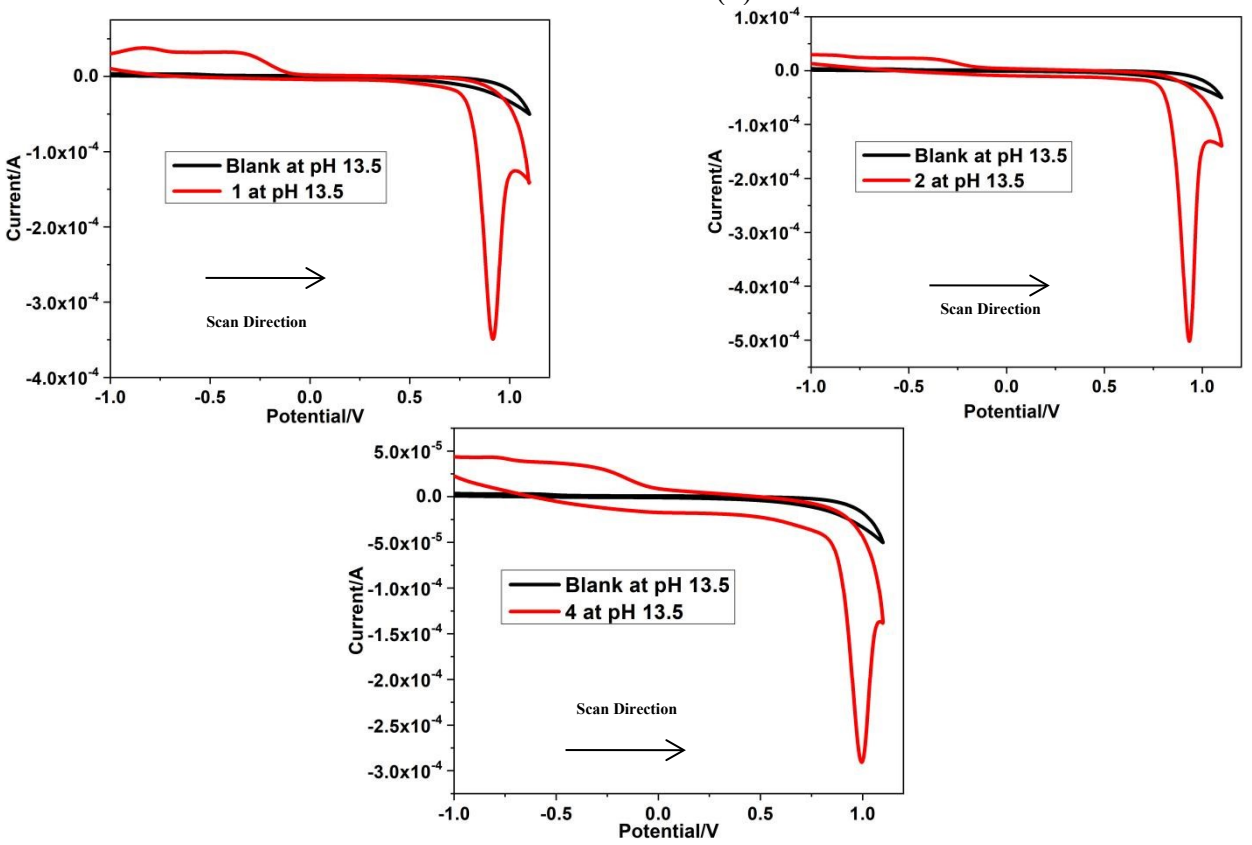


Figure S 11- The black line and red line of the CV of without-complex and with-complex respectively (0.5 mM complex) at pH 13.5 phosphate buffer solution.

Table S4: Key equations obtained for the WNA and I2M mechanisms including TOF–η relationships and TOF_{MAX} formulas[1].

WNA	I2M
$\frac{i}{i_P} = \frac{4 \times 2.24 \sqrt{\frac{RT}{Fv}} K_{WNA}}{1 + e^{\frac{F(E^\circ - E)}{RT}}}$ S1	$\frac{i}{i_P} = \frac{4 \times 2.24 \sqrt{\frac{RT}{3Fv}} K_D C^\circ_{cat}}{[1 + e^{\frac{F(E^\circ - E)}{RT}}]^{3/2}}$ S2

$TOF = \frac{4 \times 2.24 \sqrt{\frac{RT}{Fv} K_{WNA}}}{1 + e^{\frac{F(E^{\circ} - E_{H_2O/O_2} - \eta)}{RT}}}$ S3	$TOF = \frac{4 \times 2.24 \sqrt{\frac{RT}{3Fv} K_D C^{\circ}_{cat}}}{[1 + e^{\frac{F\left(E^{\circ} - E_{H_2O/O_2} - \eta\right)}{RT}}]^{3/2}}$ S4
$TOF_{MAX} = K_{WNA}$ S5	$TOF_{MAX} = \frac{1}{3} K_D C^{\circ}_{cat}$ S6
where R is the gas constant, T is temperature, F is the Faraday constant, v is the scan rate, and $E°$ is the apparent standard potential for the redox couple which onsets water oxidation $E(Ru^{V/IV})$. η is overpotential, and $E_{H2O/O2}$ is the standard potential of water oxidation at the working pH. i is the current intensity from the CV and i_p is the peak current intensity of the one-electron redox process of the catalyst.	

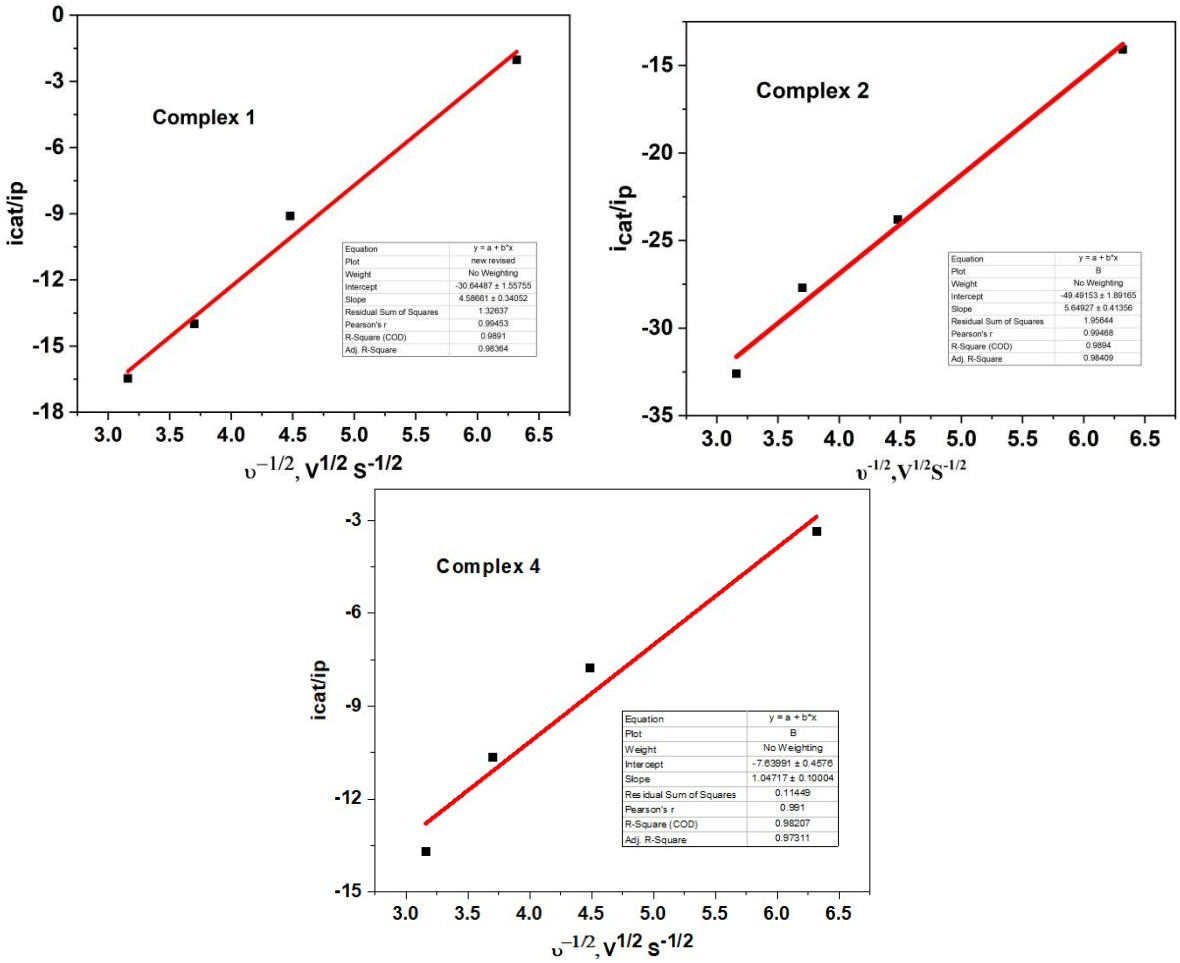


Figure S12- The plot of i_{cat} /i_p as a function of the inverse of the square root of the scan rate.

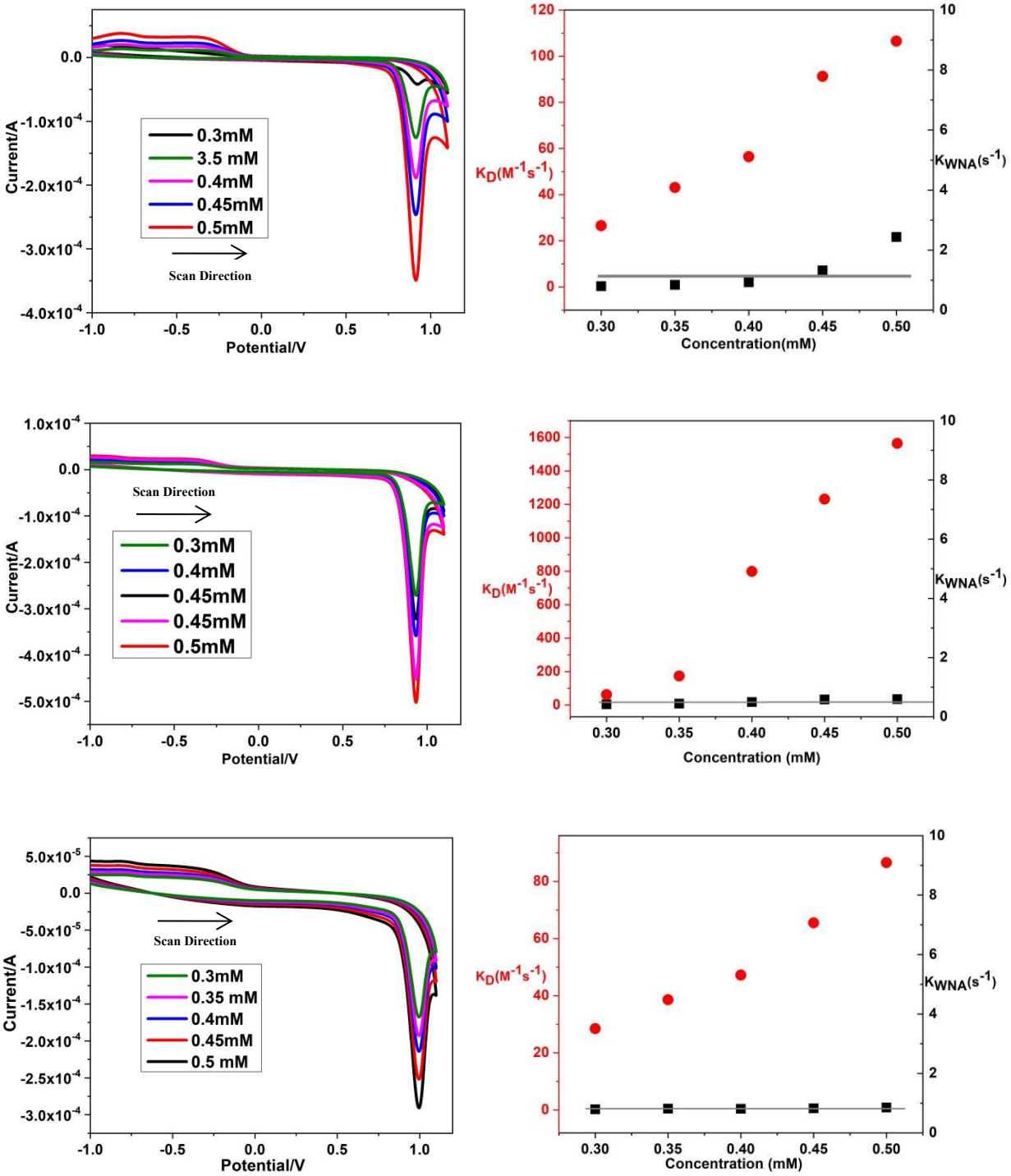


Figure S13 - CV of complex **1,2 and 4** at different concentrations at pH 13.5 and plot of calculated KD and KWNA vs. [**conc.cat.**]

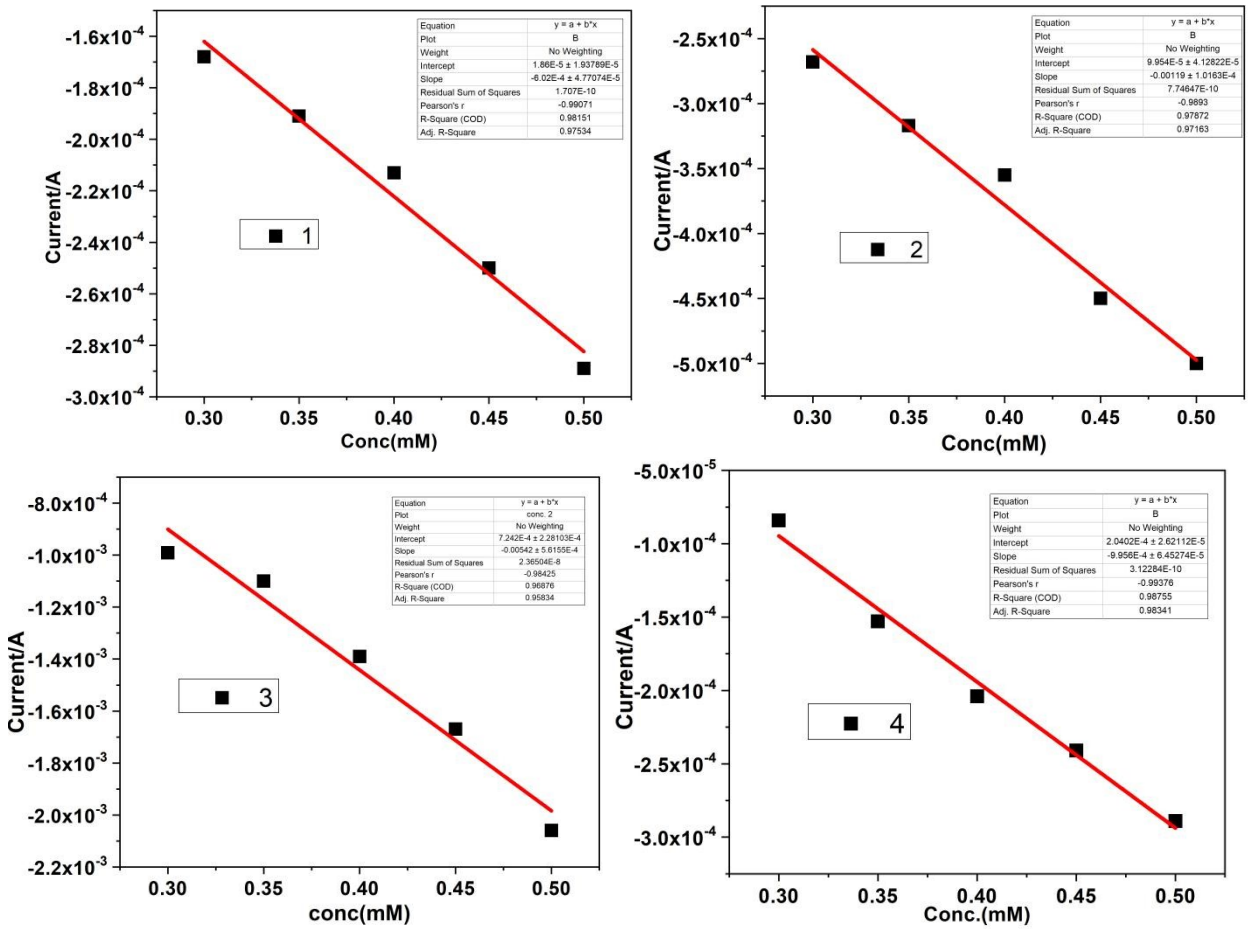


Figure S14- Linear regression of $i_{CoIII/IV}$ vs catalyst concentration (a) complex 1 (b) complex 2 (c) complex 3 (c) complex 4

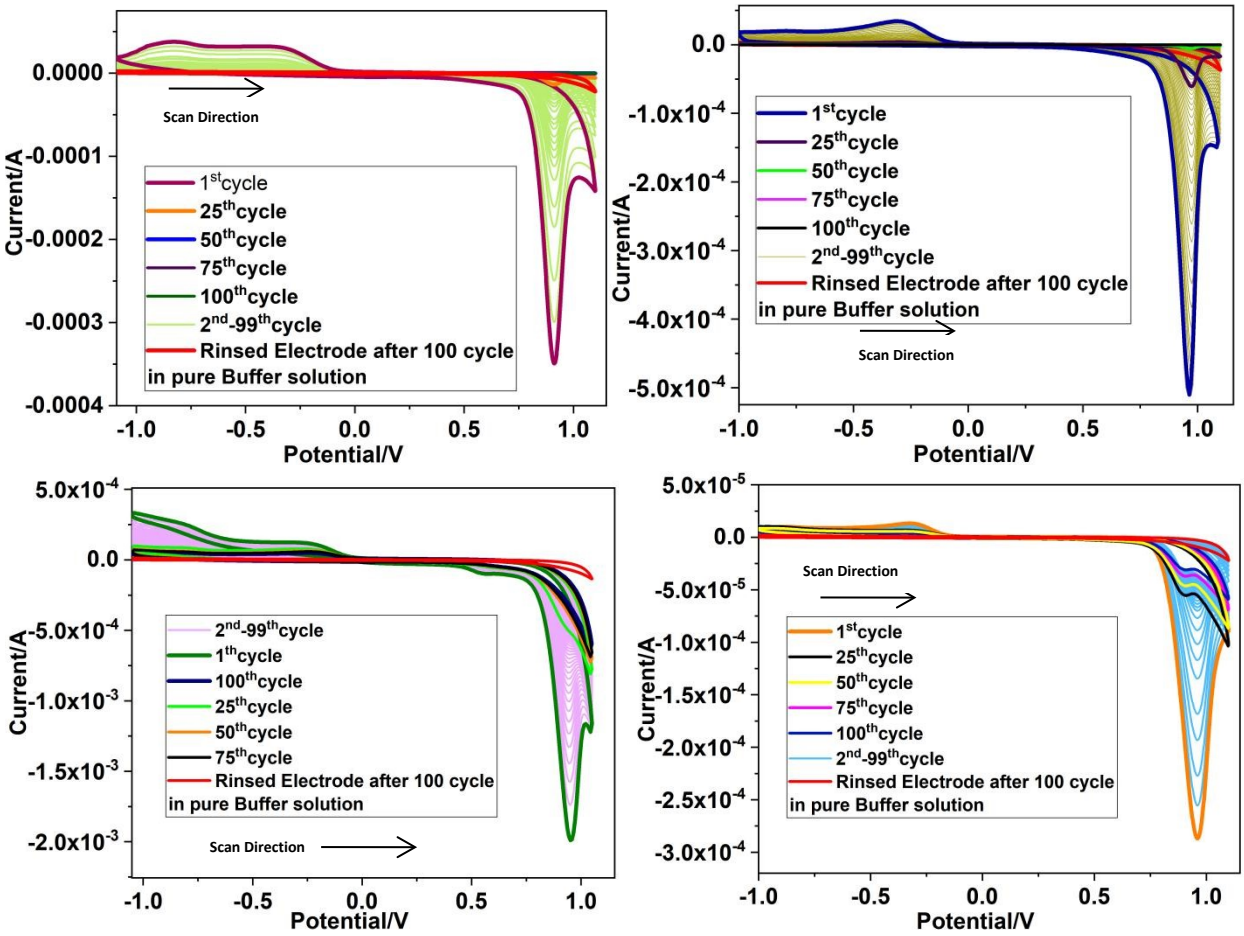
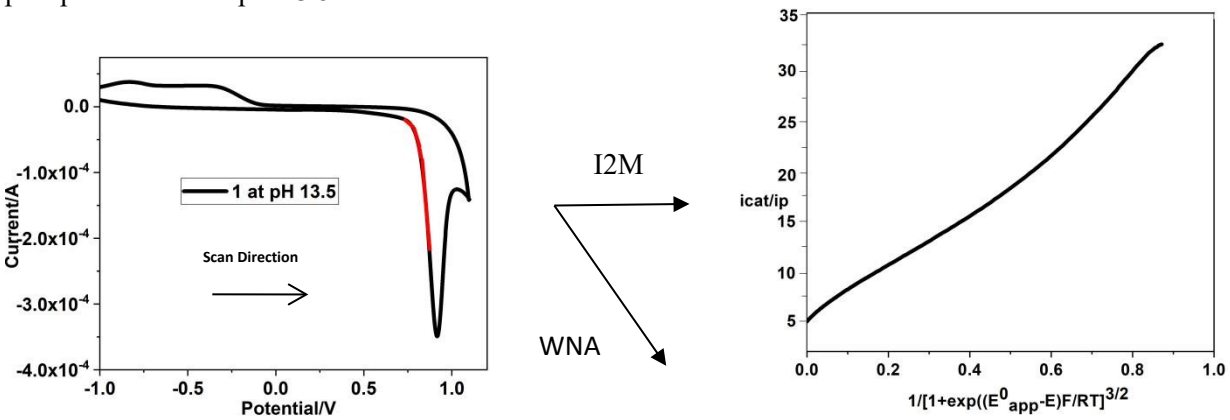
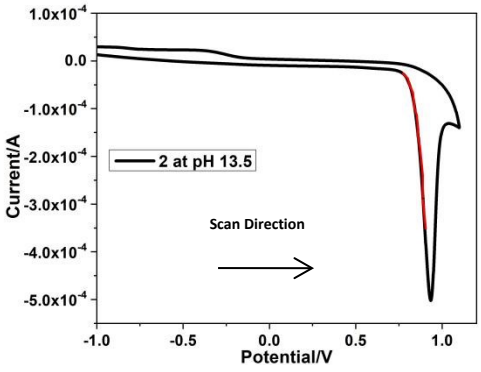


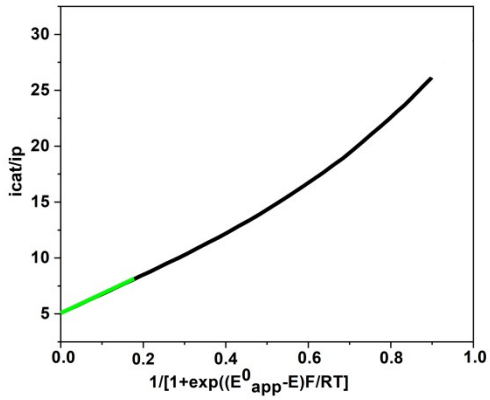
Figure S15 - 100 cycles CV of Complexes 1-4 and CV after rinsing working electrode and using in phosphate buffer at pH 13.5.

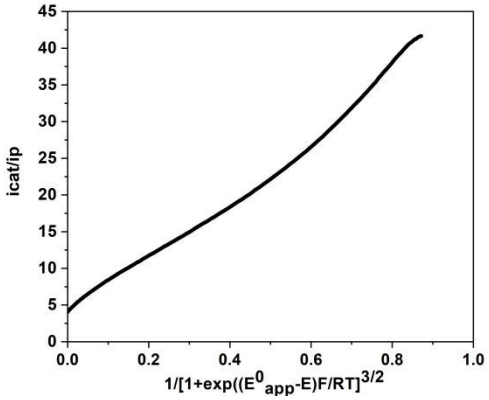


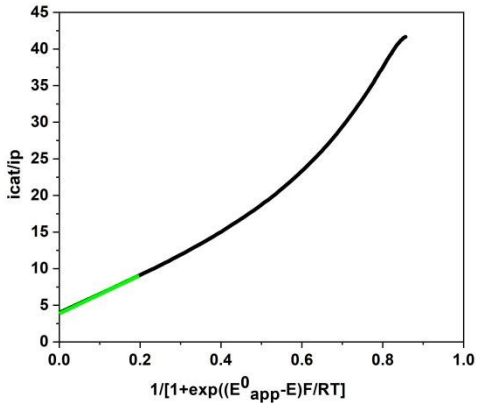

Current/A
Potential/V
2 at pH 13.5
Scan Direction

I2M

WNA


icat/ip
1/[1+exp((E0app-E)F/RT]


icat/ip
1/[1+exp((E0app-E)F/RT]3/2


icat/ip
1/[1+exp((E0app-E)F/RT]

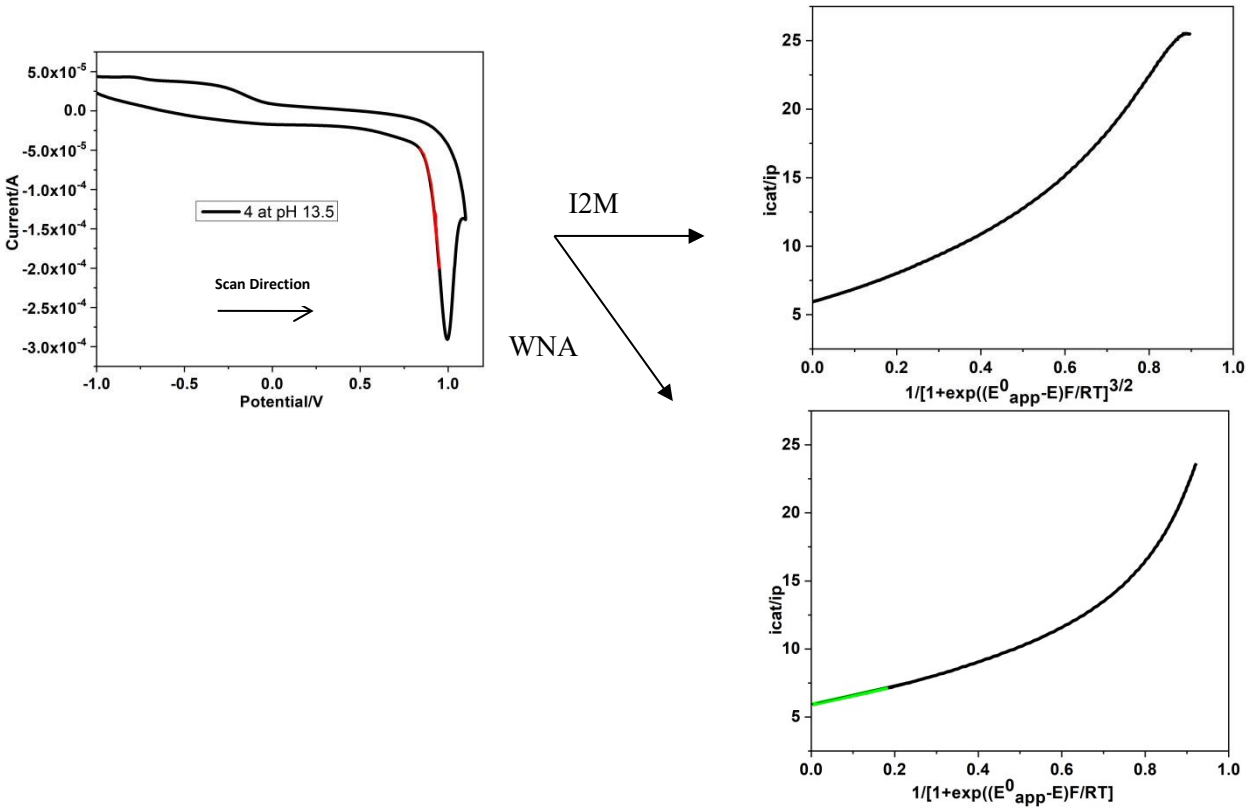


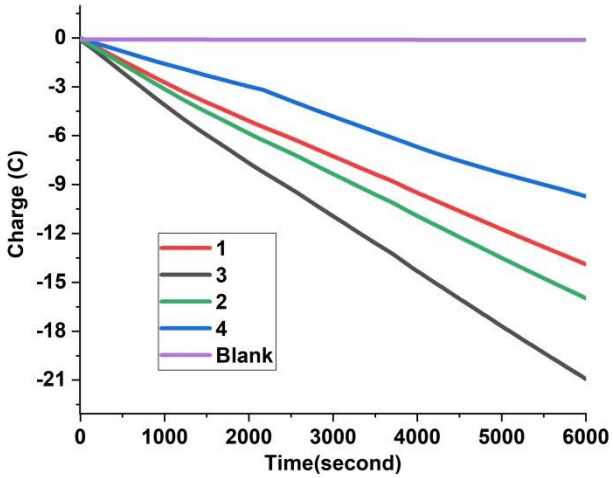
Figure S16-Solid black lines represent the CV of Complex **3**(0.5mM) at pH 13.5 buffer solution(left) .Red Line is the designated foot zone used for the calculation in *FOWA* (A) i/ip vs. $1/\{1 + e[(E^{0,ap} - E)(F/RT)]\}^{3/2}$ plot assuming a I2M. (B) i/ip vs. $1/\{1 + e[(E^{0,ap} - E)(F/RT)]\}$ plot assuming a WNA. Green line in the plot depicts the points used in the linear fitting used for TOF calculation in FOWA.

Calculation of Faradaic Efficiency *(F.E)* and *TON* from total accumulated charge during Control Potential Electrolysis

F. E= 4 x amount of O_2 (moles) x 100 / n (moles of electron)

n= Q (charge) / F (Faraday Constant)

At 1.3 V vs NHE all the complexes were subjected to CPE for 100 minutes total charge consumed was 13.95 C, 16.04 C, 21.02 C and 9.96 C for Complexes **1,2,3** and **4** . With the production of 0.5 ml, 0.6 ml , 0.8 ml and 0.2 ml of O_2 for Complexes **1,2,3** and **4**. Total moles of O_2 produced in CPE equals $2.23x10^{-5}$,$2.67x10^{-5}$, $3.57x10^{-5}$and $8.92x10^{-6}$ for complexes **1,2,3**and**4**.



Using the amount of catalyst used, number of moles of O_2 generated and the charge accumulated during the CPE for 100 minutes at 1.3 V in pH 13.5 phosphate buffer solution we calculated the TON of each catalyst[2].

For complex **3**- $TON_3 = (0.8/22400) \times (10^3 / 0.5 \times 10^{-3} \times 4) = \sim 18$

Likewise, TON calculated are as follows:-
$TON_1 = \sim 11$
$TON_2 = \sim 13$
$TON_4 = \sim 5$

Figure S17 - Total accumulated charge during control potential electrolysis from a solution containing 1 mM catalyst **1,2,3,4** and the buffer only using a GC electrode at +1.30 V vs. NHE for 6000 sec.

UV-visible Spectroscopy and FTIR analysis

The electronic absorption spectra of the mononuclear Co(II) Complexes in ACN at room temperature shows electronic transition in both UV and visible regions. UV region peaks for the complexes 1 (283 nm, 332 nm), 2 (282 nm and 319 nm), 3 (284 nm, 320 nm) and 4 (286 nm and 322) are due to the ligand centered transitions or the LMCT [3-5]. Other peaks observed for **1,2,3,4** in the spectra are 516 nm, 518 nm, 518 nm, and 513 nm respevtively due to d-d transition in the complexes (Figure S18(a)). The synthesized complexes were analyzed on FTIR and the spectra were recorded for the detection of functional groups and substitution (Figure S18(b)). Between 2936 and 2835 cm^{-1} peaks were recorded for sp^2 C-H stretching. At 1582 Cm^{-1} C=C stretching was observed and at 1466 cm^{-1} alkane methylene group ($O\text{-}CH_3$) C-H stretching was observed. At 1374 cm^{-1} aromatic C-N stretching and at 1264 cm^{-1}, 1202 cm^{-1} presence of alkyl aryl ether were confirmed in the ligands. Another C=C bending was observed at 995 cm^{-1}, 729 cm^{-1} with a peak at 774 cm^{-1} for tri-substitution of complex [4].

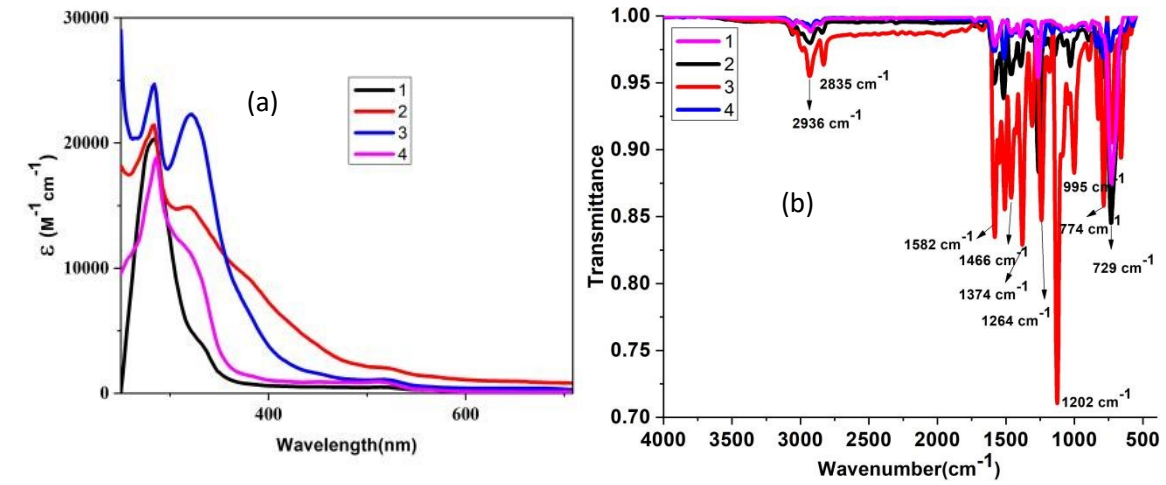


Figure S18- (a) UV Visible spectra of complex **1-4** in ACN at 0.5 mM (b) FTIR spectra of complexes **1-4**

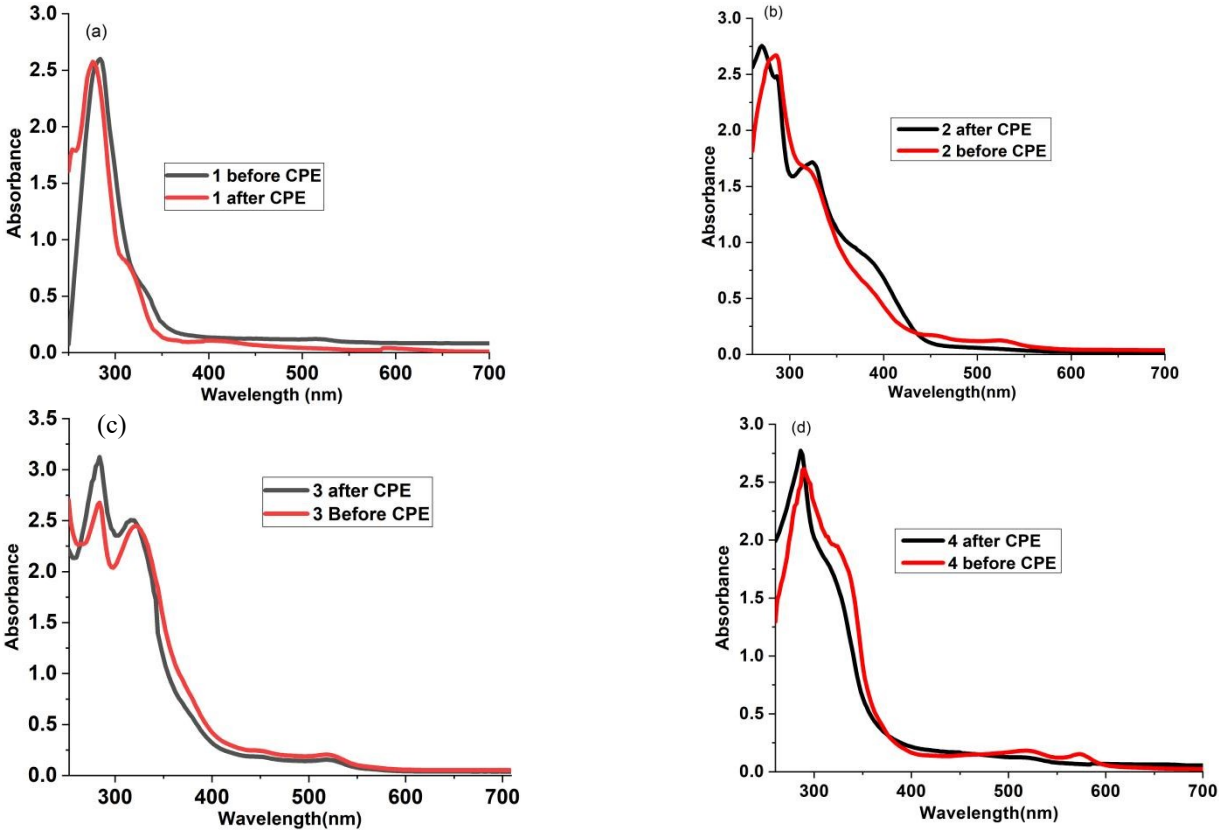


Figure S 19- UV-Vis spectra of Complexes **1,2,3** and **4** before and after CPE at pH 13.5 (at scan rate = 100 mV/s).

After CPE the catalytic solution was used for the mass spectroscopy for the detection of intermediates generated during the catalysis. Since we already used millipore water along with HPLC grade solvent for the CPE we injected the solution into LCMS after diluting it with mass grade water.

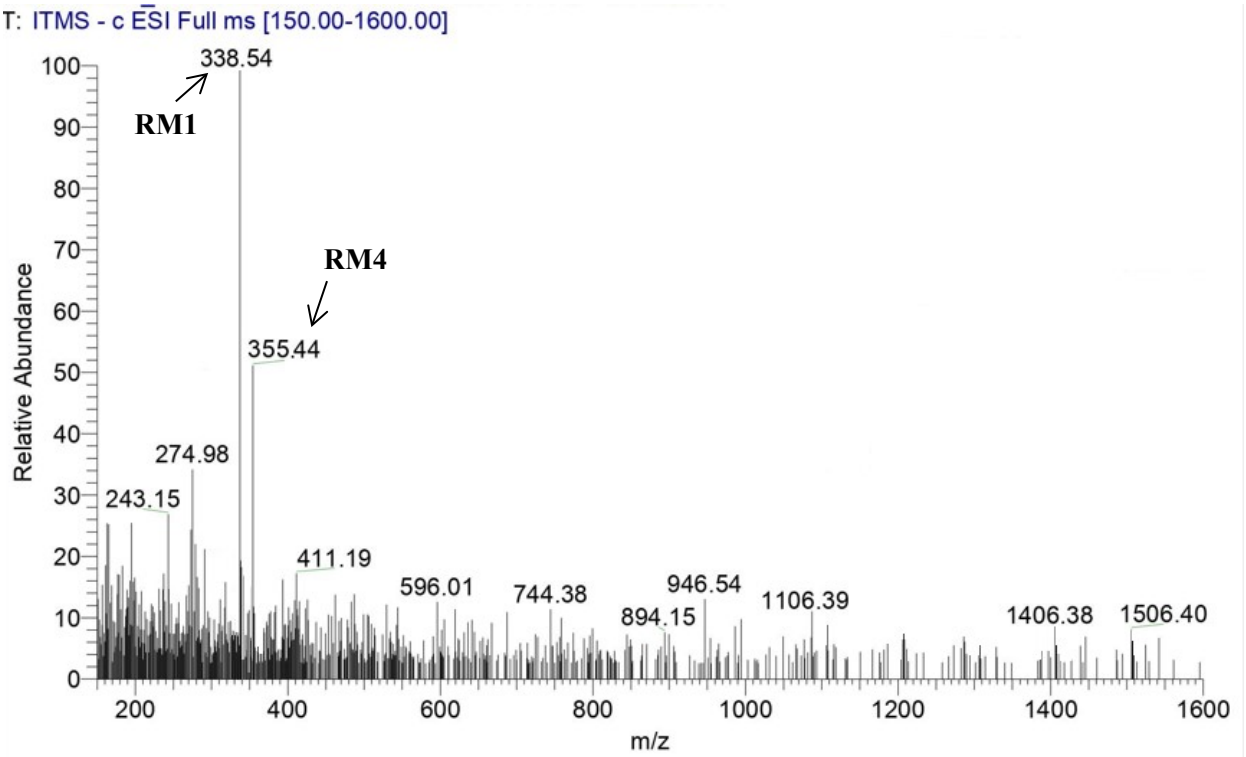


Figure S20 – Mass spectra of complex 1 observed with half mass of RM1, RM4 after CPE at 1.3 V for 100 minutes.

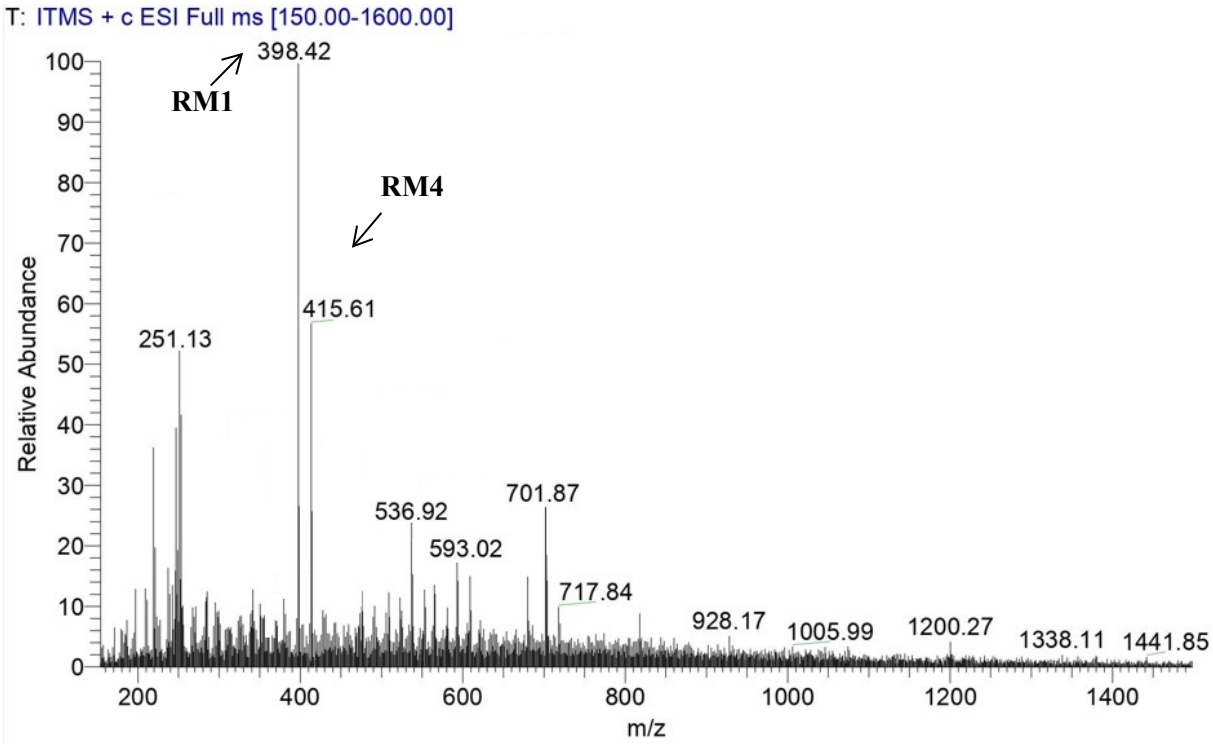


Figure S21 – Mass spectra of complex 2 observed with the half mass of RM1, RM4 after CPE at 1.3 V for 100 minutes.

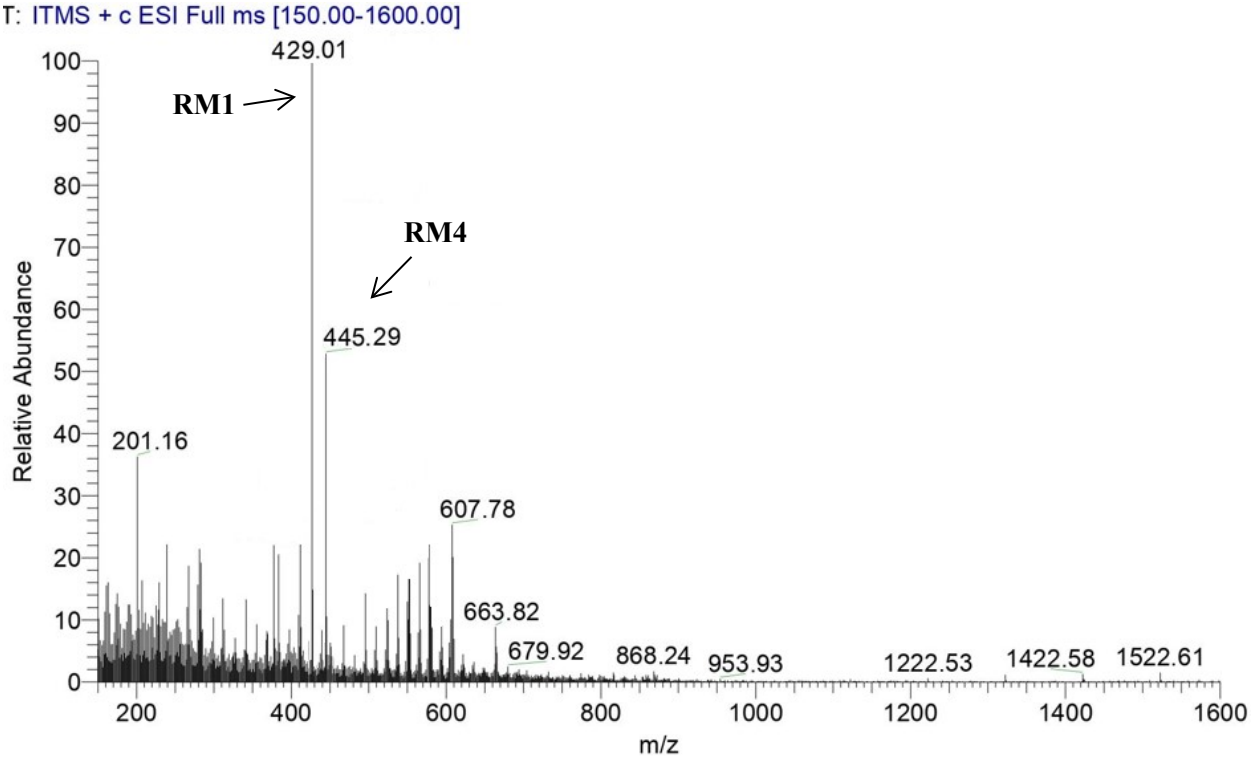


Figure S22– Mass spectra of complex 3 observed with half mass of RM1, RM4 after CPE at 1.3 V for 100 minutes.

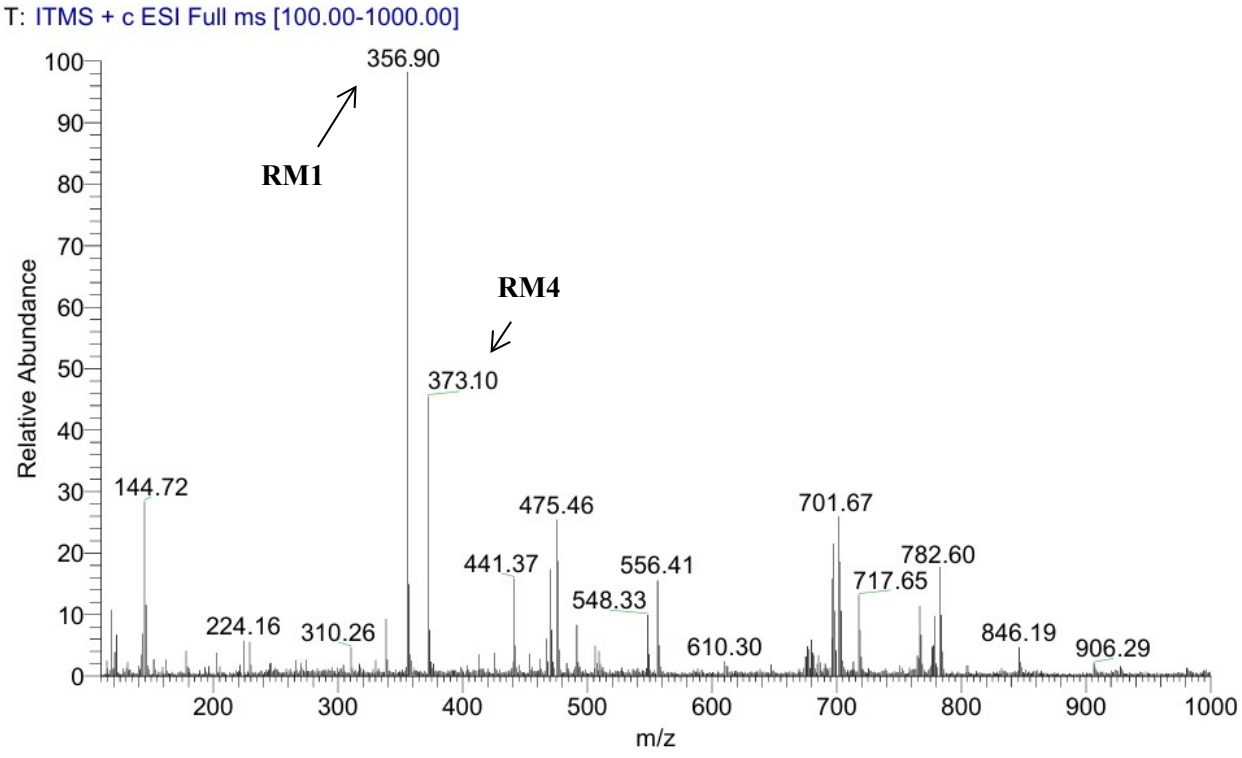


Figure S23– Mass spectra of complex 4 observed with half mass of RM1, RM4 after CPE at 1.3 V for 100 minutes.

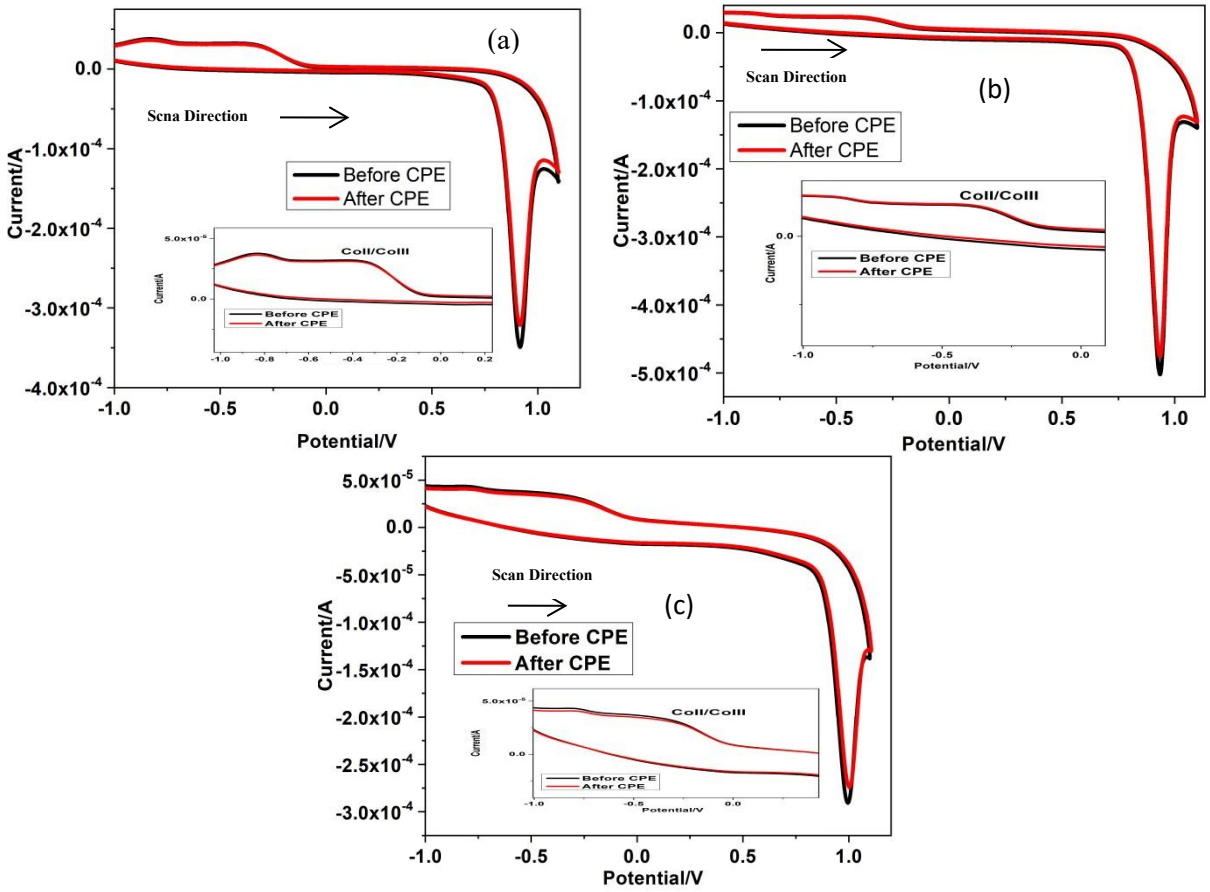
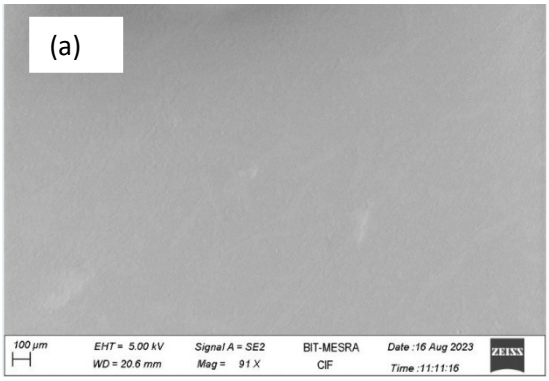


Figure S24- CV of complexes in fresh pH 13.5 buffer solution (a) **1** (b) **2** and (c) **4** after CPE with a current intensity loss of 5-8% .



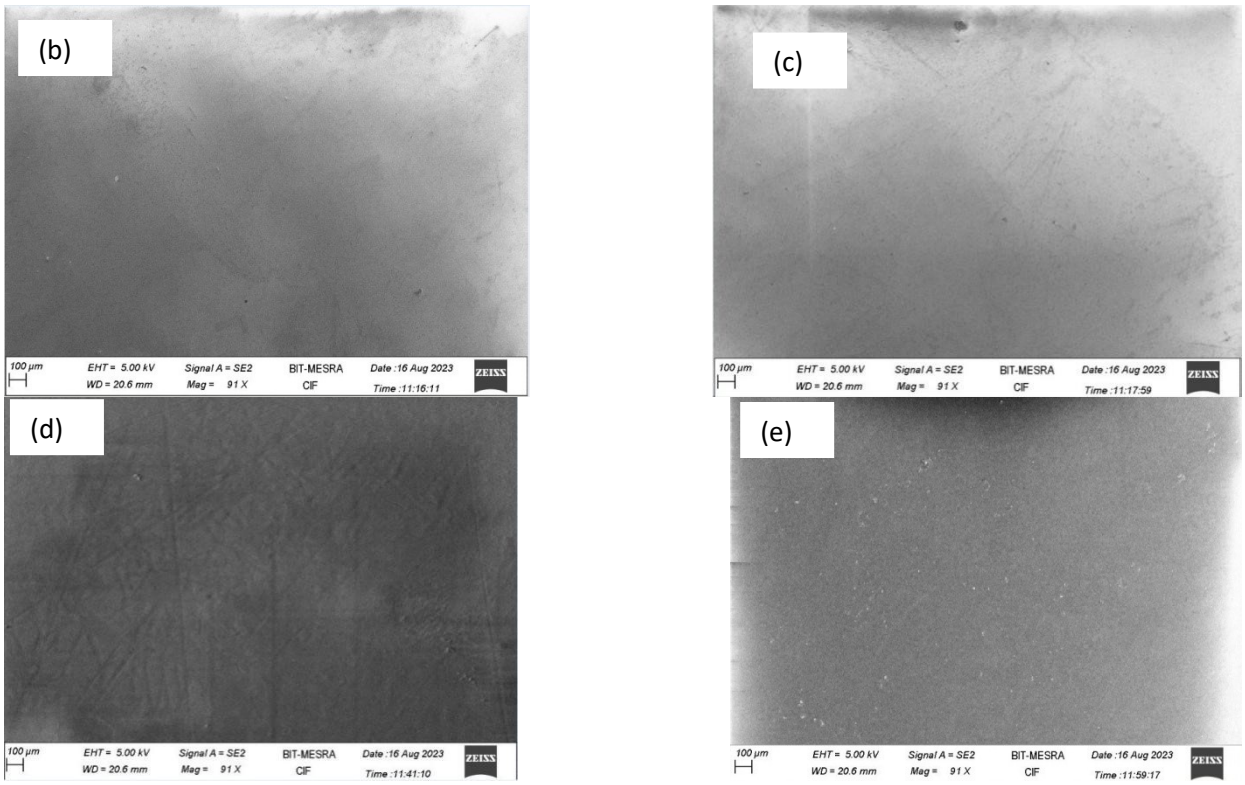
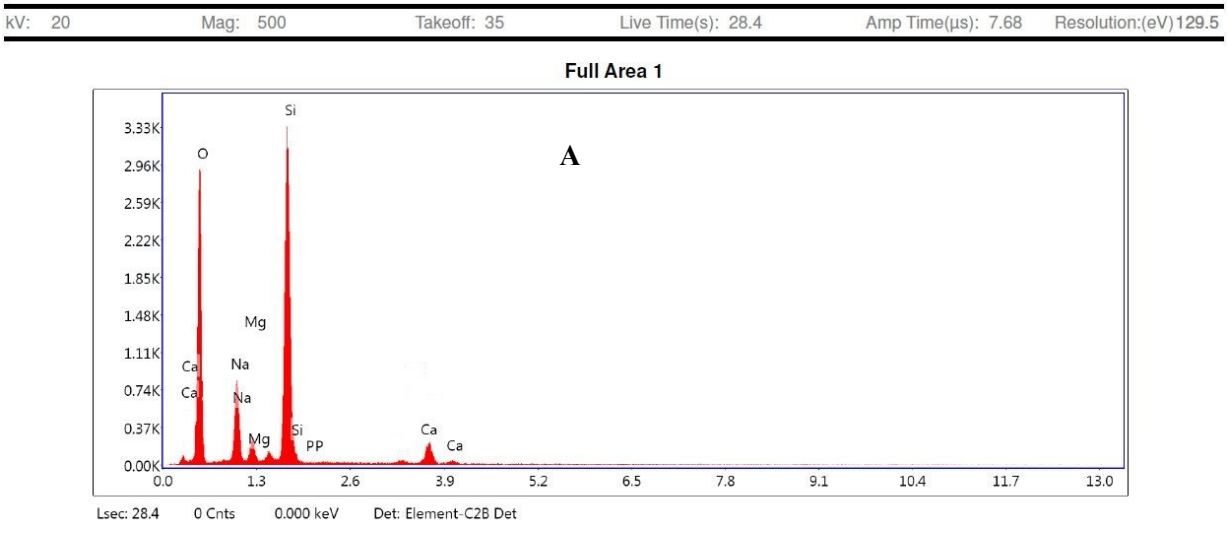
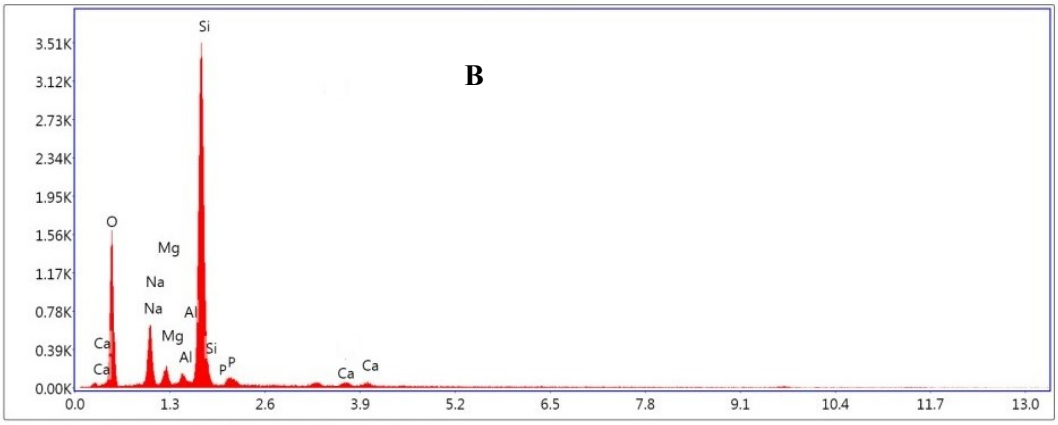


Figure-S25- FESEM images of the Working electrode (a) before CPE and (b) complex 1 (c) complex 2 (d) complex 3 (e) complex 4 after 6000 seconds of CPE.



kV: 20 Mag: 500 Takeoff: 35 Live Time(s): 28.4 Amp Time(μs): 7.68 Resolution:(eV)129.5

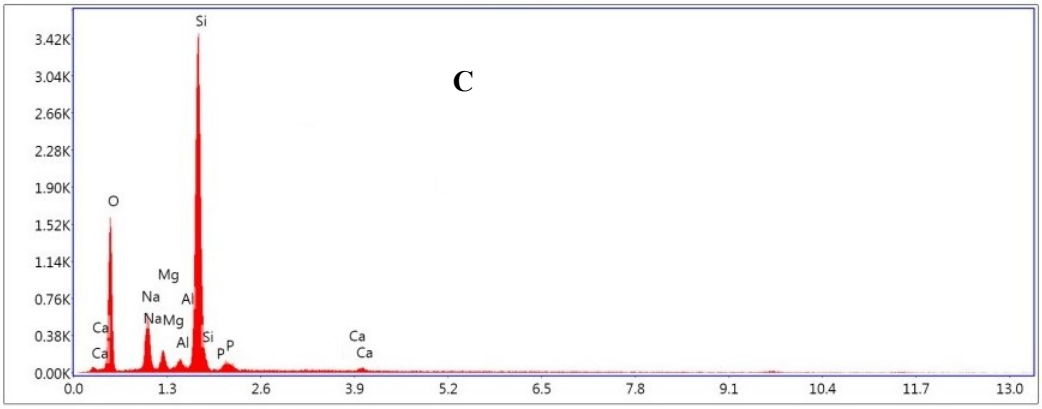
Full Area 1



Lsec: 28.4 0 Cnts 0.000 keV Det: Element-C2B Det

kV: 20 Mag: 500 Takeoff: 35 Live Time(s): 28.4 Amp Time(μs): 7.68 Resolution:(eV)129.5

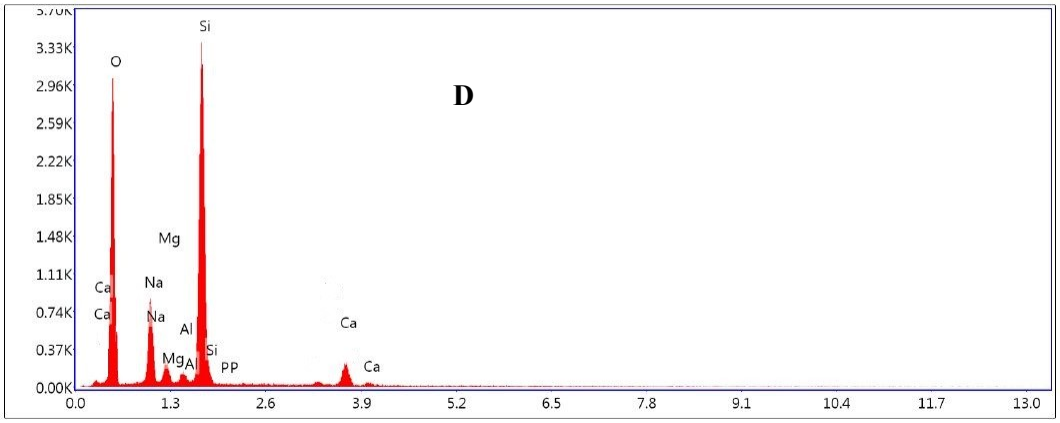
Full Area 1



Lsec: 28.4 0 Cnts 0.000 keV Det: Element-C2B Det

kV: 20 Mag: 500 Takeoff: 35 Live Time(s): 28.3 Amp Time(μs): 7.68 Resolution:(eV)129.5

Full Area 1



Lsec: 28.3 0 Cnts 0.000 keV Det: Element-C2B Det

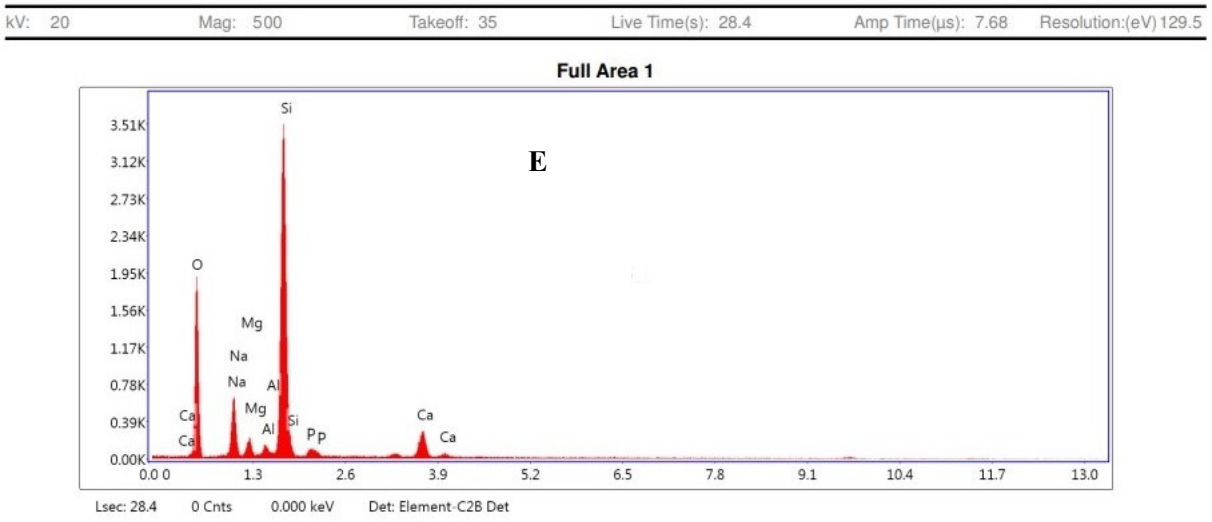


Figure S26- EDX images of working electrode (**A**) before **(B-E)** After CPE for 6000 seconds for complex **1,2,3** and **4** respectively.

Detection of Molecular Oxygen after CPE through Gas Chromatography

Through a closed reaction vessel, the generated gas after the CPE of catalyst got accumulated in the headspace (CPE at +1.3 V for 100 minutes) of vessel . Then the gas was pulled out in a gas tight syringe. The syringe was then used to inject gas into GC equipped with TCD and the amount of oxygen was measured.

Parameters and conditions maintained during GC analysis- Thermo-fisher scientific trace 1110 gas chromatograph equipped with a thermal conductivity detector and fitted with a MS-5Å 80/100 2.5m 2.0MMID 1/8INOD, calibrated with air was used for gas analysis for O_2. Inlet setting: inlet type – Packed. Temperature setting -150^{0}c. Inlet Gas type – Argon and gas flow rate 15ml/min.

Setting for GC- Max.Temperature- 250^{0}C. Initially 60^{0}C was maintained for first 5 min then for 5-13 min the temperature was ramped and raised to 100^{0}C. Next rate for rise in temperature was 5^{0}C/Min. Thus between 13-23 min temperature of 250^{0}C was attained. For the last 5 min 15^{0}C/min of ramp rate was pre-loaded.

Detector Setting- TCD detector was used, Detector bridge voltage was 5v (85mA current) and gas flow rate was 15ml/min.

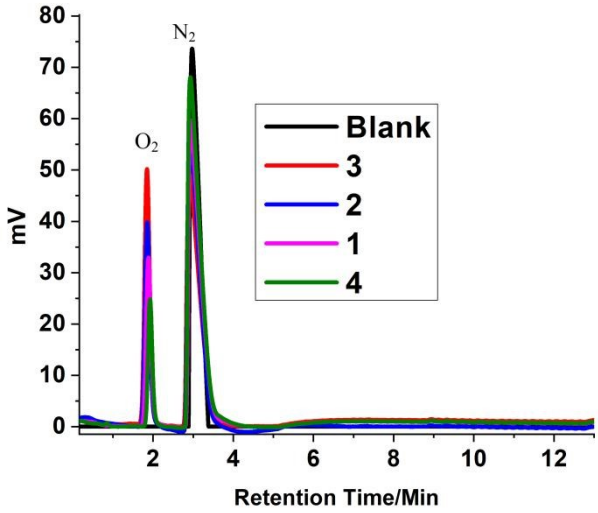


Figure S27- GC trace of electrocataltyically generated molecular oxygen by complexes **1-4** after 6000 s of CPE.

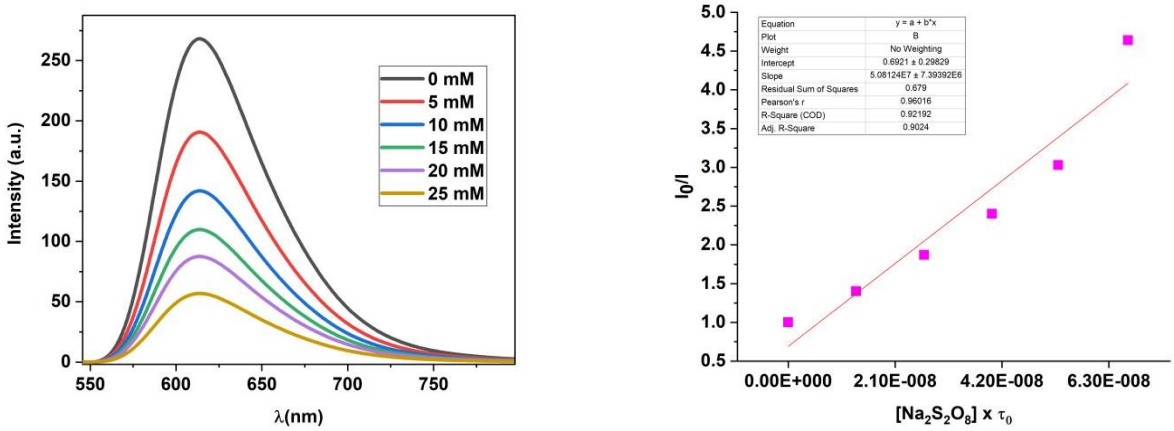
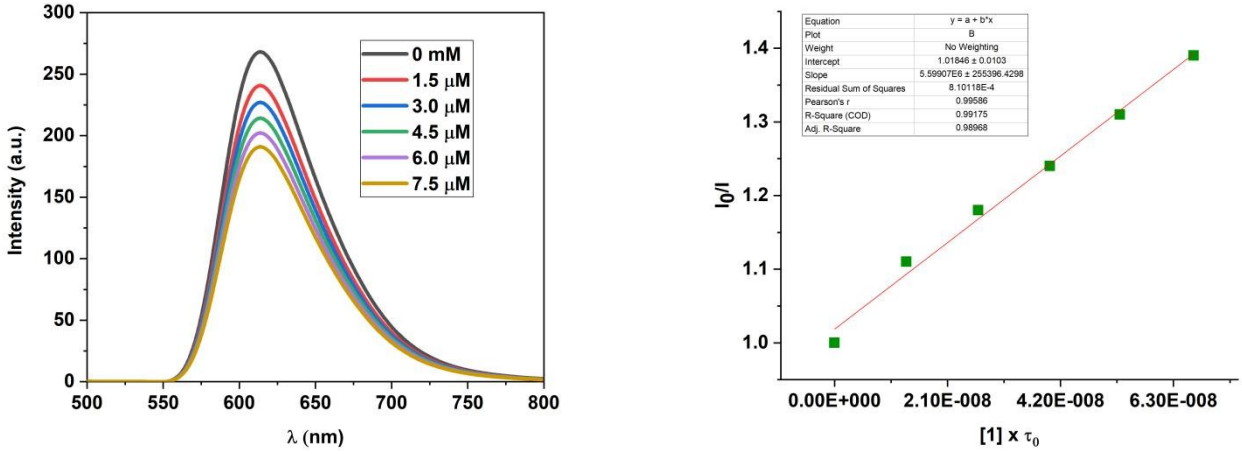


Figure S28-Emission spectra of $[Ru(bpy)_3]Cl_2$ as a function of $Na_2S_2O_8$ in 1:1 CH_3CN and Stern-Volmer plot for phosphorescence quenching of $[Ru(bpy)_3]Cl_2$ of concentration $1x10^{-6}$ M CH_3CN $Na_2S_2O_8$.



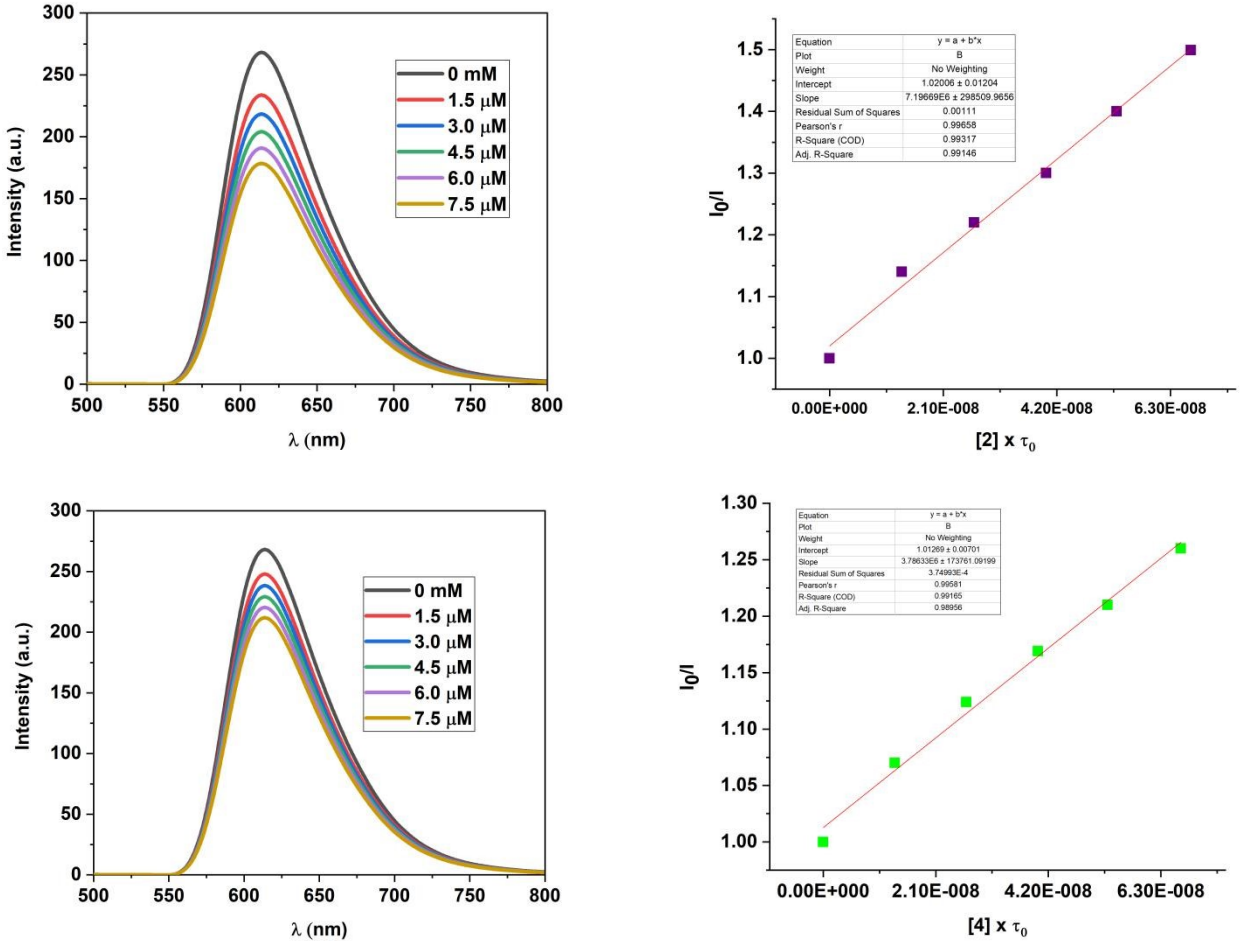
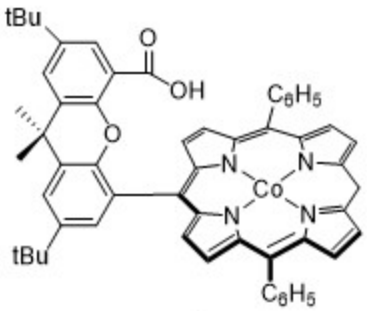


Figure S29-Emission spectra of $[Ru(bpy)_3]Cl_2$ as a function of complex **1,2** and **4** in 1:1 CH_3CN and Stern-Volmer plot for phosphorescence quenching of $[Ru(bpy)_3]Cl_2$ of concentration $1x10^{-6}$ M in 1:1 CH_3CN complex **1,2** and **4**.



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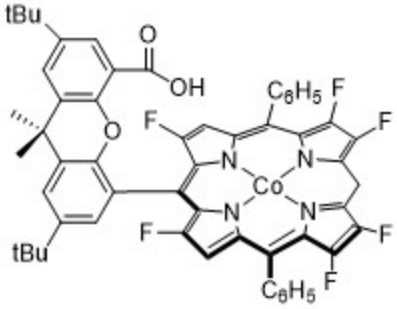
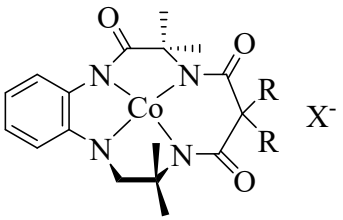


6

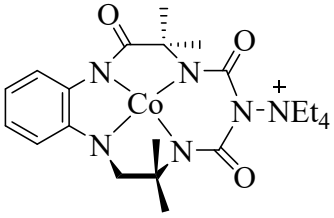


(7)

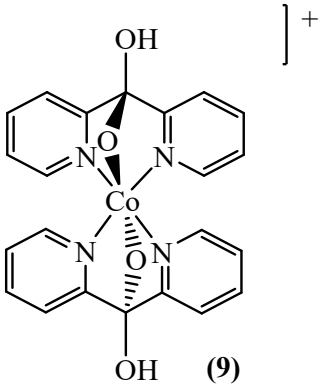
7a **7b**

R= Me Et

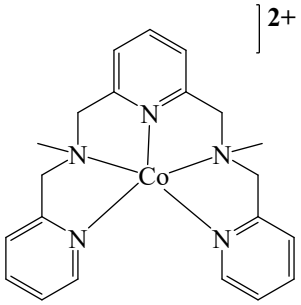
X= $Li(H_2O)_3$ Li



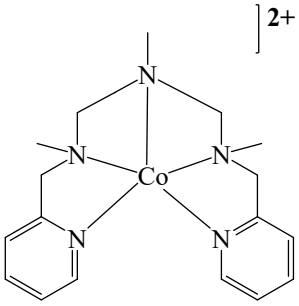
(8)



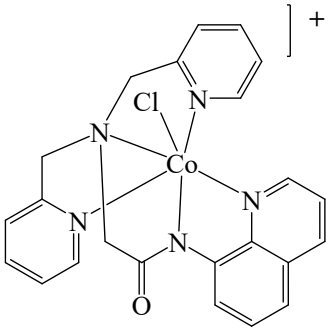
(9)



10a



10b



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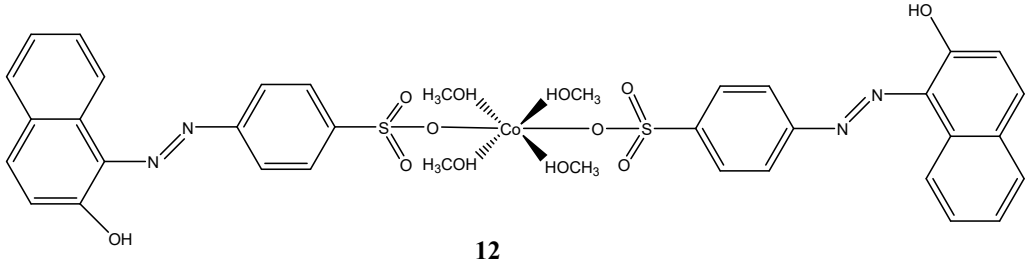

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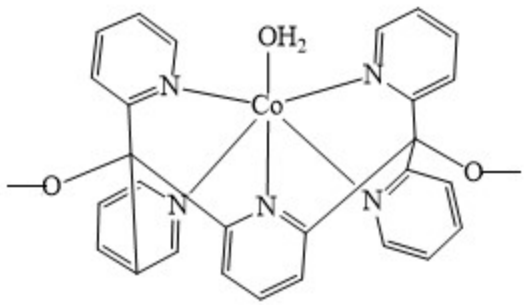


13

Figure S30- Some of the selective Cobalt based Water Oxidation homogeneous catalysts.**5-6**[55]**,7-8**[56]**, 9**[57]**,10**[47]**,11**[58]**,12**[36]**,13**[60].

References

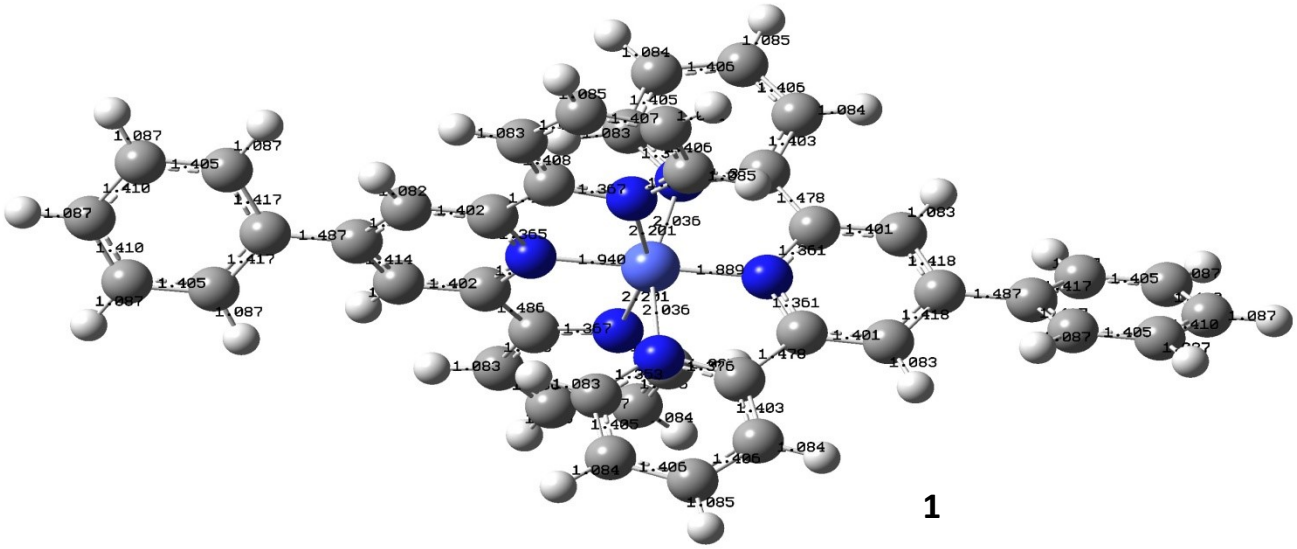
(1) R. Matheu, S. Neudeck, F. Meyer, X. Sala,A.Llobet, *chemsuschem.,* 2016, **9**, 23, 3361-3369

(2) S. Karim, A. Chakraborty, D. Samanta, E. Zangrando, T. Ghosh, D. Das, *Catal. Sci. Technol.,* 2020, **10**, 9, 2830-2837

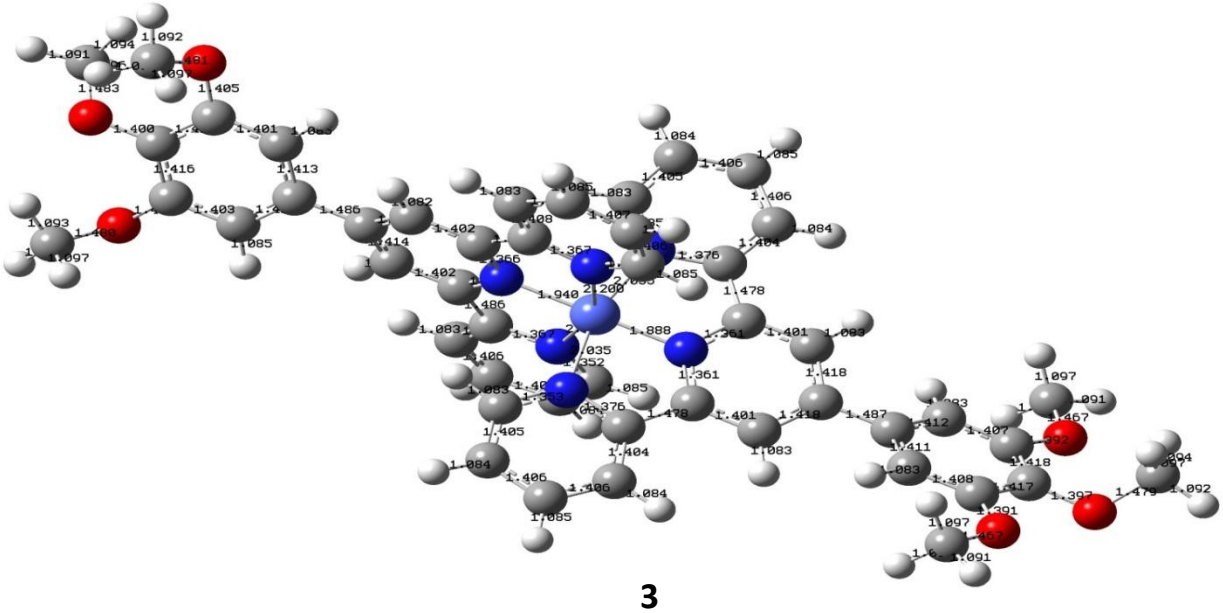
(3)R. Indumathy, M. Kanthimathi, T. Weyhermuller, B.U. Nair, Polyhedron., 2008, **27**,17, 3443-3450.

(4) D. Das, S. Pattanayak, K. K. Singh, B. Garai, S. S. Gupta, *ChemComm.,* 2016, **52,79,** 11787-11790

(5) T.I.Kasharl , S.A.Aal **,** *J. Iran. Chem.Soc.* 2021, **18**, 1625–1640



1



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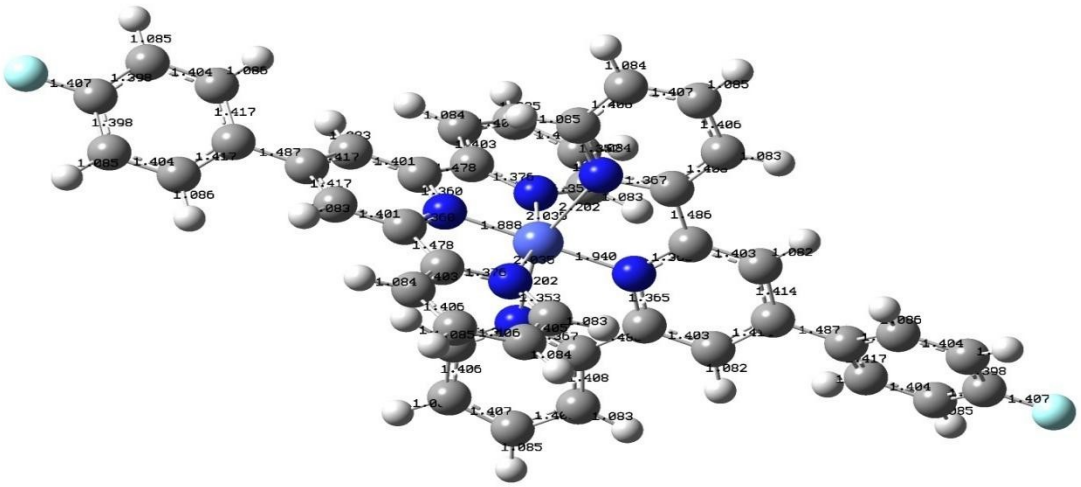
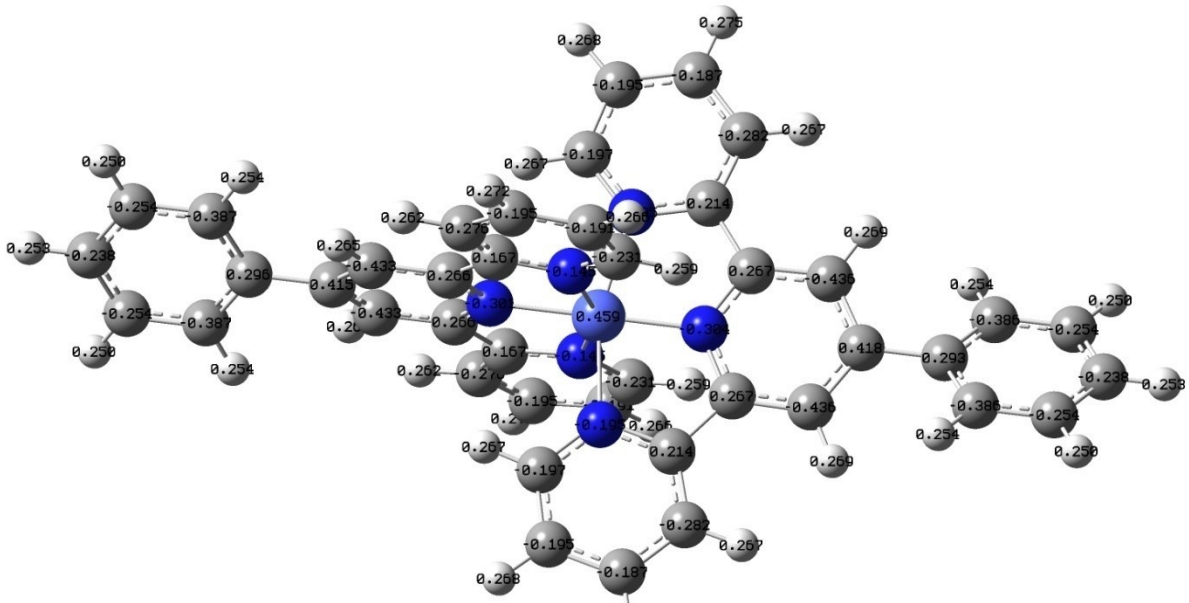


4

Figure S31- Optimized structures with Computed bond lengths of complexes **1**,**3** and **4** .



1

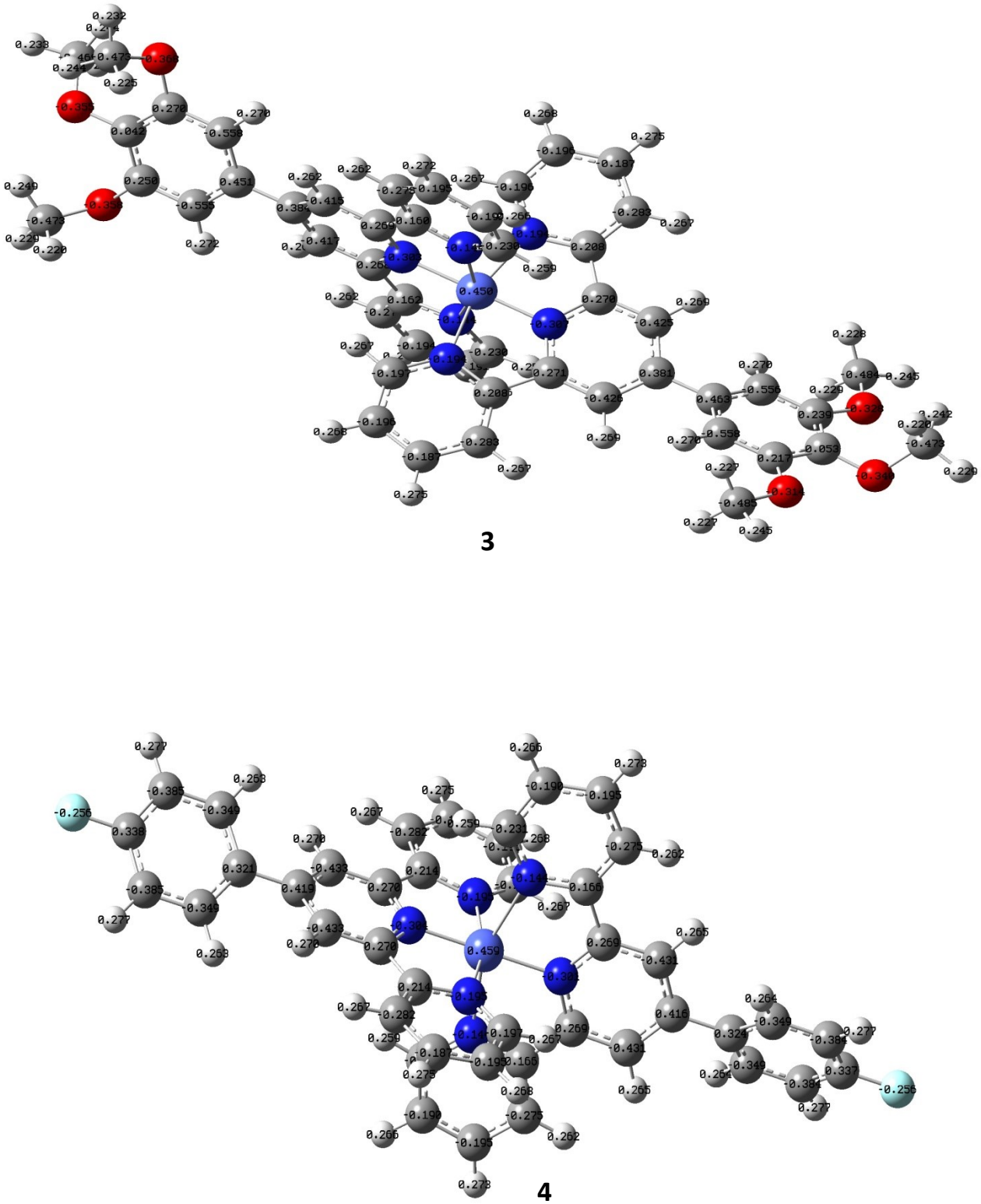


Figure S32- Mulliken Charge on individual atoms of complexes **1**, **3** and **4**

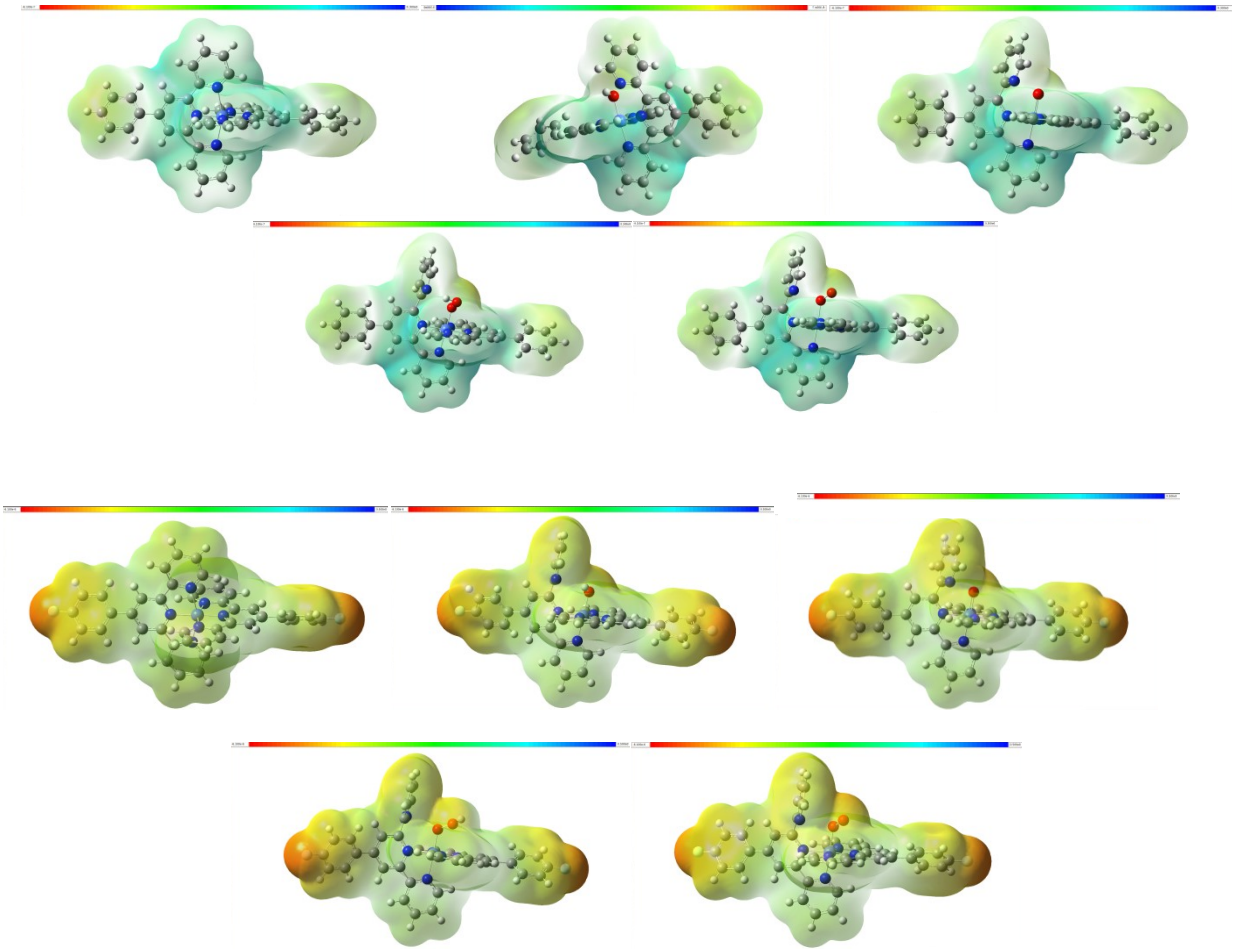


Figure S33- Electrostatic Potential Plots of complexes with their respective Key intermediates (complex **1** and **4** respectively) . ESPs are mapped onto electron density iso-value of 0.0200.

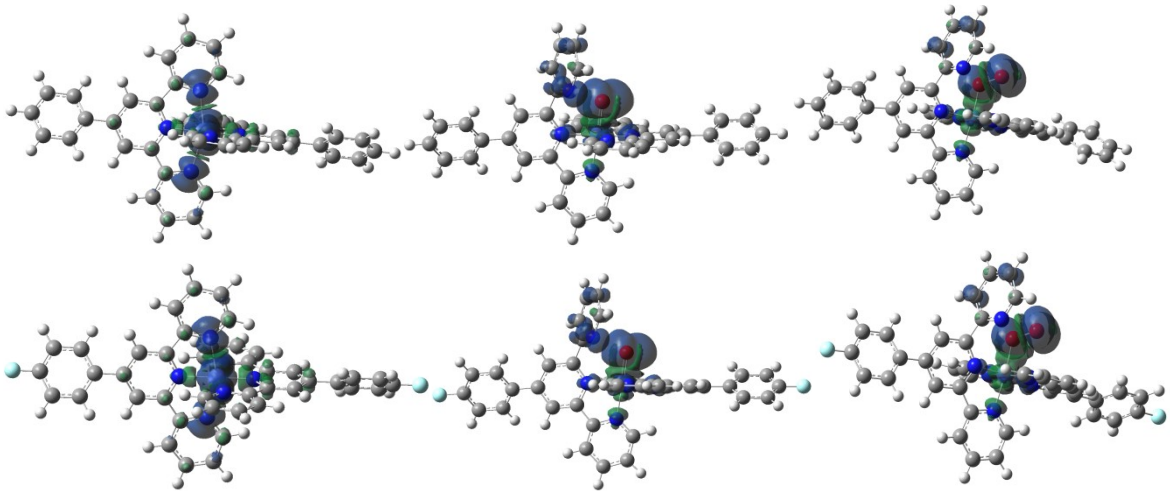


Figure S34- Spin Density of key intermediates of Complexes **1** and **4** respectively with iso value 0.0004.

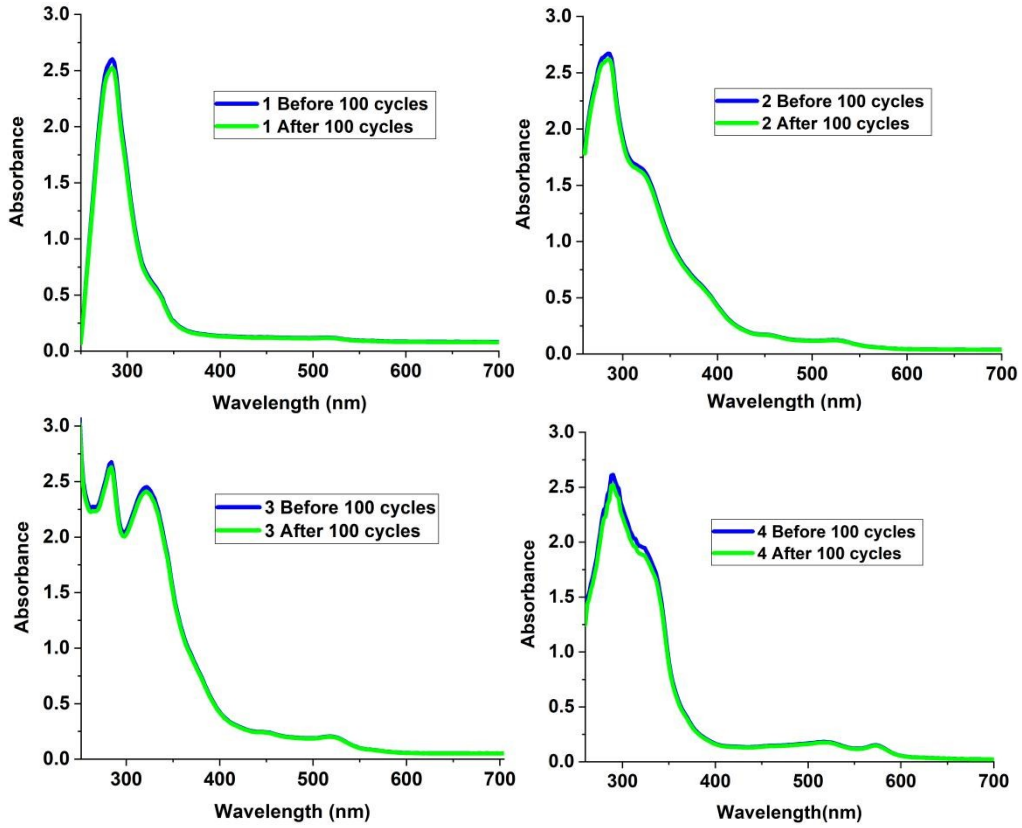


Figure S35- UV-Visible spectra of complex **1-4** before and after 100 consecutive cycles.

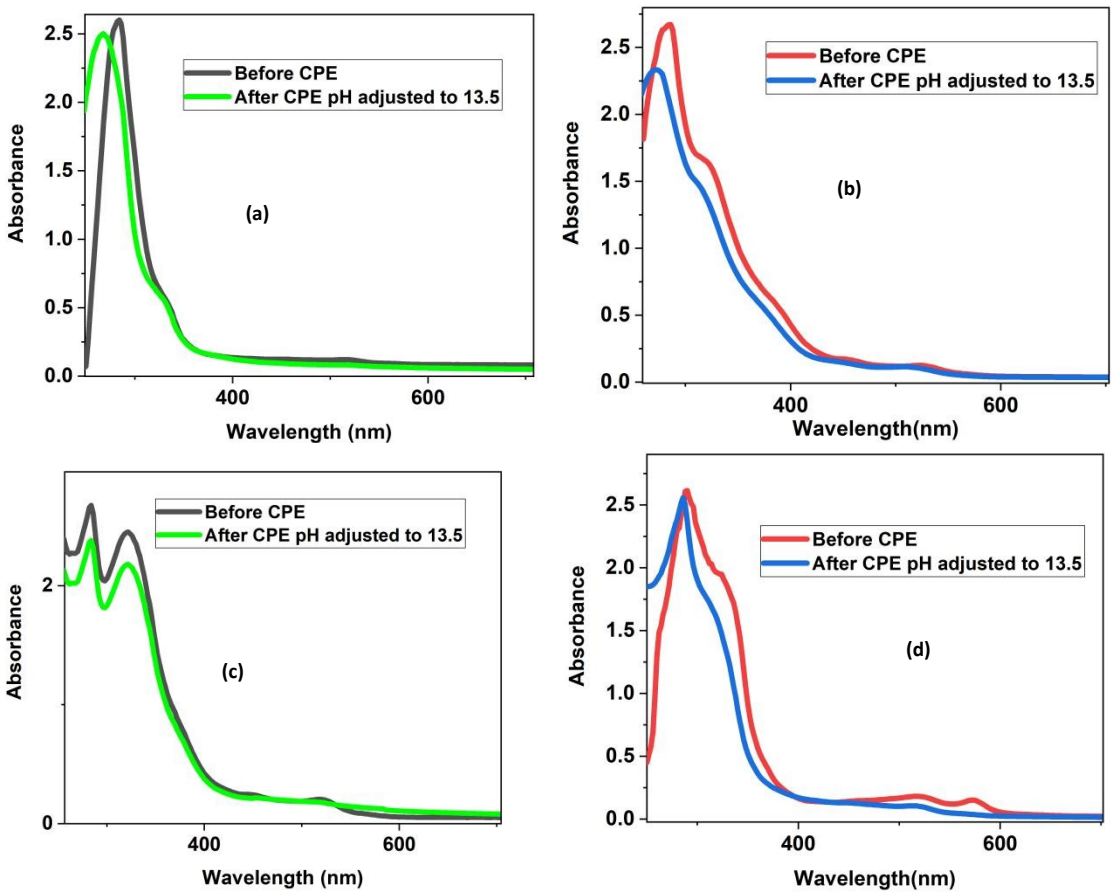
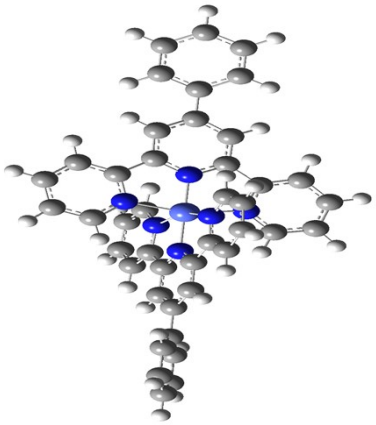


Figure S36- UV for complex (a) **1,** (b) **2,** (c) **3** and (d) **4** before CPE and after CPE when pH is adjusted to 13.5 after completion of CPE for 100 minutes at 1.3 V vs NHE

Cartesian Coordinates of steps involved in mechanistic cycle

Complex 1 Fig. 1RM1
E(UB3LYP) = - 2091.717286 Hartree
ZPE (kcal mol^{-1}) = 0.628076

C	-3.94327	1.19954	-0.00161
C	-2.54948	1.1719	-0.00412
C	-2.54962	-1.17186	0.00413
C	-3.94341	-1.19932	0.00159
C	-4.67398	0.00015	-0.00002
H	-4.46482	2.14622	0.02287
H	-4.46508	-2.14593	-0.02293
C	-1.70527	-2.39561	0.00184
C	-2.23172	-3.69194	0.00178
C	0.46439	-3.21254	-0.00053

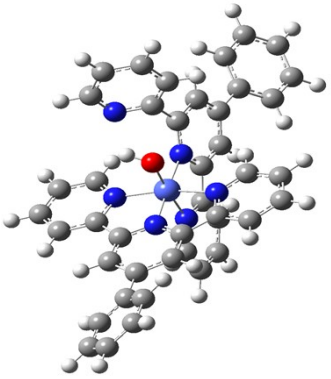


1RM1

C	-1.35364	-4.77869	-0.00038
H	-3.30025	-3.86466	0.00359
C	0.02301	-4.53803	-0.00146
H	1.52579	-2.98491	-0.00085
H	-1.73945	-5.79276	-0.00074
H	0.7402	-5.35109	-0.00277
C	-1.70496	2.39554	-0.0018
C	-2.23123	3.69194	-0.00163
C	0.46481	3.21215	0.00064
C	-1.353	4.77856	0.00062
H	-3.29974	3.8648	-0.00344
C	0.02363	4.53771	0.0017
H	1.52618	2.98437	0.00093
H	-1.73866	5.79268	0.00107
H	0.74093	5.35066	0.00309
N	-1.87305	-0.00002	0.00003
N	-0.373	-2.16969	0.00064
N	-0.37273	2.16942	-0.00064
C	-8.27309	1.01885	-0.65622
C	-6.87488	1.02183	-0.65231
C	-6.15677	0.00024	-0.00003
C	-6.87501	-1.02127	0.65224
C	-8.27322	-1.01812	0.65614
C	-8.97814	0.0004	-0.00005
H	-8.8115	1.80613	-1.17484
H	-6.34637	1.80638	-1.18393
H	-6.3466	-1.80589	1.18387
H	-8.81173	-1.80534	1.17475
H	-10.0638	0.00047	-0.00006
C	2.61792	-0.00444	-1.17405
C	4.00987	-0.00163	-1.20639
C	4.73639	-0.00003	-0.0001
C	4.00993	0.00151	1.20623
C	2.61798	0.00429	1.17397
H	4.53017	0.02306	-2.15482
H	4.5303	-0.02319	2.15462
C	-0.52904	0.00068	-2.9756
C	-0.1856	0.00167	-4.32872
C	1.16613	0.00058	-4.68017
C	2.12681	-0.00174	-3.66538
C	1.70704	-0.00201	-2.33577
H	-1.56879	0.00099	-2.67207
H	-0.96588	0.00299	-5.08097
H	1.4687	0.00106	-5.72194
H	3.18176	-0.00347	-3.91006
C	1.70718	0.00183	2.33576
C	2.12706	0.00163	3.66533
C	1.16647	-0.00071	4.68021
C	-0.1853	-0.00191	4.32886
C	-0.52884	-0.00098	2.97577
H	3.18203	0.00347	3.90993
H	1.46913	-0.00113	5.72195

H	-0.96551	-0.00325	5.08117
H	-1.56861	-0.00139	2.67233
C	6.93776	-0.65331	-1.02105
C	8.33594	-0.65702	-1.01789
C	9.0409	0.00023	-0.00009
C	8.33584	0.65739	1.0177
C	6.93766	0.65349	1.02084
C	6.2195	0.00004	-0.00011
H	6.40951	-1.18608	-1.805
H	8.87437	-1.17647	-1.80459
H	10.12655	0.0003	-0.00008
H	8.87419	1.17691	1.8044
H	6.40932	1.18621	1.80477
N	1.95547	-0.00007	-0.00002
N	0.38703	-0.00074	-1.99698
N	0.38714	0.00047	1.99707
Co	0.07522	-0.0001	-0.00001

Complex 1 Fig. 1RM2
E(UB3LYP) = - 2167.49993 Hartree
ZPE (kcal mol^{-1}) = 0.643349 Hartree



1RM2

C	3.71252	-1.21112	-0.78358
C	2.34221	-0.93487	-0.79334
C	2.66161	1.03821	0.45893
C	4.04339	0.77505	0.51367
C	4.60773	-0.36402	-0.09621
H	4.08723	-2.07693	-1.31219
H	4.67171	1.48553	1.03672
C	2.22285	2.34732	1.03986
C	2.53573	2.67365	2.37494
C	1.38004	4.48814	0.64628
C	2.2263	3.96043	2.84966
H	2.98857	1.93481	3.02834
C	1.63808	4.88922	1.97077
H	0.93692	5.17699	-0.06739
H	2.44206	4.23061	3.8789
H	1.39004	5.89507	2.29331
C	1.37211	-1.80185	-1.49338
C	1.72824	-2.88028	-2.32251
C	-0.9165	-2.18946	-1.9082
C	0.72056	-3.62601	-2.95383
H	2.76696	-3.13679	-2.48432
C	-0.62458	-3.2752	-2.74447
H	-1.9404	-1.89602	-1.72575
H	0.98187	-4.45977	-3.59676
H	-1.43422	-3.82191	-3.21334
N	1.80239	0.16262	-0.15369
N	1.6633	3.24473	0.18195
N	0.05996	-1.47314	-1.2995

C	7.91385	-2.2585	-0.03419
C	6.5374	-1.98437	-0.09633
C	6.06267	-0.65024	-0.03526
C	7.00449	0.4015	0.08726
C	8.38115	0.12679	0.14326
C	8.8419	-1.20412	0.08431
H	8.26011	-3.28759	-0.07158
H	5.83764	-2.813	-0.16203
H	6.67243	1.43557	0.10929
H	9.09035	0.94562	0.22622
H	9.9067	-1.41616	0.12972
C	-2.81841	0.60489	-0.87622
C	-4.21478	0.58437	-0.78273
C	-4.83837	-0.19521	0.22677
C	-4.01127	-0.91439	1.12863
C	-2.61909	-0.8491	0.99507
H	-4.81133	1.18284	-1.45975
H	-4.45272	-1.52441	1.90652
C	0.26368	1.86795	-2.38054
C	-0.15731	2.66402	-3.45931
C	-1.53174	2.80921	-3.70893
C	-2.45561	2.14974	-2.87698
C	-1.97856	1.36476	-1.82088
H	1.31005	1.75137	-2.14314
H	0.58457	3.15477	-4.07841
H	-1.88189	3.42036	-4.53402
H	-3.52045	2.24286	-3.05487
C	-1.59386	-1.48216	1.84557
C	-1.86058	-2.30047	2.95096
C	-0.78551	-2.81332	3.6988
C	0.52773	-2.48842	3.32048
C	0.7314	-1.6654	2.20018
H	-2.88216	-2.53137	3.22873
H	-0.97267	-3.44769	4.55864
H	1.38409	-2.85626	3.87352
H	1.73012	-1.39255	1.89076
C	-7.13704	-0.11395	-0.80724
C	-8.5369	-0.16785	-0.69974
C	-9.14494	-0.35163	0.55855
C	-8.34065	-0.48382	1.70865
C	-6.94065	-0.43547	1.60149
C	-6.31875	-0.24806	0.342
H	-6.68802	0.00169	-1.78978
H	-9.14907	-0.07401	-1.59234
H	-10.22768	-0.39123	0.64156
H	-8.80128	-0.61701	2.68351
H	-6.34003	-0.51336	2.50346
N	-2.07471	-0.11996	-0.00647
N	-0.62598	1.23583	-1.58228
N	-0.30181	-1.18112	1.47719
Co	-0.20947	0.05619	-0.06659
O	-0.41905	1.42228	1.20073

H	-0.37697	2.28441	0.73477

Complex 1 Fig. [complex 1: 7coordinate Co]
E(UB3LYP) = - 2167.491651 Hartree
ZPE (kcal mol^{-1}) = 0.644639 Hartree

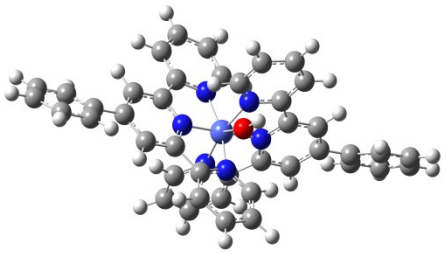


Fig. [complex 1 :7coordinate Co]

Co	0.03335	-0.11236	0.00715
C	2.57772	-0.9714	0.78964
C	2.54943	0.82058	-0.78346
C	3.97591	-0.97104	0.80654
C	3.94661	0.85885	-0.80809
C	4.68981	-0.04737	-0.00366
H	4.50804	-1.65863	1.4512
H	4.45688	1.56117	-1.4546
C	1.59754	1.66214	-1.53138
C	1.95166	2.69026	-2.41478
C	0.93743	3.41868	-3.06028
H	2.99451	2.91983	-2.59759
C	-0.7039	2.05543	-1.90803
C	-0.4069	3.09749	-2.80473
H	1.19297	4.21741	-3.74791
H	-1.72823	1.78267	-1.70246
H	-1.21818	3.62582	-3.29099
C	1.65402	-1.83558	1.54733
C	2.04037	-2.84035	2.44172
C	1.04932	-3.59612	3.094
H	3.09007	-3.03325	2.62846
C	-0.63371	-2.30275	1.92791
C	-0.30355	-3.3242	2.83258
H	1.33145	-4.37899	3.78952
H	-1.66733	-2.07236	1.71069
H	-1.09733	-3.88344	3.31327
C	6.17285	-0.02954	-0.00964
C	6.88021	1.171	-0.27059
C	6.91016	-1.21329	0.24528
C	8.2845	1.18723	-0.27247
H	6.34325	2.09996	-0.4403
C	8.31437	-1.19688	0.23571
H	6.39644	-2.15455	0.41912
C	9.00751	0.00343	-0.02126

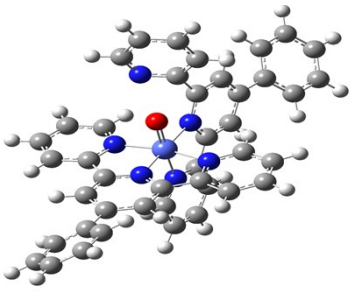
H	8.81159	2.11787	-0.46222
H	8.8645	-2.11501	0.42096
N	0.3202	-1.57631	1.30142
N	0.27447	1.35622	-1.28875
N	1.91297	-0.08603	0.00313
C	-2.49011	-0.93437	-0.87687
C	-2.50242	0.65791	0.89875
C	-3.88756	-0.95905	-0.90195
C	-3.90025	0.6625	0.92155
C	-4.62251	-0.15227	0.00862
H	-4.40369	-1.57134	-1.62998
H	-4.42582	1.26843	1.6482
C	-1.54658	-1.6797	-1.73042
C	-1.90914	-2.58367	-2.73569
C	-0.90088	-3.22316	-3.47938
H	-2.95389	-2.78783	-2.93768
C	0.75127	-2.0276	-2.17349
C	0.44522	-2.94047	-3.195
H	-1.16461	-3.92558	-4.26252
H	1.7793	-1.79426	-1.93369
H	1.25171	-3.41097	-3.74463
C	-1.57165	1.41796	1.75181
C	-1.95007	2.31159	2.75982
C	-0.95355	2.97417	3.49809
H	-2.99833	2.49172	2.96643
C	0.71846	1.81762	2.18304
C	0.39713	2.72366	3.20542
H	-1.22904	3.6701	4.28305
H	1.75036	1.60708	1.93906
H	1.19562	3.21321	3.7502
N	-0.24146	1.17979	1.47481
N	-0.21926	-1.41282	-1.45889
N	-1.84575	-0.13308	0.01093
C	-6.10588	-0.15927	0.00458
C	-6.83461	0.98618	0.41305
C	-6.8226	-1.31048	-0.40883
C	-8.23892	0.98103	0.40473
H	-6.314	1.89323	0.7069
C	-8.22696	-1.31644	-0.40995
H	-6.29291	-2.21327	-0.69965

C	-8.9412	-0.17053	-0.00502
H	-8.78202	1.87107	0.70939
H	-8.76094	-2.21064	-0.71851
H	10.09398	0.01606	-0.02573
H	-10.02774	-0.17481	-0.00884
O	-1.3127	3.95245	-0.13368
H	-1.19497	4.87583	-0.49265

Complex 1 Fig. 1RM3

E(UB3LYP) = - 2166.837078 Hartree

ZPE (kcal mol^{-1}) = 0.631621 Hartree



1RM3

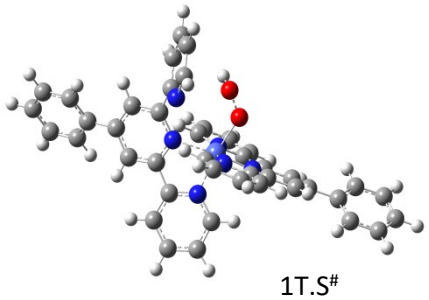
Co	0.17715	0.03218	0.07291
C	-2.3714	-0.95218	0.76936
C	-2.62656	1.03701	-0.48104
C	-3.75052	-1.17899	0.76103
C	-4.01497	0.823	-0.53741
C	-4.6156	-0.29621	0.07744
H	-4.15573	-2.03153	1.28932
H	-4.61878	1.55204	-1.06383
C	-1.41625	-1.84801	1.45327
C	-1.78527	-2.94447	2.25141
C	-0.7853	-3.71334	2.86813
H	-2.82705	-3.19773	2.39937
C	0.86823	-2.26259	1.86734
C	0.56348	-3.36668	2.67534
H	-1.05543	-4.56181	3.48774
H	1.89547	-1.97069	1.69834
H	1.36627	-3.93071	3.13543
C	-6.08039	-0.52796	0.02271
C	-6.98233	0.55977	-0.08585
C	-6.60461	-1.84374	0.07598
C	-8.36864	0.33769	-0.13625
H	-6.61118	1.58068	-0.10101
C	-7.99077	-2.06504	0.01927
H	-5.93628	-2.6987	0.1304
C	-8.87888	-0.9754	-0.08551
H	-9.04682	1.18335	-0.20846
H	-8.37564	-3.08051	0.05013
N	-0.09964	-1.52566	1.27121
N	-1.80382	0.13249	0.13552
C	2.77758	0.60963	0.88656
C	2.6074	-0.84393	-0.99139
C	4.17473	0.59687	0.80581
C	4.00058	-0.90004	-1.11114
C	4.81347	-0.17546	-0.19991
H	4.7611	1.19471	1.49206
H	4.45383	-1.50659	-1.88494
C	1.92521	1.34959	1.83527
C	2.39163	2.15448	2.88139
C	1.45848	2.79119	3.72065

H	3.45523	2.28169	3.04509
C	-0.32252	1.78956	2.41762
C	0.0864	2.60313	3.48844
H	1.79998	3.41777	4.53776
H	-1.36803	1.63865	2.19629
H	-0.66284	3.0744	4.11376
C	1.59229	-1.48206	-1.85142
C	1.87008	-2.30608	-2.94933
C	0.80237	-2.8218	-3.70591
H	2.89443	-2.53967	-3.21431
C	-0.73098	-1.66579	-2.22999
C	-0.51483	-2.49414	-3.34368
H	0.99827	-3.46077	-4.56031
H	-1.733	-1.39125	-1.93232
H	-1.36515	-2.8647	-3.9041
N	0.29539	-1.17746	-1.49875
N	0.57581	1.18022	1.61489
N	2.04731	-0.11604	0.00491
C	6.29483	-0.21677	-0.30121
C	6.92964	-0.39858	-1.55516
C	7.10141	-0.07624	0.85562
C	8.33086	-0.43483	-1.64954
H	6.33807	-0.4809	-2.46265
C	8.50248	-0.11842	0.76082
H	6.64276	0.03502	1.83417
C	9.12339	-0.29632	-0.49204
H	8.80149	-0.5635	-2.62019
H	9.1057	-0.01989	1.65895
H	-9.95112	-1.14681	-0.12677
H	10.20713	-0.32655	-0.56519
O	0.37568	1.44961	-1.08907
C	-1.95513	3.89563	-2.89245
C	-1.3106	4.78518	-2.01055
C	-1.10713	4.38205	-0.67813
C	-2.10405	2.31079	-1.06685
H	-2.13269	4.17248	-3.92725
H	-0.98198	5.76597	-2.33877
H	-0.62543	5.0444	0.03573
C	-2.36891	2.64195	-2.41229
H	-2.86293	1.93023	-3.06608
N	-1.49667	3.17222	-0.2053

Complex 1 Fig. 1T.S[#]
E(UB3LYP) = - 2242.634720 Hartree
ZPE (kcal mol^{-1}) = 0.645749

O	0.94629	1.5138	-2.1334
H	0.9125	2.4582	-2.41668
C	-3.76543	-1.30565	0.62945
C	-2.3898	-1.06441	0.68165
C	-2.65619	1.05917	-0.31168
C	-4.04235	0.84198	-0.40211

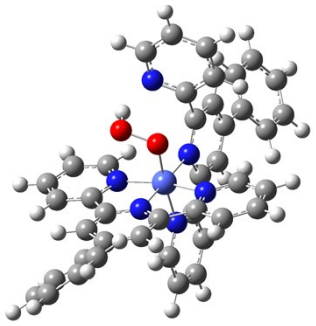
C	-4.63641	-0.35343	0.05634
H	-4.15659	-2.24387	0.99915
H	-4.6534	1.64648	-0.79319
C	-2.16521	2.42286	-0.69739
C	-2.21938	2.86088	-2.03461
C	-1.46741	4.51746	0.04288
C	-1.84456	4.18448	-2.32458
H	-2.52481	2.18076	-2.82341
C	-1.45357	5.02996	-1.26806
H	-1.19533	5.14476	0.8875
H	-1.8615	4.54795	-3.34782
H	-1.16052	6.05943	-1.44741
C	-1.43495	-2.03191	1.25876
C	-1.80539	-3.21212	1.92626
C	0.84845	-2.48914	1.63638
C	-0.80806	-4.04499	2.45751
H	-2.84772	-3.47986	2.0412
C	0.54104	-3.67725	2.31258
H	1.87577	-2.17972	1.50769
H	-1.08025	-4.95803	2.97618
H	1.34281	-4.28833	2.70998
N	-1.82451	0.09295	0.18862
N	-1.81982	3.24038	0.3327
N	-0.11801	-1.69013	1.12269
C	-8.14612	-1.64245	0.80231
C	-6.76136	-1.42393	0.89391
C	-6.09851	-0.58857	-0.03962
C	-6.86013	0.01966	-1.06842
C	-8.24382	-0.2042	-1.16281
C	-8.89318	-1.03496	-0.2272
H	-6.20946	-1.88165	1.71009
H	-6.37489	0.64439	-1.81306
C	2.76901	0.45832	1.00023
C	4.16554	0.45421	0.91686
C	4.80222	-0.21389	-0.16274
C	3.98885	-0.84575	-1.13895
C	2.59529	-0.79811	-1.01446
H	4.75445	0.97833	1.65894
H	4.44124	-1.3733	-1.96912
C	-0.33392	1.47183	2.64297
C	0.07301	2.16711	3.79503
C	1.4446	2.32623	4.04971
C	2.37991	1.78175	3.14949
C	1.91645	1.09405	2.0221
H	-1.37896	1.34979	2.40145
H	-0.67735	2.5719	4.46403
H	1.78473	2.8615	4.92991
H	3.44299	1.89043	3.32869
C	1.57829	-1.3456	-1.93043
C	1.85422	-2.06944	-3.09619
C	0.78648	-2.50003	-3.90402
C	-0.52896	-2.19045	-3.52112



1T.S#

C	-0.74264	-1.4662	-2.33689
H	2.87762	-2.29079	-3.37491
H	0.9808	-3.06068	-4.81218
H	-1.37985	-2.4962	-4.11858
H	-1.74384	-1.20819	-2.02289
C	7.09251	-0.22128	0.89367
C	8.49352	-0.25201	0.7924
C	9.11225	-0.29915	-0.47323
C	8.31756	-0.31822	-1.63734
C	6.91644	-0.29337	-1.53703
C	6.2838	-0.24303	-0.26994
H	6.63544	-0.21096	1.87932
H	6.32295	-0.28182	-2.44697
N	2.03882	-0.17457	0.05009
N	0.56681	0.94941	1.78334
N	0.28344	-1.06015	-1.55764
Co	0.17565	-0.0166	0.11811
O	0.37941	1.65284	-0.73433
H	8.78636	-0.34539	-2.61701
H	9.09847	-0.24574	1.69477
H	-8.81107	0.26151	-1.96384
H	-8.64032	-2.27705	1.53261
H	10.1959	-0.32051	-0.55107
H	-9.96389	-1.20596	-0.29906

Complex 1 Fig. 1RM4
E(UB3LYP) = - 2242.640953 Hartree
ZPE (kcal mol^{-1}) = 0.647682 Hartree



1RM4

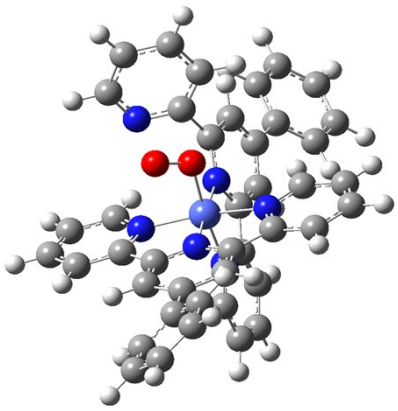
Co	0.17715	0.03218	0.07291
C	-2.3714	-0.95218	0.76936
C	-2.62656	1.03701	-0.48104
C	-3.75052	-1.17899	0.76103
C	-4.01497	0.823	-0.53741
C	-4.6156	-0.29621	0.07744
H	-4.15573	-2.03153	1.28932
H	-4.61878	1.55204	-1.06383
C	-1.41625	-1.84801	1.45327
C	-1.78527	-2.94447	2.25141
C	-0.7853	-3.71334	2.86813
H	-2.82705	-3.19773	2.39937
C	0.86823	-2.26259	1.86734
C	0.56348	-3.36668	2.67534
H	-1.05543	-4.56181	3.48774

H	1.89547	-1.97069	1.69834
H	1.36627	-3.93071	3.13543
C	-6.08039	-0.52796	0.02271
C	-6.98233	0.55977	-0.08585
C	-6.60461	-1.84374	0.07598
C	-8.36864	0.33769	-0.13625
H	-6.61118	1.58068	-0.10101
C	-7.99077	-2.06504	0.01927
H	-5.93628	-2.6987	0.1304
C	-8.87888	-0.9754	-0.08551
H	-9.04682	1.18335	-0.20846
H	-8.37564	-3.08051	0.05013
N	-0.09964	-1.52566	1.27121
N	-1.80382	0.13249	0.13552
C	2.77758	0.60963	0.88656
C	2.6074	-0.84393	-0.99139
C	4.17473	0.59687	0.80581
C	4.00058	-0.90004	-1.11114
C	4.81347	-0.17546	-0.19991
H	4.7611	1.19471	1.49206
H	4.45383	-1.50659	-1.88494
C	1.92521	1.34959	1.83527
C	2.39163	2.15448	2.88139
C	1.45848	2.79119	3.72065
H	3.45523	2.28169	3.04509
C	-0.32252	1.78956	2.41762
C	0.0864	2.60313	3.48844
H	1.79998	3.41777	4.53776
H	-1.36803	1.63865	2.19629
H	-0.66284	3.0744	4.11376
C	1.59229	-1.48206	-1.85142
C	1.87008	-2.30608	-2.94933
C	0.80237	-2.8218	-3.70591
H	2.89443	-2.53967	-3.21431
C	-0.73098	-1.66579	-2.22999
C	-0.51483	-2.49414	-3.34368
H	0.99827	-3.46077	-4.56031
H	-1.733	-1.39125	-1.93232
H	-1.36515	-2.8647	-3.9041
N	0.29539	-1.17746	-1.49875
N	0.57581	1.18022	1.61489
N	2.04731	-0.11604	0.00491
C	6.29483	-0.21677	-0.30121
C	6.92964	-0.39858	-1.55516
C	7.10141	-0.07624	0.85562
C	8.33086	-0.43483	-1.64954
H	6.33807	-0.4809	-2.46265
C	8.50248	-0.11842	0.76082
H	6.64276	0.03502	1.83417
C	9.12339	-0.29632	-0.49204
H	8.80149	-0.5635	-2.62019
H	9.1057	-0.01989	1.65895

H	-9.95112	-1.14681	-0.12677
H	10.20713	-0.32655	-0.56519
O	0.37568	1.44961	-1.08907
C	-1.95513	3.89563	-2.89245
C	-1.3106	4.78518	-2.01055
C	-1.10713	4.38205	-0.67813
C	-2.10405	2.31079	-1.06685
H	-2.13269	4.17248	-3.92725
H	-0.98198	5.76597	-2.33877
H	-0.62543	5.0444	0.03573
C	-2.36891	2.64195	-2.41229
H	-2.86293	1.93023	-3.06608
N	-1.49667	3.17222	-0.2053
O	1.59928	2.26376	-1.2855
H	2.56675	2.69305	-1.01484

Complex 1 Fig. 1RM5
E(UB3LYP) = - 2242.017746 Hartree
ZPE (kcal mol^{-1}) = 0.634896 Hartree

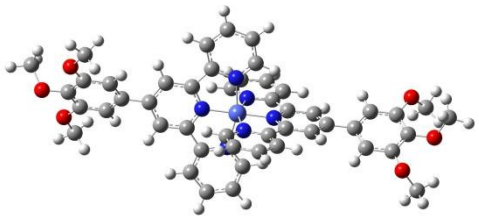
C(Fragment=1)	-3.74405	-1.23181	0.80186
C(Fragment=1)	-2.37449	-0.95437	0.82085
C(Fragment=1)	-2.69199	1.01352	-0.44201
C(Fragment=1)	-4.07083	0.74727	-0.51091
C(Fragment=1)	-4.63613	-0.39186	0.09983
H(Fragment=1)	-4.1215	-2.09371	1.33494
H(Fragment=1)	-4.69465	1.45468	-1.04365
C(Fragment=1)	-2.22905	2.32168	-1.00429
C(Fragment=1)	-2.42719	2.63624	-2.3632
C(Fragment=1)	-1.39179	4.44825	-0.55492
C(Fragment=1)	-2.06431	3.91624	-2.81839
H(Fragment=1)	-2.83371	1.89648	-3.04551
C(Fragment=1)	-1.53452	4.84146	-1.89955
H(Fragment=1)	-0.99876	5.13755	0.18718
H(Fragment=1)	-2.19319	4.18331	-3.86289
H(Fragment=1)	-1.24568	5.84109	-2.20777
C(Fragment=1)	-1.40575	-1.80629	1.53978
C(Fragment=1)	-1.76068	-2.87794	2.37737
C(Fragment=1)	0.88235	-2.15792	1.99519
C(Fragment=1)	-0.75313	-3.60089	3.03519
H(Fragment=1)	-2.79858	-3.14547	2.52637
C(Fragment=1)	0.59036	-3.23411	2.84376
H(Fragment=1)	1.90509	-1.85392	1.8251
H(Fragment=1)	-1.01356	-4.42928	3.6853
H(Fragment=1)	1.39926	-3.76201	3.33484
N(Fragment=1)	-1.83436	0.14052	0.17708
N(Fragment=1)	-1.73298	3.21529	-0.10814
N(Fragment=1)	-0.09438	-1.46567	1.35985
C(Fragment=1)	-7.9325	-2.3015	0.02217
C(Fragment=1)	-6.55809	-2.02063	0.09596
C(Fragment=1)	-6.0887	-0.68487	0.02705
C(Fragment=1)	-7.03384	0.36156	-0.11509



1RM5

C(Fragment=1)	-8.40852	0.08003	-0.18233
C(Fragment=1)	-8.86386	-1.25238	-0.11558
H(Fragment=1)	-8.27459	-3.33171	0.06558
H(Fragment=1)	-5.85562	-2.84559	0.17648
H(Fragment=1)	-6.70647	1.39693	-0.14337
H(Fragment=1)	-9.12048	0.89478	-0.28004
H(Fragment=1)	-9.92719	-1.46962	-0.16976
C(Fragment=1)	2.78837	0.60061	0.84678
C(Fragment=1)	4.18388	0.54533	0.76306
C(Fragment=1)	4.79672	-0.29232	-0.20556
C(Fragment=1)	3.96009	-1.04361	-1.07286
C(Fragment=1)	2.5699	-0.94746	-0.94879
H(Fragment=1)	4.78911	1.15945	1.41788
H(Fragment=1)	4.39311	-1.70054	-1.81628
C(Fragment=1)	-0.27465	1.90359	2.35423
C(Fragment=1)	0.16104	2.75072	3.38808
C(Fragment=1)	1.53841	2.92411	3.59751
C(Fragment=1)	2.45141	2.23852	2.77413
C(Fragment=1)	1.96003	1.40316	1.76539
H(Fragment=1)	-1.32438	1.76565	2.14714
H(Fragment=1)	-0.57304	3.25868	4.00251
H(Fragment=1)	1.89976	3.5754	4.38631
H(Fragment=1)	3.51877	2.35179	2.92249
C(Fragment=1)	1.53572	-1.60627	-1.7682
C(Fragment=1)	1.78929	-2.496	-2.81941
C(Fragment=1)	0.70708	-3.02514	-3.5457
C(Fragment=1)	-0.60004	-2.64224	-3.20269
C(Fragment=1)	-0.79205	-1.74906	-2.13578
H(Fragment=1)	2.80675	-2.76921	-3.07289
H(Fragment=1)	0.88467	-3.71565	-4.36318
H(Fragment=1)	-1.46104	-3.01873	-3.74237
H(Fragment=1)	-1.78624	-1.43206	-1.85532
C(Fragment=1)	7.09529	-0.19288	0.827
C(Fragment=1)	8.49405	-0.27386	0.72441
C(Fragment=1)	9.0998	-0.53257	-0.5218
C(Fragment=1)	8.29436	-0.71305	-1.66449
C(Fragment=1)	6.89526	-0.63854	-1.56196
C(Fragment=1)	6.27566	-0.37537	-0.3147
H(Fragment=1)	6.64791	-0.01861	1.80154
H(Fragment=1)	9.10709	-0.14247	1.6116
H(Fragment=1)	10.18185	-0.59257	-0.60123
H(Fragment=1)	8.7535	-0.90396	-2.63038
H(Fragment=1)	6.29457	-0.75488	-2.45973
N(Fragment=1)	2.03409	-0.15272	0.00899
N(Fragment=1)	0.60441	1.25021	1.56375
N(Fragment=1)	0.24744	-1.25031	-1.42934
Co(Fragment=1)	0.17013	0.03173	0.09072
O(Fragment=1)	0.31765	1.38955	-1.27189
O(Fragment=2)	1.2557	2.34922	-1.12487

Complex 3 Fig. 3RM1



E(UB3LYP) = - 2778.749302 Hartree

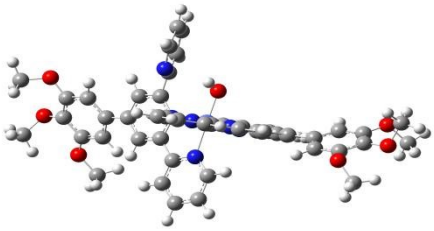
ZPE (kcal mol^{-1}) = 0.818933 Hartree

C	-4.01806	-1.17336	-0.00583	
C	-2.59452	-1.11097	-0.07469	
C	-2.57509	1.12567	0.08315	
C	-3.99721	1.22573	0.0702	
C	-4.75751	0.03258	0.10654	
H	-4.52358	-2.11534	-0.04535	3RM1
H	-4.47844	2.1811	0.05089	
C	-1.62844	2.24546	0.22418	
C	-2.05454	3.55771	0.37287	
C	0.61821	2.78854	0.36458	
C	-1.09452	4.53655	0.54468	
H	-3.09961	3.79951	0.35768	
C	0.25646	4.15364	0.53918	
H	1.64735	2.51003	0.35381	
H	-1.38163	5.55763	0.68508	
H	1.01335	4.89709	0.65794	
C	-1.66172	-2.25777	-0.26676	
C	-2.09508	-3.56697	-0.4346	
C	0.58263	-2.81613	-0.47795	
C	-1.13621	-4.55194	-0.61381	
H	-3.14026	-3.8058	-0.42978	
C	0.21683	-4.17477	-0.631	
H	1.61259	-2.53144	-0.50794	
H	-1.42611	-5.57604	-0.73669	
H	0.97021	-4.92069	-0.76611	
N	-1.92168	-0.00244	0.00889	
N	-0.33764	1.85017	0.22359	
N	-0.36418	-1.88921	-0.27435	
C	-8.39729	-1.34596	0.68568	
C	-6.98663	-1.20115	0.56714	
C	-6.34087	0.02016	0.27796	
C	-7.14185	1.17738	0.16277	
C	-8.56516	1.07214	0.27558	
C	-9.19907	-0.19406	0.49109	
H	-6.39172	-2.07576	0.67692	
H	-6.681	2.12785	-0.02964	
C	2.62223	-0.1498	1.16816	
C	4.05384	-0.16022	1.27128	
C	4.84265	-0.12542	0.08346	
C	4.09389	-0.06179	-1.13955	
C	2.65031	0.03403	-1.08152	
H	4.52428	-0.19392	2.23251	
H	4.60269	-0.05484	-2.08151	
C	-0.62025	-0.38911	2.79831	
C	-0.30117	-0.57897	4.16268	
C	1.04071	-0.59545	4.57559	
C	2.03557	-0.44582	3.61689	
C	1.64911	-0.28237	2.2928	
H	-1.64209	-0.37056	2.48728	

H	-1.0815	-0.68207	4.88587
H	1.29691	-0.73897	5.60332
H	3.07182	-0.45039	3.88835
C	1.68754	0.25859	-2.22048
C	2.07428	0.45795	-3.54649
C	1.07783	0.6591	-4.49915
C	-0.26377	0.64228	-4.08664
C	-0.58335	0.47716	-2.72161
H	3.10871	0.46786	-3.82254
H	1.3315	0.80418	-5.52994
H	-1.04247	0.785	-4.80611
H	-1.60645	0.48344	-2.40813
C	7.17668	0.13646	1.32774
C	8.59974	0.32483	1.31837
C	9.34352	0.04767	0.13633
C	8.65462	-0.27932	-1.04826
C	7.23162	-0.42026	-1.05145
C	6.45858	-0.14395	0.11824
H	6.64254	0.24754	2.2474
H	6.73861	-0.71409	-1.95404
N	1.97225	-0.05588	0.0365
N	0.36185	-0.26733	1.88886
N	0.39247	0.25843	-1.82567
Co	0.02156	-0.0291	0.02266
O	9.27848	0.84594	2.49605
O	10.7917	0.16577	0.05842
O	9.43201	-0.42142	-2.27
O	-9.37535	2.24456	0.15083
O	-10.6263	-0.31193	0.44002
O	-8.80706	-2.76322	0.92966
C	-9.64592	2.7596	1.45476
H	-8.83275	2.97336	2.11548
H	-9.54157	3.73958	1.03975
H	-10.63875	3.05897	1.72071
C	-11.26498	-0.08092	1.67583
H	-11.38144	-1.1461	1.67304
H	-11.59737	0.80839	1.18163
H	-12.25555	-0.09053	2.07745
C	9.40673	-0.02281	3.62895
H	9.92188	-0.91465	3.35295
H	9.96104	0.48549	4.39776
H	8.43403	-0.26892	3.99907
C	11.53522	-1.03157	0.35547
H	11.12707	-1.85656	-0.18813
H	11.48873	-1.23448	1.40292
H	12.56118	-0.88946	0.06593
C	9.46736	-1.71327	-2.89494
H	9.83604	-2.45685	-2.22104
H	10.1124	-1.66611	-3.7538
H	8.47864	-1.96955	-3.20474
C	-9.97642	-3.48664	1.5165
H	-9.78839	-4.50684	1.24235

H	-10.05614	-3.39219	2.61325
H	-10.90277	-3.17464	1.09621

Complex 3 Fig. 3RM2
E(UB3LYP) = - 2854.529028 Hartree
ZPE (kcal mol^{-1}) = 0.834273 Hartree



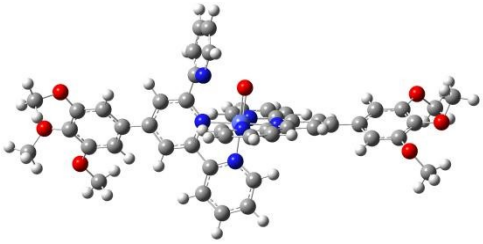
3RM2

C	-3.76563	-1.21181	0.79371
C	-2.38093	-0.99114	0.76448
C	-2.61374	0.99389	-0.43871
C	-4.03635	0.79619	-0.46925
C	-4.62277	-0.27165	0.24879
H	-4.15953	-2.09729	1.23762
H	-4.65769	1.47475	-1.01625
C	-2.11516	2.32394	-1.06849
C	-2.7048	2.78722	-2.2639
C	-0.94184	4.33026	-0.80152
C	-2.37883	4.04884	-2.74473
H	-3.40876	2.17434	-2.79413
C	-1.54079	4.86149	-1.96397
H	-0.32652	4.95072	-0.17705
H	-2.75789	4.39421	-3.68646
H	-1.36336	5.87	-2.24752
C	-1.3801	-1.85093	1.45931
C	-1.71817	-2.9574	2.2414
C	0.89167	-2.08157	1.86705
C	-0.6888	-3.62937	2.89409
H	-2.73951	-3.26155	2.34121
C	0.62893	-3.18311	2.71288
H	1.89245	-1.75648	1.71585
H	-0.90238	-4.46146	3.52448
H	1.43981	-3.68022	3.20434
N	-1.80096	0.03077	0.14063
N	-1.14555	3.03692	-0.46488
N	-0.12964	-1.45207	1.28281
C	-8.1105	-1.79778	1.17265
C	-6.70241	-1.612	1.05586
C	-6.18106	-0.43822	0.4798
C	-7.07863	0.58659	0.13784
C	-8.47135	0.44985	0.33277
C	-9.0147	-0.757	0.86396
H	-6.0281	-2.37945	1.41594
H	-6.70327	1.49	-0.26699
C	2.77671	0.51655	0.90044
C	4.19611	0.46427	0.90895
C	4.84695	-0.1247	-0.20892
C	4.03087	-0.74996	-1.18392
C	2.62233	-0.72275	-0.99483
H	4.76097	0.85339	1.71602
H	4.4707	-1.24655	-2.04984

C	-0.33677	1.83483	2.20903
C	0.05648	2.63964	3.29628
C	1.42432	2.74609	3.62934
C	2.36002	2.04964	2.87217
C	1.88631	1.27424	1.83175
H	-1.36027	1.7432	1.96119
H	-0.69142	3.14865	3.88963
H	1.73182	3.3808	4.44205
H	3.41177	2.11429	3.09462
C	1.57444	-1.40036	-1.83907
C	1.82661	-2.2364	-2.93798
C	0.73296	-2.76403	-3.62819
C	-0.56233	-2.43036	-3.19806
C	-0.73709	-1.60122	-2.07373
H	2.82731	-2.45351	-3.23922
H	0.8836	-3.39281	-4.46796
H	-1.4002	-2.82538	-3.70237
H	-1.7257	-1.35433	-1.72589
C	7.26169	0.21343	0.66151
C	8.65999	0.05654	0.50913
C	9.20504	-0.28459	-0.77168
C	8.29396	-0.28512	-1.87965
C	6.9208	-0.33408	-1.64719
C	6.39292	-0.07781	-0.39608
H	6.86676	0.54392	1.60231
H	6.26887	-0.56062	-2.45499
N	2.05139	-0.0822	0.00254
N	0.58163	1.15283	1.5213
N	0.33039	-1.12565	-1.4209
Co	0.1247	-0.02572	0.07168
O	-0.31277	1.37709	-0.99917
H	-0.0532	2.19109	-0.58726
O	-8.57314	-3.08172	1.57577
O	-10.44541	-0.91661	1.10639
O	-9.26734	1.56873	-0.06885
O	9.42245	0.254	1.72183
O	10.60953	-0.61543	-0.94302
O	8.64854	-0.23096	-3.27431
C	11.48523	0.48381	-1.22172
H	12.49337	0.11885	-1.30541
H	11.42673	1.18881	-0.4246
H	11.20367	0.94638	-2.14002
C	10.62076	1.0217	1.56352
H	11.36102	0.44793	1.04303
H	10.99119	1.28632	2.54099
H	10.40428	1.91574	1.00562
C	9.88859	-0.78661	-3.65938
H	10.10166	-1.80431	-3.4276
H	10.54535	-0.23878	-4.309
H	9.39595	-1.10693	-4.55873
C	-8.24439	-3.234	2.95228
H	-8.36745	-4.26774	3.23119

H	-7.21544	-2.93812	3.09562
H	-8.88581	-2.61508	3.55494
C	-10.82433	-0.7136	2.48895
H	-10.30945	-1.4222	3.10753
H	-10.56024	0.27704	2.79046
H	-11.88998	-0.85125	2.60405
C	-10.26644	1.89786	0.88708
H	-9.79896	2.08889	1.82778
H	-10.78818	2.77586	0.55686
H	-10.95895	1.08966	0.98801

Complex 3 Fig. 3RM3
E(UB3LYP) = - 2853.866195 Hartree
ZPE (kcal mol^{-1}) = 0.822637 Hartree



3RM3

C	3.8246	0.82111	0.78736
C	2.44751	0.58554	0.82784
C	2.66017	-1.30261	-0.56931
C	4.04652	-1.07771	-0.65508
C	4.66864	-0.00132	0.01069
H	4.2427	1.63682	1.3609
H	4.63296	-1.76822	-1.24823
C	2.16092	-2.55446	-1.22284
C	2.42339	-2.79883	-2.58606
C	1.25892	-4.68978	-0.94766
C	2.05777	-4.04015	-3.136
H	2.88089	-2.03169	-3.20269
C	1.46506	-5.00787	-2.30339
H	0.8139	-5.4113	-0.26826
H	2.23427	-4.24631	-4.1873
H	1.17441	-5.98124	-2.68467
C	1.53027	1.43023	1.62062
C	1.94973	2.43258	2.51324
C	-0.72952	1.86108	2.13903
C	0.98902	3.16249	3.23026
H	3.0015	2.64094	2.6601
C	-0.37344	2.87239	3.04126
H	-1.76895	1.61621	1.9723
H	1.29946	3.9373	3.92314
H	-1.1482	3.40944	3.57569
N	1.85045	-0.44651	0.13264
N	1.59676	-3.49034	-0.41009
N	0.20181	1.15944	1.44778
C	8.02352	1.7856	-0.03096
C	6.64512	1.54966	0.08093
C	6.12771	0.24223	-0.08609
C	7.01525	-0.81881	-0.34905
C	8.40036	-0.59228	-0.43731
C	8.92543	0.71288	-0.28523
H	5.97245	2.38303	0.24384
H	6.67057	-1.84237	-0.44797

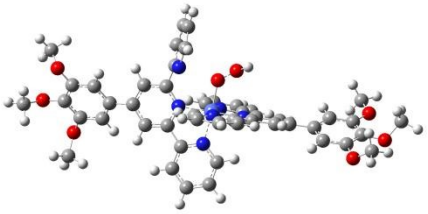
C	-2.75762	-0.80137	0.96292
C	-4.15454	-0.73428	0.91221
C	-4.78106	0.13335	-0.02041
C	-3.95746	0.89608	-0.88873
C	-2.56492	0.78347	-0.79947
H	-4.75005	-1.36241	1.56266
H	-4.39959	1.57353	-1.60804
C	0.32505	-2.25236	2.28506
C	-0.09031	-3.11635	3.31255
C	-1.46182	-3.2485	3.5846
C	-2.38811	-2.50647	2.82826
C	-1.91619	-1.65408	1.82336
H	1.36809	-2.14202	2.03059
H	0.65328	-3.66902	3.8748
H	-1.80791	-3.91227	4.36977
H	-3.45064	-2.58912	3.02417
C	-1.54456	1.44863	-1.63109
C	-1.8161	2.36006	-2.6598
C	-0.74677	2.89691	-3.39899
C	0.56532	2.50151	-3.09
C	0.77405	1.58677	-2.04422
H	-2.83712	2.64422	-2.88566
H	-0.93751	3.60332	-4.19983
H	1.41689	2.88447	-3.64018
H	1.77163	1.25864	-1.78926
C	-7.05193	0.00706	1.0576
C	-8.45201	0.07401	0.99192
C	-9.09853	0.35798	-0.23628
C	-8.30276	0.62199	-1.37888
C	-6.90523	0.54898	-1.30952
C	-6.26145	0.22791	-0.09282
H	-6.60447	-0.20014	2.02415
H	-6.34701	0.71886	-2.22444
N	-2.01596	-0.03315	0.12941
N	-0.56691	-1.54107	1.55945
N	-0.25311	1.08002	-1.32807
Co	-0.15643	-0.26888	0.11937
O	-0.44846	-1.53351	-1.2333
O	8.60437	3.04749	0.05244
O	10.28689	0.9237	-0.50592
O	9.18715	-1.70469	-0.74987
O	-9.17529	-0.22669	2.15292
O	-10.49579	0.40218	-0.2826
O	-8.89243	0.88706	-2.62546
C	-11.15338	-0.65781	-1.08568
H	-10.91392	-1.64146	-0.66634
H	-10.83117	-0.59819	-2.12952
H	-12.22365	-0.46155	-1.00301
C	-10.05374	0.8356	2.69135
H	-9.45188	1.70943	2.96986
H	-10.51947	0.40379	3.57938
H	-10.81286	1.11133	1.95485

C	-9.63869	2.16149	-2.73515
H	-8.95871	3.00494	-2.56636
H	-10.46255	2.18772	-2.0153
H	-10.02351	2.18715	-3.75618
C	7.74198	4.21437	0.2713
H	8.42001	5.06844	0.29439
H	7.02594	4.32906	-0.55125
H	7.21063	4.13412	1.22704
C	11.08861	1.5263	0.58499
H	10.72832	2.53257	0.80728
H	11.03773	0.89342	1.47913
H	12.11088	1.55627	0.2034
C	10.40552	-1.97592	0.03937
H	10.18592	-1.91614	1.11248
H	10.69225	-2.99597	-0.22505
H	11.19932	-1.27465	-0.22482

Complex 3 Fig. 3T.S#

E(UB3LYP) = - 2929.663991 Hartree

ZPE (kcal mol^{-1}) = 0.837069 Hartree



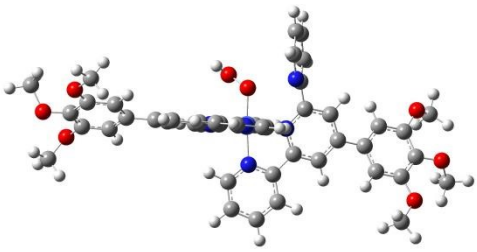
3T.S#

O	1.21218	1.27818	-2.24977
H	1.98975	1.87564	-2.13461
C	-3.78757	-0.87623	0.89743
C	-2.41217	-0.63185	0.93635
C	-2.64298	1.2661	-0.44397
C	-4.02694	1.03191	-0.53237
C	-4.63893	-0.05562	0.12551
H	-4.19887	-1.698	1.46723
H	-4.61666	1.72533	-1.11913
C	-2.13967	2.5334	-1.06351
C	-2.30495	2.77762	-2.44129
C	-1.29645	4.6753	-0.7088
C	-1.91352	4.02498	-2.95646
H	-2.70408	2.00576	-3.09195
C	-1.3941	4.99395	-2.07602
H	-0.91993	5.40249	0.00561
H	-2.01338	4.23642	-4.01693
H	-1.08459	5.97173	-2.43103
C	-1.48421	-1.46425	1.72892
C	-1.89079	-2.46245	2.63171
C	0.78103	-1.86094	2.24994
C	-0.92069	-3.17221	3.35632
H	-2.94018	-2.68131	2.78101
C	0.43776	-2.86543	3.16472
H	1.81744	-1.60567	2.08083
H	-1.22089	-3.94343	4.05765
H	1.21952	-3.38527	3.70593
N	-1.8259	0.40774	0.24459
N	-1.66335	3.47177	-0.20329
N	-0.15918	-1.17995	1.54997
C	-7.98602	-1.87789	0.12386

C	-6.60813	-1.61569	0.2091
C	-6.09612	-0.3122	0.03016
C	-7.00049	0.73883	-0.24773
C	-8.37278	0.48403	-0.34101
C	-8.89337	-0.8217	-0.1494
H	-5.95556	-2.46174	0.39833
H	-6.66739	1.76304	-0.37822
C	2.79683	0.77051	0.9796
C	4.19097	0.66959	0.92592
C	4.79466	-0.25797	0.03554
C	3.9497	-1.04463	-0.79089
C	2.56149	-0.88754	-0.71259
H	4.80307	1.31168	1.54646
H	4.37217	-1.77529	-1.46877
C	-0.25147	2.24598	2.34716
C	0.19001	3.14504	3.33413
C	1.56792	3.29639	3.55667
C	2.47515	2.53711	2.79371
C	1.97681	1.65132	1.83176
H	-1.30085	2.12296	2.12894
H	-0.54002	3.70906	3.9029
H	1.93391	3.98697	4.30908
H	3.54279	2.63214	2.95258
C	1.52142	-1.56898	-1.50515
C	1.76653	-2.53772	-2.48555
C	0.68274	-3.07545	-3.20306
C	-0.61669	-2.62323	-2.92045
C	-0.79948	-1.656	-1.91822
H	2.77867	-2.86384	-2.69392
H	0.85312	-3.82535	-3.9682
H	-1.47831	-3.00245	-3.45735
H	-1.78701	-1.28509	-1.68407
C	7.06166	-0.12907	1.10467
C	8.46127	-0.25981	1.05354
C	9.09969	-0.67046	-0.1404
C	8.29692	-0.94252	-1.28498
C	6.90179	-0.80241	-1.23018
C	6.27133	-0.39612	-0.02961
H	6.62208	0.15833	2.05366
H	6.31115	-0.98278	-2.12006
N	2.03456	-0.01001	0.17457
N	0.62182	1.52039	1.61628
N	0.24093	-1.14883	-1.22149
Co	0.1799	0.23224	0.19639
O	0.36442	1.63001	-1.07028
O	9.14154	-0.04576	2.2557
O	10.47538	-0.90557	-0.12756
O	8.99047	-1.3713	-2.41258
O	-9.24417	1.55694	-0.60484
O	-10.24719	-1.10335	-0.31351
O	-8.36399	-3.21594	0.24932
C	10.34486	0.81015	2.26736

H	10.53008	1.02248	3.32247
H	11.19489	0.28531	1.82743
H	10.15354	1.74507	1.72637
C	11.32388	-0.13317	-1.06553
H	12.34528	-0.45857	-0.85955
H	11.22163	0.94	-0.86423
H	11.04688	-0.35721	-2.09758
C	8.2366	-1.72142	-3.62195
H	7.53831	-2.54258	-3.42089
H	8.98955	-2.04239	-4.34287
H	7.69542	-0.85106	-4.01167
C	-9.78937	1.60275	-1.98021
H	-10.44659	2.47368	-2.00869
H	-8.97158	1.72318	-2.70093
H	-10.35585	0.69133	-2.20011
C	-11.23399	-0.38744	0.53422
H	-10.74253	0.35359	1.16833
H	-11.73947	-1.14144	1.1456
H	-11.95031	0.10439	-0.1285
C	-9.54284	-3.57468	1.06401
H	-9.45163	-4.65026	1.22983
H	-9.52046	-3.04557	2.0244
H	-10.46542	-3.34463	0.52794

Complex 3 Fig. 3RM4
E(UB3LYP) = - 2929.670054 Hartree
ZPE (kcal mol^{-1}) = 0.837849 Hartree



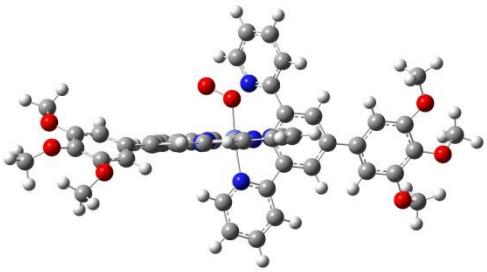
3RM4

C	3.82687	-0.89529	0.75936
C	2.44666	-0.68391	0.80747
C	2.65684	1.39099	-0.29777
C	4.04661	1.19893	-0.38718
C	4.67178	0.04219	0.1258
H	4.2417	-1.8022	1.17763
H	4.63883	1.99771	-0.81628
C	2.13405	2.72146	-0.74202
C	2.35333	3.17636	-2.0574
C	1.16258	4.74643	-0.12338
C	1.92413	4.46915	-2.4039
H	2.82204	2.52945	-2.79211
C	1.3128	5.27095	-1.42103
H	0.71283	5.34024	0.66766
H	2.06456	4.84112	-3.41432
H	0.97076	6.27623	-1.6448
C	1.52109	-1.63786	1.44795
C	1.92614	-2.7613	2.18842
C	-0.74755	-2.12625	1.87942

C	0.95606	-3.58109	2.78534
H	2.97576	-2.99442	2.30973
C	-0.40273	-3.25616	2.63208
H	-1.78401	-1.85588	1.74254
H	1.25637	-4.45019	3.36069
H	-1.18537	-3.85704	3.0797
N	1.84855	0.42929	0.25465
N	1.56489	3.49774	0.21817
N	0.19398	-1.34068	1.30048
C	8.20823	-1.13185	0.88396
C	6.82064	-0.94892	0.98116
C	6.13528	-0.16472	0.02181
C	6.86023	0.41569	-1.0367
C	8.24687	0.21406	-1.15357
C	8.94269	-0.55822	-0.19352
H	6.28491	-1.36779	1.82441
H	6.37204	0.9941	-1.8136
C	-2.51503	-0.75779	-0.90493
C	-3.90075	-0.90887	-1.01722
C	-4.75603	-0.2781	-0.07596
C	-4.16614	0.49976	0.95592
C	-2.77403	0.60905	1.02749
H	-4.31814	-1.47709	-1.83858
H	-4.78432	0.98716	1.69913
C	0.86024	-1.29977	-2.19502
C	0.689	-2.08233	-3.34832
C	-0.60706	-2.47888	-3.7178
C	-1.6992	-2.07239	-2.93084
C	-1.4671	-1.28362	-1.79777
H	1.84518	-0.97774	-1.8891
H	1.55675	-2.36633	-3.93198
H	-0.76811	-3.08755	-4.60117
H	-2.70816	-2.36016	-3.2015
C	-1.96465	1.35652	2.0073
C	-2.46963	2.06725	3.10117
C	-1.56969	2.71884	3.96569
C	-0.19175	2.63944	3.70885
C	0.25806	1.91834	2.58896
H	-3.53694	2.10898	3.28302
H	-1.94148	3.27248	4.82132
H	0.53254	3.12492	4.35235
H	1.30699	1.85691	2.34536
C	-6.79312	-1.59861	-0.71599
C	-8.18722	-1.73819	-0.8151
C	-9.04757	-0.70534	-0.37963
C	-8.47858	0.46717	0.19071
C	-7.08437	0.60434	0.28743
C	-6.22964	-0.42558	-0.17355
H	-6.17814	-2.42962	-1.0446
H	-6.6643	1.51892	0.68851
N	-2.00103	-0.03116	0.11562
N	-0.18986	-0.91826	-1.43457

N	-0.60877	1.2952	1.7613
Co	-0.14741	0.22824	0.17438
O	-0.32139	1.74718	-0.96676
O	-1.46713	1.66291	-2.14812
O	-10.42822	-0.89109	-0.46835
O	-8.686	-2.90279	-1.41454
O	-9.38969	1.42489	0.62258
O	8.96692	-1.83027	1.81815
O	10.33361	-0.63485	-0.26742
O	8.8782	0.87129	-2.21338
C	-11.17287	0.02628	-1.36275
H	-12.21139	-0.3065	-1.31507
H	-10.79333	-0.06384	-2.38728
H	-11.08246	1.05607	-1.00804
C	-9.51606	-3.78654	-0.5668
H	-10.40355	-3.25291	-0.2166
H	-8.92484	-4.14968	0.28309
H	-9.79992	-4.62264	-1.20907
C	-8.88503	2.6597	1.23488
H	-9.77585	3.23115	1.49836
H	-8.27483	3.22776	0.52281
H	-8.30385	2.43658	2.13751
C	8.29571	-2.42032	2.98195
H	9.09002	-2.90077	3.55458
H	7.81571	-1.64371	3.58931
H	7.55664	-3.16771	2.66981
C	10.95662	-1.97554	-0.37168
H	10.60108	-2.48254	-1.27677
H	12.02914	-1.78588	-0.44392
H	10.72713	-2.56913	0.51532
C	9.81646	0.12251	-3.07382
H	9.37163	-0.83122	-3.38351
H	9.97134	0.76118	-3.946
H	10.76058	-0.05083	-2.55397
H	-2.15272	2.55625	-1.93655

Complex 3 Fig. 3RM5
E(UB3LYP) = - 2929.050103 Hartree
ZPE (kcal mol^{-1}) = 0.826442 Hartree



3RM5

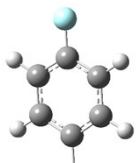
C(Fragment=1)	3.78412	-1.09188	-0.75404
C(Fragment=1)	2.41001	-0.84066	-0.79159
C(Fragment=1)	2.69218	1.21957	0.32381
C(Fragment=1)	4.07601	0.98772	0.40274
C(Fragment=1)	4.66214	-0.18361	-0.12314
H(Fragment=1)	4.17008	-2.00765	-1.18044
H(Fragment=1)	4.69312	1.76651	0.83377
C(Fragment=1)	2.20814	2.56087	0.78151
C(Fragment=1)	2.3963	2.97988	2.1133
C(Fragment=1)	1.34615	4.63631	0.16981

C(Fragment=1)	2.01466	4.28554	2.46956
H(Fragment=1)	2.81014	2.29888	2.85016
C(Fragment=1)	1.47721	5.13158	1.48152
H(Fragment=1)	0.94821	5.26265	-0.62371
H(Fragment=1)	2.13536	4.63235	3.49138
H(Fragment=1)	1.17399	6.14769	1.71234
C(Fragment=1)	1.45495	-1.76866	-1.4304
C(Fragment=1)	1.82677	-2.90113	-2.17566
C(Fragment=1)	-0.82766	-2.19972	-1.84333
C(Fragment=1)	0.83086	-3.69611	-2.76429
H(Fragment=1)	2.86898	-3.16071	-2.30719
C(Fragment=1)	-0.51859	-3.33879	-2.59859
H(Fragment=1)	-1.85539	-1.90032	-1.69609
H(Fragment=1)	1.10463	-4.57199	-3.34274
H(Fragment=1)	-1.31928	-3.92097	-3.0392
N(Fragment=1)	1.84972	0.28808	-0.22804
N(Fragment=1)	1.70489	3.37757	-0.18163
N(Fragment=1)	0.13799	-1.43867	-1.27319
C(Fragment=1)	8.14902	-1.46969	-0.93431
C(Fragment=1)	6.76405	-1.23663	-1.00372
C(Fragment=1)	6.11981	-0.43638	-0.04054
C(Fragment=1)	6.88159	0.12612	1.01197
C(Fragment=1)	8.25894	-0.12456	1.10104
C(Fragment=1)	8.917	-0.92052	0.11973
H(Fragment=1)	6.22978	-1.65868	-1.84801
H(Fragment=1)	6.39332	0.71127	1.78177
C(Fragment=1)	-2.77309	0.62139	-0.94383
C(Fragment=1)	-4.16773	0.54966	-0.86502
C(Fragment=1)	-4.77509	-0.20585	0.17239
C(Fragment=1)	-3.9325	-0.86144	1.10987
C(Fragment=1)	-2.5435	-0.76461	0.97835
H(Fragment=1)	-4.77613	1.05317	-1.60551
H(Fragment=1)	-4.36106	-1.40947	1.93915
C(Fragment=1)	0.27923	1.8392	-2.5411
C(Fragment=1)	-0.16237	2.58885	-3.6453
C(Fragment=1)	-1.54076	2.71701	-3.87947
C(Fragment=1)	-2.44853	2.0864	-3.00774
C(Fragment=1)	-1.95125	1.34957	-1.92773
H(Fragment=1)	1.32931	1.7378	-2.31547
H(Fragment=1)	0.56785	3.0578	-4.29438
H(Fragment=1)	-1.90678	3.29214	-4.7234
H(Fragment=1)	-3.51638	2.16595	-3.17334
C(Fragment=1)	-1.50379	-1.32892	1.8595
C(Fragment=1)	-1.74974	-2.11791	2.98997
C(Fragment=1)	-0.663	-2.56771	3.76156
C(Fragment=1)	0.64116	-2.21128	3.38079
C(Fragment=1)	0.82574	-1.41997	2.23505
H(Fragment=1)	-2.76459	-2.37608	3.26832
H(Fragment=1)	-0.83491	-3.1792	4.64086
H(Fragment=1)	1.50533	-2.53168	3.95076
H(Fragment=1)	1.81765	-1.12612	1.92257
C(Fragment=1)	-7.0769	0.74286	-0.19253

C(Fragment=1)	-8.47197	0.65016	-0.07825
C(Fragment=1)	-9.07964	-0.50712	0.48831
C(Fragment=1)	-8.2468	-1.55465	0.94764
C(Fragment=1)	-6.84769	-1.44593	0.85199
C(Fragment=1)	-6.25123	-0.30572	0.28051
H(Fragment=1)	-6.63219	1.64434	-0.59617
H(Fragment=1)	-6.25793	-2.29077	1.19088
N(Fragment=1)	-2.01304	-0.04881	-0.04319
N(Fragment=1)	-0.59507	1.23821	-1.70526
N(Fragment=1)	-0.21845	-0.99416	1.4889
Co(Fragment=1)	-0.15194	0.15437	-0.13419
O(Fragment=1)	-0.32554	1.61996	1.10805
O(Fragment=2)	-1.2799	2.54735	0.87923
O(Fragment=1)	-9.35109	1.65971	-0.45686
O(Fragment=1)	-10.45464	-0.58724	0.71025
O(Fragment=1)	-8.72995	-2.70626	1.57401
O(Fragment=1)	9.0655	0.33157	2.13909
O(Fragment=1)	10.26303	-1.27048	0.22838
O(Fragment=1)	8.68116	-2.3166	-1.91102
C(Fragment=1)	-8.80812	2.90187	-1.01877
H(Fragment=1)	-8.25668	2.70317	-1.94541
H(Fragment=1)	-9.67958	3.52243	-1.23114
H(Fragment=1)	-8.15931	3.40613	-0.29278
C(Fragment=1)	-11.35699	-0.52261	-0.46351
H(Fragment=1)	-12.36361	-0.6293	-0.05507
H(Fragment=1)	-11.13761	-1.35052	-1.14832
H(Fragment=1)	-11.24574	0.43628	-0.97353
C(Fragment=1)	-9.84995	-3.45309	0.96676
H(Fragment=1)	-9.86039	-4.41509	1.48356
H(Fragment=1)	-10.7929	-2.92519	1.12035
H(Fragment=1)	-9.6702	-3.60695	-0.10434
C(Fragment=1)	8.46033	1.12951	3.21178
H(Fragment=1)	8.03529	2.05912	2.8151
H(Fragment=1)	7.6883	0.55425	3.73667
H(Fragment=1)	9.2807	1.35762	3.89342
C(Fragment=1)	11.27092	-0.18376	0.23235
H(Fragment=1)	11.20731	0.3874	-0.70163
H(Fragment=1)	11.11798	0.47079	1.09252
H(Fragment=1)	12.23537	-0.69076	0.29786
C(Fragment=1)	9.90202	-1.90935	-2.63547
H(Fragment=1)	10.77983	-2.00259	-1.99322
H(Fragment=1)	9.97169	-2.59709	-3.4809
H(Fragment=1)	9.80345	-0.8792	-2.99937

Complex 4 Fig. 4RM1
E(UB3LYP) = - 2290.206633 Hartree
ZPE (kcal mol^{-1}) = 0.610741 Hartree

C	3.95757	-1.20925	0.01504
C	2.55528	-1.18578	0.0106
C	2.55529	1.18578	-0.0106

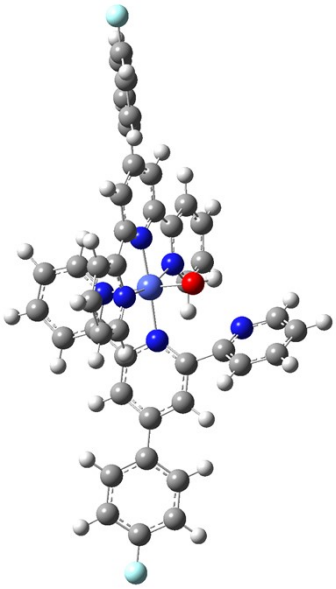


C	3.95758	1.20925	-0.01505
C	4.69084	-0.00001	0.
H	4.47949	-2.15646	0.05264
H	4.4795	2.15645	-0.05264
C	1.70174	2.40188	-0.02514
C	2.20923	3.71496	-0.0376
C	-0.50942	3.20008	-0.03504
C	1.30848	4.79438	-0.04989
H	3.27608	3.9033	-0.03714
C	-0.07466	4.53721	-0.04868
H	-1.56667	2.95703	-0.033
H	1.6811	5.81363	-0.05986
H	-0.80003	5.34324	-0.05769
C	1.70173	-2.40188	0.02513
C	2.20922	-3.71496	0.03759
C	-0.50943	-3.20007	0.03504
C	1.30846	-4.79438	0.04989
H	3.27607	-3.90331	0.03714
C	-0.07468	-4.5372	0.04867
H	-1.56668	-2.95701	0.033
H	1.68108	-5.81363	0.05986
H	-0.80005	-5.34323	0.05768
N	1.87826	0.	0.
N	0.35578	2.16127	-0.02393
N	0.35577	-2.16126	0.02393
C	8.3064	-1.05184	-0.61452
C	6.90104	-1.05324	-0.61262
C	6.17778	-0.00001	0.
C	6.90104	1.05322	0.61262
C	8.3064	1.05182	0.61453
C	9.01552	-0.00001	0.
H	8.84465	-1.86242	-1.09806
H	6.37366	-1.86015	-1.11401
H	6.37367	1.86013	1.11402
H	8.84465	1.8624	1.09806
C	-2.61473	-0.01062	-1.18719
C	-4.01536	-0.01468	-1.21523
C	-4.74521	0.	0.
C	-4.01536	0.01468	1.21523
C	-2.61473	0.01063	1.18719
H	-4.53638	-0.05168	-2.16387
H	-4.53638	0.05168	2.16387
C	0.56286	-0.03365	-2.99268
C	0.21453	-0.04976	-4.35382
C	-1.14643	-0.05362	-4.70766
C	-2.11846	-0.04099	-3.6916
C	-1.704	-0.02567	-2.35092
H	1.60094	-0.02965	-2.68441
H	0.99427	-0.05872	-5.10699
H	-1.44677	-0.06588	-5.75025
H	-3.17265	-0.04285	-3.94297
C	-1.704	0.02567	2.35092

C	-2.11846	0.041	3.6916
C	-1.14642	0.05364	4.70766
C	0.21453	0.04978	4.35382
C	0.56286	0.03366	2.99267
H	-3.17265	0.04286	3.94297
H	-1.44676	0.0659	5.75025
H	0.99428	0.05874	5.10698
H	1.60094	0.02966	2.6844
C	-6.95579	0.61536	-1.05164
C	-8.36114	0.61712	-1.05026
C	-9.0703	-0.00001	0.
C	-8.36113	-0.61714	1.05027
C	-6.95578	-0.61537	1.05165
C	-6.23241	0.	0.
H	-6.4285	1.11901	-1.8572
H	-8.89932	1.10272	-1.85964
H	-8.89931	-1.10274	1.85965
H	-6.42849	-1.11902	1.8572
N	-1.95011	0.	0.
N	-0.37026	-0.02232	-2.01236
N	-0.37026	0.02233	2.01236
Co	-0.06156	0.	0.
F	10.36552	-0.00002	0.
F	-10.4203	-0.00001	0.00001

Complex 4 Fig. 4RM2
E(UB3LYP) = - 2365.988932 Hartree
ZPE (kcal mol^{-1}) = 0.625896 Hartree

C	-3.71306	-1.21032	0.78361
C	-2.34262	-0.93469	0.79337
C	-2.661	1.03804	-0.45977
C	-4.04288	0.77547	-0.51454
C	-4.60777	-0.36311	0.09574
H	-4.08825	-2.07571	1.31258
H	-4.67085	1.48603	-1.0379
C	-2.22163	2.34692	-1.04075
C	-2.53389	2.67332	-2.37594
C	-1.37855	4.48752	-0.64677
C	-2.22393	3.96003	-2.85051
H	-2.98669	1.93462	-3.02953
C	-1.63589	4.88867	-1.97137
H	-0.93564	5.17627	0.06714
H	-2.43919	4.23028	-3.87985
H	-1.38748	5.89448	-2.29378
C	-1.37288	-1.80176	1.49379
C	-1.72941	-2.88008	2.32288
C	0.91555	-2.18959	1.90944

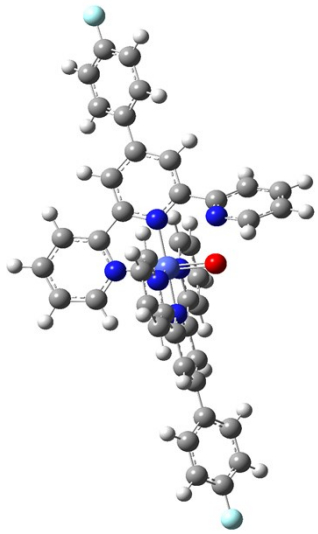


4RM2

C	-0.72203	-3.62588	2.9546
H	-2.76821	-3.13649	2.48434
C	0.62322	-3.2752	2.74573
H	1.93954	-1.89622	1.72738
H	-0.98366	-4.45958	3.59747
H	1.43264	-3.82194	3.21497
N	-1.8023	0.16228	0.15325
N	-1.66226	3.24419	-0.1826
N	-0.06062	-1.47327	1.30027
C	-7.9147	-2.25614	0.03323
C	-6.53812	-1.98261	0.09557
C	-6.06283	-0.64868	0.03466
C	-7.00417	0.40349	-0.08787
C	-8.38095	0.12937	-0.14404
C	-8.84227	-1.20134	-0.08527
H	-8.26141	-3.28508	0.07048
H	-5.83872	-2.81153	0.16126
H	-6.67164	1.43741	-0.10978
H	-9.08978	0.94852	-0.227
C	2.81819	0.60514	0.87607
C	4.21455	0.58519	0.78238
C	4.83831	-0.19494	-0.22658
C	4.0114	-0.91521	-1.12775
C	2.6192	-0.85031	-0.9941
H	4.81099	1.18439	1.45886
H	4.45302	-1.52562	-1.90524
C	-0.26424	1.86743	2.3803
C	0.15651	2.66377	3.45896
C	1.53091	2.80965	3.70836
C	2.45499	2.15051	2.87637
C	1.97815	1.36516	1.82046
H	-1.31059	1.75031	2.14307
H	-0.5855	3.1542	4.07816
H	1.88089	3.42102	4.53335
H	3.51979	2.24407	3.05418
C	1.5941	-1.48395	-1.84435
C	1.86104	-2.30287	-2.94922
C	0.7861	-2.81628	-3.69687
C	-0.52721	-2.4913	-3.3189
C	-0.7311	-1.66761	-2.19912
H	2.88267	-2.53383	-3.22676
H	0.97342	-3.45113	-4.55631
H	-1.38347	-2.85956	-3.87182
H	-1.72989	-1.39464	-1.89
C	7.13706	-0.11234	0.80708
C	8.53693	-0.16584	0.69944
C	9.14486	-0.34998	-0.55885
C	8.34048	-0.48296	-1.70879
C	6.94048	-0.43505	-1.60148
C	6.31868	-0.24728	-0.34199
H	6.68811	0.0036	1.78963
H	9.14918	-0.0714	1.59192

H	8.80103	-0.61642	-2.68365
H	6.33976	-0.51356	-2.50332
N	2.07466	-0.12066	0.00698
N	0.62561	1.23565	1.58201
N	0.30199	-1.1828	-1.47632
Co	0.20932	0.05544	0.0667
O	0.41903	1.42074	-1.20133
H	0.37852	2.28309	-0.73559
F	-10.16522	-1.46419	-0.14187
F	10.49002	-0.39877	-0.66213

Complex 4 Fig. 4RM3
E(UB3LYP) = - 2365.326030 Hartree
ZPE (kcal mol^{-1}) = 0.614213 Hartree

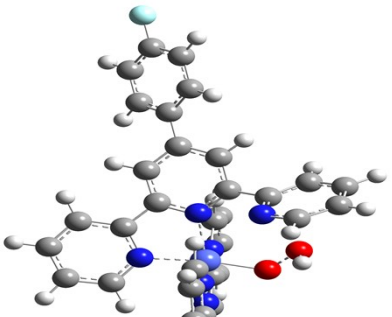


4RM3

C	-3.8466	-0.8301	0.7794
C	-2.46407	-0.63116	0.81967
C	-2.62985	1.25614	-0.59222
C	-4.02002	1.06908	-0.67856
C	-4.66794	0.01363	-0.0011
H	-4.28693	-1.63196	1.35636
H	-4.58776	1.76728	-1.28097
C	-2.05682	2.46563	-1.26064
C	-2.2702	2.69221	-2.63663
C	-1.01869	4.53751	-1.00676
C	-1.80909	3.89277	-3.20186
H	-2.76129	1.94112	-3.24729
C	-1.16951	4.83561	-2.37331
H	-0.54245	5.24411	-0.33275
H	-1.9467	4.08891	-4.26089
H	-0.80511	5.77846	-2.76819
C	-1.55406	-1.48876	1.60647
C	-1.97649	-2.49908	2.48744
C	0.70572	-1.92671	2.12098
C	-1.01613	-3.23796	3.19673
H	-3.02909	-2.70696	2.63033
C	0.34701	-2.94734	3.01236
H	1.74546	-1.67822	1.95841
H	-1.3275	-4.02016	3.88083
H	1.12009	-3.49094	3.54263
N	-1.84915	0.38548	0.12086
N	-1.45451	3.37962	-0.45135
N	-0.22414	-1.21882	1.43574
C	-8.07005	-1.68164	-0.03469
C	-6.68551	-1.4835	0.07429
C	-6.13324	-0.19049	-0.09358
C	-6.99201	0.89474	-0.35334
C	-8.38302	0.70613	-0.43833
C	-8.94295	-0.58455	-0.28657
H	-6.03532	-2.33508	0.23455

H	-6.6193	1.90855	-0.45156
C	2.72409	0.80373	0.95157
C	4.12168	0.74777	0.90862
C	4.76178	-0.12071	-0.01407
C	3.95083	-0.90092	-0.87948
C	2.55754	-0.80007	-0.79982
H	4.70797	1.38397	1.55951
H	4.40339	-1.58199	-1.58876
C	-0.37743	2.17725	2.30795
C	0.02862	3.06652	3.31798
C	1.39985	3.24485	3.56279
C	2.33469	2.52156	2.79894
C	1.87075	1.64188	1.81376
H	-1.42142	2.03033	2.07679
H	-0.72187	3.60274	3.88697
H	1.73942	3.92953	4.33272
H	3.39757	2.63991	2.97366
C	1.54611	-1.48276	-1.62908
C	1.8273	-2.40788	-2.64242
C	0.76441	-2.95911	-3.38047
C	-0.55121	-2.56441	-3.0856
C	-0.77089	-1.6357	-2.05486
H	2.85078	-2.69171	-2.85731
H	0.96285	-3.67616	-4.16983
H	-1.39765	-2.95904	-3.63537
H	-1.77162	-1.30869	-1.81079
C	7.02604	0.03867	1.07294
C	8.42696	-0.01321	1.01339
C	9.08161	-0.29815	-0.21046
C	8.29355	-0.58009	-1.35426
C	6.89505	-0.52347	-1.2907
C	6.24293	-0.20011	-0.07899
H	6.57233	0.24821	2.03606
H	6.34245	-0.70684	-2.20642
N	1.99459	0.02446	0.11625
N	0.52252	1.48499	1.57759
N	0.25036	-1.1131	-1.34025
Co	0.12831	0.22714	0.12274
O	0.39639	1.54117	-1.14256
F	-10.26559	-0.75229	-0.49868
F	10.43079	-0.3246	-0.24941
H	8.74878	-0.78331	-2.30103
H	8.97314	0.22901	1.90104
H	-8.96243	1.57412	-0.67449
H	-8.54273	-2.6394	0.02983

Complex 4 Fig. 4T.S[#]
E(UB3LYP) = - 2441.123665 Hartree
ZPE (kcal mol^{-1}) = 0.62809 Hartree



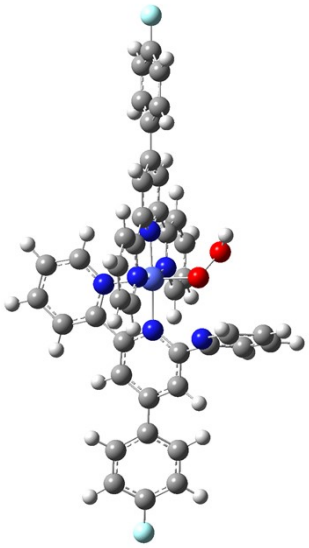
O	1.46618	0.64952	-0.05911
H	1.43104	1.54012	-0.48217
C	-3.25476	-1.7234	3.06448
C	-1.8793	-1.4764	3.09319
C	-2.13805	0.49449	1.82111
C	-3.52264	0.26069	1.74223
C	-4.11832	-0.86159	2.35422
H	-3.65683	-2.57536	3.59625
H	-4.12357	0.97744	1.19551
C	-1.64122	1.78991	1.25344
C	-1.70574	2.04914	-0.12916
C	-0.91393	3.95508	1.70576
C	-1.32116	3.3191	-0.59365
H	-2.02561	1.2753	-0.8198
C	-0.91	4.29127	0.33889
H	-0.62558	4.68427	2.45808
H	-1.34559	3.54531	-1.65554
H	-0.60871	5.28492	0.02311
C	-0.92944	-2.34638	3.81516
C	-1.30572	-3.41167	4.65097
C	1.35109	-2.74091	4.27264
C	-0.31263	-4.1545	5.30888
H	-2.34891	-3.65911	4.79808
C	1.03772	-3.81286	5.11904
H	2.37963	-2.45453	4.10538
H	-0.58923	-4.97842	5.95798
H	1.836	-4.3565	5.61034
N	-1.31127	-0.39471	2.45347
N	-1.2758	2.73121	2.16369
N	0.38868	-2.02911	3.63733
C	-7.45723	-2.6963	2.2278
C	-6.0793	-2.44207	2.31045
C	-5.57763	-1.11716	2.2713
C	-6.49399	-0.04313	2.14909
C	-7.87576	-0.27734	2.07191
C	-8.3204	-1.60239	2.11216
H	-5.39956	-3.28594	2.37495
H	-6.14104	0.9832	2.14313
C	3.2951	0.04055	3.1803
C	4.69122	0.0016	3.09357
C	5.30922	-0.82883	2.12197
C	4.48135	-1.58674	1.25481
C	3.08947	-1.4999	1.37711
H	5.29094	0.62124	3.74843
H	4.91954	-2.24081	0.51172
C	0.21895	1.31978	4.68137
C	0.64496	2.16877	5.71793
C	2.02049	2.34798	5.93491
C	2.94107	1.66883	5.11454
C	2.45891	0.83057	4.10302

4T.S

H	-0.82963	1.17704	4.46844
H	-0.09449	2.67382	6.32835
H	2.37472	3.00068	6.72573
H	4.00713	1.78987	5.26648
C	2.05958	-2.16437	0.5587
C	2.31791	-3.06173	-0.48386
C	1.23938	-3.58927	-1.21649
C	-0.06831	-3.19796	-0.88555
C	-0.26399	-2.29993	0.17652
H	3.3362	-3.34132	-0.72719
H	1.41976	-4.28478	-2.02919
H	-0.92701	-3.57168	-1.43089
H	-1.25875	-1.976	0.44614
C	7.60718	-0.72694	3.15561
C	9.0062	-0.7926	3.06107
C	9.56886	-1.02477	1.80237
C	8.80613	-1.19621	0.64313
C	7.40868	-1.13345	0.75848
C	6.78929	-0.89694	2.01098
H	7.16096	-0.57229	4.13285
H	6.80946	-1.24031	-0.14022
N	2.54971	-0.71449	2.33771
N	1.10557	0.66886	3.89815
N	0.77171	-1.80344	0.88734
Co	0.68921	-0.52532	2.39398
O	0.89895	0.99772	1.30289
F	-9.70248	-1.84653	2.03247
F	10.96913	-1.08902	1.69711
H	9.28764	-1.36523	-0.31415
H	9.63843	-0.67452	3.93467
H	-8.58458	0.53978	1.98973
H	-7.84852	-3.70796	2.24585

Complex 4 Fig. 4RM4
E(UB3LYP) = - 2441.126442 Hartree
ZPE (kcal mol^{-1}) = 0.629214 Hartree

C	3.75667	-1.14979	0.8087
C	2.38787	-0.86764	0.8538
C	2.68415	1.10888	-0.39943
C	4.0637	0.84629	-0.48411
C	4.63638	-0.30017	0.10492
H	4.13111	-2.04667	1.2832
H	4.68855	1.58386	-0.97286
C	2.22093	2.43136	-0.92778
C	2.42859	2.78088	-2.27695
C	1.40641	4.55471	-0.42502
C	2.07374	4.07291	-2.7007
H	2.83183	2.05565	-2.97676
C	1.54769	4.97899	-1.75946
H	1.0233	5.23011	0.33524

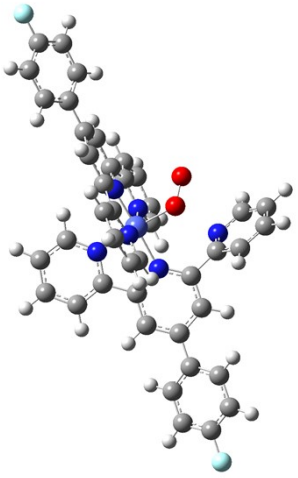


4RM4

H	2.20669	4.36597	-3.73787
H	1.26584	5.98795	-2.04303
C	1.42806	-1.7292	1.57355
C	1.79686	-2.79248	2.41603
C	-0.8539	-2.10427	2.03308
C	0.79854	-3.52515	3.07708
H	2.83844	-3.04409	2.5682
C	-0.54917	-3.17455	2.88482
H	-1.88062	-1.81226	1.86508
H	1.06902	-4.3473	3.73102
H	-1.35166	-3.70971	3.37862
N	1.83793	0.2291	0.22441
N	1.73754	3.30775	-0.00837
N	0.11323	-1.40237	1.39347
C	8.12998	-1.57931	0.94469
C	6.75548	-1.3078	1.02953
C	6.0895	-0.58519	0.00844
C	6.83643	-0.13867	-1.11012
C	8.21032	-0.40588	-1.21565
C	8.82141	-1.12044	-0.18069
H	6.21668	-1.63908	1.91154
H	6.34831	0.39551	-1.91917
C	-2.55366	-0.91946	-0.88606
C	-3.94305	-1.03963	-1.00486
C	-4.78778	-0.29385	-0.14261
C	-4.1883	0.55964	0.8201
C	-2.79317	0.64147	0.89653
H	-4.36737	-1.67338	-1.77321
H	-4.80134	1.12725	1.50879
C	0.81384	-1.65995	-2.08904
C	0.63281	-2.55903	-3.15328
C	-0.66806	-2.97433	-3.48171
C	-1.75496	-2.46702	-2.74684
C	-1.51118	-1.56472	-1.7048
H	1.80286	-1.31924	-1.8187
H	1.49714	-2.91561	-3.70119
H	-0.83726	-3.6723	-4.29471
H	-2.7682	-2.76547	-2.98868
C	-1.97411	1.44794	1.82021
C	-2.47491	2.28218	2.82585
C	-1.56891	2.96989	3.65545
C	-0.19008	2.80183	3.45233
C	0.25427	1.95933	2.41765
H	-3.54358	2.3928	2.96685
H	-1.93682	3.61903	4.44298
H	0.539	3.31123	4.07161
H	1.30538	1.82913	2.2125
C	-6.87399	-1.60715	-0.67387
C	-8.26958	-1.71652	-0.7766
C	-9.0415	-0.59627	-0.45381
C	-8.48983	0.6179	-0.03377
C	-7.09278	0.70632	0.06877

C	-6.26572	-0.39951	-0.24963
H	-6.26825	-2.47946	-0.89842
H	-6.65454	1.6529	0.36881
N	-2.02999	-0.10299	0.05929
N	-0.22954	-1.18299	-1.37593
N	-0.61771	1.30199	1.62356
Co	-0.17144	0.1015	0.13037
O	-0.30418	1.58164	-1.04549
O	-1.12915	1.31949	-2.26409
H	-1.89835	1.92394	-2.13084
H	-9.12865	1.46373	0.19717
H	-8.74304	-2.6409	-1.08991
H	8.64896	-2.12238	1.72737
H	8.7868	-0.07679	-2.07371
F	10.19766	-1.39042	-0.27609
F	-10.43977	-0.69542	-0.55689

Complex 4 Fig. 4RM5
E(UB3LYP) = - 2440.506772 Hartree
ZPE (kcal mol^{-1}) = 0.617789 Hartree



4RM5

C(Fragment=1)	-3.78417	-1.09158	0.75445
C(Fragment=1)	-2.41006	-0.84031	0.79206
C(Fragment=1)	-2.6922	1.21963	-0.32388
C(Fragment=1)	-4.07601	0.98772	-0.40288
C(Fragment=1)	-4.66214	-0.1835	0.12323
H(Fragment=1)	-4.17016	-2.00725	1.18105
H(Fragment=1)	-4.69311	1.76639	-0.83413
C(Fragment=1)	-2.20811	2.56079	-0.78184
C(Fragment=1)	-2.39629	2.97958	-2.11369
C(Fragment=1)	-1.34601	4.6363	-0.1705
C(Fragment=1)	-2.01459	4.28517	-2.47018
H(Fragment=1)	-2.81019	2.29847	-2.85042
C(Fragment=1)	-1.47708	5.13136	-1.48231
H(Fragment=1)	-0.94802	5.26275	0.6229
H(Fragment=1)	-2.1353	4.6318	-3.49206
H(Fragment=1)	-1.17382	6.1474	-1.71332
C(Fragment=1)	-1.45504	-1.7681	1.43122
C(Fragment=1)	-1.82691	-2.90032	2.17684
C(Fragment=1)	0.82755	-2.19906	1.84439
C(Fragment=1)	-0.83103	-3.69511	2.76579
H(Fragment=1)	-2.86912	-3.15983	2.30842
C(Fragment=1)	0.51843	-3.33787	2.60002
H(Fragment=1)	1.85528	-1.89971	1.69708
H(Fragment=1)	-1.10483	-4.57079	3.34451
H(Fragment=1)	1.31909	-3.91991	3.04085
N(Fragment=1)	-1.84975	0.28829	0.22825
N(Fragment=1)	-1.70481	3.37765	0.18113
N(Fragment=1)	-0.13807	-1.43819	1.27395

C(Fragment=1)	-8.14911	-1.46928	0.93445
C(Fragment=1)	-6.76415	-1.23615	1.00398
C(Fragment=1)	-6.11979	-0.43634	0.04053
C(Fragment=1)	-6.8814	0.12564	-1.01239
C(Fragment=1)	-8.25872	-0.12511	-1.10155
C(Fragment=1)	-8.91692	-0.92062	-0.11997
H(Fragment=1)	-6.22999	-1.65779	1.84855
H(Fragment=1)	-6.39298	0.71042	-1.78237
C(Fragment=1)	2.77313	0.62169	0.94375
C(Fragment=1)	4.16777	0.54992	0.86487
C(Fragment=1)	4.77505	-0.20593	-0.17232
C(Fragment=1)	3.93239	-0.86183	-1.10953
C(Fragment=1)	2.5434	-0.76495	-0.97794
H(Fragment=1)	4.77622	1.05367	1.60516
H(Fragment=1)	4.36088	-1.4101	-1.93868
C(Fragment=1)	-0.27909	1.84	2.54083
C(Fragment=1)	0.16258	2.58995	3.6448
C(Fragment=1)	1.54099	2.71816	3.87886
C(Fragment=1)	2.44871	2.08731	3.00726
C(Fragment=1)	1.95136	1.35019	1.92747
H(Fragment=1)	-1.32917	1.73855	2.31527
H(Fragment=1)	-0.56759	3.05908	4.2938
H(Fragment=1)	1.90705	3.29352	4.72261
H(Fragment=1)	3.51656	2.16689	3.17279
C(Fragment=1)	1.50363	-1.32955	-1.85884
C(Fragment=1)	1.74951	-2.11895	-2.98904
C(Fragment=1)	0.66272	-2.56898	-3.76043
C(Fragment=1)	-0.64141	-2.21236	-3.37973
C(Fragment=1)	-0.82591	-1.42065	-2.23426
H(Fragment=1)	2.76434	-2.37726	-3.26733
H(Fragment=1)	0.83457	-3.18079	-4.63951
H(Fragment=1)	-1.50562	-2.53293	-3.94955
H(Fragment=1)	-1.8178	-1.12664	-1.92186
C(Fragment=1)	7.07693	0.74286	0.19204
C(Fragment=1)	8.47199	0.65009	0.07761
C(Fragment=1)	9.07955	-0.50738	-0.48869
C(Fragment=1)	8.24664	-1.55506	-0.94752
C(Fragment=1)	6.84755	-1.44627	-0.85172
C(Fragment=1)	6.25118	-0.30585	-0.28056
H(Fragment=1)	6.63229	1.64449	0.59542
H(Fragment=1)	6.25773	-2.29124	-1.1902
N(Fragment=1)	2.01301	-0.04881	0.04339
N(Fragment=1)	0.59517	1.23879	1.70511
N(Fragment=1)	0.21832	-0.99461	-1.4883
Co(Fragment=1)	0.15193	0.15447	0.1344
O(Fragment=1)	0.32559	1.61962	-1.10838
O(Fragment=2)	1.28001	2.54702	-0.87991
F(Fragment=1)	10.41006	-0.58497	-0.70366
F(Fragment=1)	-10.21949	-1.25933	-0.22519
H(Fragment=1)	-8.55652	-2.11718	1.68221
H(Fragment=1)	-8.87884	0.22525	-1.90005
H(Fragment=1)	8.61658	-2.43721	-1.42695

H(Fragment=1)	9.14823	1.42663	0.36846