Supplementary Information

Water Oxidation by Ni(II) Amido-Quinoline Complexes

Monika[a], Vasanthapandiyan Mari[a], Pankaj Kumar[b], Naiwrit Karmodak[a], Basab Bijayi Dhar[a]*

[a]Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence Deemed to be University, Gautam Buddha Nagar, Dadri, UP-201314, India.

[b]Department of Chemistry, Ashoka University, Sonipat, Delhi NCR, Haryana-131029, India.

Email: basab.dhar@snu.edu.in, basabbijayi@gmail.com

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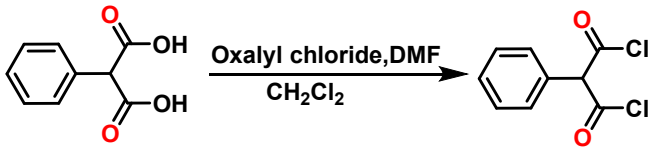
Experimental

Synthesis of dimethyl N, N'-Bis(8-quinolyl)malonamide (**H_2L1**) and *methyl N; N'-Bis(8-quinolyl)formylamide* (**H_2L2**): First 8-aminoquinoline (1 g, 7 mmol) and trimethylamine (462 mg, 3.5 mmol) were first dissolved in dry THF at 0° C under inert atmosphere and stirred for 15 minutes. Then the acid chloride (7 mmol) (N, N'-formyl methylamine in the case of **H_2L1** and 2,2'-dimethyl malonyl chloride in the case of **H_2L2**) was added slowly over a period of 15 minutes. After that, the reaction was brought to room temperature and stirred for 12 hours. The reaction was filtered, and the solvent was evaporated to dryness. The ligands were purified by column chromatography using 40% Ethyl acetate/ hexane.

Synthesis of 2-phenylmalonyl dichloride:[1]



2-phenylmalonyl dichloride was synthesis according to the reported method.[10] To a solution of phenylmalonic acid (2.2 g, 12 mmol) in DCM (25 mL), 100 µL (1.25 mmol) of N, N-dimethylformamide (DMF) was added. This was then placed in an ice bath and oxlyl chloride (2.6 mL, 30 mmol) was added carefully using a dropping funnel over a period of 30 minutes. After addition, the reaction was allowed to warm to room temperature, and the reaction was kept on stirring for an additional 4 hours to ensure a complete reaction. Then, the solvent was removed under reduced pressure, resulting in the formation of a colourless liquid (9.2 mmol, 75% yield).

2-phenyl-N, N'-di(quinoline-8-yl)malonamide (**H_2L3**): First, 2-phenylmalonyl dichloride was prepared by following the above procedure. Then a solution of 8-amino quinoline (1 g, 7 mmol) in dry THF (30 mL), triethylamine (1.16 mL, 8.4 mmol) was stirred under an N2 atmosphere at 0 °C, and the reaction was stirred for 15 minutes. Then the phenylmalonyl dichloride (548

μL, 3.5 mmol) 2) predissoved in 10 mL of dry THF was added dropwise at 0 ℃ over a period of 20 minutes. Over time, the formation of white precipitates of triethylammonium chloride started, indicating the progress of amide coupling. After this, the reaction mixture was brought to room temperature (RT) and kept overnight. After 12 hours, the reaction mixture was filtered over celite. The filtrate was then evaporated to dryness, and the residue was re-dissolved in 150 mL of DCM and washed with aqueous sodium bicarbonate (3 × 50 mL), and the solvent was evaporated to dryness. The purified ligand **H_2L3** was obtained after column chromatography using 5% Ethyl acetate/ hexane to afford a pure yellowish powder. Yield: 650 mg (43%).

Dark orange crystals; ^{1}H NMR (400 MHz, DMSO) δ 11.10 (s, 2H), 8.96 – 8.90 (m, 2H), 8.67 (d, *J* = 7.7 Hz, 2H), 8.42 (dd, *J* = 8.3, 1.6 Hz, 2H), 7.71 (d, *J* = 7.9 Hz, 4H), 7.66 – 7.57 (m, 5H), 7.42 (d, *J* = 7.5 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 1H), 5.79 (s, 1H). 13C NMR (101 MHz, DMSO) δ 167.69, 149.38, 138.57, 136.84, 135.91, 134.36, 129.02, 128.78, 128.10, 127.13, 122.84, 122.44, 117.37, 60.01.

Elemental analysis for Ligand **H_2L3** (fw = 433.1620 g/mol): analytically calculated elements for C, 74.98; H, 4.66; N, 12.95. Found: C, 74.08; H, 4.78; N, 12.5.

[Ni^{II} (NMe)L1] **NiL1** and [Ni^{II} (Me_2)L2] **NiL2**: The ligand (0.2 mmol) was dissolved in dry DMF, and two equivalents of triethylamine/sodium hydride (0.4 mmol) were added to it. The solution color immediately changed to yellow and was stirred for 15 minutes. Then, $NiCl_2.6H_2O$ (0.23mmol) was added to it, and a color change occurred immediately from yellow to dark brown. After 3 hours, the solution was filtered and was kept directly for crystallization. The complex crystals were then obtained by slow evaporation.

Dark orange crystals; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.93 (s, 2H), 8.84 (ddd, *J* = 9.0, 5.6, 1.9 Hz, 4H), 8.13 (dd, *J* = 8.3, 1.7 Hz, 2H), 7.57 – 7.47 (m, 4H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 2H), 1.92 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 171.76, 148.71, 139.11, 136.29, 134.57, 128.05, 127.36, 122.01, 121.76, 116.87, 52.86, 24.23.

Dark brown crystals; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.61 (s, 2H), 8.91 (dd, *J* = 4.2, 1.7 Hz, 2H), 8.76 (dd, *J* = 7.6, 1.4 Hz, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 2H), 7.58 (t, *J* = 7.9 Hz, 2H), 7.51 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 2H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.88, 148.72, 139.29, 136.43, 128.21, 127.46, 121.68, 121.50, 116.74, 30.85.

[Ni^{II} (PhH)L3] **NiL3**: To a solution of ligand (100 mg, 0.23 mmol) in 3 mL dry THF, two equivalents of triethylamine as a base were added, and the solution was stirred for 15 minutes. Then $NiCl_2$.dme (62 mg, 0.27 mmol) under argon was added, and immediately dark brown coloration was observed. The reaction mixture was kept stirring for 4 hours at room temperature under argon. After completion of the reaction, the solution was filtered over celite and evaporated under reduced pressure. After evaporation, the residue was dissolved in CH_2Cl_2, the deep-orange solution was filtered through a Celite pad, and the insoluble part was discarded. A recrystallized sample was collected after the addition of diethyl ether as a precipitant to the dichloromethane solution of the crude. Yield: 73mg (~65%). Single crystals suitable for X-ray diffraction studies were obtained by slow diffusion of diethyl ether into the dimethylformamide solution of complex **3.**

Dark orange brownish crystals; ^{1}H NMR (400 MHz, CDCl3) δ 11.02 (s, 2H), 8.88 (t, *J* = 4.6 Hz, 4H), 8.17 (d, *J* = 8.2 Hz, 2H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 4.5 Hz, 4H), 7.50 – 7.43 (m, 4H), 7.39 (d, *J* = 7.3 Hz, 1H), 5.01 (s, 1H).

Elemental analysis for complex **NiL3** (fw = 489.1604 g/mol): analytically calculated elements for C, 66.30; H, 3.71; N, 11.45. Found: C, 67.88; H, 3.30; N, 12.56.

Synthesis of Zinc complex:

The ligand **H_2L1** (0.13 mmol, 50 mg) was dissolved in ethanol, and 2 equivalents of NaH (0.26 mmol, 2 mg) were added. The solution was stirred for 15 minutes under reflux conditions. Then zinc acetate dihydrate (0.15 mmol, 29 mg) was added, and the mixture was refluxed for 12 hours. After cooling to room temperature, the solution was filtered, and the solvent was evaporated under reduced pressure. After evaporation, the residue was dissolved in CH_2Cl_2, the pale-yellow colour solution was filtered through a Celite pad, and the insoluble part was discarded. Then the solution was kept for crystallization. A yellow colour semi-crystalline material was obtained. Characterization was carried out by NMR, HR-MS and cyclic voltammetry.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.93 (s, 1H), 8.94 – 8.74 (m, 4H), 8.14 (dd, J = 8.2, 1.7 Hz, 2H), 7.57 – 7.47 (m, 4H), 7.44 (dd, J = 8.3, 4.2 Hz, 2H), 1.92 (s, 6H).

Calculation of Faradaic efficiency:

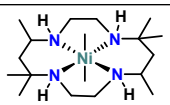
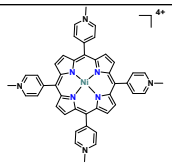
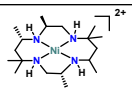
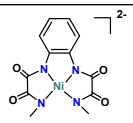
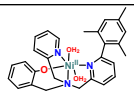
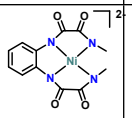
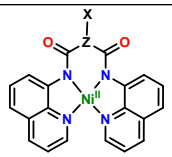
The equation was used to calculate Faradaic efficiency for all 3 Ni(II) complexes:

$$\text{Faradaic efficiency} = \frac{moles\ of\ O2\ experimental}{moles\ of\ O2\ charge} \times 100\ \%$$

The moles of oxygen (O_2) experimentally determined show the percentage of O_2 present in the headspace of the electrochemical cell. These values were determined by the total charge passed during controlled potential electrolysis (CPE) at specific potentials 1.21V, 1.19V, and 1.18V for **NiL1**, **NiL2**, and **NiL3**, respectively. The total charge passed belongs to the theoretical amount of oxygen produced for the electron oxidation process. To calculate the moles of O_2 produced from the total charge can be calculated by the following relation:

The moles of O_2 charge (n) = Q/4F, F is the Faraday constant.

Table S1. Comparison of electrocatalytic activity of water oxidation based on various Ni (II) based catalysts.

Year wise Ni (II) complex reported	Angew. Chem. Int. Ed. 2014, 53, 13042 – 13048	Inorg. Chem. 2015, 54, 5604−5613	*Catal. Sci. Technol.*, 2017,7, 5585-5593	*Electrochim. Acta*, 2017, 258, 353–359	Inorg. Chem. 2017, 56, 13638-13641	ACS Catal. 2019, 9, 3936−3945	Our work
Complex and Ligand	[Ni(meso-L)](ClO4) Meso-L = meso-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane	Ni(II) porphyrin complex Porphyrin based ligand	NilJMe6L)]IJClO4)2	(Me4N)2[Ni(II)L$_i$] L1 = o-phenylenebis(N′-methyloxamidate)	Nickel phenolate complex	[(L1)NiII]$^{2-}$ (L1 = ophenylenebis(oxamidate)) (Tetra Amido ligand)	Ni(II)-Amido-quinoline (Di Amido ligand)
Structure							
TOF	Not reported	0.67	15	0.5	0.15	High in case of	1.75

						heterogeneous	
TON	15, however no supportive data given in manuscript and SI	Not reported				3.81	16.4
Ligand participation	No	No	No		Redox active	Redox active ligand framework, however during electrochemical study at alkaline pH likely undergoes $[Ni(III)(OH)_4]^-$ (speculation)	Redox active ligand
Mechanism pathway	No experimental proof for high valent Ni(IV) formation; No spectroelectrochemical study; No HR-MS data; No O^{18} labelling experiment; Only DFT study supports the mechanism	No experimental proof for Ni(IV) species, no spectroelectrochemical study; No HR-MS data; No O^{18} labelling experiment; Only DFT study supports mechanism	Showing influence of steric effect; No spectroelectrochemistry; No HR-MS data, DFT study confirmed the mechanism	One complex (Ni(II)L1) homogeneous, other two complexes (Ni(II)L2 and Ni(II)L3) formed NiO_x during the electrochemical process; no mechanistic proof	No experimental proof for any reactive intermediate, To prove redox active ligand, the study with Zn complex was not done; No DFT study	The borderline between homogeneous and heterogeneous active form; The dominant path way is NiO_x.	Experimental proof of Ni(III) and ligand oxidation; Spectroelectrochemistry study; HR-MS confirmed Ni(III) generation, Raw data also supplied after reviewer's query, O^{18} label study supports oxygen is coming from water, FE-SEM, EDAX, XPS analysis supported homogeneity of the catalyst, DFT study supports mechanism
CPE	1.55 V	1.32 V	1.55 V	1.06V	1.5 V	0.85 V (not truly for homogeneous catalyst)	1.28
Overpotential	170 mv (onsidering pH contribution) co	Not mentioned	Not mentioned	Not mentioned	Not mentioned	170 mv to 220 mV (not truly for homogeneous	Performed water oxidation in non-aqueous medium, with water as the limiting reagent; Therefore,

						catalyst)	overpotential not calculated.

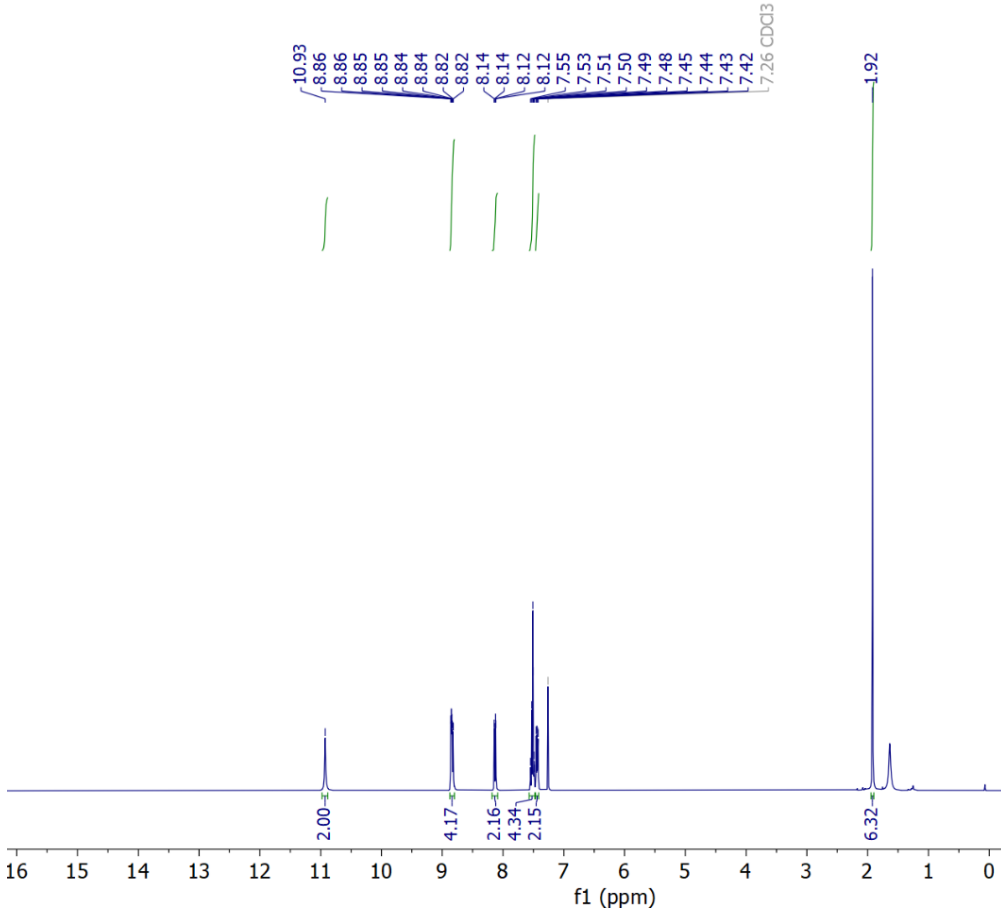


Figure S1a: ^{1}H NMR spectrum (400 MHz) of **H_2L1** recorded in $CDCl_3$ at 25°C.

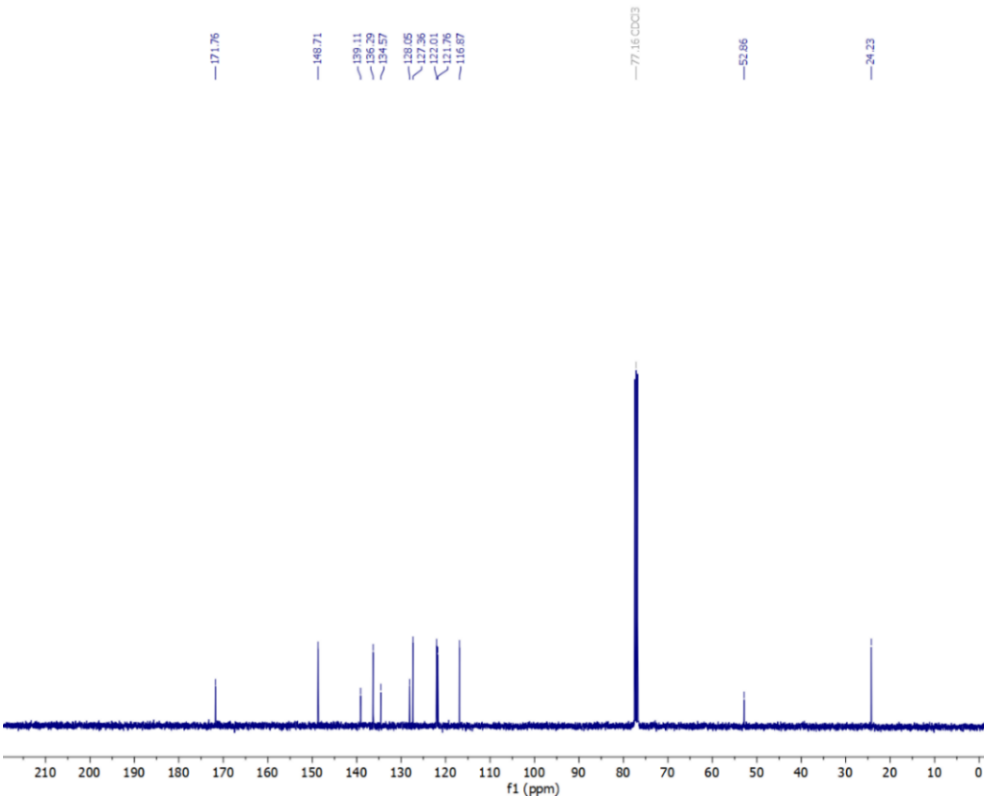


Figure S1b: ^{13}C NMR spectrum (400 MHz) of **H_2L1** recorded in $CDCl_3$ at 25°C.

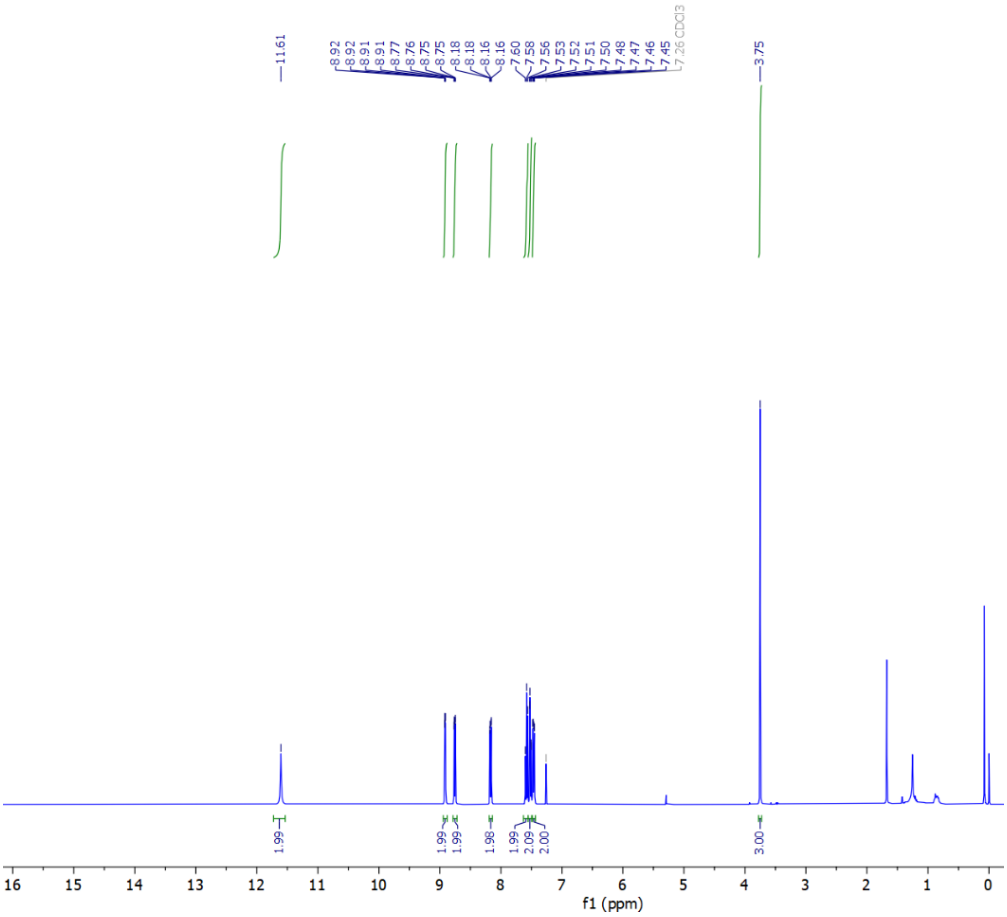


Figure S1c: ^{1}H NMR spectrum (400 MHz) of **H_2L2** recorded in $CDCl_3$ at 25°C.

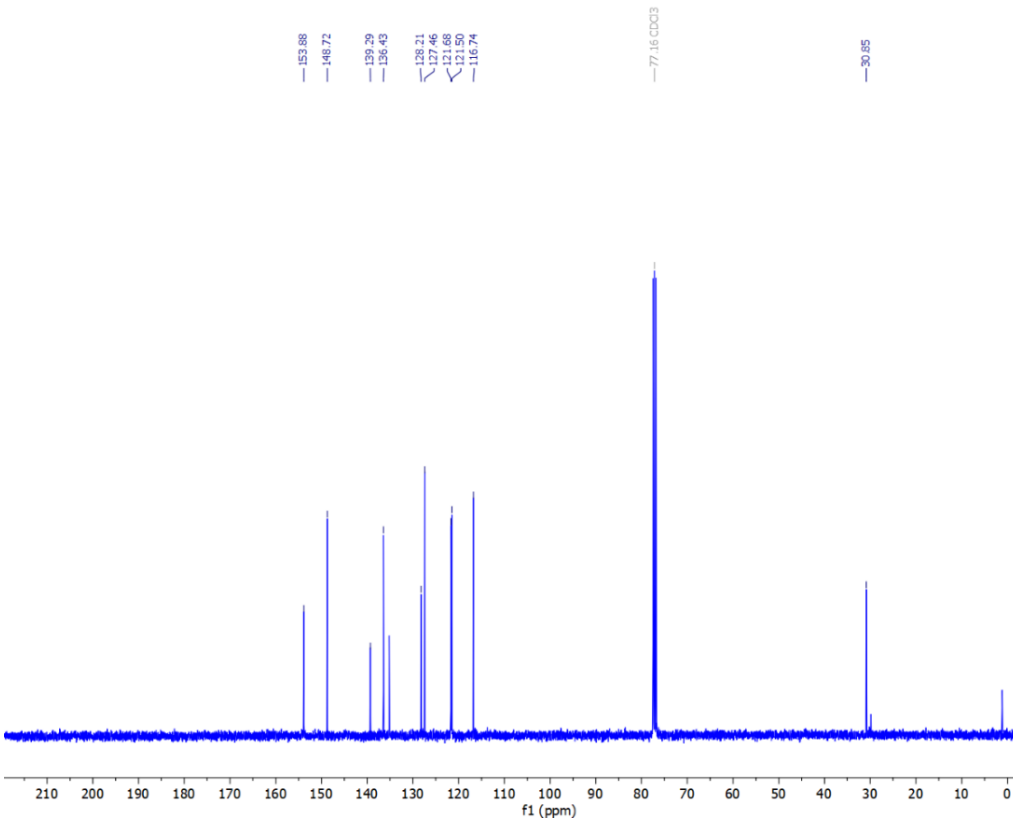


Figure S1d: ^{13}C NMR spectrum (400 MHz) of **H_2L2** recorded in $CDCl_3$ at 25°C.

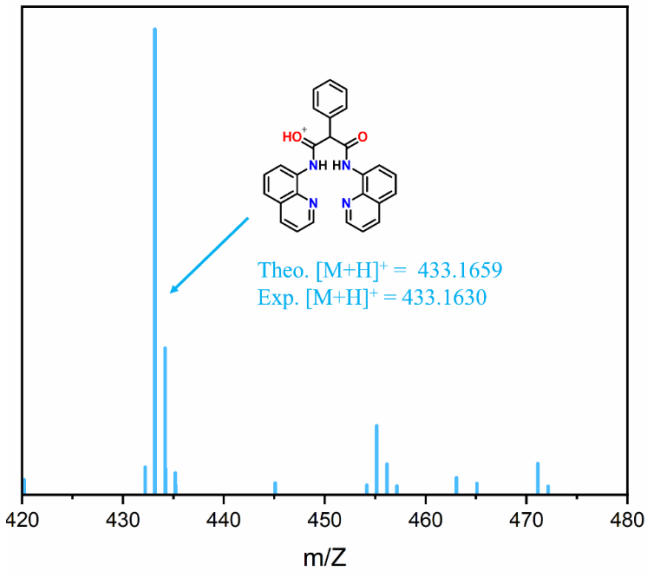


Figure S2: HR-MS of ligand **H_2L3**.

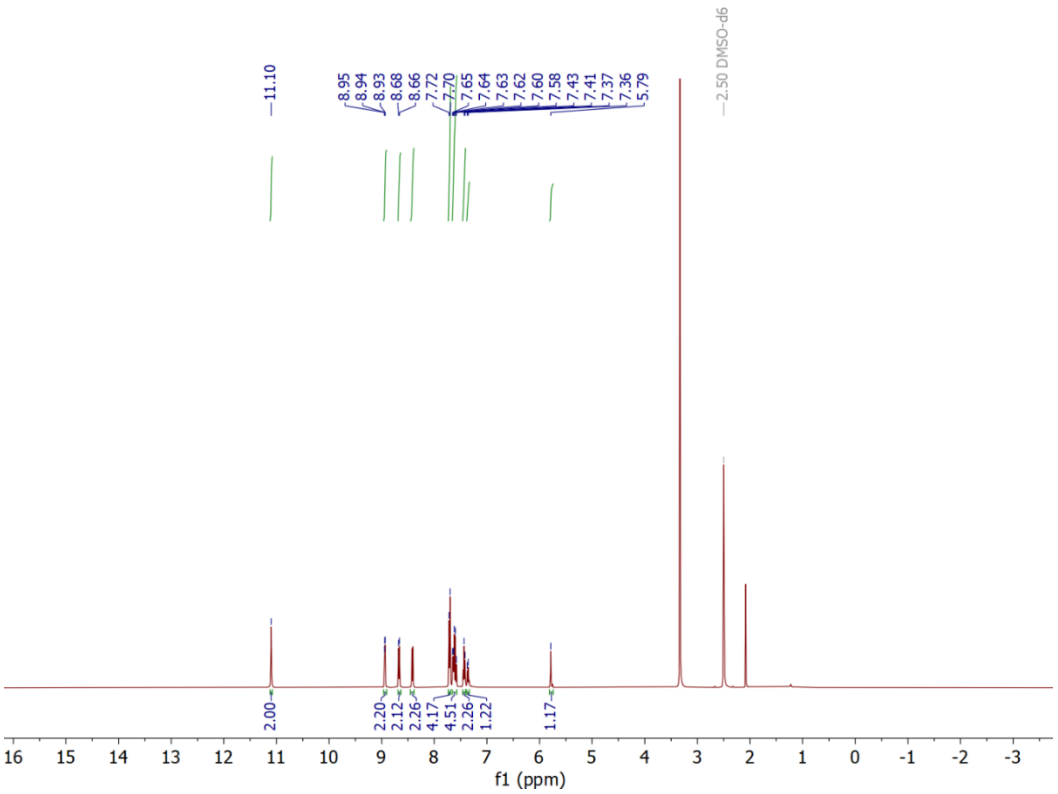


Figure S3: ^{1}H NMR spectrum (400 MHz) of ligand **H_2L3** recorded in DMSO-d_6 at 25°C.

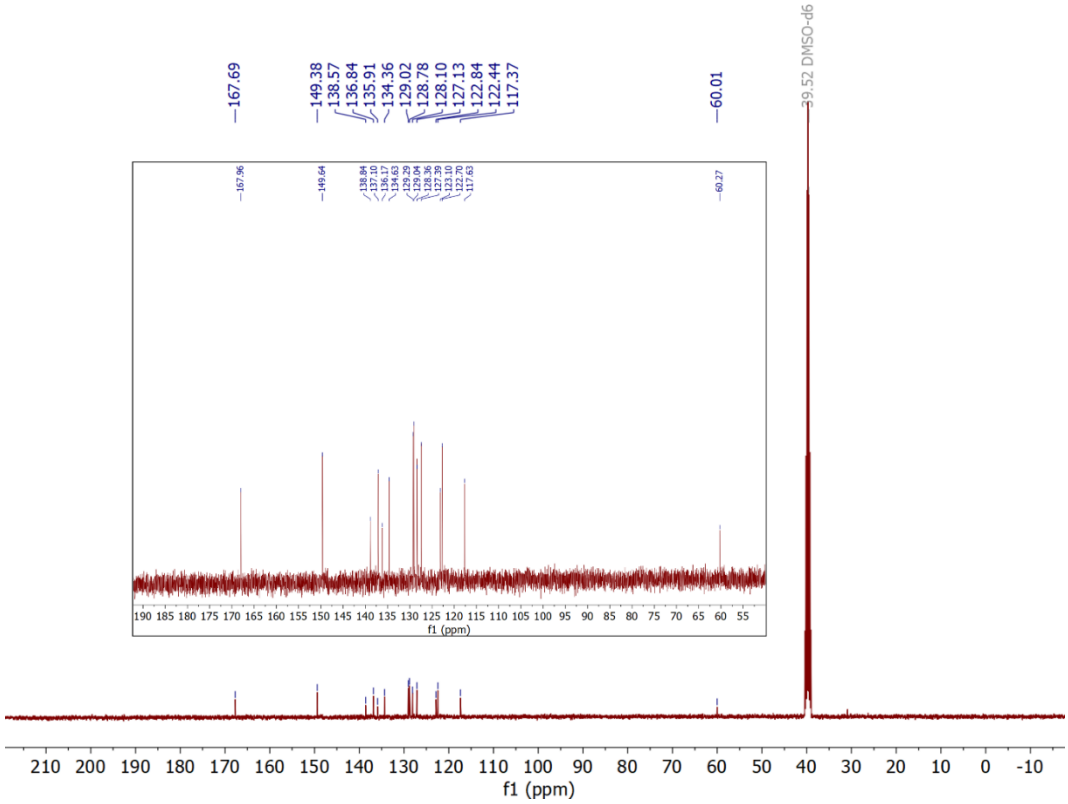


Figure S4: ^{13}C NMR spectrum (400 MHz) of **H_2L3** recorded in DMSO-d_6 at 25°C. The zoomed-in region highlights the low-intensity signals for clarity.

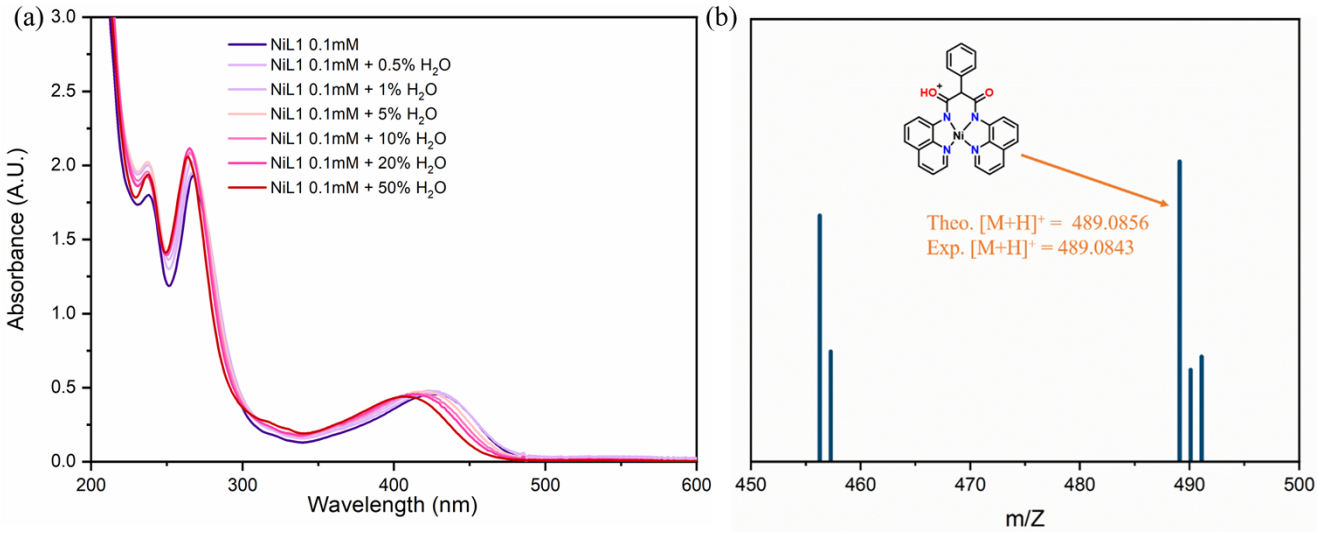


Figure S5: (a) UV-Vis spectra of **NiL1** (0.1 mM) upon addition of increasing amounts of water, as indicated by the percentages. (b) HR-MS of **NiL3**.

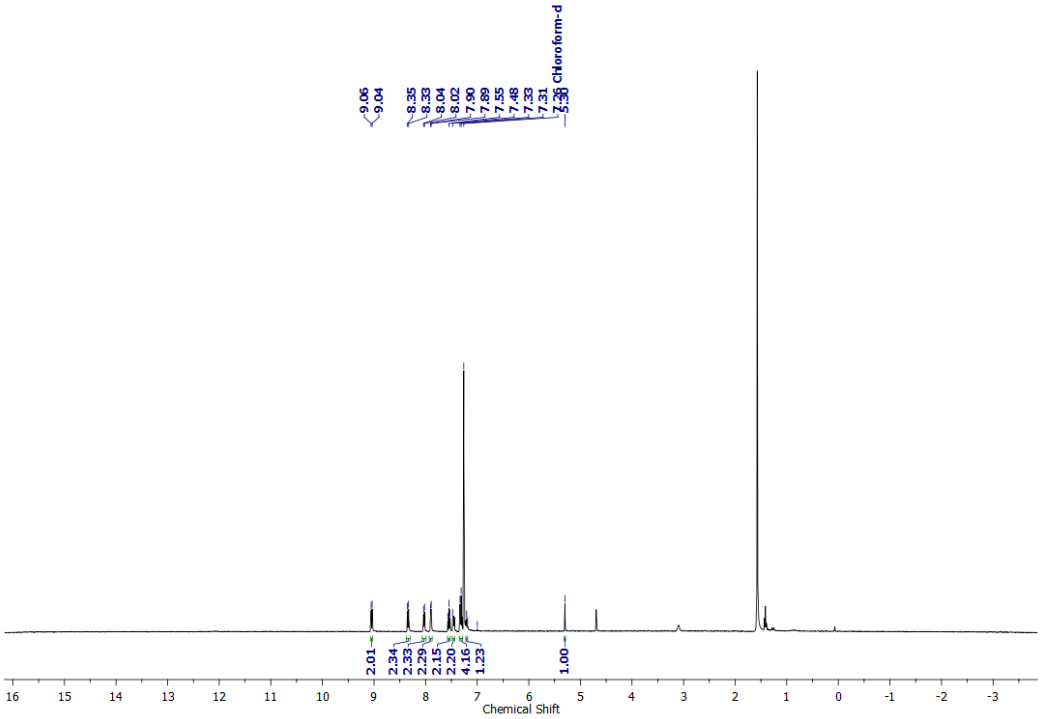


Figure S6: ^{1}H NMR spectrum (400 MHz) of **NiL3** recorded in $CDCl_3$ at 25°C.

Table S2. Crystal data and structural refinement parameters of **H_2L3** and **NiL3**

Compounds	**H_2L3**	**NiL3**
Empirical formula	C_{27} H_{20} N_4 O_2	$C_{27}H_{18}N_4NiO_2$ 1[CH_2Cl_2]
Formula weight	432.47	574.09
Temperature (K)	293	293
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	Tricilinic
Space group	*$P2_1/c$*	*P^{-1}*
a (Å)/α (°)	8.4075(6)/90	9.3561(7)/73.38(3)
b (Å)/β (°)	14.8165(10)/ 99.102(2)	10.5101(9)/88.773)
c (Å)/γ (°)	17.5707(11)/90	12.3184(10)/89.545(3)
Volume (Å^3)	2161.2(3)	1160.44(16)
Z	4	2
Density (calc) (Mg/m^{-3})	1.329	1.643
Absorption coefficient (μ) (mm^{-1})	0.086	1.104
F(000)	904	588
Crystal size (mm^3)	0.324 x 0.214 x 0.052	0.2 x 0.12 x 0.05
Theta ranges for data collection	2.35-25.99	2.022 - 26.494°
Index ranges	-10<=h<=10, -18<=k<=18, -21<=l<=18	-11<=h<=11, -13<=k<=13, -15<=l<=15
Reflections collected	38816	19972
Independent reflections	4252 [R(int) = 0.0525]	4768 [R(int) = 0.0414]
Data/restraints/parameters	4252/0/303	4768/0/308
Goodness-of-fit on F^2	1.084	1.04588
Final R indices [I>2sigma(I)]	R1 = 0.0695 wR_2 = 0.1932	R1 = 0.0779 wR_2 = 0.1606
R indices (all data)	R1 = 0.0993 wR_2 = 0.2217	R1 = 0.1172 wR_2 = 0.1978
Largest diff peak and hole (e Å^{-3})	0.248 and -0.215	0.703 and -0.772
CCDC No.	2444267	2419464

τ_4 and τ_δ value equation for four-coordinate complexes[2]:

Table S3. Selected bond lengths (Å) and bond angles (°) for calculating the distortion parameter of **NiL3** complex.

Bond Length [Å]
NiL3
1.906 [Ni(1)-N(2)]
1.885 [Ni(1)-N(3)]
1.881 [Ni(1)-N(4)]
1.909 [Ni(1)-N(5)]

Bond Angle [°]
ML1
83.8 [N(2)-Ni(1)-N(3)]
173.1 [N(2)-Ni(1)-N(4)]
97.9 [N(2)-Ni(1)-N(5)]
95.6 [N(3)-Ni(1)-N(4)]
162.9 [N(3)-Ni(1)-N(5)]
84.7 [N(4)-Ni(1)-N(5)]
τ_4 = 0.171
τ_δ = 0.159

Equation for the calculation of τ_4 and τ_δ [8-9]

$$\tau_4 = \frac{360° - (\alpha + \beta)}{141°}$$

Where α and β are the two largest bond angles in the four-coordinate species

and, $$\tau_\delta = \frac{360° - (\alpha + \beta)}{141°}\delta$$

Where, $\delta = \frac{\beta}{\alpha}$

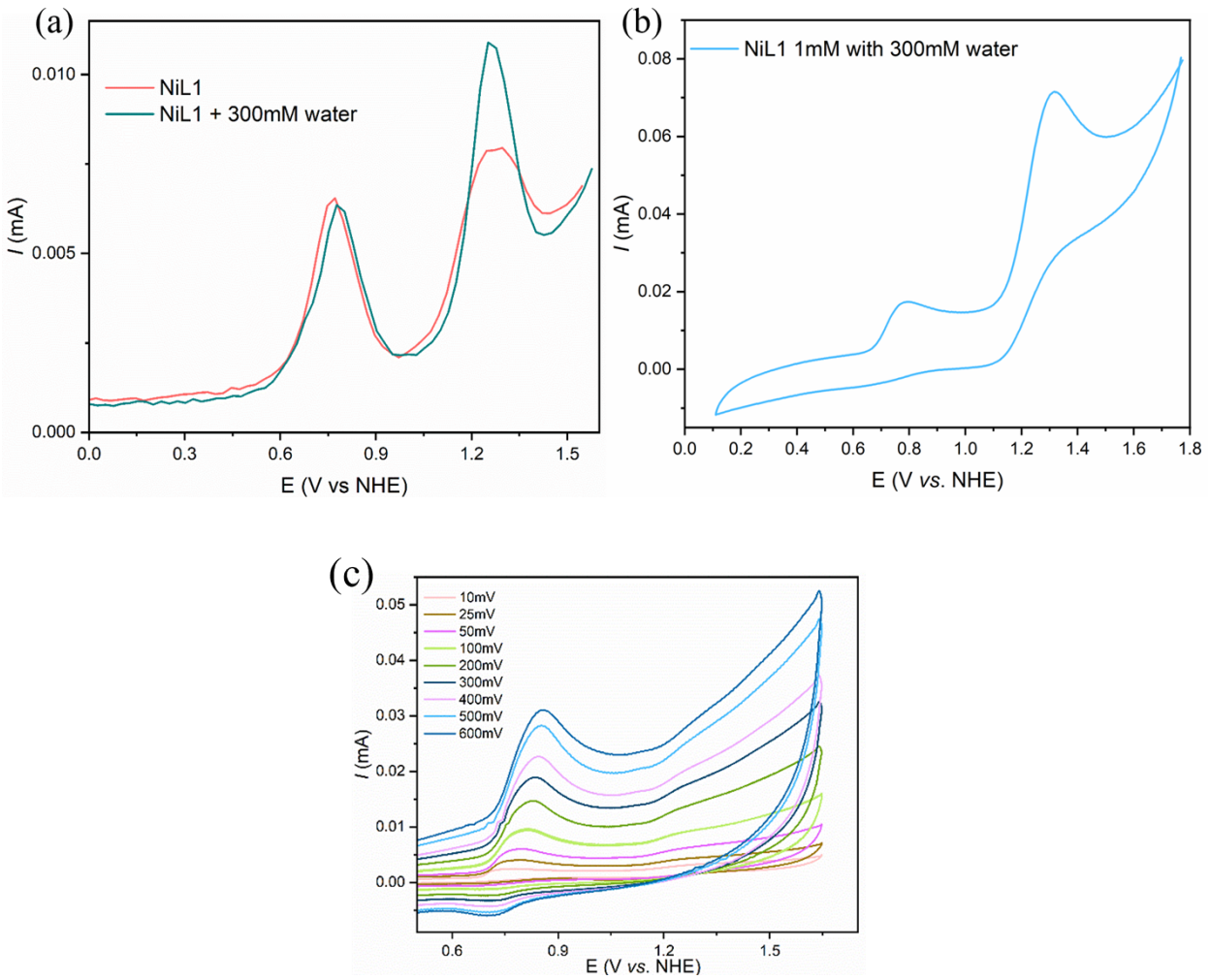


Figure S7: (a) DPV of **NiL1** and **NiL1** with 300 mM of H_2O in ACN solution with 0.05 M nBu$_4$NPF$_6$ as a supporting electrolyte (scan rate 50 mV/s). (b) CV of **NiL1** (1 mM) with 300 mM water added. (c) Scan rate dependence study for **NiL1** in the absence of water, no catalytic current generation observed at 1.3 V.

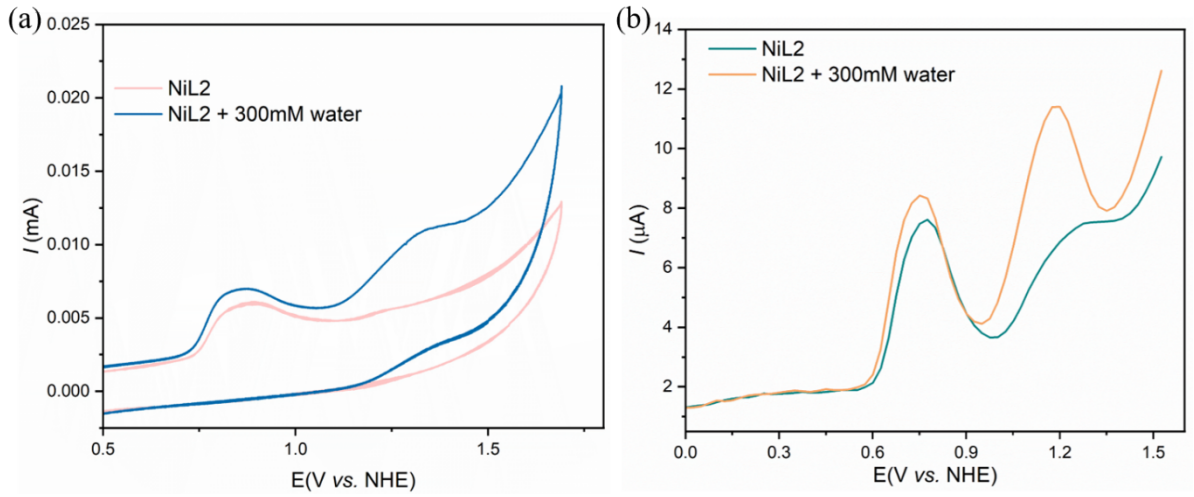


Figure S8: (a) Cyclic voltammograms of complex **NiL2** (0.2 mM) and electrocatalytic water oxidation upon addition of 300 mM of H_2O at a scan rate of 100 mV/s. (b) similarly, DPV of **NiL2** and **NiL2** with 300 mM of H_2O in ACN solution with 0.05 M nBu_4NPF_6 as a supporting electrolyte at scan rate 50 mV/s.

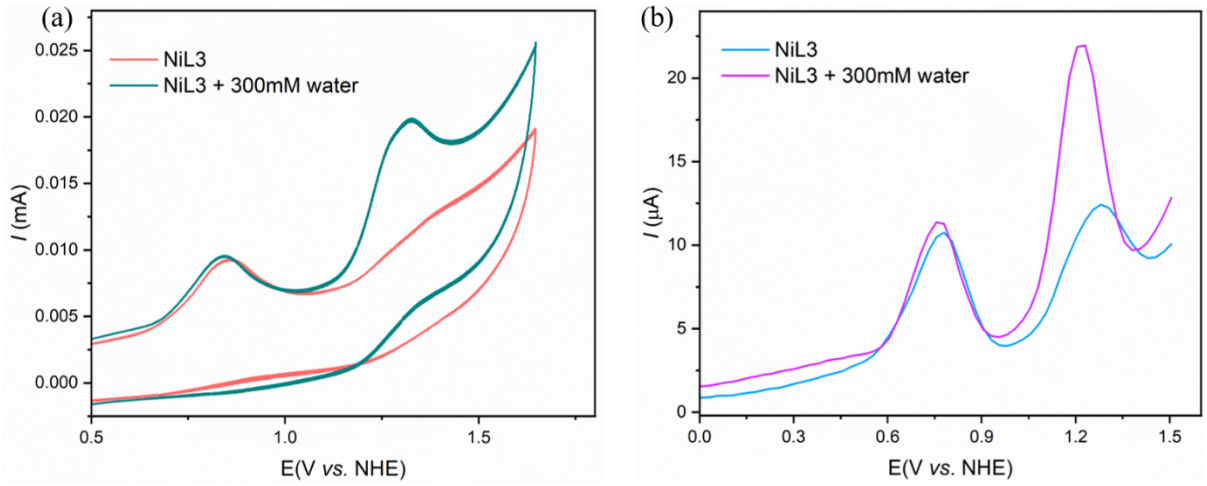


Figure S9: (a) Cyclic voltammograms of complex **NiL3** (0.2 mM) and electrocatalytic water oxidation upon addition of 300 mM of H_2O at a scan rate of 100 mV/s. (b) similarly, DPV of **NiL3** and **NiL3** with 300 mM of H_2O in ACN solution with 0.05 M nBu_4NPF_6 as a supporting electrolyte at scan rate 50 mV/s.

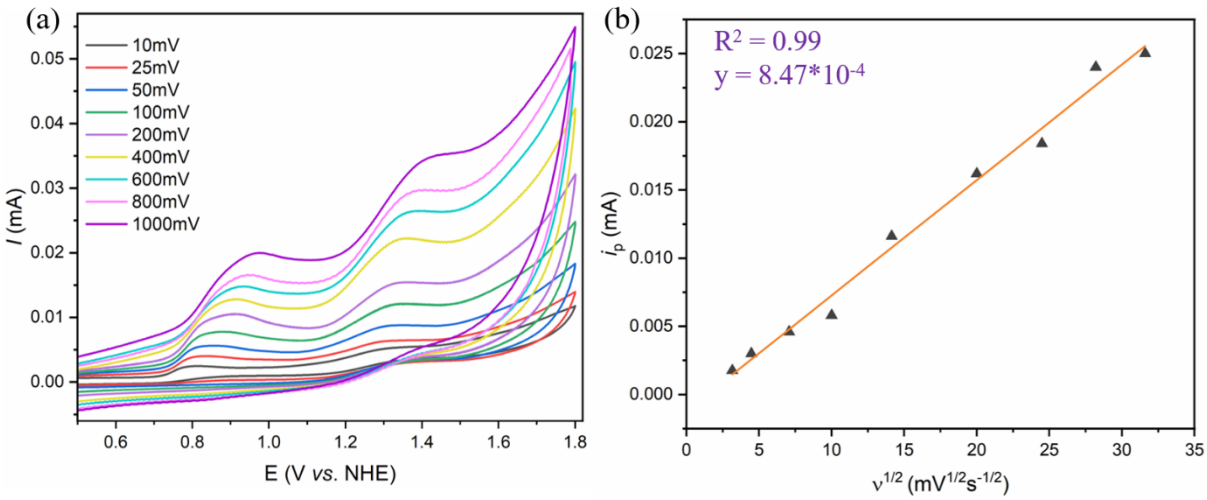


Figure S10: (a) CV of scan rate variation of **NiL2** (0.2 mM) with 300 mM water added to it. (b) peak catalytic current response with respect to $\nu^{1/2}$.

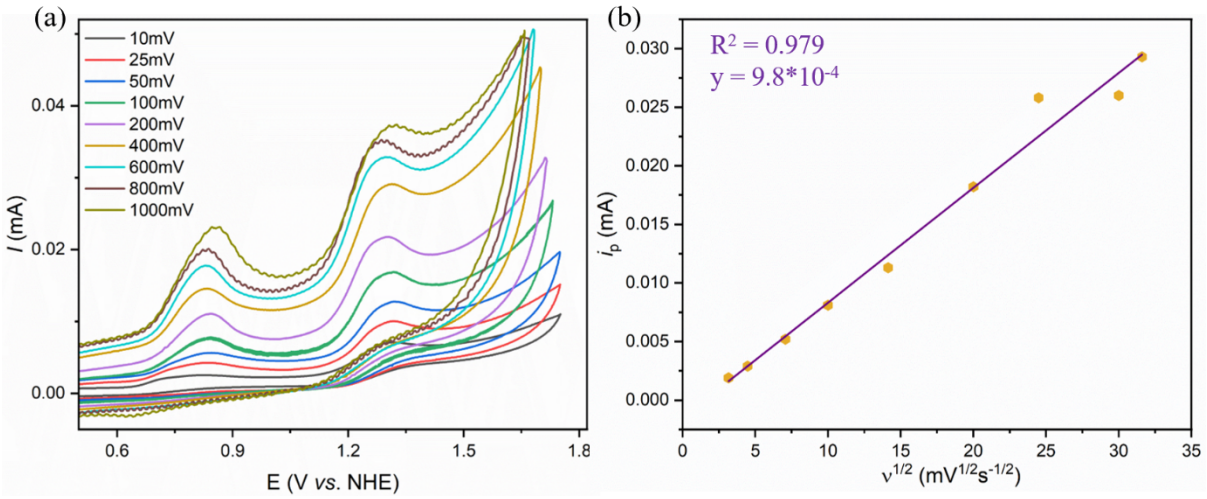


Figure S11: (a) CV of scan rate variation of **NiL3** (0.2 mM) with 300 mM water added to it. (b) peak catalytic current response with respect to $\nu^{1/2}$.

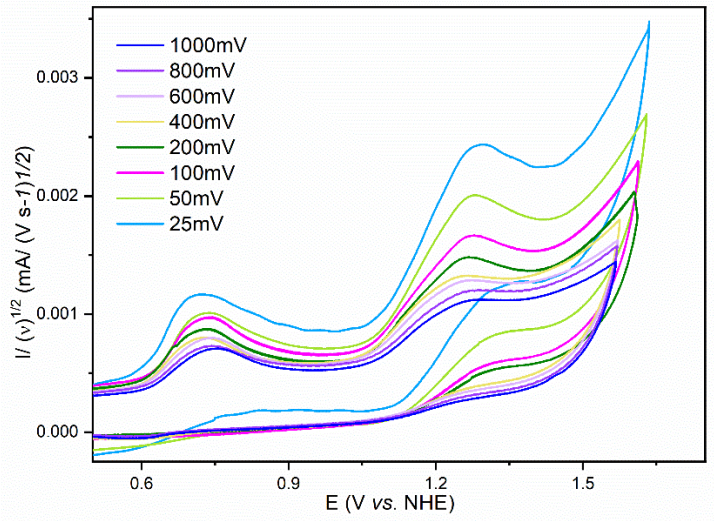


Figure S12a: Normalized CVs of 0.2 mM **NiL1** in 0.05 M supporting electrolyte ($^{n}Bu_4NPF_6$) at different scan rates.

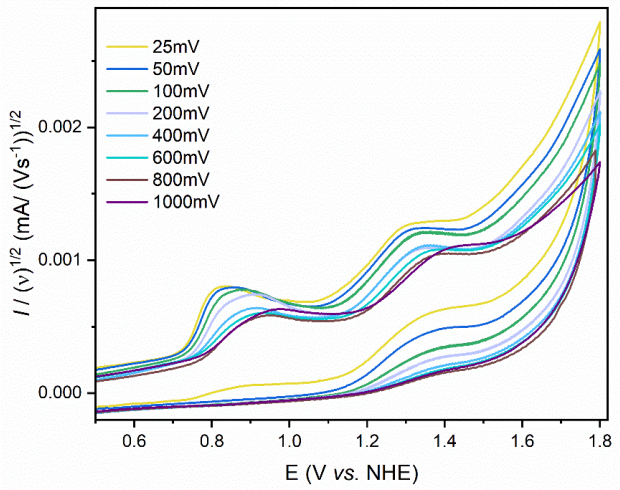


Figure S12b: Normalized CVs of 0.2 mM **NiL2** in 0.05 M supporting electrolyte ($^{n}Bu_4NPF_6$) at different scan rates.

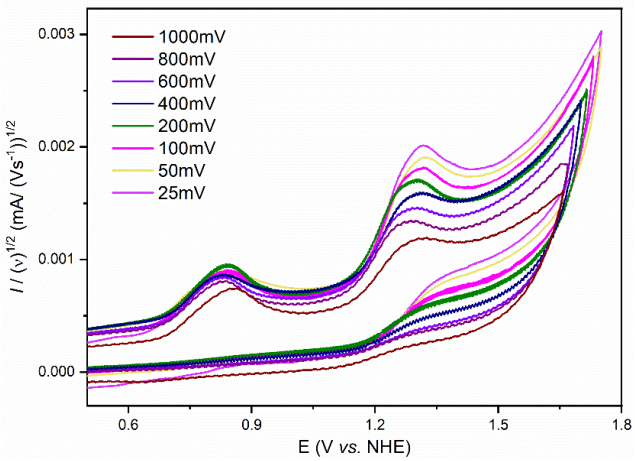


Figure S12c: Normalized CVs of 0.2 mM **NiL3** in 0.05 M supporting electrolyte ($^{n}Bu_4NPF_6$) at different scan rates.

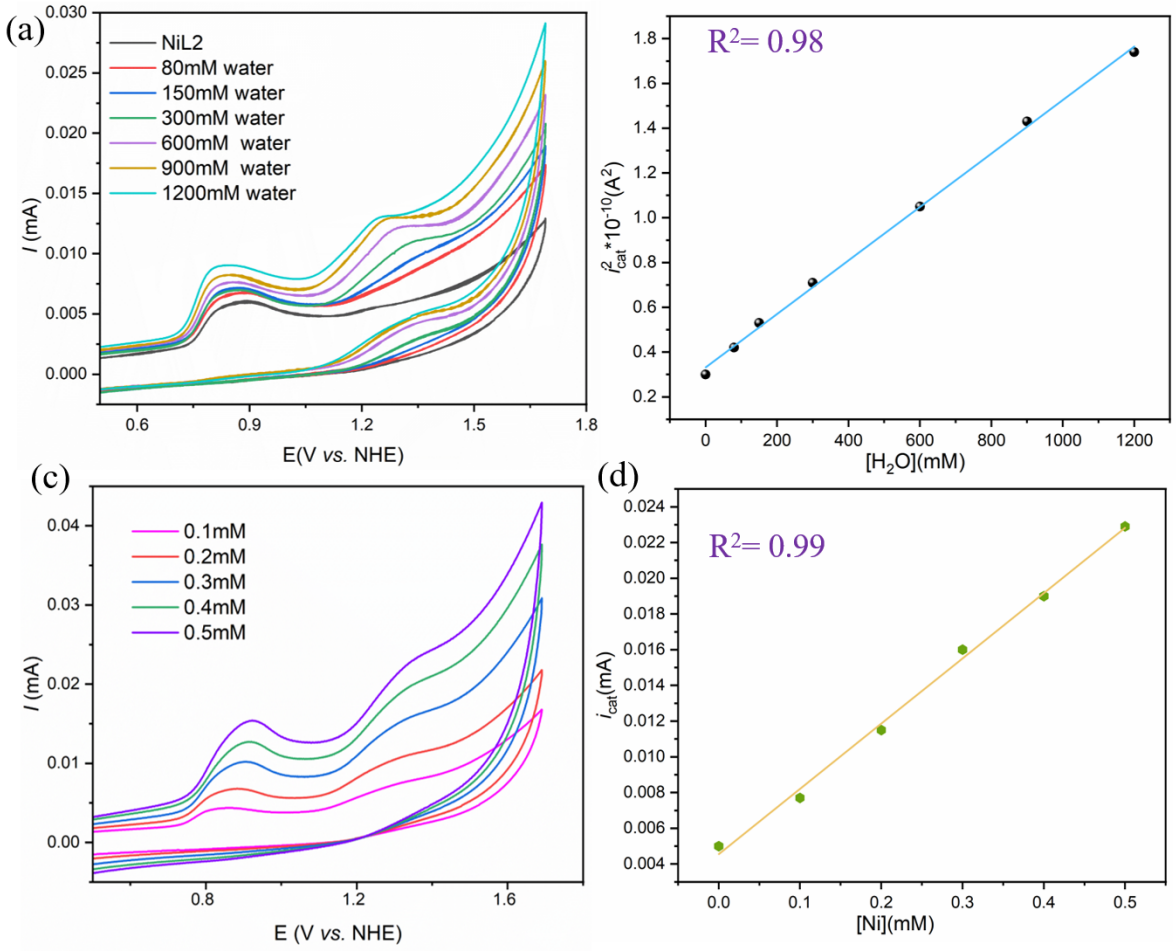


Figure S13: (a) CV for **NiL2** (0.2 mM) upon adding different amounts of water. (b) plot of i_{cat}^2 at 1.31V (*vs*. NHE) *vs.* [H_2O]. (c) CVs of complex concentration variation of **NiL2**. (d) plot of i_{cat} at 1.31V (*vs.* NHE) *vs.* [**NiL2**].

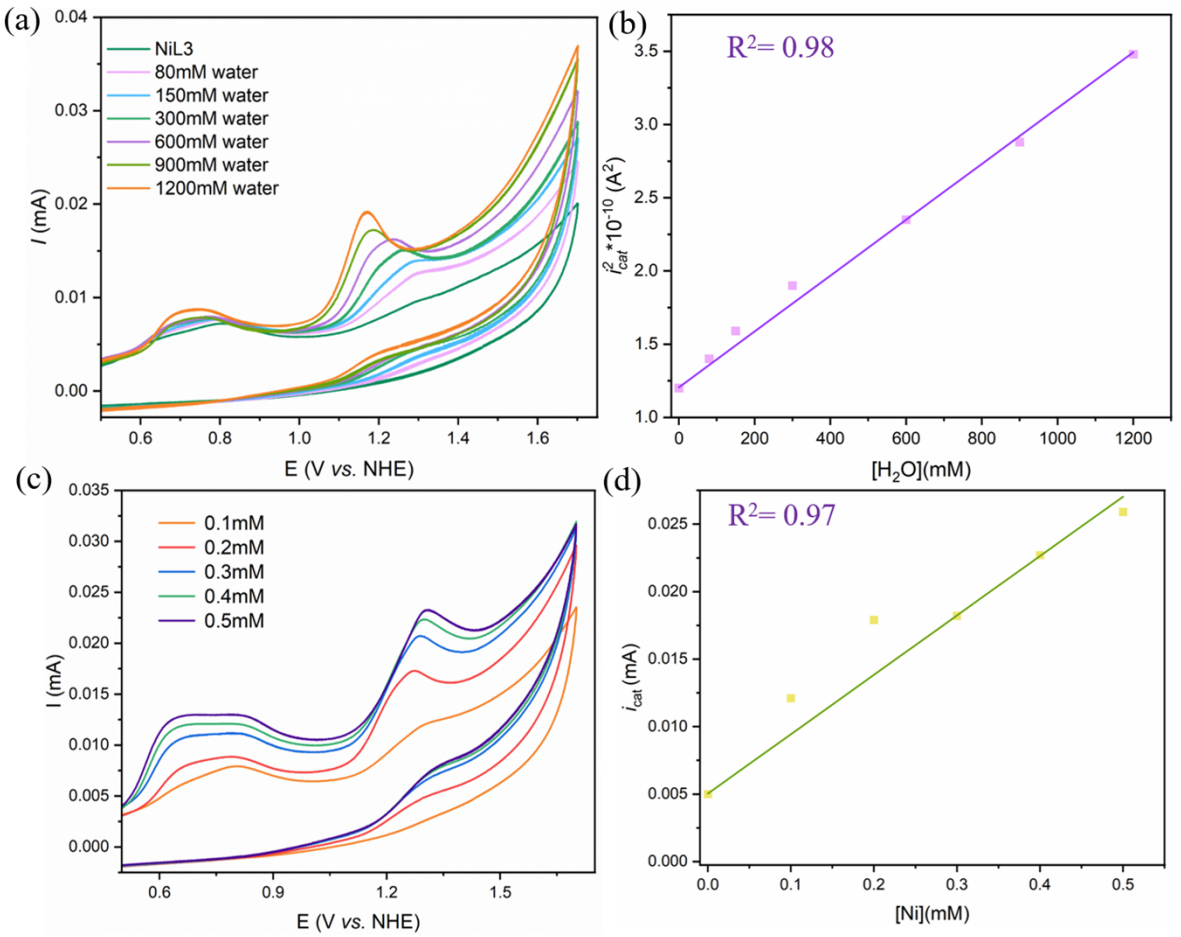


Figure S14: (a) CV for **NiL3** (0.2 mM) upon adding different amounts of water. (b) plot of i_{cat}^2 at 1.28 V (*vs*. NHE) *vs.* [H_2O]. (c) CVs of complex concentration variation of **NiL3**. (d) plot of i_{cat} at 1.28 V (*vs*. NHE) *vs.* [**NiL3**].

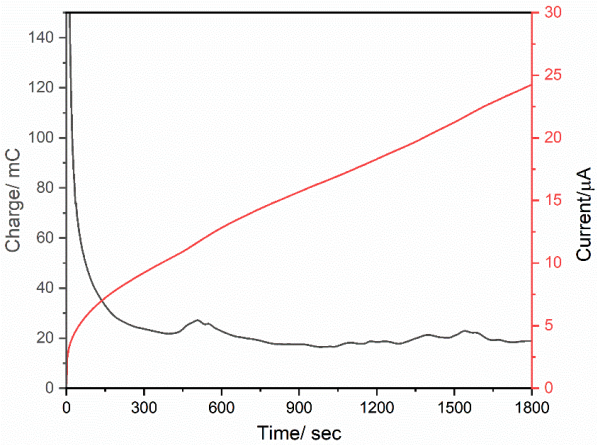


Figure S15: Plot of charge and current versus time during the CPE of **NiL1** (0.05 mM) at 0.78 V vs. NHE obtained from spectroelectrochemical analysis. *Note:* [Ni(II)L1] = 0.05 mM for the spectroelectrochemistry experiment and the total volume was 2.5 ml, reaction completion time = 1800 sec, total charge pass = 21.7 mC.

So according to the given condition, 1.25×10^{-7} moles of **NiL1** was present in the solution. Ni(II) → Ni(III) + e-; Therefore theoretically 1.25×10^{-7} moles of electrons is required for the

transformation, i.e. 12.1 mC charge should pass through the solution. Assuming 100% current efficiency, all the electrons should go towards the desired oxidation. However, in experimental conditions extra charge needs to be used to guarantee complete oxidation. Several practical reasons are:

1. Some side reactions like solvent oxidation
2. Solution resistance which was not compensated during the experiment.
3. Mass transport limitation where uneven current is distributed in bulk solution.

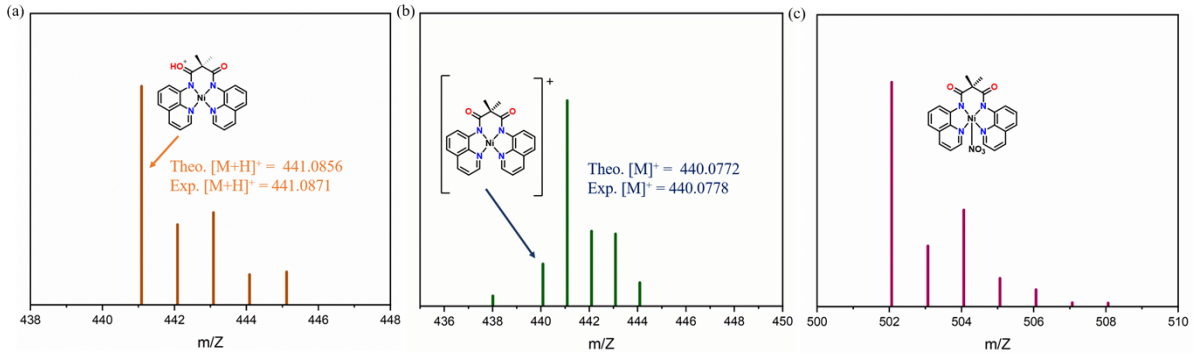


Figure S16: (a) HRMS spectrum of **NiL1** (observed m/Z [$C_{23}H_{18}N_4NiO_2$+H]: 441.0871, theoretical m/Z: 441.0856). (b) HRMS spectrum of **NiL1** with 1 eq. of CAN added to it (observed m/Z $[C_{23}H_{18}N_4NiO_2]^+$: 440.0772, theoretical m/Z: 440.0778). (c) Theoretical mass calculated by Isotope Distribution Calculator for [$C_{23}H_{18}N_4NiO_2 + NO_3$] of **NiL1** with 1 eq. of CAN added to it.

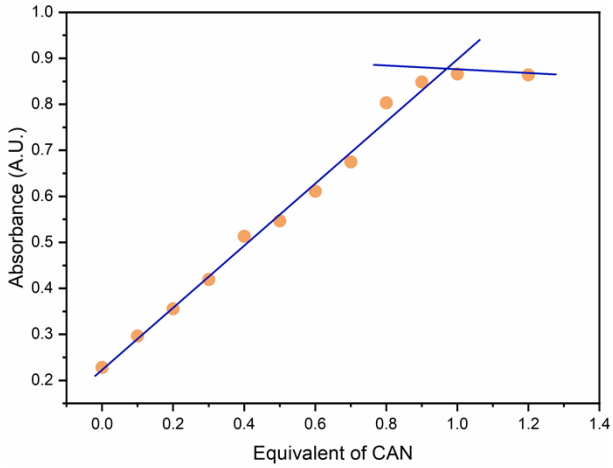


Figure S17: plot of absorbance vs. equivalent of CAN added to **NiL1**.

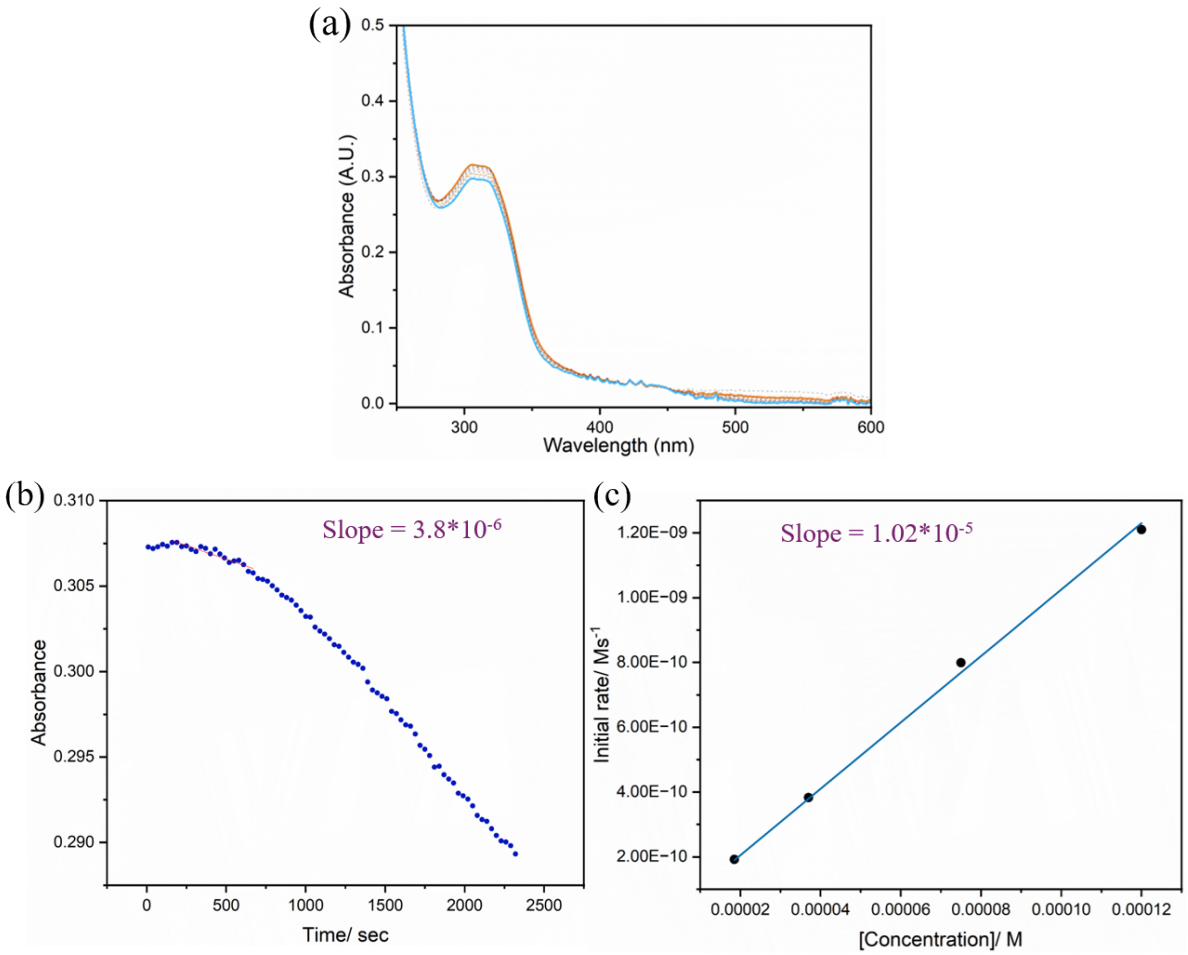


Figure S18: (a) UV-Vis spectral changes of **NiL1** with 1 equivalent of CAN added to it at RT for measurement of kinetic stability constant of chemically synthesized $[Ni(III)L1]NO_3$. (b) The spontaneous decay of $[Ni(III)L1]NO_3$ at 320 nm at RT. (c) Initial rate *vs*. [Ni(III) species]; The first order rate constants for the decay were found 1.02×10^{-5} s^{-1}.

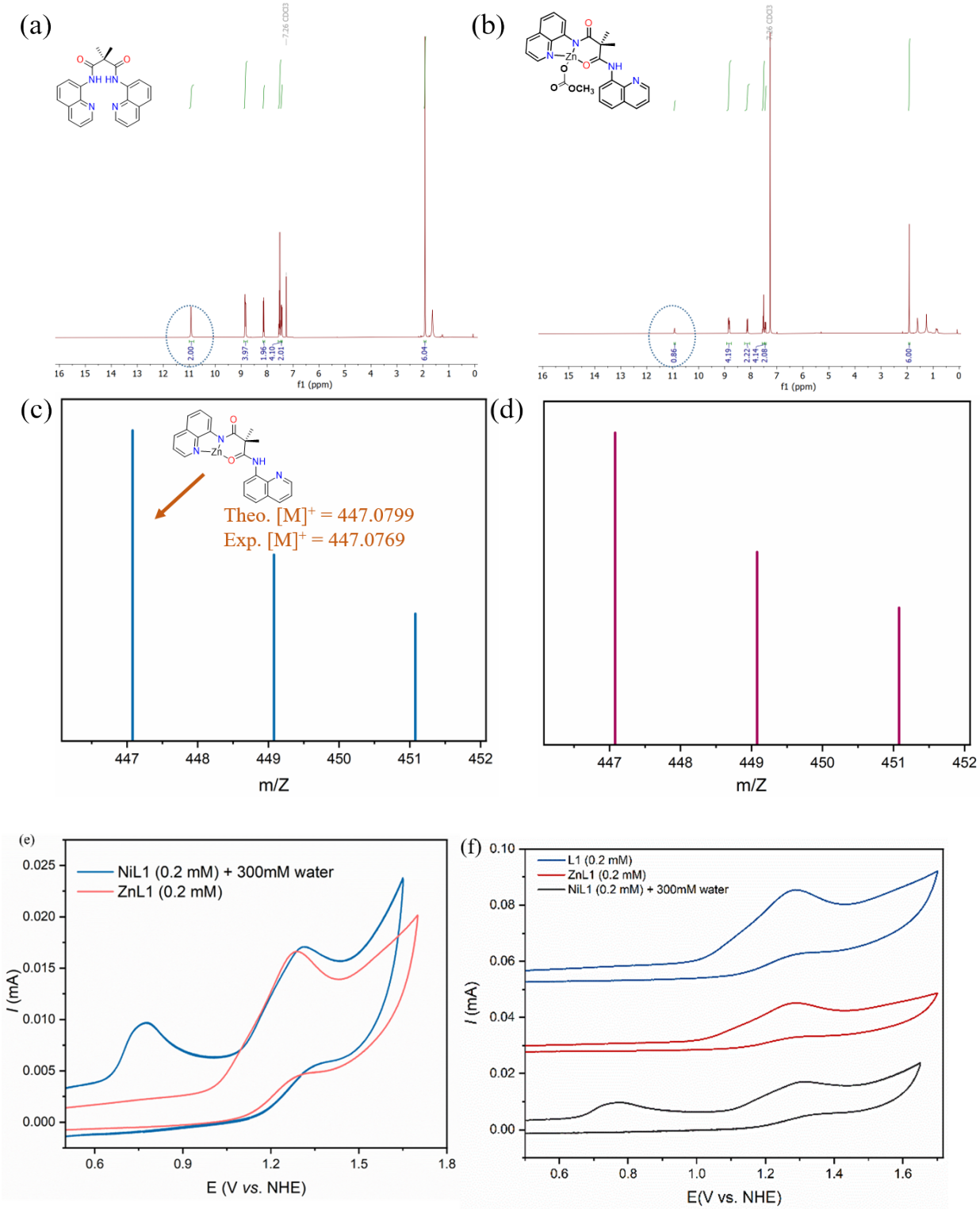


Figure S19: (a) ^{1}H NMR spectrum (400 MHz) of **H_2L1** recorded in $CDCl_3$ at 25°C. 11 ppm corresponds to two amide protons. (b) ^{1}H NMR spectrum (400 MHz) of Zn**L1** recorded in $CDCl_3$ at 25°C. 11 ppm corresponds to one amide proton. (c) HR-MS of Zn(II)L1 (chemical formula: $C_{23}H_{19}N_4O_2Zn$); Theo. $[M]^+$ = 447.0799, Exp. $[M]^+$ = 447.0769. (d) Theoretical *m/z* values of chemical formula: $C_{23}H_{19}N_4O_2Zn$ were calculated using Isotope Distribution Calculator under MassHunter software. (e) cyclic voltammogram of **NiL1** (blue) with 300 mM water and 0.05 M $^{n}Bu_4NPF_6$ as a supporting electrolyte added to it and **ZnL1** recorded at a scan rate of 100 mV/s. Conditions: glassy carbon as working electrode, Pt wire as counter

electrode and Ag/ $AgNO_3$ as reference electrode. (f) Comparison of CV of **NiL1** (0.2 mM) with 300 mM water added, **ZnL1**(0.2 mM) and **H_2L1** (0.2 mM).

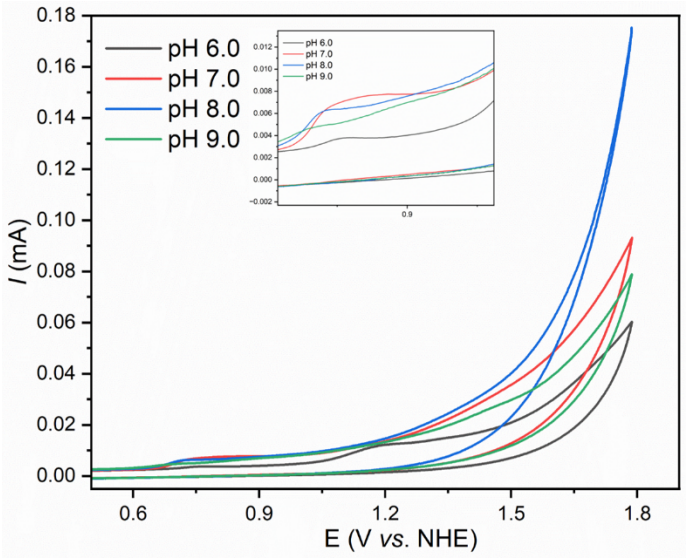


Figure S20: CV of the complex **NiL1** (0.2 mM) in various 0.1 M pH (scan rate 100 mV/s).

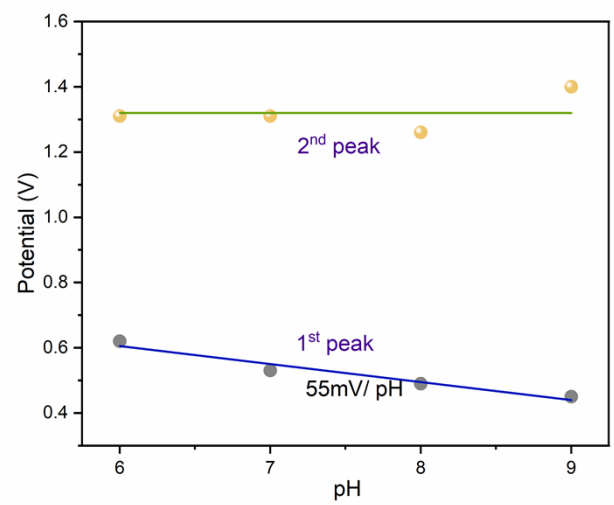


Figure S21: Pourbaix diagram (Plot of Potential of two oxidation peaks *vs*. pH) for complex **NiL2** (0.2 mM) in 0.1 M PBS using glassy carbon working electrode and Pt wire counter electrode.

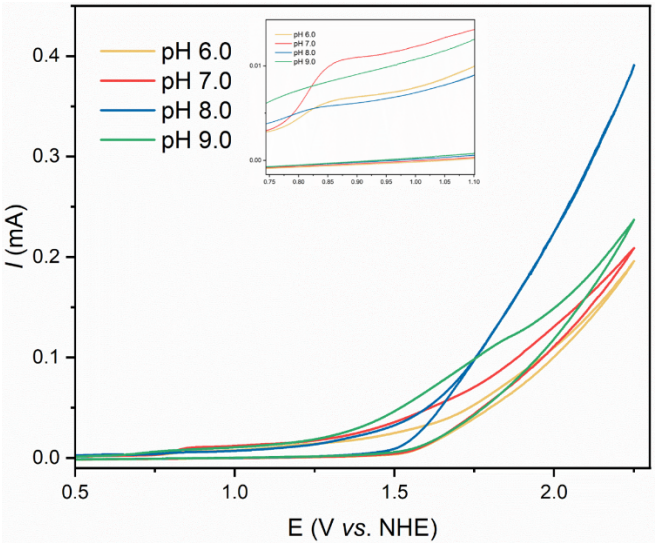


Figure S22: CV of the complex **NiL2** (0.2 mM) in various 0.1M pH (scan rate 100 mV/s).

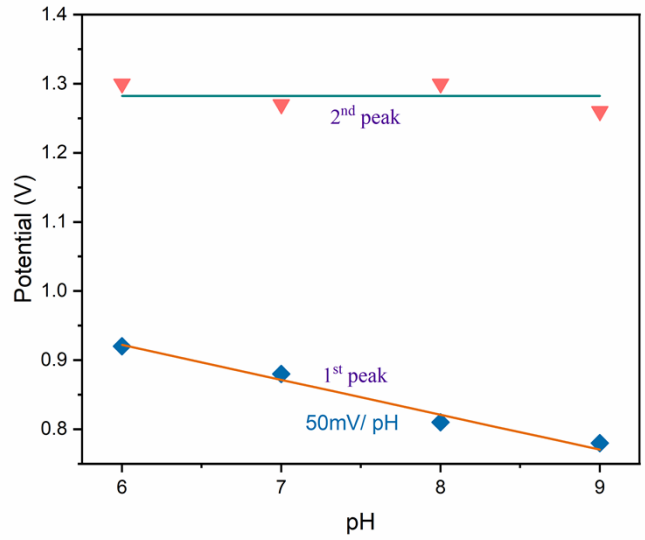


Figure S23: Pourbaix diagram (Plot of Potential of two oxidation peaks *vs*. pH) for complex **NiL3** (0.2 mM) in 0.1M PBS using glassy carbon working electrode and Pt wire counter electrode.

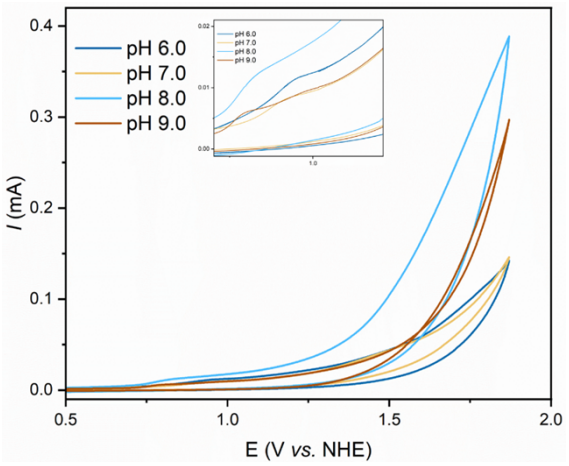


Figure S24: CV of the complex **NiL3** (0.2 mM) in various 0.1 M pH (scan rate 100 mV/s).

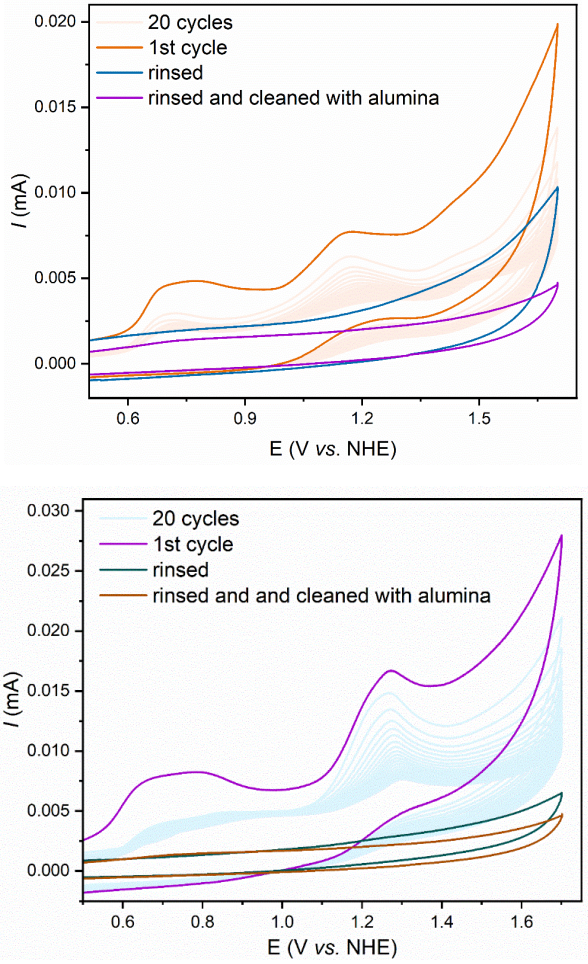
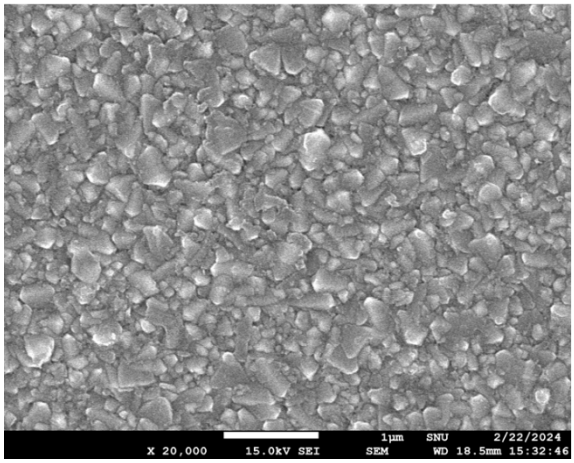


Figure S25: Consecutive 20 CV scans of 0.2 mM (top) **NiL2** and (bottom) **NiL3** in 0.05 M $^{n}Bu_4NF_6$/ ACN at a scan rate of 100 mV/s and 300 mM water added to it using GC working electrode. After 20th cycle, the GC electrode was rinsed with CAN, and the CV data was recorded in fresh 0.05 M $^{n}Bu_4NF_6$/ ACN solution. The electrode was then polished with alumina powder washed with water and ACN and CV data was collected again in a fresh 0.05 M $^{n}Bu_4NF_6$/ ACN solution.

Blank



After bulk electrolysis

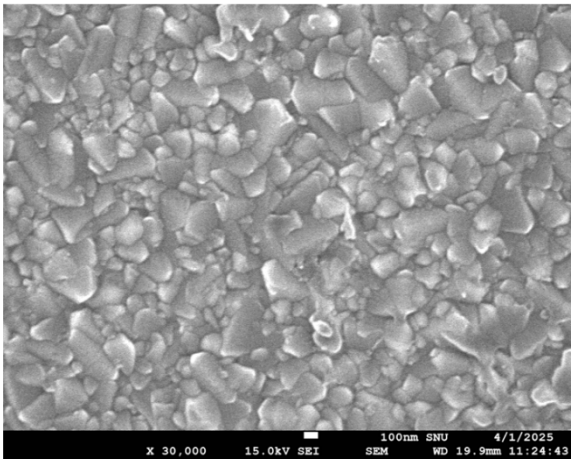
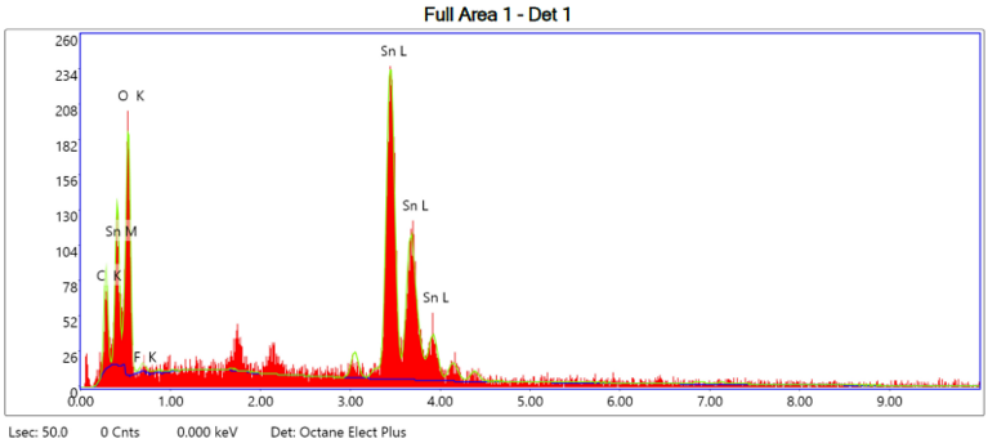


Figure S26a: FE-SEM images of the FTO working electrode before and after bulk electrolysis.



Element	Weight %	Atomic %
C K	2.78	15.58
O K	8.05	33.86
F K	0.01	0.04
SnL	89.16	50.53

Figure S26b: EDX of the FTO working electrode after bulk electrolysis.

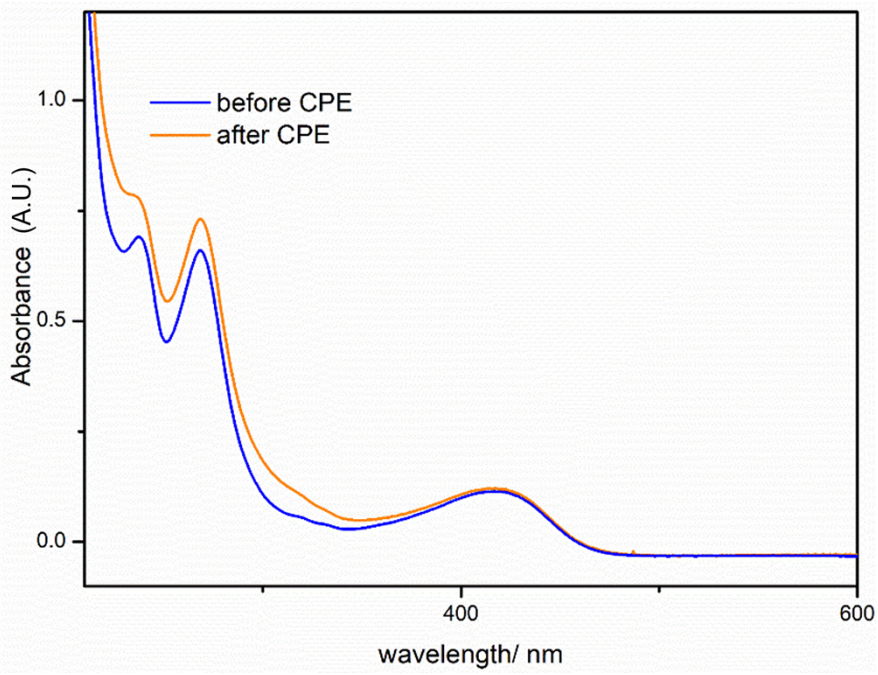


Figure S27: UV-Vis spectra of **NiL1** before and after bulk electrolysis (CPE).

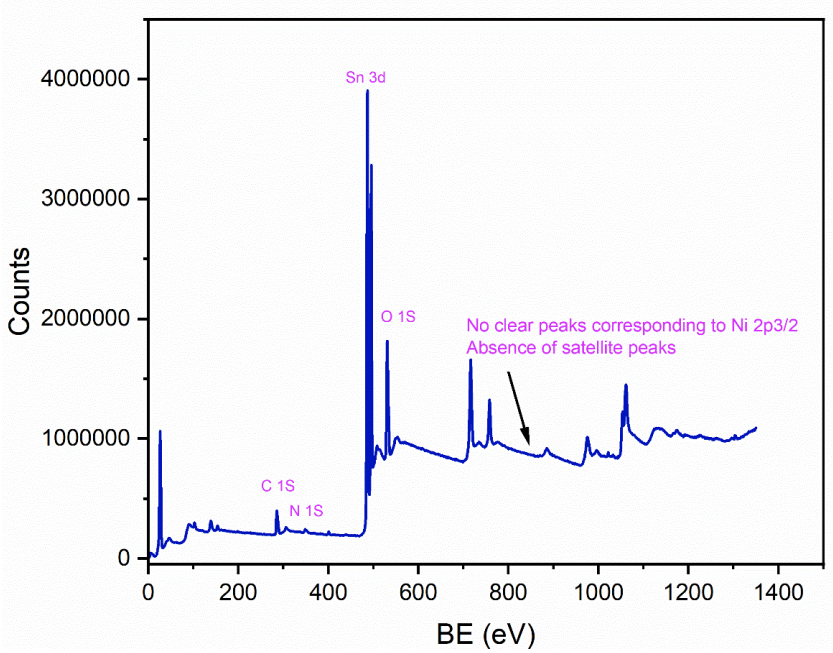


Figure S28: XPS spectrum of FTO electrode after bulk electrolysis of **NiL1**.

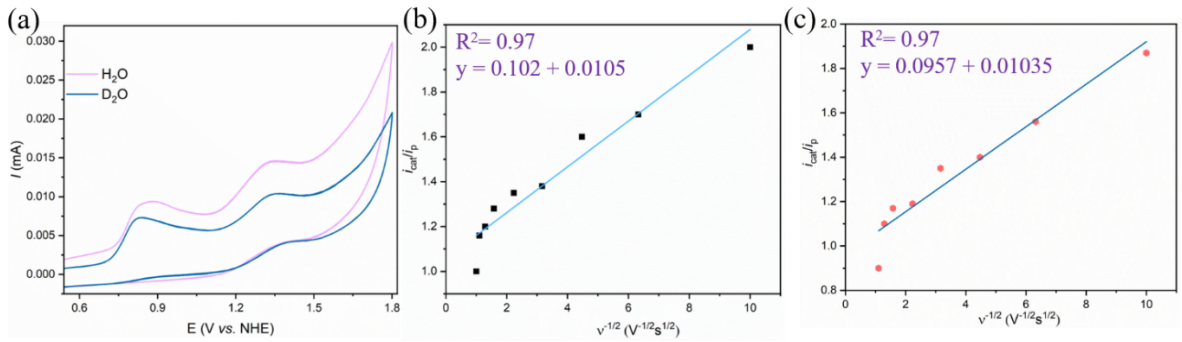


Figure S29: CVs of **NiL2** (0.2 mM) with added 300 mM of H_2O (blue) and D_2O (orange) (scan rate 100 mV/s). (b) plot of i_{cat} / i_p as a function of the inverse of the square root of scan rate in the case of H_2O for **NiL2**. (c) plot of i_{cat} / i_p as a function of the inverse of the square root of scan rate in the case of D_2O for **NiL2**.

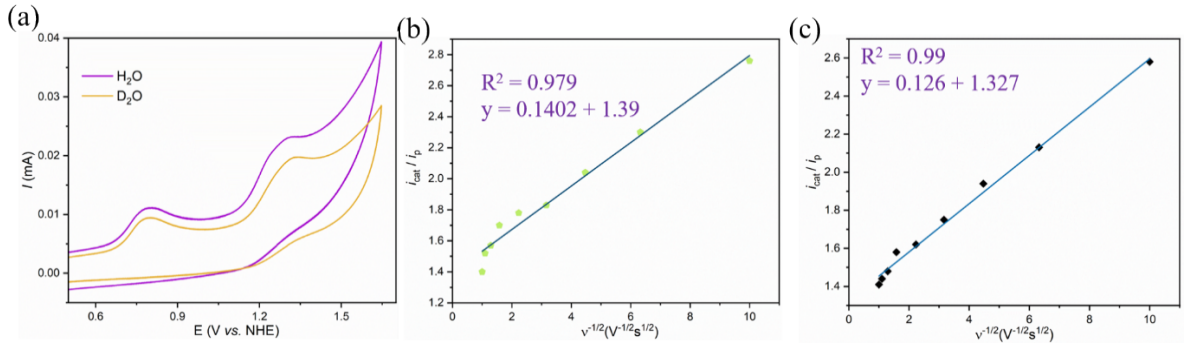


Figure S30: CVs of **NiL3** (0.2 mM) with added 300 mM of H_2O (blue) and D_2O (orange) (scan rate 100 mV/s). (b) plot of i_{cat} / i_p as a function of the inverse of the square root of scan rate in the case of H_2O for **NiL3**. (c) plot of i_{cat} / i_p as a function of the inverse of the square root of scan rate in the case of D_2O for **NiL3**.

Faradaic efficiencies Calculations for Ni(II) complexes:

For **NiL1**

Total charge passed for catalytic oxygen = 1.73 C

Amount of oxygen expected =

$$\frac{1.73\ C}{96485\ \times 4\ C} mol = 4.48\ \mu moles = \left(22.4 \frac{\mu l}{\mu moles} \times 4.48\ \mu moles\right) = 100.41\ \mu l$$

Amount of oxygen detected in the headspace (calibrated by control) = 95 μl

$$\%\ \text{of faradaic efficiency of } \textbf{NiL2} = \frac{95}{100.41} \times 100 = 94.6$$

For **NiL2**

Total charge passed for catalytic oxygen = 1.4 C

Amount of oxygen expected =

$$\frac{1.4\ C}{96485\ \times 4\ C} mol = 3.63\ \mu moles = \left(22.4 \frac{\mu l}{\mu moles} \times 3.63\ \mu moles\right) = 81.26\ \mu l$$

Amount of oxygen detected in the headspace (calibrated by control) = 70 μl

% of faradaic efficiency of **NiL2** = $\frac{70}{81.26} \times 100 = 86.14$

For **NiL3**

Total charge passed for catalytic oxygen = 3.85 C

Amount of oxygen expected =

$$\frac{3.85\ C}{96485\ \times 4\ C} mol = 9.3\ \mu moles = \left(22.4 \frac{\mu l}{\mu moles} \times 9.94\ \mu moles\right) = 208.3\ \mu l$$

Amount of oxygen detected in the headspace (calibrated by control) = 210 μl

% of faradaic efficiency of **NiL2** = $\frac{208.3}{210} \times 100 = 99.04$

TON value calculations for Ni(II) complexes:

$$TON = \frac{Qcat - Qblank}{moles\ of\ catalyst \text{ x } n \text{ x } F}$$

Q_{cat} = Charge passed with catalyst (in Coulombs)

Q_{blank} = Charge passed without catalyst (in Coulombs)

n = number of electrons transferred

F = Faraday constant (96485 C/mol)

For **NiL1**

Total charge passed for catalytic oxygen = 1.73 C

Charge passed without catalyst = 0.04 C

moles of catalyst = $(0.2 \times 10^{-6} \times 3) = 0.6 \times 10^{-6}$

$$TON = \frac{1.73 - 0.04}{0.0000006 \times 4 \times 96485}$$

$$TON = 7.29$$

For **NiL2**

Total charge passed for catalytic oxygen = 1.4 C

Charge passed without catalyst = 0.04 C

moles of catalyst = $(0.2 \times 10^{-6} \times 3) = 0.6 \times 10^{-6}$

$$TON = \frac{1.4 - 0.04}{0.0000006 \times 4 \times 96485}$$

$$TON = 5.86$$

For **NiL3**

Total charge passed for catalytic oxygen = 3.85 C

Charge passed without catalyst = 0.04 C

moles of catalyst = $(0.2 \times 10^{-6} \times 3) = 0.6 \times 10^{-6}$

$$TON = \frac{3.85 - 0.04}{0.0000006 \times 4 \times 96485}$$

$$TON = 16.4$$

Table S4. Total charge passed during bulk electrolysis for 3 hours for all the complexes.

Entry	Complex	Total charge passed	TON
1	**NiL1**	1.73 C	7.29
2	**NiL2**	1.4 C	5.86

3	**NiL3**	3.6 C	16.4

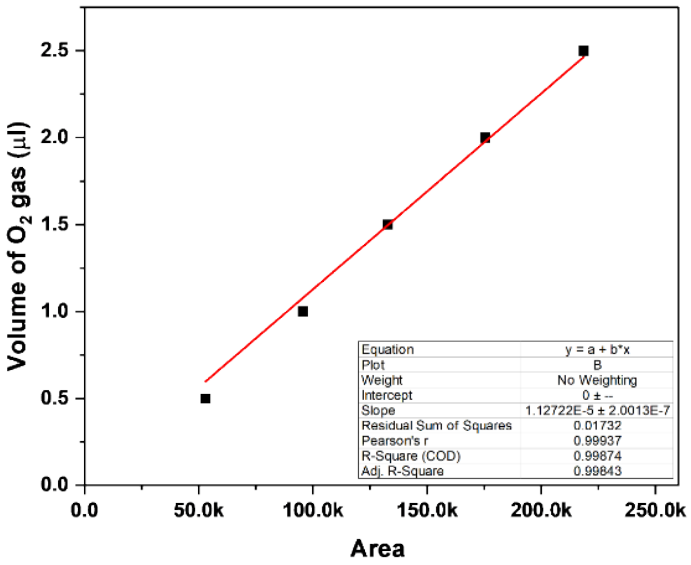


Figure S31a. Calibration curve for the quantitative analysis of oxygen gas during CPE experiments.

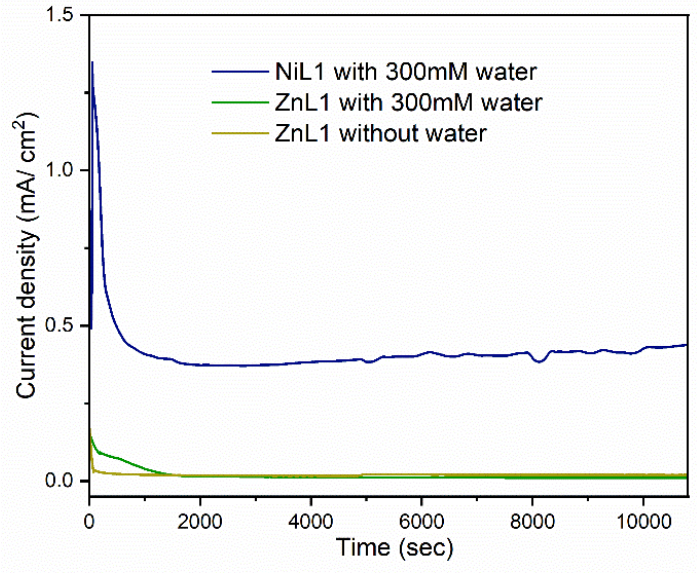


Figure S31b: Plot of the catalytic current density vs reaction time comparing **NiL1** (with 300 mM water) and **ZnL1** (with and without 300 mM water).

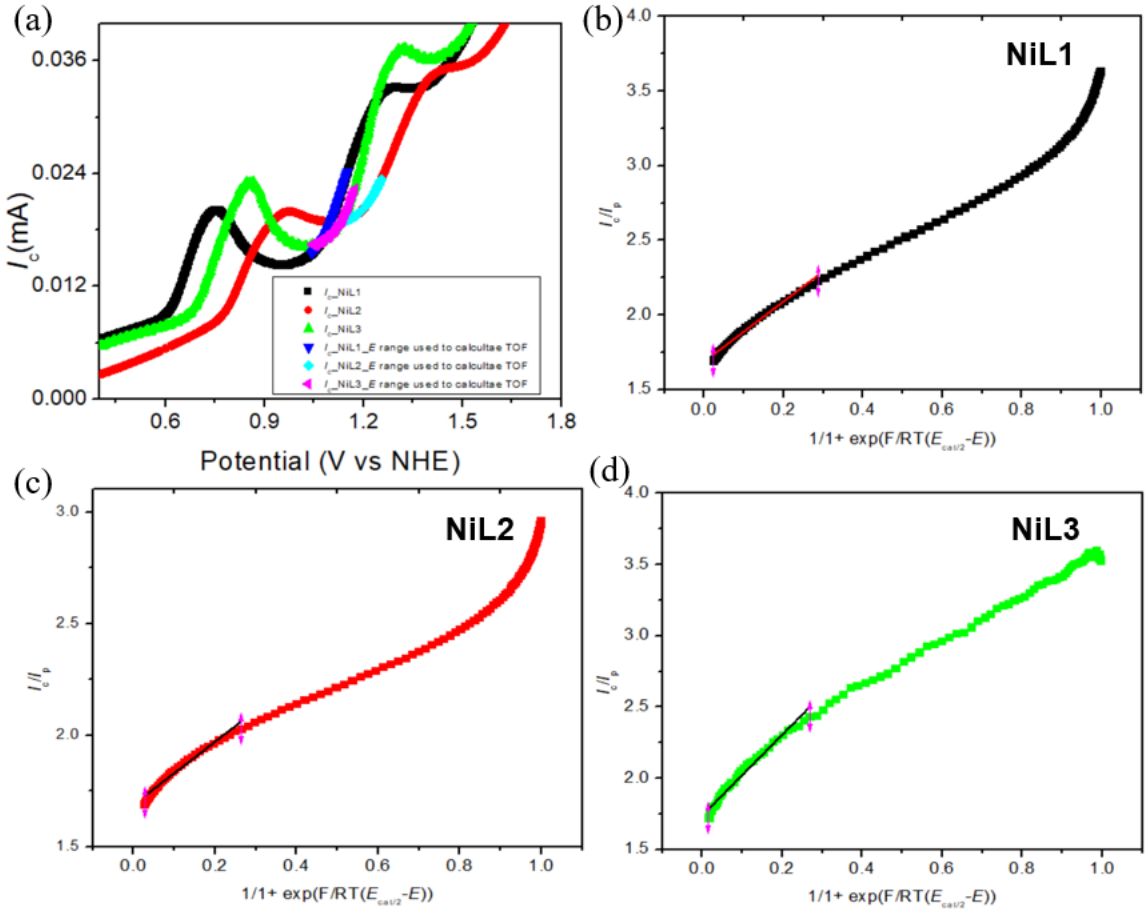


Figure S32: (a) Forward trace CV of **NiL1, NiL2 and NiL3** in MeCN with 300 mM H_2O recorded at 1000 mV/s. The potential range used to calculate TOF is highlighted in each case. (b) Plot of Normalized current from the anodic sweep of CV of **NiL1** *vs*. 1/(1+ exp(F/RT($E_{cat/2}$-E)). (c) Plot of Normalized current from the anodic sweep of CV of **NiL2** *vs*. 1/(1+ exp(F/RT($E_{cat/2}$-E)). (d) Plot of Normalized current from the anodic sweep of CV of **NiL3** *vs*. 1/(1+ exp(F/RT($E_{cat/2}$-E)).

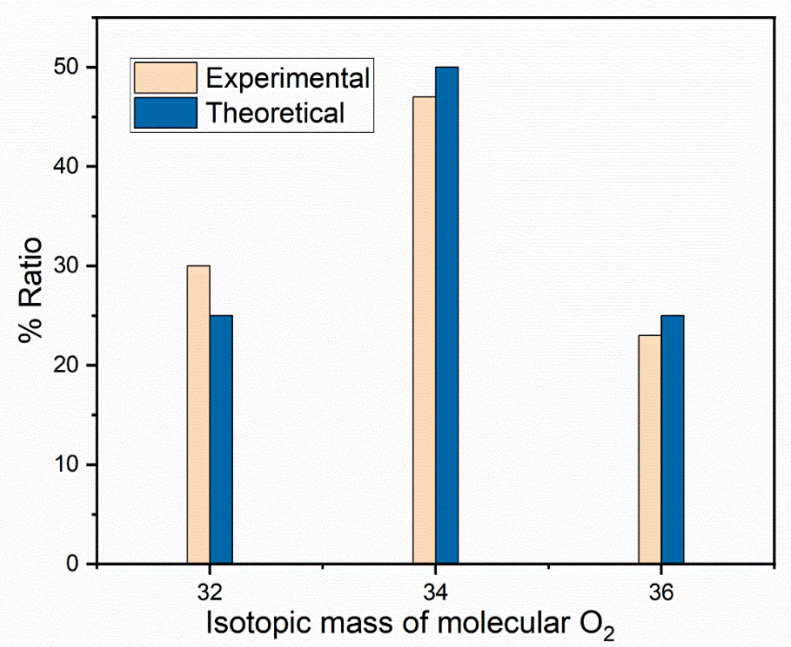


Figure S33. Comparison for the ratio of $^{32}O_2$, $^{34}O_2$ and $^{36}O_2$ molecular oxygen evolved (theoretical and observed) during electrochemical WO oxidation using 1:1 $H_2{}^{18}O$ in $H_2{}^{16}O$.

Computational Details:

Theoretical calculations (DFT) were carried out using the Gaussian 16 program to study the water oxidation mechanism (O-O bond formation via WNA or intramolecular O-O coupling process) of quinoline-based nickel catalysts.[3] Geometry optimizations and frequency calculations were performed with no symmetry and spin constraints (spin polarized) using the M06L functional with the def2TZVP basis set for all atoms. [4, 5] A polarized continuum model (PCM) was utilized to incorporate implicit solvent effect (acetonitrile) on the geometries and energy of the optimized structures.[6] The nature of all stationary points as minima (no imaginary frequency) or transition states (one imaginary frequency) are confirmed through vibrational frequency calculations. For the transition state calculations, bond/angle scans were performed, and the transition states were confirmed using Chemcraft visualization software by animating the vibration modes.[7] All reaction-free energies relative to reactant energies at 298.15 K, including zero-point and entropic corrections. Spin density and charge calculations (Natural Bonding Orbital-NBO) were performed to quantify the radical behaviour of oxyl radicals and amino quinoline ligand oxidation.[8, 9, 10] In the current study, to construct a free energy diagram, we used experimental standard solvation free energies for the electron (-4.28 eV) from standard free energy change of NHE and proton in aqueous solution (-272.2 kcal/mol) for protonation and deprotonation during the electrochemical reactions.

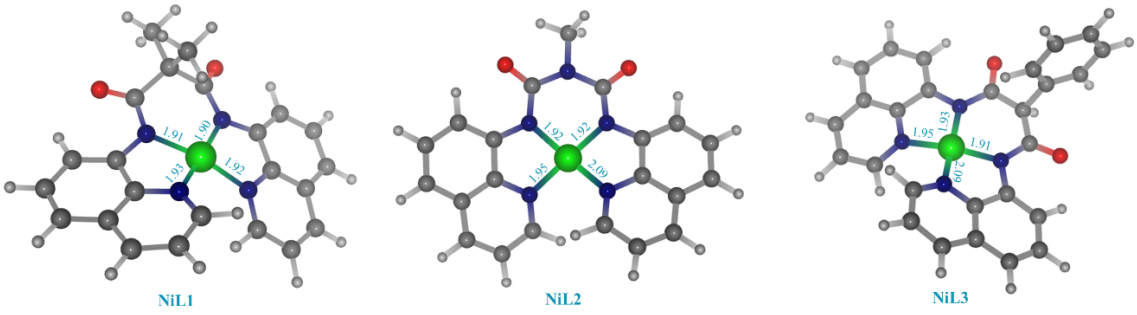


Figure S34: DFT optimized structures for **NiL1**, **NiL2** and **NiL3** complexes in singlet spin as a ground state (M-N Bond lengths in Å).

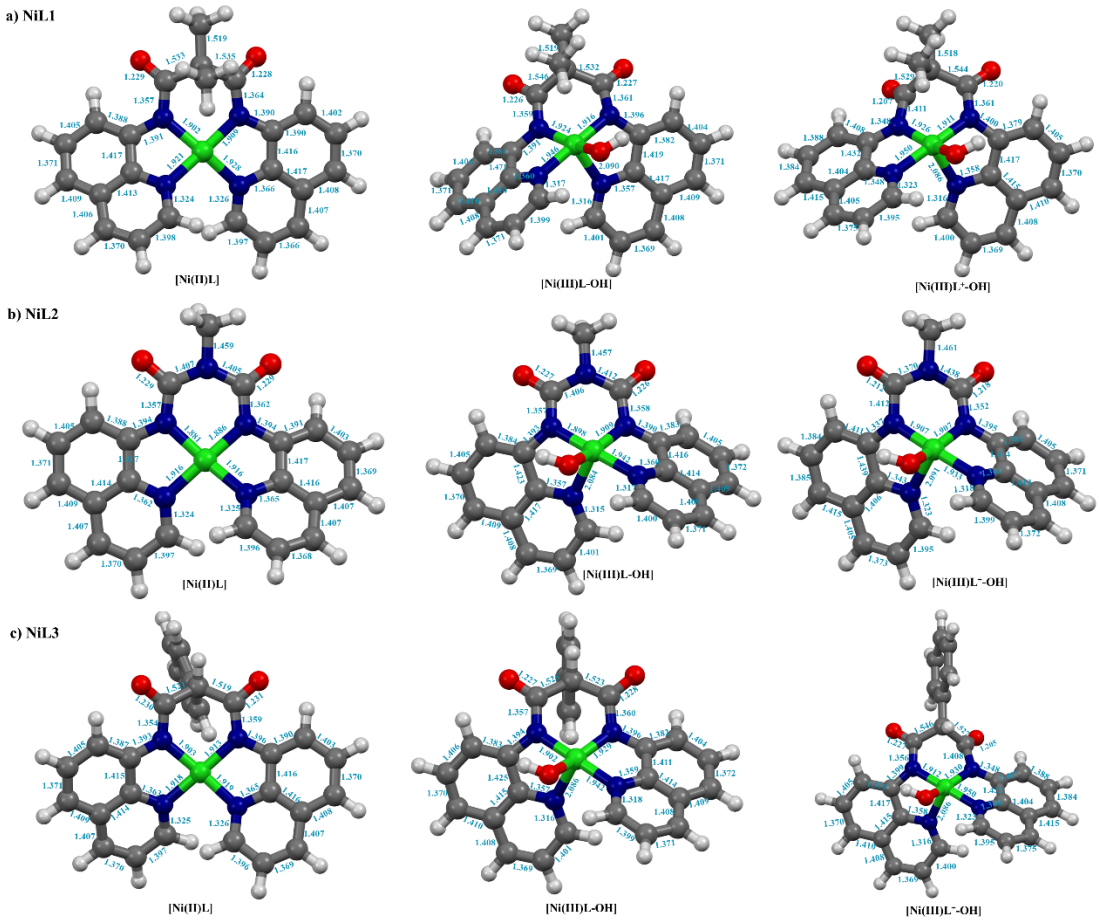


Figure S35: Optimized structural parameters of **NiL1**, **NiL2** and **NiL3**. (All the bond lengths in Å)

Table S5. NBO charge distribution analysis of [Ni(II)L], [Ni(III)L-OH] and [Ni(III)$L^{\cdot+}$-OH] intermediates.

Complexes	[Ni(II)L]		[Ni(III)L-OH]		[Ni(III)L$^{\cdot+}$-OH]	
Charge	**Metal**	**Ligand**	**Metal**	**Ligand**	**Metal**	**Ligand**
NiL1	0.612	-0.612	0.820	-0.820	0.811	0.189
NiL2	0.601	-0.601	0.859	-0.859	0.857	0.143
NiL3	0.611	-0.611	0.857	-0.857	0.873	0.127

Table S6. Spin density analysis for [Ni(III)L-O$^{\cdot}$]and [Ni(III)L-OHO$^{\cdot}$] intermediates

Spin density of [Ni(III)L-O$^{\cdot}$] intermediate		
Complexes	**Metal**	**O$^{\cdot}$**
NiL1	1.607	1.400
NiL2	1.606	1.390
NiL3	1.612	1.435
Spin density of [Ni(III)L-OHO$^{\cdot}$] intermediate		
Complexes	**Metal**	**O$^{\cdot}$**
NiL1	-0.051	0.982
NiL2	-0.057	0.996
NiL3	-0.062	0.935

Table S7. NBO charge distribution analysis of [Ni(III)L-O$^{\cdot}$] intermediate.

NBO charges [Ni(III)L-O•] intermediate			
Complexes	**Metal**	**Ligand**	**O•**
NiL1	0.883	-0.514	-0.369
NiL2	0.872	-0.499	-0.374
NiL3	0.892	-0.553	-0.339

Alternative Pathway for NiL3 complex:

Our proposed pathway for the water oxidation process involves the formation of highly reactive Ni-O• intermediate species. In the optimized Ni-O• intermediate structure shows a Ph-C-H proton with the distance between O of Ni-O• approximately 2.6 Å away from H of Ph-C-H moiety. We explored the possibility of proton abstraction from the Ph-CH moiety via the radical pathway (Figure S33, step 4). Figure 33a shows the reaction energy scheme for O_2 evolution following the proton abstraction, and the corresponding calculated Gibbs free energy profile for the **NiL3** complex is shown in Figure S33b.

While following this pathway, we found that proton abstraction needs a Kinetic energy barrier of 8 kcal/mol. The initial steps G1-G3 are similar to the other two pathways (path I and path II). In the later steps G6-G8, compared to the most feasible mechanism (pathway II) in the main text, we found one of the reaction steps with high endothermicity. The formation of the dihydroxide intermediate [$Ni(OH)_2$] shows a Gibbs free energy of 28 kcal/mol. On the other hand, in O-OH coupling pathway (pathway II), the formation of Ni-O•(OH) intermediate following Ni-O• is an electrochemical step without a subsequent barrier under an applied potential. Therefore, the rate of Ni-O•(OH) intermediate formation would be faster than the proton abstraction. Therefore, we conclude that this pathway is energetically less favourable.

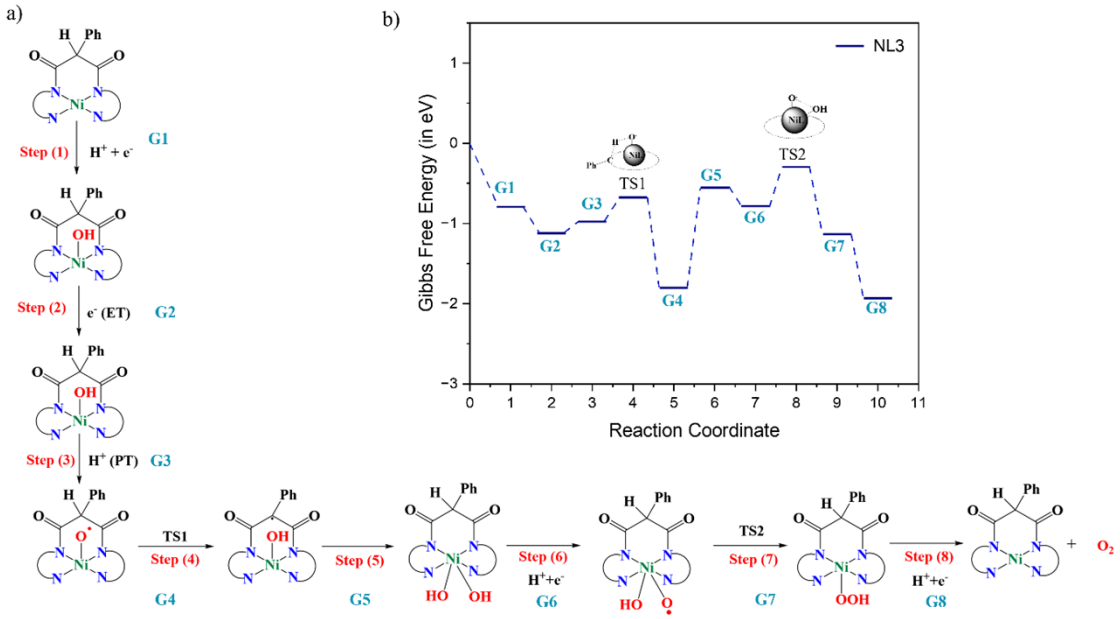


Figure S36: (a) Alternative Mechanistic pathway for **NiL3** complex. (b) Gibbs free energy pathway for **NiL3** complex.

Computed structures xyz coordinates

NiL1 complex

1. NiL1-S							
N	1.37589	-1.51382	-0.06059	H	-0.61971	-2.79657	1.66694
N	-1.35474	1.10184	-0.20629	C	3.95654	1.02058	-0.16977
N	1.45297	1.05916	0.01494	H	4.05601	2.09108	-0.14249
N	-1.48522	-1.33512	0.51203	C	-2.68520	-3.26493	1.23254
O	-2.03156	3.22716	-0.71920	H	-2.66081	-4.19455	1.78207
O	2.23043	3.18570	-0.33605	C	-4.94768	-1.04193	-0.71926
C	-3.82599	-1.60263	-0.07612	H	-5.86683	-1.60987	-0.77506
C	-2.63049	-0.84917	-0.04496	C	-0.12174	2.60402	2.00710
C	2.62540	-0.97005	-0.15168	H	-1.04335	3.01147	2.42367
C	-2.55996	0.48328	-0.52038	H	0.71328	3.01288	2.57684
C	2.69261	0.44418	-0.11142	H	-0.13294	1.52385	2.14315
C	-1.21646	2.45163	-0.22537	C	3.58846	-3.16152	-0.45815
C	1.33326	2.41742	0.00023	H	4.44967	-3.80442	-0.59113
C	0.00855	2.99097	0.52293	C	5.03754	-1.14607	-0.36745
C	-3.81500	-2.84895	0.57821	H	5.92727	-1.74973	-0.48759
H	-4.71258	-3.45477	0.58162	C	5.10270	0.21989	-0.27868
C	1.23504	-2.81786	-0.25248	H	6.06645	0.71235	-0.31503
H	0.22971	-3.21029	-0.25575	C	-4.85352	0.21989	-1.24720
C	3.77911	-1.77481	-0.31979	H	-5.71210	0.65336	-1.74472
C	2.31970	-3.67407	-0.45395	C	0.03738	4.50540	0.40875

H	2.13379	-4.72868	-0.59574	H	0.13546	4.83003	-0.62437
C	-3.68825	0.99815	-1.14291	H	0.87847	4.90805	0.96851
H	-3.67525	2.00223	-1.52954	H	-0.88296	4.92701	0.80699
C	-1.52902	-2.48191	1.17324	Ni	0.00519	-0.17642	0.15830

1. NiL1_H_2O_S							
N	1.30472	-1.50632	-0.22641	H	3.97409	2.10610	-0.35431
N	-1.43796	1.10215	-0.28516	C	-2.71044	-3.26854	1.19066
N	1.38293	1.06537	-0.09258	H	-2.66805	-4.19668	1.74154
N	-1.54055	-1.33615	0.43362	C	-5.03447	-1.05804	-0.70422
O	-2.13352	3.22384	-0.79006	H	-5.95256	-1.62949	-0.73554
O	2.11912	3.18645	-0.55403	C	-0.16860	2.62612	1.89409
C	-3.89380	-1.61386	-0.09100	H	-1.03850	3.10758	2.34121
C	-2.70157	-0.85491	-0.09291	H	0.71594	2.96432	2.43603
C	2.54912	-0.95852	-0.36046	H	-0.27482	1.55119	2.03489
C	-2.64889	0.47799	-0.56881	C	3.50518	-3.14352	-0.72633
C	2.61851	0.45398	-0.30095	H	4.36200	-3.78242	-0.90029
C	-1.30534	2.45309	-0.31278	C	4.95088	-1.12406	-0.67307
C	1.24728	2.42508	-0.15015	H	5.83629	-1.72384	-0.83659
C	-0.06348	3.00013	0.40512	C	5.01828	0.24032	-0.56837
C	-3.85882	-2.85894	0.56487	H	5.97887	0.73525	-0.63620
H	-4.75297	-3.46917	0.59312	C	-4.95953	0.20419	-1.23425
C	1.16108	-2.80935	-0.42057	H	-5.83290	0.63406	-1.70856
H	0.15793	-3.20589	-0.38374	C	-0.03563	4.51359	0.27815
C	3.69717	-1.75769	-0.58198	H	0.05116	4.82886	-0.75862
C	2.23933	-3.66024	-0.67329	H	0.81205	4.92096	0.82488
H	2.05088	-4.71431	-0.81534	H	-0.95111	4.93818	0.68376
C	-3.79548	0.98806	-1.16060	Ni	-0.06684	-0.17482	0.04600
H	-3.79788	1.99247	-1.54656	O	1.76620	-0.20221	2.86671
C	-1.55956	-2.48086	1.09930	H	1.59511	0.35013	2.09097
H	-0.63497	-2.78728	1.57041	H	1.50216	0.35483	3.60565
C	3.87550	1.03600	-0.39945				

2. NiL1OH_D							
N	0.73929	-1.47790	-0.35224	C	4.00518	0.02635	0.07558
N	-0.93082	1.23490	-0.37596	H	4.43999	0.95616	0.40595
N	1.69635	0.85633	0.42433	C	-3.29653	-2.40499	1.73921
N	-1.75151	-0.75404	1.03832	H	-3.53105	-3.19932	2.43256
O	-1.22904	3.29956	-1.29973	C	-4.65007	-0.56870	-1.21656
O	2.88454	2.58751	-0.46293	H	-5.60290	-1.04989	-1.39221
C	-3.83783	-1.01163	-0.15306	C	0.24002	3.11022	1.70309
C	-2.59330	-0.36949	0.04191	H	-0.66980	3.69534	1.83567
C	2.09090	-1.35449	-0.36865	H	1.03504	3.59102	2.27293
C	-2.15481	0.70537	-0.77093	H	0.07526	2.12982	2.15060
C	2.63097	-0.11589	0.06448	C	2.29264	-3.58664	-1.25320
C	-0.58813	2.53219	-0.58946	H	2.89905	-4.41517	-1.59812
C	1.84926	2.14901	0.02801	C	4.32244	-2.21768	-0.79011

C	0.62539	3.05170	0.21608	H	4.97106	-3.01769	-1.12206
C	-4.16385	-2.05365	0.73668	C	4.83372	-1.02556	-0.34746
H	-5.10691	-2.57281	0.61783	H	5.90591	-0.87891	-0.32277
C	0.17632	-2.59033	-0.77192	C	-4.21352	0.45817	-2.01368
H	-0.90597	-2.64002	-0.73702	H	-4.83402	0.79348	-2.83496
C	2.92686	-2.40931	-0.81201	C	0.96303	4.45593	-0.25491
C	0.92649	-3.67500	-1.24473	H	1.20921	4.47458	-1.31353
H	0.41584	-4.56441	-1.58427	H	1.81887	4.83924	0.29672
C	-2.98202	1.10336	-1.80689	H	0.11639	5.11940	-0.09385
H	-2.68188	1.91475	-2.44895	Ni	-0.00055	0.07070	0.84084
C	-2.07742	-1.72914	1.86208	O	0.60012	-0.71166	2.40833
H	-1.33998	-1.97218	2.61792	H	1.52876	-0.48022	2.52640

4. NiL1OH_T (+1 charge)							
N	0.87140	-1.41446	-0.47535	C	4.00747	0.20789	0.33311
N	-1.01662	1.12951	-0.36805	H	4.36221	1.12626	0.77284
N	1.62801	0.89952	0.50630	C	-3.21072	-2.70018	1.55283
N	-1.71733	-0.97367	0.92315	H	-3.39369	-3.57161	2.16343
O	-0.83549	2.89556	-1.82291	C	-4.80465	-0.47623	-0.98827
O	2.80366	2.75551	-0.08077	H	-5.78048	-0.92165	-1.12947
C	-3.89596	-1.08217	-0.08852	C	-0.15831	3.04747	1.64501
C	-2.63371	-0.48659	0.06257	H	-1.15030	3.49653	1.64684
C	2.21206	-1.22231	-0.37953	H	0.48282	3.64296	2.29246
C	-2.25968	0.69485	-0.65516	H	-0.23336	2.06095	2.10000
C	2.65180	-0.00103	0.18814	C	2.59843	-3.35391	-1.42901
C	-0.52212	2.38718	-0.77424	H	3.27191	-4.11947	-1.79346
C	1.74601	2.22324	0.21420	C	4.51076	-1.93466	-0.68639
C	0.43372	3.03596	0.22816	H	5.22599	-2.67073	-1.02874
C	-4.16408	-2.22552	0.68349	C	4.92215	-0.76475	-0.10488
H	-5.12354	-2.71777	0.59279	H	5.97921	-0.57095	0.02076
C	0.39909	-2.51014	-1.03116	C	-4.45584	0.67965	-1.66434
H	-0.67795	-2.61645	-1.08371	H	-5.16994	1.13289	-2.33755
C	3.13322	-2.19246	-0.84052	C	0.71184	4.45969	-0.21993
C	1.24184	-3.50745	-1.53669	H	1.12812	4.49059	-1.22250
H	0.80630	-4.38503	-1.99124	H	1.42084	4.92777	0.45821
C	-3.21530	1.28120	-1.50649	H	-0.20894	5.04000	-0.21364
H	-2.96924	2.18282	-2.04373	Ni	-0.01692	-0.02714	0.80373
C	-1.98397	-2.04409	1.65441	O	0.56782	-0.83073	2.32821
H	-1.19486	-2.36493	2.32387	H	1.46847	-0.54503	2.52911

5. NiL1O_Q							
N	1.27419	-1.54247	-0.29556	C	4.07813	0.73111	0.08042
N	-1.27992	1.13286	-0.15532	H	4.27154	1.76636	0.30507

N	1.60981	1.02782	0.18324	C	-3.10029	-3.27353	0.88861
N	-1.71599	-1.37458	0.50621	H	-3.18268	-4.27549	1.28371
O	-1.37854	2.96489	-1.52324	C	-5.08550	-0.58982	-0.75287
O	2.55908	3.05959	-0.30503	H	-6.05603	-1.05367	-0.86879
C	-4.03211	-1.32761	-0.17723	C	-0.10226	2.99369	1.75408
C	-2.76133	-0.71422	-0.04278	H	-1.06093	3.47479	1.94994
C	2.55711	-1.09456	-0.27022	H	0.66009	3.53217	2.31704
C	-2.53724	0.63675	-0.44119	H	-0.14881	1.97787	2.13732
C	2.76360	0.28680	0.01090	C	3.33844	-3.29330	-0.88870
C	-0.88154	2.38772	-0.56798	H	4.14735	-3.98027	-1.10542
C	1.59332	2.37144	0.01658	C	4.95674	-1.46068	-0.46838
C	0.22712	3.05549	0.25520	H	5.78945	-2.12291	-0.66510
C	-4.16614	-2.64343	0.30140	C	5.15028	-0.14268	-0.14715
H	-5.12394	-3.14119	0.21294	H	6.15706	0.24922	-0.07645
C	1.02209	-2.79044	-0.64748	C	-4.86257	0.70642	-1.13918
H	-0.01755	-3.08618	-0.68838	H	-5.67050	1.28242	-1.57180
C	3.64406	-1.96490	-0.54350	C	0.32660	4.51453	-0.16372
C	2.03308	-3.70144	-0.96158	H	0.59265	4.61651	-1.21209
H	1.76906	-4.70988	-1.24470	H	1.08615	5.01980	0.42791
C	-3.61537	1.32537	-0.98544	H	-0.62716	5.01543	-0.00598
H	-3.49037	2.34992	-1.29357	Ni	-0.00325	-0.16258	0.59409
C	-1.88074	-2.59716	0.97558	O	0.16995	-0.33716	2.30846
H	-1.01767	-3.06005	1.43998				

6. NiL1_OHO_D							
N	0.63335	-1.40745	-0.43622	H	4.50470	0.54952	0.67991
N	-0.81709	1.19760	-0.43477	C	-3.37344	-2.37840	1.66168
N	1.75158	0.74977	0.48116	H	-3.64165	-3.17958	2.33448
N	-1.74935	-0.80798	0.97595	C	-4.66201	-0.38455	-1.21548
O	-1.26373	3.32821	-1.06795	H	-5.64410	-0.80549	-1.38378
O	3.11110	2.29435	-0.43816	C	0.68445	3.60126	1.35390
C	-3.86262	-0.89323	-0.17489	H	-0.10496	4.35199	1.34503
C	-2.57800	-0.32711	0.01600	H	1.60987	4.07842	1.67671
C	1.99055	-1.42886	-0.40604	H	0.42455	2.83556	2.08670
C	-2.09087	0.73727	-0.77627	C	1.99178	-3.56832	-1.50323
C	2.62374	-0.29915	0.15171	H	2.51728	-4.42473	-1.90703
C	-0.49459	2.51522	-0.56588	C	4.13284	-2.48090	-0.80847
C	1.99503	1.99262	-0.02851	H	4.71551	-3.31252	-1.18189
C	0.86811	3.02229	-0.05799	C	4.73593	-1.39786	-0.22509
C	-4.23508	-1.94028	0.69062	H	5.81392	-1.37142	-0.13292
H	-5.21039	-2.39620	0.57377	C	-4.17317	0.62442	-2.00505
C	-0.03139	-2.39772	-0.99481	H	-4.77884	1.00814	-2.81586
H	-1.11197	-2.33590	-0.99906	C	1.30082	4.16618	-0.97605

C	2.72740	-2.52058	-0.91945	H	1.44524	3.82660	-2.00046
C	0.62464	-3.49897	-1.55736	H	2.23883	4.58854	-0.62659
H	0.03585	-4.28401	-2.00835	H	0.53997	4.94131	-0.97816
C	-2.90523	1.19087	-1.80019	O	0.72218	-1.14284	2.16255
H	-2.56557	1.98605	-2.44216	H	0.89299	-0.52540	2.88696
C	-2.11040	-1.78518	1.77777	Ni	0.02380	0.01032	0.85536
H	-1.36592	-2.09511	2.50131	O	-0.39989	1.10215	2.21996
C	3.99678	-0.29957	0.25094				

7. NiL1OOH_D							
N	0.77447	-1.38632	-0.49128	H	4.36919	1.22958	0.18545
N	-1.02395	1.30307	-0.34120	C	-3.32290	-2.51503	1.54176
N	1.63580	0.97893	0.30891	H	-3.55563	-3.34021	2.19879
N	-1.77415	-0.81405	0.94218	C	-4.65783	-0.57495	-1.34353
O	-1.42522	3.41670	-1.10280	H	-5.59352	-1.07451	-1.55647
O	2.73282	2.83404	-0.44248	C	0.15337	3.04299	1.84221
C	-3.84929	-1.04851	-0.29086	H	-0.77817	3.56494	2.06049
C	-2.62148	-0.39112	-0.03947	H	0.94688	3.51588	2.42076
C	2.11668	-1.18577	-0.55315	H	0.05747	2.02201	2.21331
C	-2.21612	0.74611	-0.78276	C	2.40569	-3.39060	-1.48382
C	2.60422	0.07365	-0.11089	H	3.04358	-4.17937	-1.86353
C	-0.73657	2.62528	-0.46707	C	4.37488	-1.92223	-1.07176
C	1.73179	2.30376	0.03166	H	5.05209	-2.68036	-1.44241
C	0.47859	3.13084	0.34206	C	4.83652	-0.71181	-0.62404
C	-4.17557	-2.13788	0.53859	H	5.89970	-0.50788	-0.63381
H	-5.10658	-2.66654	0.37487	C	-4.24231	0.50370	-2.08051
C	0.25692	-2.52082	-0.91266	H	-4.85934	0.86325	-2.89406
H	-0.81876	-2.63056	-0.83606	C	0.73504	4.58540	-0.01338
C	2.99154	-2.18681	-1.04622	H	0.93867	4.70809	-1.07414
C	1.04734	-3.55473	-1.42993	H	1.59336	4.96045	0.54001
H	0.57482	-4.46604	-1.76651	H	-0.13345	5.19132	0.23513
C	-3.03755	1.17321	-1.81223	Ni	-0.01304	0.07655	0.75181
H	-2.75322	2.02992	-2.40022	O	0.88142	-0.66015	2.23977
C	-2.11536	-1.82930	1.71387	O	0.76478	-2.05977	2.42220
H	-1.40080	-2.12139	2.46961	H	1.60609	-2.38902	2.06777
C	3.97029	0.28612	-0.15011				

8. NiL1_TS1_T							
O	-0.35647	0.73718	2.05332	C	-2.06244	3.12842	-1.29644
O	-1.94823	1.34311	2.19998	C	0.11029	4.15333	-1.16420
H	-1.86488	1.75943	3.07090	H	0.77132	5.00300	-1.25639

H	-2.47421	0.45111	2.33983	C	3.54999	-1.57523	-1.66680
H	-3.47080	-1.40567	1.92792	H	3.22401	-2.32518	-2.36759
H	-2.41893	-1.32199	3.11103	C	2.56886	1.49148	1.79950
O	-3.13811	-0.83891	2.65849	H	1.78642	1.91466	2.41759
O	-4.22328	-2.47498	0.71777	C	-3.56755	0.77590	-1.04737
H	-5.17655	-2.36806	0.65119	H	-4.17054	-0.11333	-0.96003
H	-3.88450	-2.34543	-0.18947	C	3.90033	1.90277	1.91044
O	-0.71188	-1.35396	3.87309	H	4.16594	2.65425	2.63992
H	-0.43644	-0.58706	3.32596	C	5.36452	-0.24931	-0.74713
H	-0.64519	-1.04969	4.78284	H	6.40782	0.03704	-0.72512
N	-0.12056	1.84012	-0.63691	C	-0.61931	-2.92251	0.88252
N	1.27396	-1.29136	-0.68024	H	0.13253	-3.67315	1.12882
N	-1.46612	-0.41968	-0.46718	H	-1.57534	-3.26313	1.28353
N	2.18488	0.57556	0.92828	H	-0.35602	-2.00974	1.41407
O	1.22204	-3.18038	-1.99409	C	-1.23098	4.25844	-1.41636
O	-2.77439	-1.92898	-1.59614	H	-1.66798	5.20502	-1.71055
C	4.46209	0.36738	0.14182	C	-3.45126	3.14817	-1.53508
C	3.09353	-0.00468	0.09812	H	-3.92525	4.07802	-1.82145
C	-1.45014	1.90736	-0.91495	C	-4.17436	1.99236	-1.39735
C	2.61665	-1.00461	-0.80972	H	-5.24342	2.00590	-1.56889
C	-2.20490	0.70117	-0.81143	C	4.89911	-1.19275	-1.62534
C	0.69541	-2.40134	-1.20001	H	5.58774	-1.66475	-2.31533
C	-1.75405	-1.63758	-0.94567	C	-1.18659	-4.04905	-1.24684
C	-0.71756	-2.73697	-0.63909	H	-1.26556	-3.98609	-2.32889
C	4.83767	1.34607	1.08159	H	-2.16524	-4.31714	-0.85233
H	5.87606	1.65007	1.13633	H	-0.48500	-4.84555	-1.00715
C	0.62818	2.91728	-0.76023	Ni	0.28876	0.08767	0.39119
H	1.68126	2.80893	-0.52677				

9. NiL1OHO_D_TS2							
H	5.63610	-0.84696	-1.40261	C	-4.71870	-1.37740	-0.29784
O	1.05752	3.25747	-1.47602	H	-5.79650	-1.33266	-0.20942
C	2.94328	1.21992	-1.79853	C	3.86306	-0.88741	-0.17690
H	2.62351	2.03007	-2.43033	C	0.03152	-2.48185	-1.02475
C	4.19461	0.61828	-2.01145	H	1.11467	-2.43622	-1.03761
H	4.80334	0.98724	-2.82712	C	-0.64118	-3.60238	-1.52900
C	3.36530	-2.34013	1.68140	H	-0.07002	-4.42163	-1.94082
H	3.62525	-3.13687	2.36265	C	-2.00893	-3.64022	-1.47367
C	4.22347	-1.93425	0.69322	H	-2.55423	-4.50179	-1.83885
H	5.18727	-2.41237	0.56984	C	-4.12779	-2.49051	-0.83525
C	4.66618	-0.40154	-1.22667	H	-4.71973	-3.32915	-1.17757
N	0.88395	1.28269	-0.36560	C	-1.31185	4.28265	-0.77930
N	-1.71560	0.75303	0.38651	H	-0.53161	5.03931	-0.77480

N	-0.60575	-1.44943	-0.51397	H	-1.56104	4.05984	-1.81468
N	1.75880	-0.74611	0.99166	O	-3.10707	2.36210	-0.38012
C	-1.96386	-1.45056	-0.47374	H	-2.19897	4.68816	-0.29936
C	-2.58908	-0.29049	0.04813	O	-0.66329	-0.93885	2.36102
C	2.12276	0.78653	-0.76741	H	-1.54388	-0.59485	2.57131
C	0.44104	2.52003	-0.71224	Ni	-0.00444	0.04810	0.83386
C	2.59259	-0.29462	0.02003	O	0.06098	0.73365	2.59881
C	-1.98456	2.02783	-0.01604	C	-0.83737	3.04276	-0.03086
C	-3.96590	-0.27527	0.14238	C	-0.47251	3.46185	1.40253
H	-4.46300	0.59189	0.54600	H	0.31799	4.21185	1.37314
C	2.11835	-1.71767	1.80459	H	-1.34056	3.90598	1.89015
H	1.39681	-2.00711	2.55757	H	-0.13851	2.62054	2.00778
C	-2.72336	-2.55193	-0.93746				

NiL2 complex

10. NiL2							
H	5.91691	-1.46721	-0.54058	C	-1.30258	2.49114	0.28879
O	2.13979	3.31604	-0.36393	C	-3.93560	1.13546	0.04119
C	3.73793	1.14033	-0.91235	H	-4.03045	2.20040	0.14572
H	3.74405	2.15925	-1.25608	C	1.47732	-2.46807	1.08378
C	4.91304	0.37458	-0.98978	H	0.54169	-2.81758	1.49828
H	5.79186	0.83661	-1.42198	C	-3.78735	-1.64281	-0.30039
C	2.63526	-3.24501	1.17417	C	-5.09070	0.35042	-0.09385
H	2.58562	-4.20516	1.66656	H	-6.04960	0.85335	-0.07549
C	3.79969	-2.78326	0.61924	C	3.83871	-1.50256	0.03692
H	4.70191	-3.38166	0.64422	C	-1.25076	-2.69983	-0.41735
C	4.99130	-0.90787	-0.51238	H	-0.24708	-3.09068	-0.49295
Ni	-0.00230	-0.10451	0.13237	C	-2.34835	-3.53502	-0.63381
N	1.33968	1.18650	-0.13186	H	-2.17723	-4.57704	-0.86132
N	-1.41325	1.14684	0.09805	C	-3.61184	-3.01659	-0.54664
N	-1.37750	-1.41391	-0.12252	H	-4.48298	-3.64322	-0.69191
N	1.46466	-1.28446	0.48957	C	-5.04255	-1.00715	-0.26644
N	-0.02396	3.07204	0.26227	H	-5.94049	-1.59658	-0.39571
C	-2.62331	-0.85730	-0.11530	C	-0.03181	4.51046	0.50775
C	-2.67255	0.55274	0.03013	H	0.98120	4.82942	0.71468
C	2.57943	0.59676	-0.37452	H	-0.40641	5.06541	-0.35312
C	1.22104	2.53809	-0.11771	O	-2.25395	3.24456	0.48436
C	2.63667	-0.75768	0.03658	H	-0.67662	4.72600	1.35295

11. NiL2_H_2O

H	5.95131	-1.63677	0.07193	C	1.27317	-2.72112	0.49361
O	2.23761	3.22165	-0.31417	H	0.27517	-3.10432	0.64752
C	3.91731	1.07042	-0.38379	C	-3.84662	-1.57894	-0.10248
H	4.00399	2.12555	-0.56635	C	-4.95311	0.36006	0.76719
C	5.07930	0.28740	-0.30166	H	-5.84366	0.84586	1.14538
H	6.03298	0.78044	-0.44275	C	3.79742	-1.67960	0.15029
C	2.38389	-3.54216	0.69744	C	-1.45503	-2.60452	-1.01522
H	2.22946	-4.56709	1.00135	H	-0.50809	-2.97948	-1.37831
C	3.63872	-3.03434	0.49423	C	-2.60851	-3.39077	-1.08199
H	4.51747	-3.65482	0.61825	H	-2.54262	-4.38286	-1.50395
C	5.04551	-1.05332	-0.02530	C	-3.78896	-2.89701	-0.59230
N	1.39670	1.09179	-0.23319	H	-4.68820	-3.50023	-0.59879
N	-1.35427	1.13004	-0.01510	C	-5.01416	-0.95174	0.37394
N	-1.46049	-1.38170	-0.50709	H	-5.93924	-1.51118	0.41445
N	1.38176	-1.45626	0.11350	C	0.04023	4.46063	-0.66672
N	0.00316	3.01946	-0.43244	H	0.36379	4.99840	0.22422
C	-2.64700	-0.83017	-0.12440	H	0.73987	4.68285	-1.46614
C	-2.60818	0.54587	0.19496	O	-2.24969	3.21774	-0.26191
C	2.66148	0.49791	-0.21697	H	-0.95522	4.78597	-0.93692
C	1.28423	2.44790	-0.31564	Ni	-0.00420	-0.17355	-0.20189
C	2.62326	-0.90174	0.00401	O	0.17395	1.33152	2.80408
C	-1.27469	2.47336	-0.23144	H	1.02542	1.14133	2.39398
C	-3.77700	1.12131	0.66739	H	-0.44312	1.20774	2.06900
H	-3.79244	2.16083	0.94549				

12. NiL2OH_D

H	5.60929	-0.93011	-1.36879	H	-4.39462	1.21622	0.45915
O	1.40258	3.46870	-0.82722	C	2.04411	-1.78368	1.80091
C	3.00594	1.26081	-1.67650	H	1.29878	-2.06573	2.53516
H	2.71971	2.11351	-2.27056	C	-3.02983	-2.17017	-0.87283
C	4.23590	0.62366	-1.91005	C	-4.87131	-0.71372	-0.37926
H	4.86794	1.00672	-2.70105	H	-5.93540	-0.51513	-0.36059
C	3.26026	-2.45928	1.64895	C	3.82988	-0.95778	-0.15032
H	3.48319	-3.29527	2.29560	C	-0.29100	-2.48445	-0.82381
C	4.14004	-2.05389	0.67829	H	0.78790	-2.58402	-0.78372
H	5.08140	-2.57087	0.53829	C	-1.08797	-3.51525	-1.33795
C	4.65704	-0.45513	-1.17440	H	-0.61823	-4.41595	-1.70575
N	0.92272	1.29841	-0.29466	C	-2.44810	-3.36001	-1.35213
N	-1.64357	0.97285	0.49028	H	-3.09082	-4.14523	-1.73098
N	-0.80546	-1.36252	-0.36905	C	-4.41500	-1.91319	-0.85915
N	1.73195	-0.75917	1.03415	H	-5.09728	-2.66838	-1.22655
N	-0.58942	3.05074	0.17778	C	-0.76657	4.49604	0.21144
C	-2.14905	-1.17412	-0.38350	H	0.15382	4.95654	0.55386
C	-2.63292	0.07552	0.09527	H	-1.01265	4.90494	-0.76939

C	2.16315	0.80239	-0.67990	O	-2.85586	2.88209	0.16861
C	0.64163	2.62484	-0.36665	H	-1.57554	4.72874	0.89459
C	2.58650	-0.32142	0.07059	Ni	0.00001	0.10399	0.87377
C	-1.77813	2.30639	0.27573	O	-0.62171	-0.74835	2.39882
C	-4.00130	0.28095	0.09656	H	-1.55116	-0.52052	2.51638

13. NiL2OH_T (+1 charge)							
H	5.52988	-0.54183	-1.64232	H	-4.34169	1.13566	-0.04564
O	0.83051	3.40372	-1.23482	C	2.33591	-1.46462	1.88287
C	2.68895	1.33455	-1.90924	H	1.68271	-1.75716	2.69620
H	2.26687	2.09573	-2.54448	C	-2.81278	-2.36040	-0.90717
C	3.95888	0.80439	-2.19473	C	-4.70076	-0.83062	-0.83297
H	4.48005	1.17123	-3.06920	H	-5.74607	-0.63175	-1.02347
C	3.60726	-2.01425	1.68712	C	3.86776	-0.63301	-0.27250
H	3.97008	-2.75788	2.38095	C	-0.11830	-2.66627	-0.46864
C	4.36005	-1.60890	0.61464	H	0.94650	-2.75337	-0.29194
H	5.33997	-2.03473	0.43899	C	-0.84187	-3.72344	-1.02199
C	4.55080	-0.14761	-1.40594	H	-0.32967	-4.64002	-1.27410
N	0.74978	1.31427	-0.32332	C	-2.18867	-3.57309	-1.24260
N	-1.68300	0.79114	0.52522	H	-2.77405	-4.37145	-1.67940
N	-0.68888	-1.51805	-0.14313	C	-4.18062	-2.07820	-1.13335
N	1.85463	-0.55795	1.05667	H	-4.81154	-2.84811	-1.55795
N	-0.91043	2.95773	0.15550	C	-1.15888	4.39698	0.17064
C	-2.00865	-1.35772	-0.33640	H	-0.21259	4.91509	0.27166
C	-2.56047	-0.07290	0.00333	H	-1.64109	4.72428	-0.74943
C	1.98949	0.89116	-0.80377	O	-2.98818	2.61471	1.03364
C	0.28011	2.56174	-0.54764	H	-1.80573	4.62377	1.00998
C	2.58240	-0.11256	-0.00323	Ni	0.03875	0.09963	0.96367
C	-1.94154	2.17660	0.60757	O	-0.38026	-0.71191	2.56051
C	-3.91938	0.17252	-0.28632	H	-1.32818	-0.64741	2.72773

14. NiL2O_Q							
H	5.73828	-1.07626	-1.50787	H	-4.18238	1.88924	-0.37023
O	1.82951	3.41373	-0.38600	C	2.02170	-2.31862	1.29835
C	3.28366	1.29164	-1.46077	H	1.26035	-2.71808	1.95846
H	3.07721	2.26162	-1.88074	C	-3.53928	-1.92622	-0.63461
C	4.47567	0.63217	-1.79355	C	-5.01992	-0.04812	-0.78243
H	5.15780	1.12029	-2.47780	H	-6.00171	0.36503	-0.97648
C	3.22311	-3.00102	1.08671	C	3.90117	-1.22462	-0.38942
H	3.39757	-3.94029	1.59087	C	-0.97640	-2.79392	-0.15021
C	4.14760	-2.46347	0.22986	H	0.04106	-3.10860	0.03579

H	5.07979	-2.97669	0.02816	C	-1.94788	-3.72495	-0.51847
C	4.80276	-0.58950	-1.26606	H	-1.67549	-4.76589	-0.61304
N	1.15158	1.23172	-0.17996	C	-3.22721	-3.29194	-0.74719
N	-1.57337	1.08356	0.14266	H	-4.00786	-3.98919	-1.02562
N	-1.23747	-1.50413	-0.01948	C	-4.82133	-1.39990	-0.88584
N	1.74965	-1.16886	0.71088	H	-5.62315	-2.07087	-1.16388
N	-0.29206	3.04705	0.30921	C	-0.33739	4.48066	0.56924
C	-2.49176	-1.04303	-0.26765	H	0.59808	4.78278	1.02639
C	-2.70260	0.36534	-0.17087	H	-0.47620	5.06040	-0.34429
C	2.36614	0.71169	-0.59662	O	-2.55023	3.16881	0.16499
C	0.96274	2.58545	-0.13018	H	-1.16666	4.68701	1.23554
C	2.67154	-0.58456	-0.09214	Ni	-0.01392	-0.03898	0.76168
C	-1.56559	2.43682	0.19514	O	-0.13539	0.06572	2.47898
C	-3.98780	0.83271	-0.43483				

15. NiL2OHO_D							
H	5.52010	-0.89943	-1.52084	C	2.14678	-1.53381	1.90174
O	1.23333	3.31059	-1.14322	H	1.44708	-1.75314	2.69967
C	2.75333	1.03904	-2.01290	C	-2.85658	-2.35013	-0.86612
H	2.37899	1.77542	-2.70642	C	-4.79865	-0.97003	-0.56695
C	4.01881	0.46383	-2.21161	H	-5.86935	-0.82627	-0.63466
H	4.59262	0.77364	-3.07538	C	3.79383	-0.87492	-0.23084
C	3.40527	-2.13817	1.78767	C	-0.11053	-2.50213	-0.61537
H	3.71355	-2.85487	2.53454	H	0.96500	-2.54201	-0.50480
C	4.21430	-1.81679	0.72898	C	-0.81513	-3.59284	-1.13835
H	5.18574	-2.28251	0.61876	H	-0.26835	-4.47588	-1.43448
C	4.54301	-0.46743	-1.35142	C	-2.17736	-3.52070	-1.25263
N	0.72411	1.15324	-0.58039	H	-2.74438	-4.35696	-1.64217
N	-1.71982	0.89405	0.43028	C	-4.25044	-2.16295	-0.95922
N	-0.72156	-1.39861	-0.23680	H	-4.86709	-2.96728	-1.33726
N	1.73548	-0.66083	1.00889	C	-0.84331	4.40140	0.04529
N	-0.68699	2.95471	0.01373	H	0.09798	4.85200	0.34133
C	-2.07123	-1.29077	-0.35480	H	-1.12972	4.80247	-0.92739
C	-2.64703	-0.05763	0.03113	O	-2.95768	2.77395	0.10439
C	1.98571	0.66979	-0.92539	H	-1.61637	4.64753	0.76450
C	0.49026	2.49720	-0.61509	O	-0.70903	-0.82189	2.33043
C	2.51336	-0.30050	-0.04444	H	-0.94764	-0.11200	2.94139
C	-1.86984	2.21854	0.18375	Ni	-0.04189	0.13923	0.86250
C	-4.01730	0.08810	-0.07337	O	0.36196	1.47602	1.99665
H	-4.47619	1.01904	0.21688				

16. NiL2OOH_D							
H	5.82775	-1.40031	-1.25247	C	1.66764	-2.39745	1.00294
O	2.14750	3.37526	-0.33195	H	0.80752	-2.71430	1.57797
C	3.60806	1.19458	-1.34406	C	-3.73844	-1.55850	-0.72746
H	3.55550	2.21199	-1.69267	C	-4.93929	0.49850	-0.95799
C	4.76896	0.43630	-1.56943	H	-5.85229	1.03866	-1.17456
H	5.58059	0.89722	-2.11789	C	3.85173	-1.43972	-0.38961
C	2.82491	-3.17786	0.91763	C	-1.29555	-2.73226	-0.25954
H	2.84847	-4.13633	1.41493	H	-0.32381	-3.17631	-0.09979
C	3.89613	-2.71743	0.19805	C	-2.39305	-3.54147	-0.56499
H	4.79279	-3.31609	0.09648	H	-2.25752	-4.61143	-0.62378
C	4.91374	-0.84269	-1.09788	C	-3.61066	-2.95788	-0.78541
N	1.33934	1.23563	-0.27804	H	-4.48068	-3.55768	-1.02227
N	-1.35141	1.18783	-0.11234	C	-4.93782	-0.87104	-0.98964
N	-1.38227	-1.41826	-0.16334	H	-5.83076	-1.43391	-1.22648
N	1.57254	-1.22378	0.40515	C	0.03418	4.44689	0.81956
N	0.01664	3.05756	0.38111	H	1.01873	4.67624	1.20931
C	-2.57651	-0.80942	-0.41028	H	-0.18642	5.13591	0.00317
C	-2.58749	0.60731	-0.37070	O	-2.23137	3.21411	0.48716
C	2.54029	0.64451	-0.65488	H	-0.71571	4.58002	1.59106
C	1.23901	2.57839	-0.12232	Ni	0.03048	-0.05724	0.21265
C	2.65792	-0.69918	-0.22830	O	-0.24512	0.08252	2.20687
C	-1.26195	2.49762	0.26081	O	-0.53333	-1.17052	2.79017
C	-3.78889	1.24197	-0.66007	H	-1.50319	-1.19815	2.77991
H	-3.83739	2.31644	-0.66151				

17. NiL2_TS1_T							
O	0.02142	-0.07829	1.91786	H	0.43292	3.40628	0.34286
O	-1.32307	0.72125	2.76337	C	-3.01591	2.56393	-1.09275
H	-0.85281	0.87289	3.59533	C	-1.46343	4.21760	-0.29145
H	-1.93211	-0.10563	2.91394	H	-1.18193	5.23889	-0.07942
H	-3.38556	-1.47957	2.35420	C	3.83096	-1.33194	-1.52552
H	-2.07389	-2.05083	2.99983	H	3.61135	-2.22838	-2.07968
O	-2.75549	-1.35457	3.10140	C	2.45772	2.14289	1.35375
O	-4.42543	-1.70389	0.96279	H	1.63443	2.56495	1.91987
H	-4.72669	-0.85558	0.61946	C	-3.49158	-0.13355	-1.66146
H	-3.77276	-2.00911	0.29212	H	-3.69678	-1.16009	-1.91897
O	-0.40435	-2.71659	2.66068	C	3.74434	2.68404	1.44152
H	-0.13978	-1.81956	2.35806	H	3.92181	3.54343	2.07190
H	0.11114	-2.86785	3.45835	C	5.47674	0.31809	-0.84625
N	-0.83225	1.91660	-0.27068	H	6.48724	0.70496	-0.85817
N	1.51039	-1.13969	-0.62779	C	-2.68973	3.90382	-0.81112

N	-1.23884	-0.65075	-0.73424	H	-3.41737	4.67736	-1.02478
N	2.17668	1.10165	0.59686	C	-4.23677	2.17355	-1.67517
O	1.89444	-3.32148	-1.24231	H	-4.98030	2.92567	-1.90312
O	-2.46692	-2.60108	-0.71386	C	-4.44408	0.84932	-1.96099
C	4.49367	0.97513	-0.08091	H	-5.36810	0.54061	-2.43398
C	3.16623	0.47260	-0.08490	C	5.12777	-0.79779	-1.55999
C	-2.04242	1.57560	-0.78871	H	5.87315	-1.30288	-2.16176
C	2.82510	-0.73137	-0.77995	Ni	0.33145	0.26024	0.13241
C	-2.28313	0.18839	-1.04837	N	-0.21639	-2.76756	-0.64234
C	1.14104	-2.41908	-0.88461	C	-0.44264	-4.20457	-0.53731
C	-1.38361	-1.99126	-0.70296	H	0.42917	-4.66543	-0.08813
C	4.74964	2.11284	0.70751	H	-1.31534	-4.37880	0.07983
H	5.75387	2.51831	0.73350	H	-0.61104	-4.66537	-1.51199
C	-0.55378	3.18586	-0.04348				

18. NiL2OHO_TS2_D							
H	5.54403	-0.98692	-1.51918	C	-3.99420	0.17819	-0.13179
O	1.32434	3.37874	-1.09731	H	-4.41268	1.13129	0.14536
C	2.88210	1.11274	-1.93026	C	2.09988	-1.64095	1.82479
H	2.55905	1.91088	-2.57930	H	1.40203	-1.87245	2.61953
C	4.12020	0.48668	-2.14638	C	-2.95056	-2.32311	-0.87275
H	4.72287	0.81920	-2.98180	C	-4.82705	-0.85754	-0.58475
C	3.32837	-2.29902	1.69241	H	-5.89185	-0.66962	-0.63839
H	3.59391	-3.06458	2.40647	C	3.79976	-0.95450	-0.25274
C	4.16392	-1.96500	0.65851	C	-0.21523	-2.59514	-0.66168
H	5.11377	-2.47002	0.53398	H	-0.47640	-4.58713	-1.41900
C	4.58571	-0.51925	-1.33769	C	-2.33318	-3.53521	-1.23615
N	0.83948	1.22686	-0.50601	H	-2.94687	-4.35271	-1.59400
N	-1.66473	0.91482	0.33961	C	-4.33634	-2.08274	-0.95215
N	-0.76130	-1.45061	-0.30532	H	-4.99149	-2.87082	-1.29888
N	1.73094	-0.70698	0.97257	C	-0.82016	4.44187	-0.01108
N	-0.64179	2.99708	-0.02645	H	0.11550	4.90884	0.27689
C	-2.10649	-1.28551	-0.40652	H	-1.11505	4.83005	-0.98668
C	-2.62596	-0.01407	-0.04424	O	-2.90420	2.80978	0.07767
C	2.07782	0.71583	-0.87782	H	-1.59522	4.68626	0.70674
C	0.57169	2.55536	-0.59069	O	-0.61934	-0.49851	2.54307
C	2.54447	-0.33286	-0.05104	H	-1.49183	-0.10565	2.69350
C	-1.81526	2.25005	0.13388	Ni	-0.01021	0.13860	0.81633
H	0.86121	-2.67847	-0.56831	O	0.16487	1.13848	2.41810
C	-0.97430	-3.66997	-1.13976				

3. NiL3 complex

19. NiL3							
H	4.87162	-3.82729	-0.42819	C	-4.35936	-0.92741	0.08765
O	2.54174	1.62196	-2.20250	C	-5.05905	1.32518	-0.32023
C	3.51199	-0.96088	-1.69960	H	-5.84241	2.06709	-0.41156
H	3.76218	-0.17613	-2.39182	C	2.96331	-3.00652	0.15224
C	4.39874	-2.03284	-1.50200	C	-2.22364	-2.65611	0.22226
H	5.31457	-2.04814	-2.07946	H	-1.37642	-3.32503	0.24362
C	1.46969	-3.76660	1.87491	C	-3.51923	-3.15912	0.35619
H	1.20982	-4.42766	2.68866	H	-3.65608	-4.22172	0.49345
C	2.63278	-3.92315	1.16770	C	-4.58118	-2.29650	0.32188
H	3.31738	-4.72999	1.39797	H	-5.59512	-2.65539	0.44701
C	4.15878	-3.03040	-0.59319	C	-5.38661	0.02828	-0.02608
Ni	-0.27064	-0.50950	-0.18417	H	-6.41506	-0.28076	0.10565
N	1.36177	0.10845	-0.94120	O	-1.53319	3.21375	-1.30354
N	-1.31880	1.02974	-0.62227	C	0.66560	2.44915	-1.02769
N	-1.97075	-1.36485	0.06041	H	0.82200	3.24805	-1.75030
N	0.83783	-1.89888	0.53556	C	1.15924	2.96670	0.31254
C	-3.01856	-0.50068	-0.07327	C	2.01203	4.06772	0.34422
C	-2.68656	0.82862	-0.42886	C	0.81501	2.35438	1.51598
C	2.32258	-0.89969	-0.98777	C	2.51091	4.54549	1.54705
C	1.59418	1.33101	-1.47436	H	2.28490	4.55121	-0.58650
C	2.03865	-1.96847	-0.10454	C	1.31029	2.83341	2.71929
C	-0.83924	2.24114	-1.00749	H	0.15084	1.49670	1.50841
C	-3.73466	1.73432	-0.53985	C	2.16156	3.92946	2.73966
H	-3.52959	2.75481	-0.80798	H	3.17161	5.40320	1.55111
C	0.58612	-2.74187	1.52608	H	1.02848	2.34830	3.64535
H	-0.34687	-2.60864	2.05637	H	2.54715	4.30253	3.67968

20. NiL3_H_2O							
H	5.41772	-2.86107	-0.03071	C	3.37411	-2.34527	0.42763
O	2.32858	2.05928	-2.15266	C	-1.80303	-2.82664	0.26393
C	3.68415	-0.28913	-1.46619	H	-0.86566	-3.36582	0.23999
H	3.84039	0.50477	-2.17512	C	-3.01266	-3.50690	0.43074
C	4.72076	-1.19601	-1.18796	H	-2.99390	-4.57831	0.56829
H	5.65633	-1.07794	-1.72015	C	-4.18808	-2.80550	0.42882
C	1.92636	-3.30936	2.08576	H	-5.13607	-3.30545	0.58426
H	1.72961	-3.99050	2.90073	C	-5.32639	-0.61784	0.09621
C	3.13950	-3.28396	1.44991	H	-6.29760	-1.06618	0.25860
H	3.93271	-3.96181	1.74010	O	-2.00772	2.97964	-1.52065
C	4.59609	-2.19461	-0.25735	C	0.27748	2.62080	-1.13377

N	1.34925	0.43480	-0.85767	H	0.32468	3.37115	-1.92072
N	-1.45895	0.93543	-0.62861	C	0.60540	3.33147	0.16842
N	-1.74808	-1.51162	0.10042	C	1.07447	4.64225	0.13377
N	1.08107	-1.59111	0.66739	C	0.46909	2.70380	1.40562
C	-2.91147	-0.80858	-0.01417	C	1.39970	5.31179	1.30458
C	-2.77956	0.54769	-0.39496	H	1.18461	5.13868	-0.82323
C	2.46413	-0.40173	-0.81438	C	0.79099	3.37293	2.57618
C	1.40281	1.65001	-1.45280	H	0.10626	1.68236	1.44964
C	2.31015	-1.47682	0.09303	C	1.25868	4.67915	2.53052
C	-1.17298	2.16718	-1.12280	H	1.76229	6.33082	1.25688
C	-3.94563	1.29799	-0.47860	H	0.67612	2.87130	3.52881
H	-3.89457	2.33387	-0.76239	H	1.50993	5.20025	3.44533
C	0.91036	-2.44906	1.66077	Ni	-0.19661	-0.41345	-0.13688
H	-0.06213	-2.46459	2.13304	O	0.78500	-4.23314	-1.18077
C	-4.17244	-1.41956	0.18517	H	0.32057	-4.68060	-1.89453
C	-5.19226	0.71021	-0.21307	H	1.56000	-4.78337	-1.03147
H	-6.07437	1.33425	-0.28297				

21. NiL3_OHD							
H	2.92245	-5.02165	1.22997	H	-3.72599	4.06480	1.71207
O	3.18523	0.23818	-2.02455	C	1.36867	-3.53542	1.06525
C	2.94439	-2.41940	-0.97960	C	-3.43666	-1.36242	-0.83259
H	3.56489	-2.00361	-1.75620	H	-3.06661	-2.24956	-1.33269
C	3.34831	-3.57784	-0.29278	C	-4.76013	-1.22574	-0.39870
H	4.28679	-4.03859	-0.57354	H	-5.45497	-2.03517	-0.56785
C	-0.64941	-3.35703	2.36594	C	-5.14762	-0.07394	0.23666
H	-1.31350	-3.69893	3.14646	H	-6.16538	0.04609	0.58687
C	0.51985	-4.01131	2.08337	C	-4.50632	2.19242	1.07857
H	0.80520	-4.89776	2.63648	H	-5.50310	2.37556	1.45702
C	2.59547	-4.13198	0.70805	O	-0.10480	3.43680	-1.14943
N	1.24931	-0.59523	-1.15163	C	1.62132	1.84132	-1.27657
N	-0.65192	1.34189	-0.41680	H	1.93606	2.45372	-2.12108
N	-2.55426	-0.40160	-0.64719	C	2.44555	2.26668	-0.06773
N	-0.22197	-1.75839	0.65875	C	3.39821	3.27324	-0.17516

C	-2.90804	0.75873	-0.03444	C	2.24978	1.64710	1.16594
C	-1.89219	1.72977	0.09187	C	4.14417	3.65652	0.93045
C	1.75272	-1.79663	-0.65587	H	3.55401	3.75716	-1.13191
C	2.05972	0.41024	-1.56833	C	2.99622	2.02964	2.26949
C	0.95102	-2.37698	0.36873	H	1.50480	0.86358	1.25628
C	0.19042	2.25905	-0.96375	C	3.94592	3.03585	2.15494
C	-2.21137	2.91519	0.72772	H	4.88266	4.44217	0.83317
H	-1.46000	3.68027	0.84685	H	2.83576	1.54078	3.22202
C	-0.99511	-2.22611	1.61513	H	4.52830	3.33458	3.01693
H	-1.92330	-1.69685	1.79942	Ni	-0.64087	-0.50952	-0.95930
C	-4.22358	0.96879	0.44013	O	-0.91709	-1.99193	-2.05000
C	-3.51100	3.12747	1.21530	H	-0.06042	-2.32452	-2.34187

22. NiL3_OH_T (+1 Charge)							
H	-4.96580	-3.01625	1.17766	H	6.11847	-0.12892	0.50920
O	-1.27385	1.55552	3.14498	C	-3.43233	-1.99536	0.05674
C	-2.58457	-1.01042	2.56794	C	0.88372	-2.86204	-0.59069
H	-2.28390	-0.62878	3.53077	H	-0.16454	-3.09367	-0.73456
C	-3.68366	-1.87041	2.45475	C	1.85752	-3.85440	-0.72599
H	-4.21246	-2.15260	3.35510	H	1.55601	-4.86168	-0.97237
C	-3.06657	-1.96476	-2.32396	C	3.17676	-3.52611	-0.54321
H	-3.32950	-2.25609	-3.32993	H	3.95462	-4.27246	-0.64001
C	-3.79159	-2.39998	-1.24222	C	4.84848	-1.76565	0.00995
H	-4.64617	-3.05053	-1.37775	H	5.65988	-2.47446	-0.09054
C	-4.11045	-2.35717	1.24100	O	2.50607	2.36845	1.91847
N	-0.81956	0.23250	1.32153	C	0.15066	2.45714	1.42063
N	1.64154	0.87434	0.39273	H	0.17614	3.29876	2.11112
N	1.18657	-1.61430	-0.28307	C	-0.40597	2.88469	0.07367
N	-1.60234	-0.75408	-0.91239	C	-1.73030	2.64213	-0.29513
C	2.47711	-1.26752	-0.10464	C	0.42497	3.55795	-0.82467
C	2.74381	0.08991	0.26787	C	-2.20277	3.04449	-1.53697
C	-1.88105	-0.64211	1.42984	H	-2.40616	2.14710	0.39187
C	-0.70620	1.36702	2.08770	C	-0.04809	3.95860	-2.06158
C	-2.31005	-1.15174	0.17726	H	1.45265	3.76860	-0.55074
C	1.56747	1.94370	1.27960	C	-1.36285	3.69637	-2.42463
C	4.07231	0.47468	0.48881	H	-3.23189	2.84535	-1.80559
H	4.29068	1.49973	0.73820	H	0.61245	4.47387	-2.74636
C	-1.95987	-1.13448	-2.12440	H	-1.73010	4.00353	-3.39480
H	-1.33749	-0.77264	-2.93433	Ni	0.03658	0.15192	-0.40173
C	3.52473	-2.20365	-0.21960	O	0.51518	0.37864	-2.15707
C	5.09926	-0.45332	0.35122	H	1.33707	0.88218	-2.20700

23. NL3_O_Q							
H	5.52566	-2.93162	0.71239	H	-5.56714	1.88385	0.73623
O	2.71391	2.02236	-1.80507	C	3.40387	-2.55440	0.69238
C	4.02283	-0.30346	-0.86126	C	-2.24584	-3.01915	-0.19425
H	4.28461	0.56242	-1.44511	H	-1.44370	-3.70589	-0.43818
C	5.02474	-1.17574	-0.41123	C	-3.51546	-3.49180	0.15132
H	6.05136	-0.95791	-0.67740	H	-3.69640	-4.55633	0.17911
C	1.69090	-3.81984	1.81167	C	-4.50003	-2.58867	0.45533
H	1.36561	-4.62607	2.45263	H	-5.48962	-2.92357	0.74090
C	3.01294	-3.63341	1.50492	C	-5.19237	-0.20777	0.65094
H	3.77148	-4.30221	1.89287	H	-6.19129	-0.49570	0.95078
C	4.74313	-2.27482	0.35625	O	-1.77629	2.68528	-1.75529
N	1.59211	0.26836	-0.82105	C	0.49083	2.43894	-1.16253
N	-1.27497	0.80422	-0.54309	H	0.57156	3.16850	-1.96619
N	-1.95964	-1.73202	-0.24083	C	0.66448	3.19193	0.14843
N	1.07324	-1.94121	0.48273	C	0.81445	4.57548	0.13987
C	-2.92981	-0.81772	-0.00019	C	0.66546	2.52101	1.37092
C	-2.58694	0.54976	-0.17537	C	0.96515	5.27719	1.32728
C	2.68663	-0.53046	-0.55306	H	0.81314	5.10286	-0.80672
C	1.69984	1.51651	-1.32645	C	0.81487	3.22311	2.55682
C	2.38250	-1.69857	0.20771	H	0.55117	1.44331	1.38623
C	-0.95450	1.96578	-1.20268	C	0.96514	4.60315	2.53937
C	-3.55969	1.49764	0.10384	H	1.08257	6.35313	1.30333
H	-3.32803	2.54577	-0.00395	H	0.81519	2.68976	3.49900
C	0.74285	-2.94994	1.26956	H	1.08215	5.14964	3.46625
H	-0.30940	-3.07542	1.48710	Ni	-0.14535	-0.78962	-0.73000
C	-4.23776	-1.20844	0.38274	O	-0.08830	-1.48226	-2.31527
C	-4.83963	1.11143	0.52294				

24. NiL3_OHO_D							
H	-0.10777	5.92432	0.97740	C	-0.23383	4.06464	-0.10516
O	2.09952	0.47499	2.79051	C	-2.98487	0.88162	0.11395
C	0.67476	2.86146	2.27237	H	-2.62648	1.90242	0.08110
H	1.02374	2.42748	3.19370	C	-4.35389	0.60821	0.21767
C	0.47388	4.24877	2.17924	H	-5.04979	1.43225	0.27319
H	0.67419	4.85187	3.05545	C	-4.78087	-0.69301	0.22737
C	-0.94413	3.70241	-2.38124	H	-5.83662	-0.92736	0.28327
H	-1.29825	4.06279	-3.33584	C	-4.16815	-3.11438	0.17719
C	-0.69696	4.55856	-1.34017	H	-5.20761	-3.41107	0.22205
H	-0.85630	5.62359	-1.45387	O	0.68369	-3.43408	1.47083

C	0.03946	4.85390	1.02883	C	1.91953	-1.40218	1.35161
N	0.61933	0.67172	1.06730	H	2.34861	-1.87219	2.23904
N	-0.16565	-1.81673	0.12366	C	3.01468	-1.37647	0.29997
N	-2.08742	-0.08004	0.04638	C	3.77246	-0.22907	0.05865
N	-0.31743	1.85261	-1.05401	C	3.33342	-2.54672	-0.39131
C	-2.48014	-1.37967	0.08923	C	4.81047	-0.24935	-0.86141
C	-1.45469	-2.35088	0.07238	H	3.55062	0.68690	0.59245
C	0.43275	2.04721	1.17826	C	4.36643	-2.56372	-1.31013
C	1.53330	-0.00164	1.81149	H	2.76159	-3.44819	-0.20476
C	-0.04252	2.66572	-0.00378	C	5.10871	-1.41275	-1.55138
C	0.76514	-2.31341	0.97763	H	5.38448	0.65100	-1.03863
C	-1.80886	-3.68290	0.07859	H	4.59669	-3.47846	-1.84123
H	-1.04268	-4.44112	0.06173	H	5.91716	-1.42811	-2.27077
C	-0.74439	2.32819	-2.20315	O	-0.84739	-0.60018	-2.21273
H	-0.93726	1.58937	-2.97190	H	-0.11120	-1.11542	-2.57023
C	-3.84438	-1.74151	0.16627	Ni	-0.15765	-0.03331	-0.56534
C	-3.16654	-4.04739	0.12518	O	1.44677	-0.15121	-1.36636
H	-3.41607	-5.10050	0.12720				

25. NiL3_OOH_D

H	3.36827	-4.87542	1.17250	C	1.70869	-3.49942	1.10629
O	3.15625	0.46112	-1.98906	C	-3.28826	-1.58414	-0.42505
C	3.15478	-2.17486	-0.90642	H	-2.85023	-2.50000	-0.80512
H	3.72927	-1.67999	-1.67130	C	-4.61981	-1.50525	-0.00460
C	3.65392	-3.33353	-0.28730	H	-5.24317	-2.38540	-0.06232
H	4.61713	-3.71017	-0.60783	C	-5.10474	-0.31631	0.47633
C	-0.28529	-3.52975	2.45702	H	-6.13054	-0.23521	0.81386
H	-0.90201	-3.95404	3.23605	C	-4.66010	2.08113	1.01698
C	0.92209	-4.08120	2.11911	H	-5.67171	2.22465	1.37248
H	1.28647	-4.96676	2.62531	O	-0.33200	3.43249	-1.29625
C	2.96630	-3.98931	0.69901	C	1.51310	1.97272	-1.23372
N	1.33754	-0.46734	-0.95713	H	1.81015	2.56927	-2.09532
N	-0.73649	1.37860	-0.37459	C	2.27787	2.50123	-0.02791
N	-2.48471	-0.53821	-0.37670	C	3.15994	3.56772	-0.16389
N	-0.01841	-1.83177	0.81385	C	2.10413	1.92255	1.22880
C	-2.93886	0.65687	0.08517	C	3.85789	4.04939	0.93438
C	-2.00966	1.72016	0.08296	H	3.29889	4.02006	-1.13863
C	1.92887	-1.65097	-0.53363	C	2.80176	2.40435	2.32544
C	2.04627	0.56397	-1.47268	H	1.41778	1.09020	1.34149
C	1.19263	-2.34202	0.47353	C	3.68091	3.46931	2.18174
C	0.04961	2.30713	-0.98862	H	4.54179	4.87989	0.81348
C	-2.43269	2.94406	0.56874	H	2.65888	1.94635	3.29596
H	-1.74972	3.77857	0.59001	H	4.22531	3.84454	3.03864

C	-0.73204	-2.39872	1.76410	Ni	-0.56075	-0.51390	-0.71102
H	-1.69323	-1.95040	1.98884	O	-0.66961	-2.09709	-1.72398
C	-4.27005	0.81540	0.53726	O	-0.83339	-1.55786	-3.02538
C	-3.74820	3.10603	1.03181	H	-1.79851	-1.54119	-3.13777
H	-4.04373	4.07684	1.40833				

26. NiL3_TS1_T							
O	0.99158	0.89314	2.18875	H	4.94177	2.72369	-1.29889
O	0.27304	2.42538	2.48467	C	1.40359	-3.45737	-1.71878
H	0.60385	2.55728	3.38548	H	0.56345	-3.64126	-2.36852
H	-0.72844	2.15507	2.57206	C	3.42966	-0.92378	1.72712
H	-2.80809	1.80827	2.08146	H	3.32057	-0.07593	2.39260
H	-2.03997	0.73024	2.94520	C	-1.05615	3.52296	-0.95737
O	-2.14020	1.69007	2.79276	H	-2.12568	3.44384	-0.84494
O	-4.12924	2.02511	0.89869	C	4.58006	-1.71866	1.73302
H	-4.41751	2.93930	0.82002	H	5.37807	-1.49350	2.42568
H	-3.80799	1.78275	0.00876	C	3.62426	-4.09076	-0.96961
O	-1.00293	-0.78512	3.19419	H	4.49293	-4.73324	-1.02916
H	-0.17949	-0.27616	3.04070	C	3.11468	3.83237	-1.44294
H	-0.90338	-1.18869	4.06122	H	3.57942	4.75045	-1.78154
N	1.92467	1.48786	-0.55359	C	0.86389	4.88165	-1.54349
N	0.29859	-1.53259	-0.58503	H	1.29172	5.81815	-1.87676
N	-0.67464	1.16685	-0.27817	C	-0.48819	4.73787	-1.37049
N	2.42075	-1.14985	0.90436	H	-1.14478	5.57723	-1.56225
O	-1.38075	-2.69046	-1.66357	C	2.53850	-4.27975	-1.78485
O	-2.71209	1.17519	-1.34825	H	2.54741	-5.08774	-2.50594
C	3.61234	-3.03459	-0.03651	Ni	0.83718	0.06929	0.50166
C	2.47562	-2.18882	0.02589	C	-3.40656	-1.32177	-0.29143
C	1.14879	2.56794	-0.84057	C	-4.07672	-1.65654	0.88128
C	1.33929	-2.40361	-0.81760	C	-4.08955	-1.43198	-1.50197
C	-0.26135	2.41983	-0.69445	C	-5.39653	-2.08775	0.85449
C	-0.98333	-1.78381	-0.93726	H	-3.55413	-1.57228	1.82843
C	-1.82898	0.61855	-0.67629	C	-5.40630	-1.86203	-1.53352
C	-1.99121	-0.84006	-0.22105	H	-3.58175	-1.17333	-2.42097
C	4.67084	-2.76225	0.85079	C	-6.06552	-2.19117	-0.35521
H	5.55315	-3.39025	0.82482	H	-5.89999	-2.34158	1.77892
C	3.22991	1.56228	-0.71983	H	-5.92320	-1.94135	-2.48192
H	3.80385	0.67440	-0.48146	H	-7.09474	-2.52625	-0.38255
C	1.71637	3.79029	-1.28295	H	-1.68353	-0.85504	0.82898
C	3.86835	2.72156	-1.17592				

27. NiL3OHO_TS2_D							
H	-0.39114	5.91992	1.04757	C	-0.35320	4.06269	-0.04655
O	2.18413	0.61360	2.82306	C	-3.12358	0.78001	-0.11650
C	0.51111	2.90311	2.37186	H	-2.82256	1.81960	-0.18162
H	0.85010	2.48474	3.30513	C	-4.47945	0.42921	-0.13870
C	0.23167	4.27676	2.27289	H	-5.22672	1.20551	-0.21670
H	0.35552	4.88860	3.15721	C	-4.82650	-0.89344	-0.07124
C	-0.89487	3.67135	-2.36200	H	-5.86627	-1.19543	-0.09960
H	-1.20543	4.01529	-3.33759	C	-4.08100	-3.26402	0.11521
C	-0.76946	4.53594	-1.30584	H	-5.10346	-3.61678	0.08444
H	-0.98529	5.59000	-1.42839	O	0.80317	-3.35599	1.60896
C	-0.18414	4.85960	1.10337	O	-0.34676	-0.63228	-2.29133
N	0.62921	0.72446	1.15247	H	-0.20340	-1.58914	-2.29545
N	-0.14475	-1.76153	0.28638	Ni	-0.10359	-0.02013	-0.47413
N	-2.16390	-0.11616	-0.02075	O	1.39108	-0.39395	-1.59161
N	-0.24993	1.84516	-1.00036	C	1.98598	-1.29346	1.41435
C	-2.48359	-1.43396	0.06765	C	3.01728	-1.26554	0.30002
C	-1.40715	-2.34943	0.20275	C	3.43983	-0.08136	-0.31125
C	0.36165	2.08478	1.26634	C	3.58644	-2.46915	-0.11202
C	1.58794	0.10202	1.87852	C	4.40331	-0.11075	-1.31650
C	-0.09044	2.67713	0.06300	H	3.03959	0.87074	0.01358
C	0.83025	-2.23981	1.09959	C	4.54004	-2.49425	-1.11465
C	-1.69804	-3.69897	0.26656	H	3.27131	-3.39171	0.36147
H	-0.89552	-4.41195	0.36132	C	4.95021	-1.31316	-1.72464
C	-0.62468	2.31076	-2.17410	H	4.71866	0.81686	-1.77646
H	-0.71864	1.58395	-2.97092	H	4.96933	-3.43946	-1.42197
C	-3.82752	-1.87978	0.03685	H	5.69696	-1.33567	-2.50745
C	-3.03155	-4.13821	0.22081	H	2.47079	-1.75217	2.27708
H	-3.22377	-5.20217	0.27267				

Water (H_2O)			
O	0.00000	-0.00000	0.11884
H	-0.00000	0.75553	-0.47535
H	-0.00000	-0.75553	-0.47535

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