Electronic Supplementary Material (ESI) for Materials Advances.

Mononuclear nickel(II) complexes as electrocatalyst in hydrogen evolution reactions: Effect of alkyl side chain length

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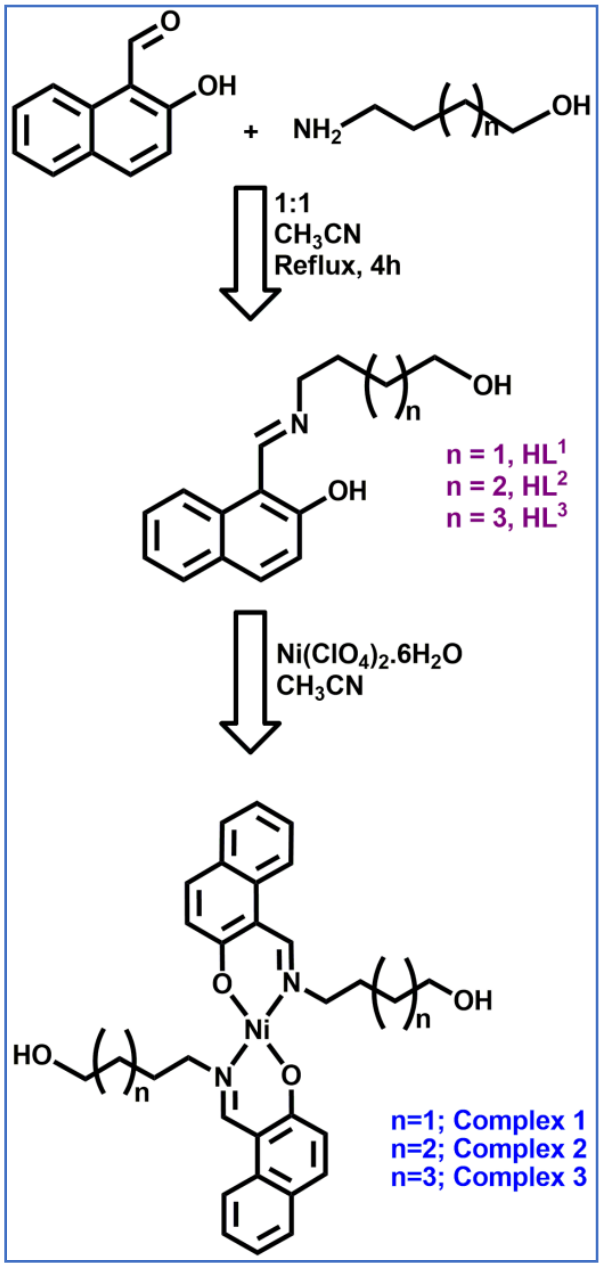


Scheme S1: Synthetic route to Complexes **1**, **2** and **3**.

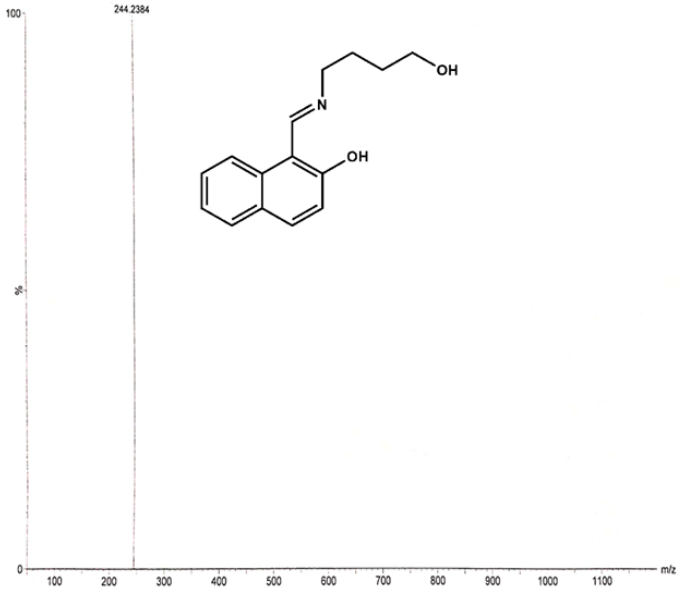


Fig. S1 Mass spectrum of HL^1 in methanol.

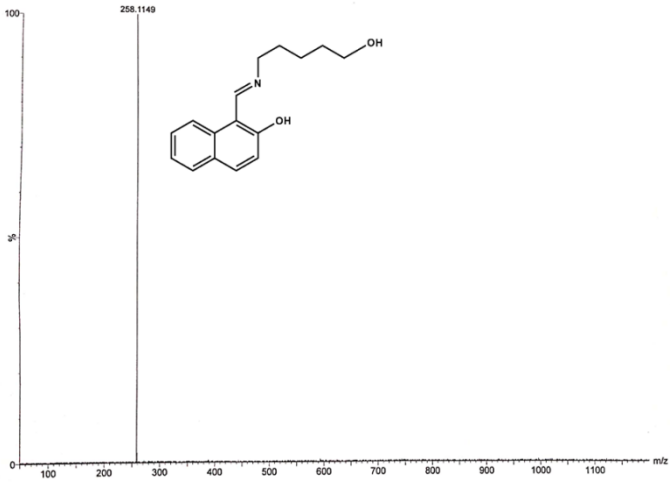


Fig. S2 Mass spectrum of HL^2 in methanol.

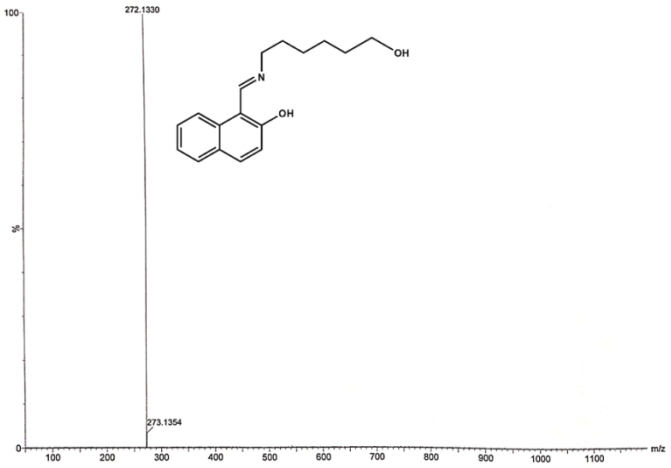


Fig. S3 Mass spectrum of HL^3 in methanol.

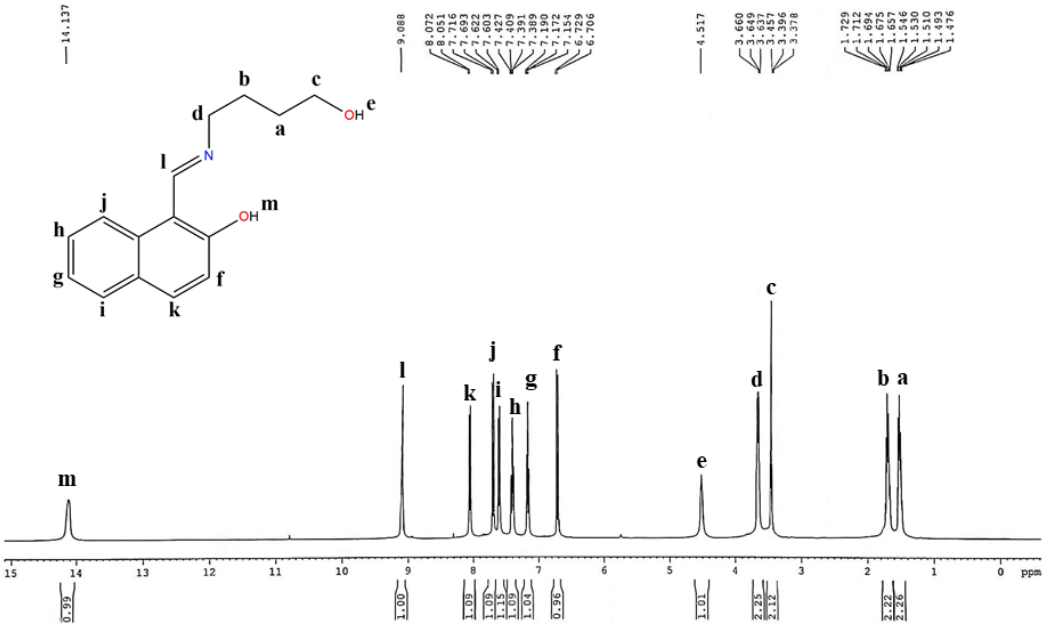


Fig. S4 ^{1}H NMR spectrum of HL^1 in DMSO-d_6.

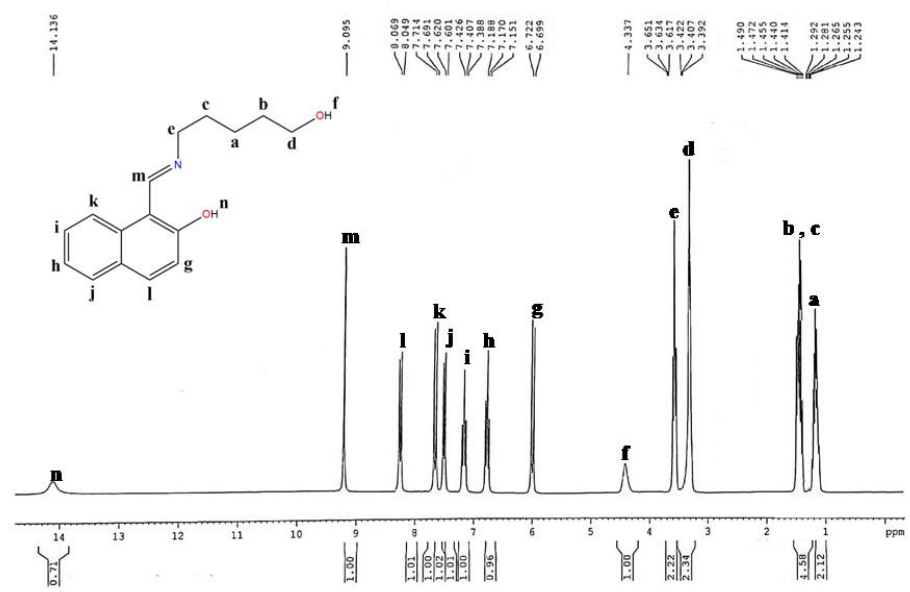


Fig. S5 ^{1}H NMR spectrum of HL^{2} in DMSO-d_6.

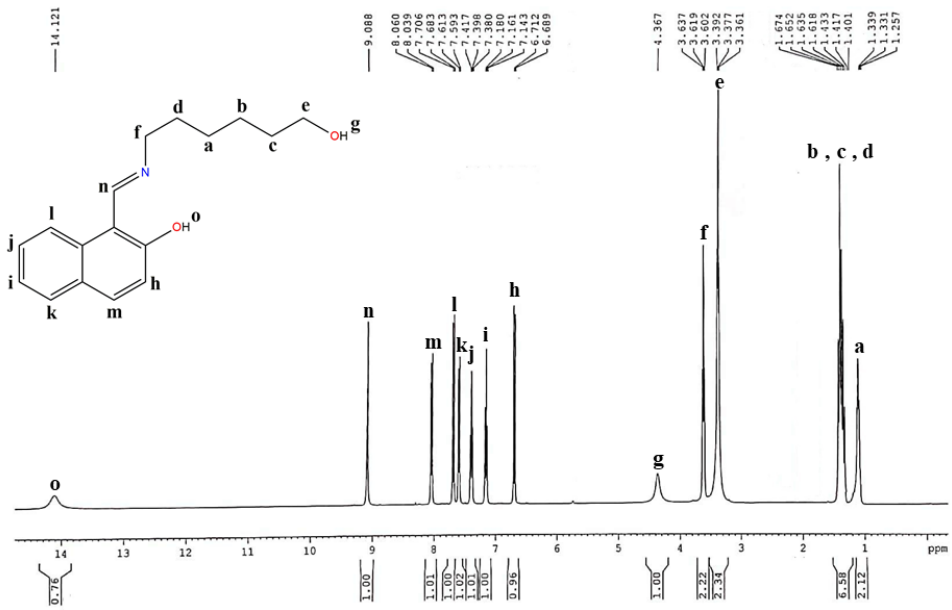


Fig. S6 ^{1}H NMR spectrum of HL^{3} in DMSO-d_6.

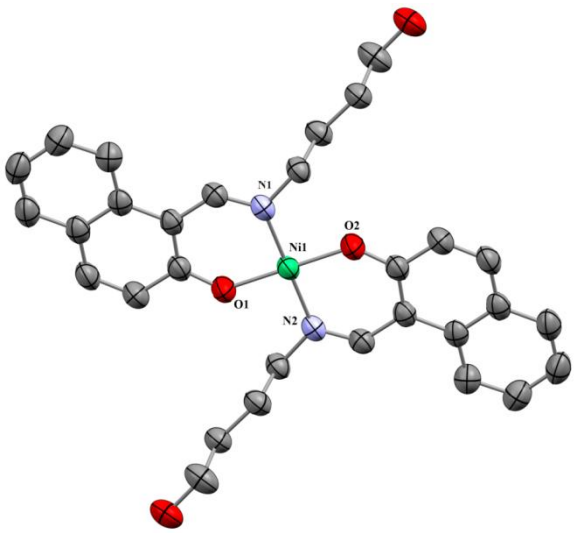


Fig. S7 A perspective view of complex **1** with displacement ellipsoids drawn at the 50% probability level. Symmetry code; (a) –x, 1-y, 1-z

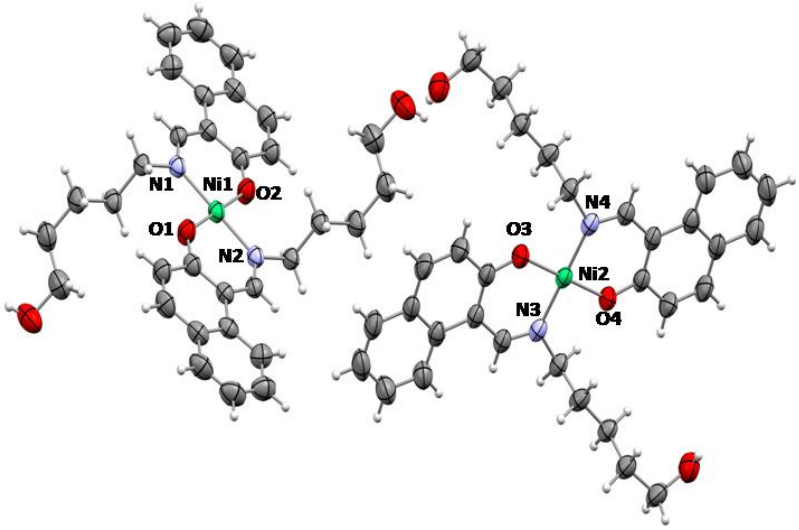


Fig. S8 A perspective view of complex **2** with displacement ellipsoids drawn at the 50% probability level. Symmetry code; (a) –x, 1-y, 1-z

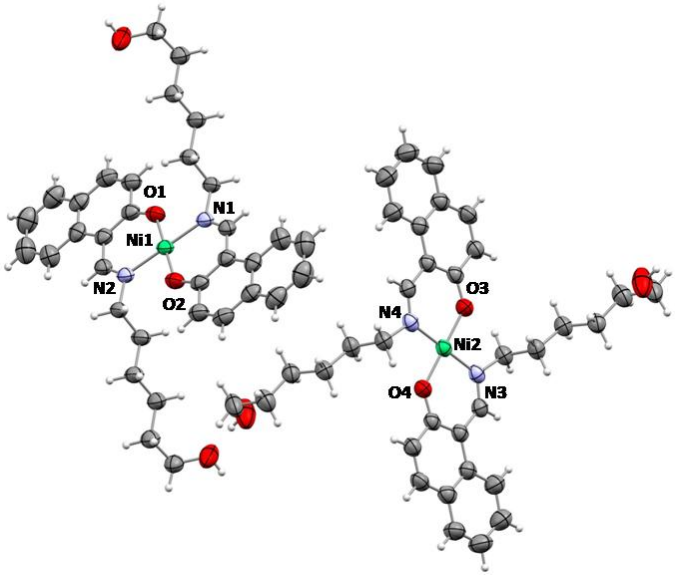


Fig. S9 A perspective view of complex **3** with displacement ellipsoids drawn at the 50% probability level. Symmetry code; (a) 1 –x, -y, 2-z

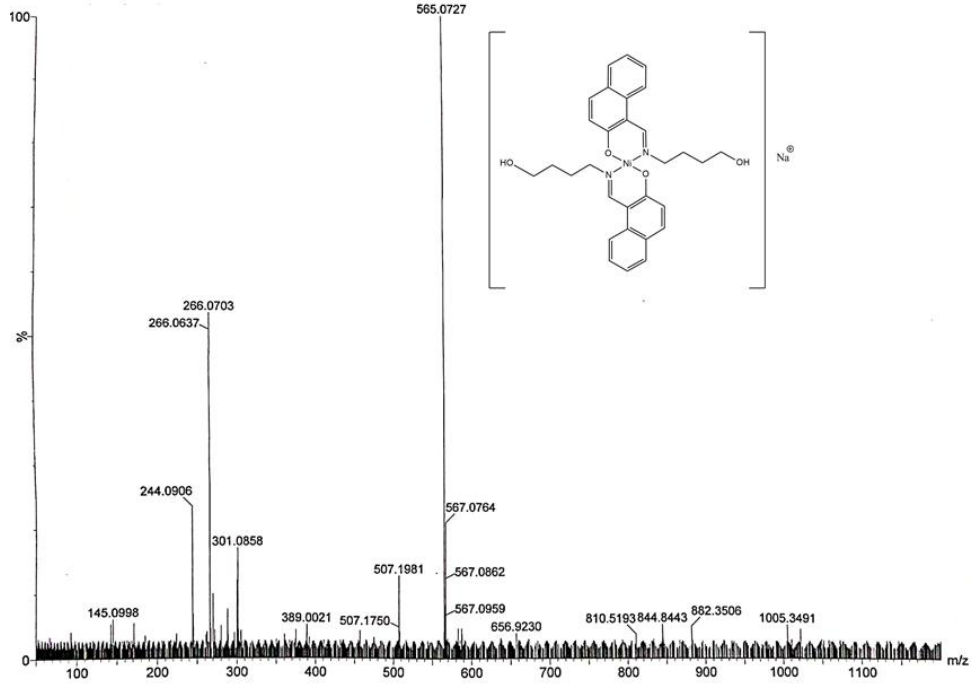


Fig. S10 Mass spectrum of Complex **1** in methanol.

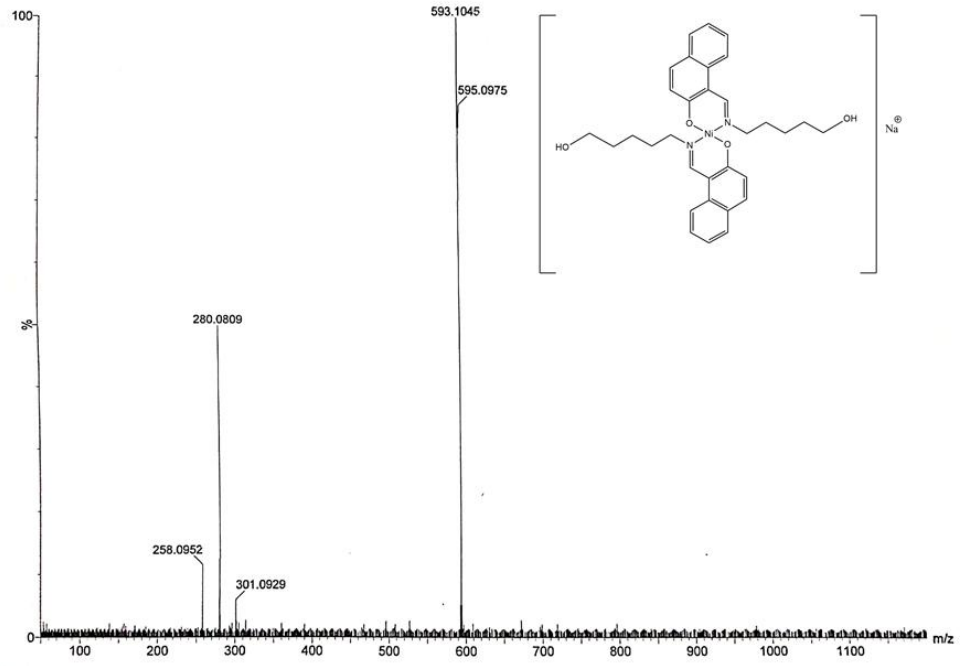


Fig. S11 Mass spectrum of Complex **2** in methanol.

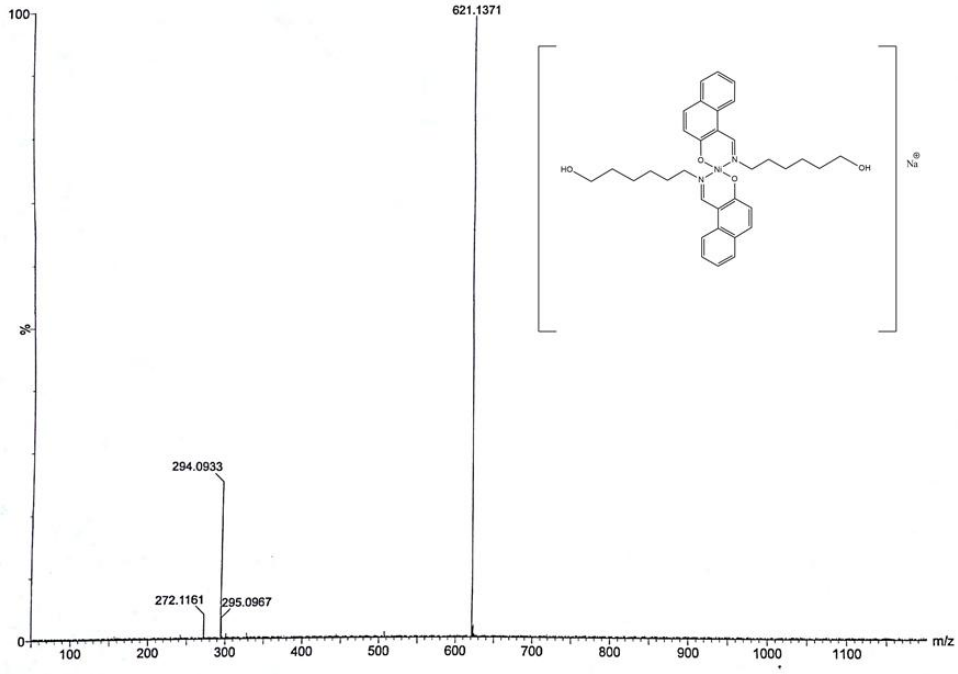


Fig. S12 Mass spectrum of Complex **3** in methanol.

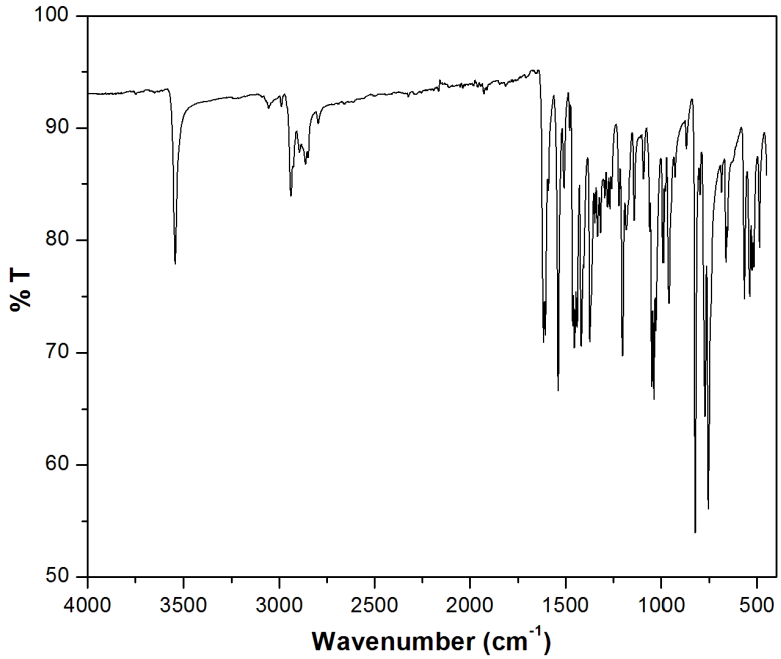


Fig. S13 FT-IR spectrum of Complex **1**.

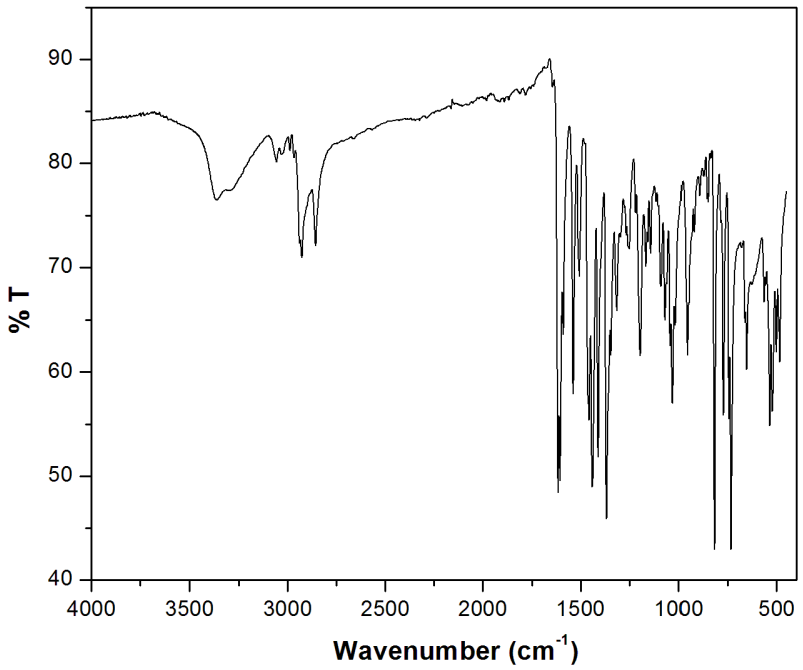


Fig. S14 FT-IR spectrum of Complex **2**.

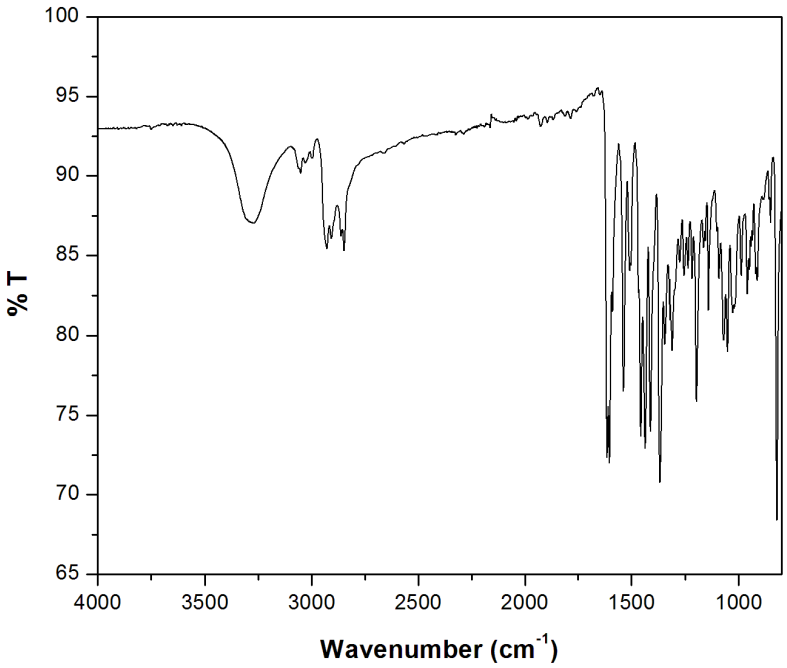


Fig. S15 FT-IR spectrum of Complex **3**.

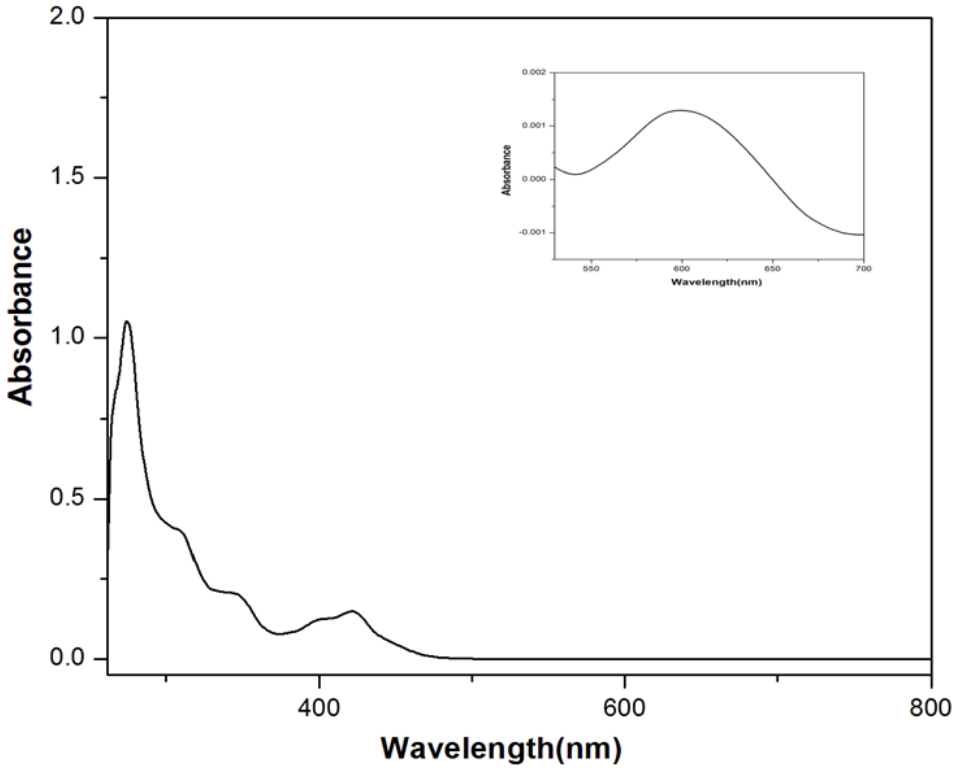


Fig. S16 UV-vis spectrum of complex **1** in DMF

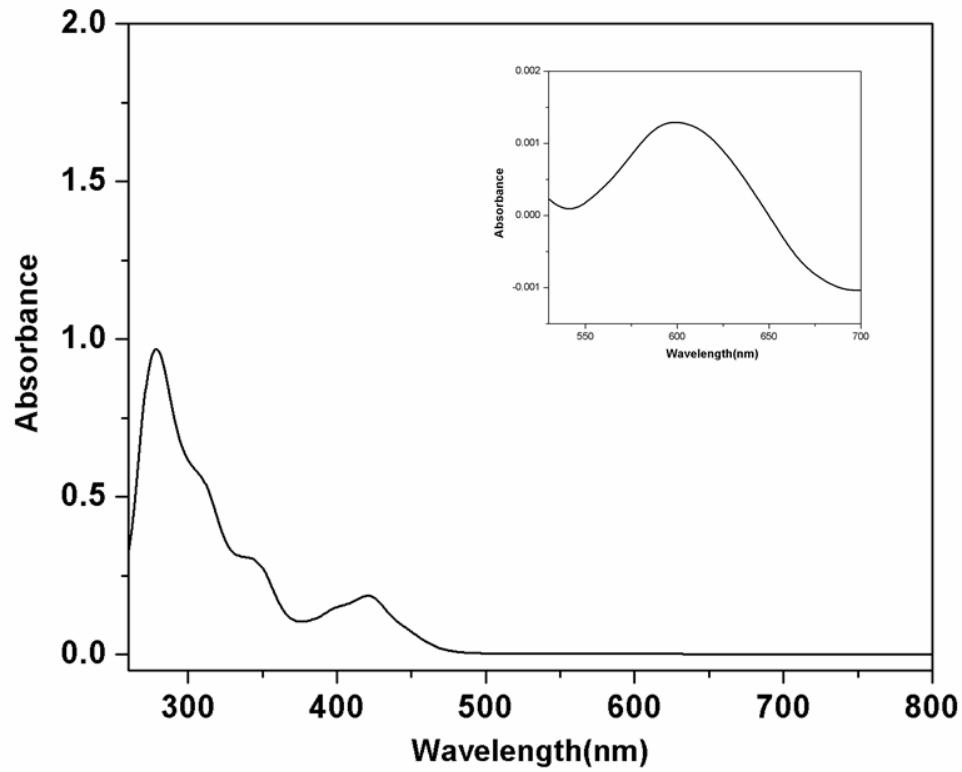


Fig. S17 UV-vis spectrum of complex **2** in DMF

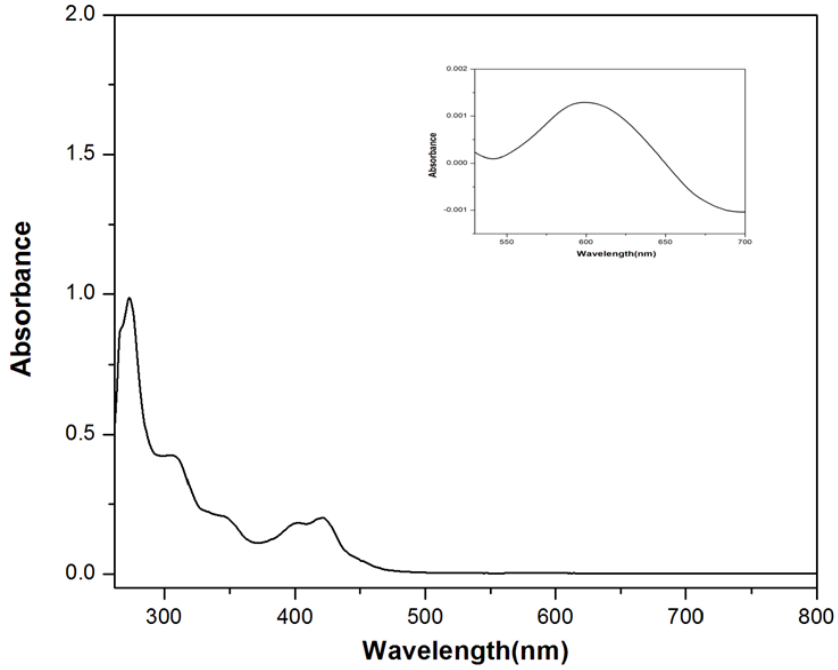


Fig. S18 UV-vis spectrum of complex **3** in DMF

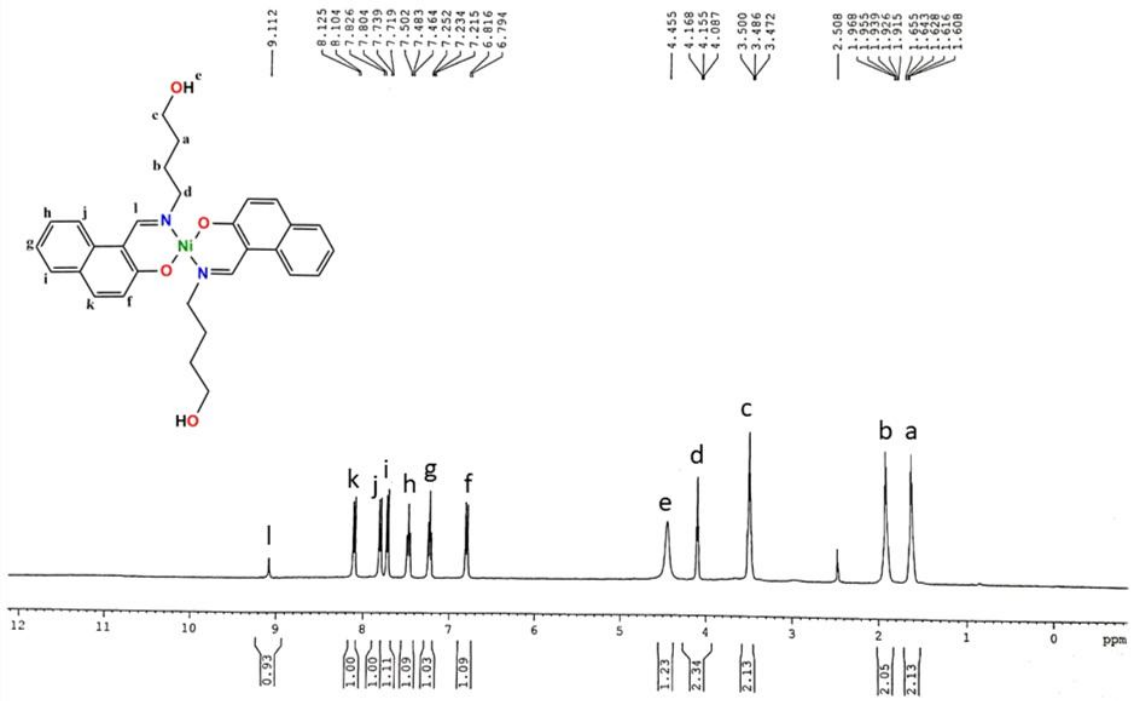


Fig. S19 ^{1}H NMR spectrum of complex **1** in DMSO-d_6.

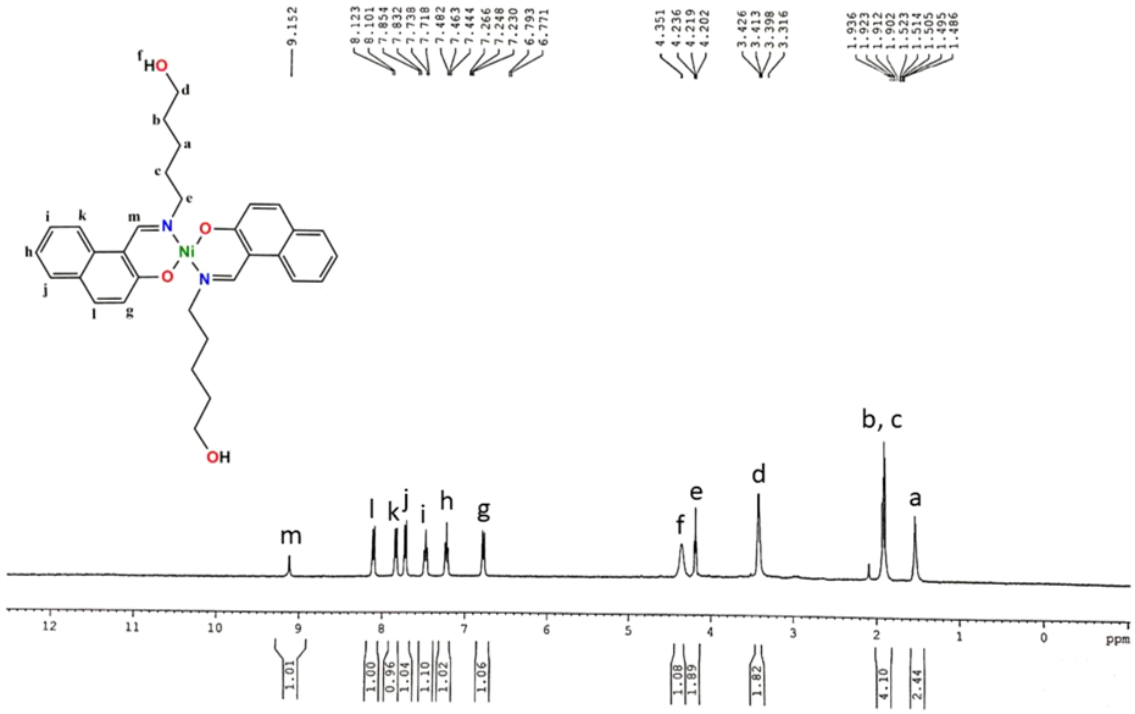


Fig. S20 ^{1}H NMR spectrum of complex **2** in DMSO-d_6.

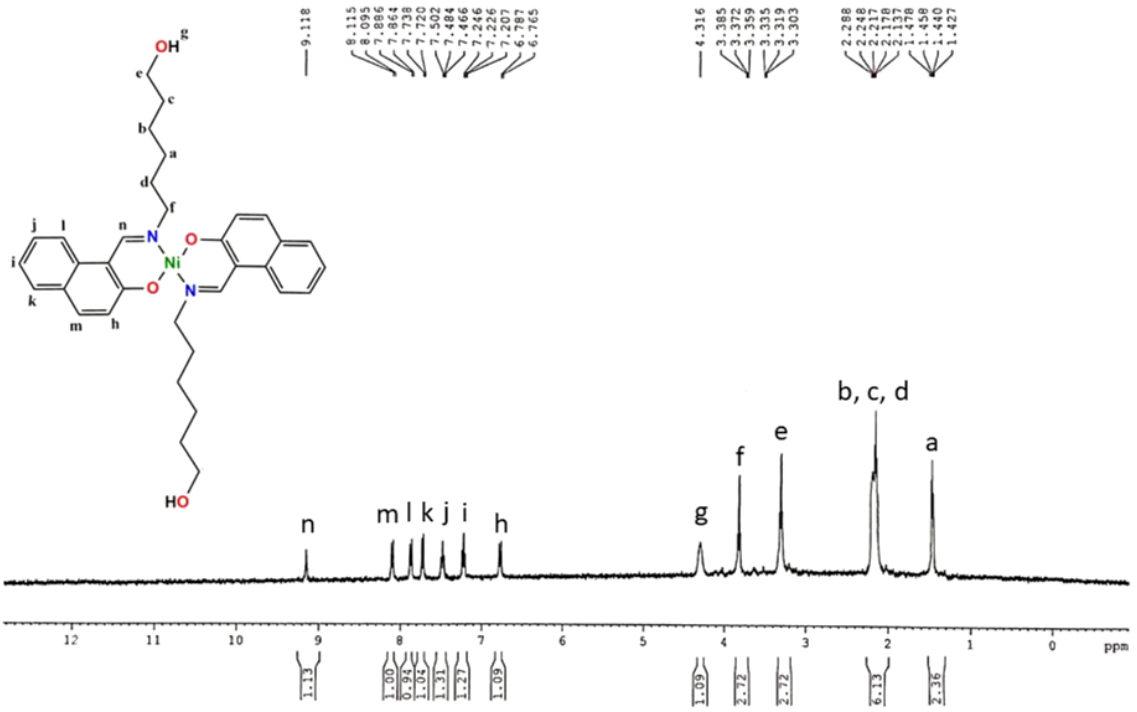


Fig. S21 ^{1}H NMR spectrum of complex **3** in DMSO-d_6.

Calculation of $E_{1/2}$ with respect to nHE of Fc/Fc^+

E vs. nHE = [value obtained against Ag/AgCl, Cl^- + 0.224 V (Potential of Ag/AgCl, Cl^-electrode) – 0.200 V (Liquid junction potential of saturated aqueous KCl solution with DMF)]

= [0.535 + 0.224 – 0.200] V

= 0.559 V

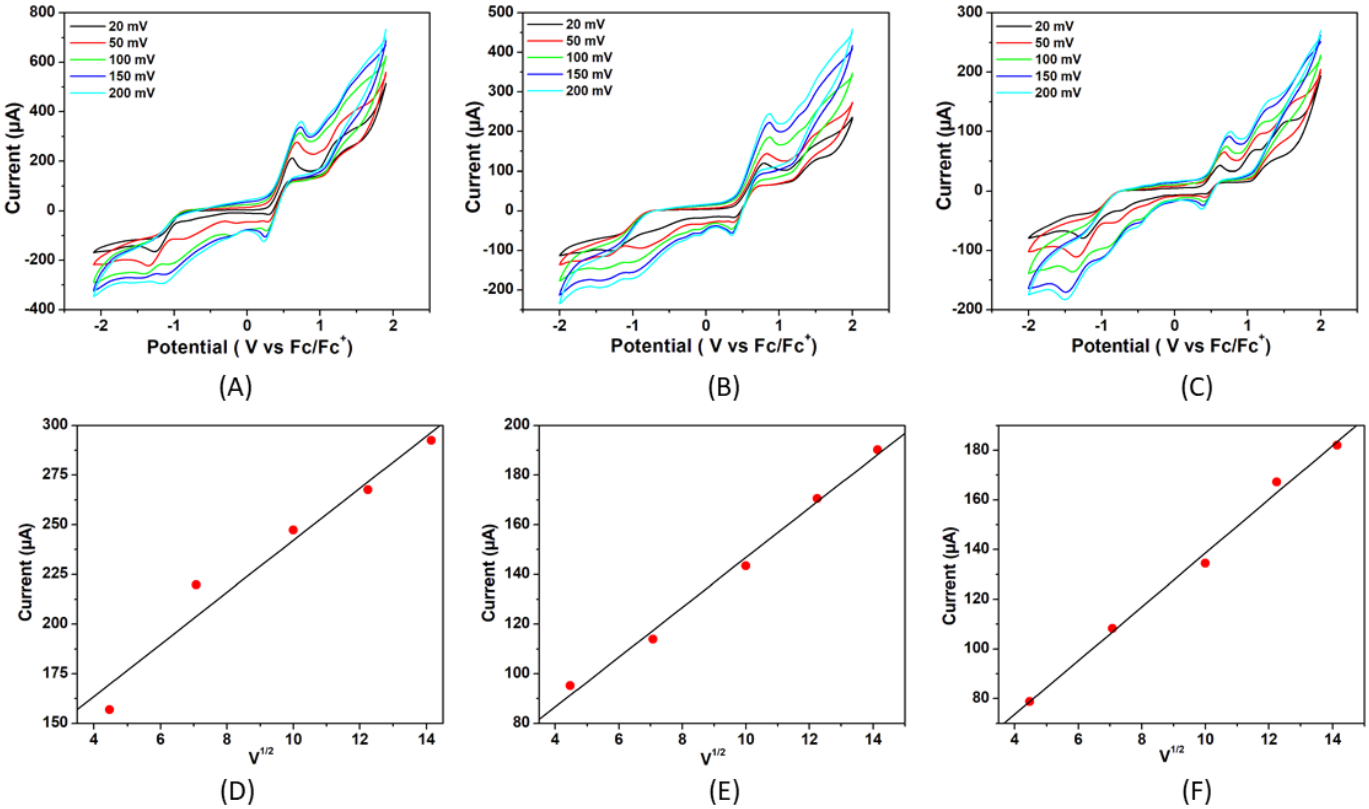


Fig. S22 Scan rate dependence of precatalytic waves for 5.36 µM solutions of complexes (A)**1**, (B)**2** and (C)**3** at scan rate from 20 to 200 mV/s inair free DMF solutions with 0.1M [n-Bu_4N]Bras supporting electrolyte and Cottrell plot of peak current versus the square root of scan rate for complexes (D) **1**, (E) **2** and (F) **3**.

Determination of Diffusion Coefficient (D) for complex 1, 2 and 3

Using the Randles-Sevcik equation,

$$i_P = 0.4463\left(\frac{n^3F^3}{RT}\right)^{1/2} A[cat](Dv)^{1/2} \ldots\ldots\ldots(1)$$

Where, i_p = Peak current (amperes), n = Number of electrons transferred in a redox cycle, F = Faraday's constant (96485C/mol), R = Universal gas constant (8.314 $J.K^{-1}.mol^{-1}$), T = Absolute temperature (298 K), A = The electrode surface area in working (0.07 cm^2), C = Molar concentration of redox-active species (mol/cm^3), D = The diffusion coefficient (cm^2/s), v = Scan rate in V/s.

Plotting peak current (i_p) versus the square root of the scan rate $(v)^{1/2}$

$$Slope = 0.4463\left(\frac{n^3F^3}{RT}\right)^{1/2} A[cat](D)^{1/2} \ldots\ldots\ldots(2)$$

Complex	Slope	Diffusion coefficient (cm^2/s)
1	1.31×10^{-5}	1.07×10^{-5}
2	1.11×10^{-5}	0.77×10^{-5}
3	1.08×10^{-5}	0.72×10^{-5}

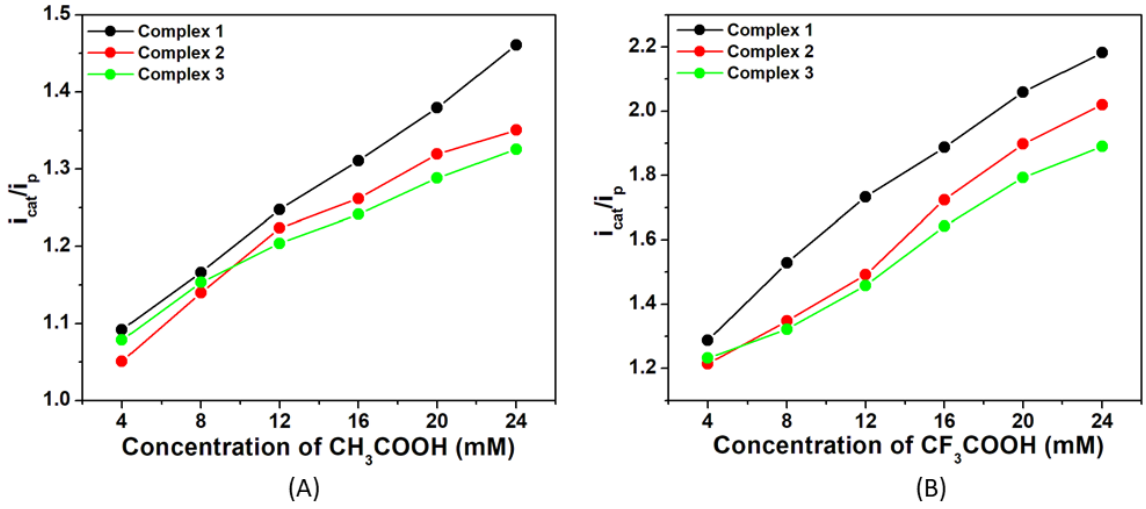


Fig. S23 Plot of i_{cat}/i_p vs [Acid] for 5.36 µM of complexes **1**, **2** and **3**.

Over potential Calculations:

Calculations of $E^{T}_{1/2}$ (= E_{ref}) and η using $E^{0}_{H^+/H_2}$, pKa, $\mathcal{E}_D$ and $C^{0}_{H_2}$ using Fourmond's approach.[1]

$$E^{T}_{1/2} = E^{0}_{H^+/H_2} - 2.303\frac{RT}{F}pK_a + \mathcal{E}_D - \frac{RT}{2F}ln\frac{C_0}{C^{0}_{H_2}}$$

$E^{T}_{1/2}$ for Complexes **1**, **2**, **3** with 24.00 mM CH_3COOH in DMF

$$E^{T}_{1/2} = (-0.62) - 2.303\frac{8.314 \times 298}{96485}13.5 + 0.04 - \frac{8.314 \times 298}{2 \times 96485}ln\frac{24}{1.9}$$

$$E^{T}_{1/2} = -1.41\ vs\ Fc^{+}/Fc$$

Complex	**Overpotential**
1	–1.41 – (–0.888) = –0.52
2	–1.41 – (–0.853) = –0.55
3	–1.41 – (–0.849) = –0.56

$E^{T}_{1/2}$ for Complexes **1**, **2**, **3** with 24.00 mM CF_3COOH in DMF

$$E^{T}_{1/2} = (-0.62) - 2.303\frac{8.314 \times 298}{96485}6.0 + 0.04 - \frac{8.314 \times 298}{2 \times 96485}ln\frac{24}{1.9}$$

$$E^{T}_{1/2} = -0.96\ vs\ Fc^{+}/Fc$$

Complex	**Overpotential**
1	–0.96 – (–0.733) = –0.22
2	–0.96 – (–0.723) = –0.23
3	–0.96 – (–0.713) = –0.24

Fig. S24 Photograph of the customized, one-compartment, three-neck cell with a glassy carbon working electrode. H_2 gas bubbles are appeared on the surface of the working electrode.

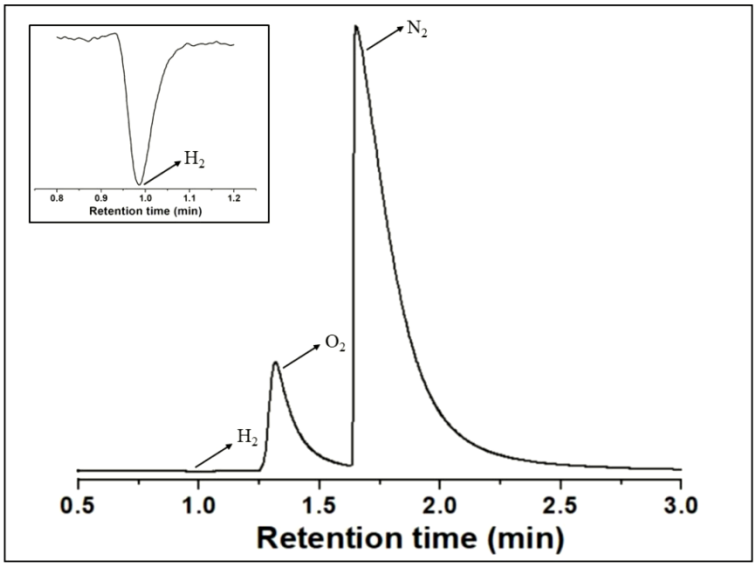


Fig. S25 Gas chromatogram of the headspace gas obtained after bulk electrolysis of a N_2 saturated 0.5 mM solution of complex **1** containing 24 mM TFA. The headspace gas was analyzed after 30 min of electrolysis. Inset: Detection region of evolved H_2 gas.

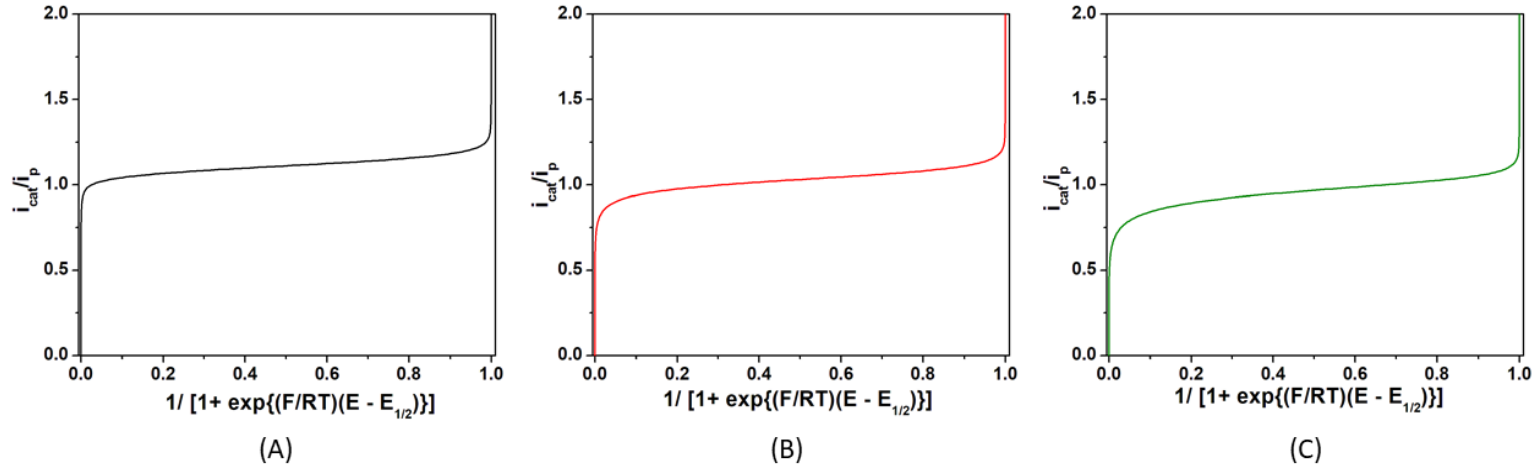


Fig. S26 Plot of i_{cat}/i_p vs. 1/(1+exp[(F/RT)(E-$E_{1/2}$)] using FOWA of 5.36 µM of (A) complex **1** (B) complex **2** and (C) complex **3** with 24 mM CH_3COOH in DMF.

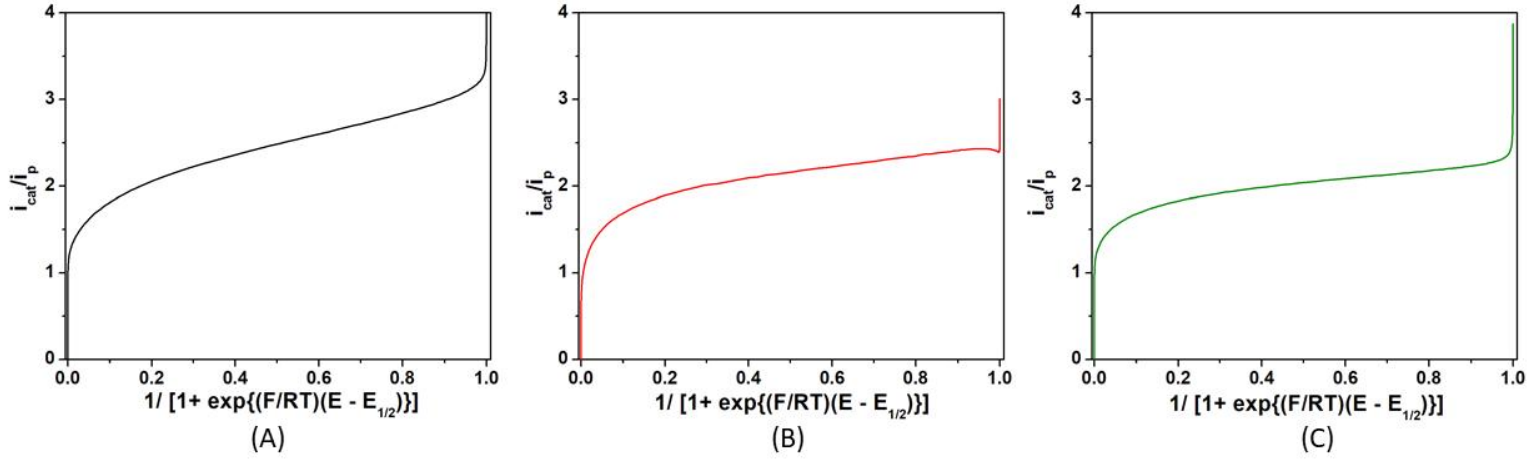


Fig. S27 Plot of i_{cat}/i_p vs. 1/(1+exp[(F/RT)(E-$E_{1/2}$)] using FOWA of 5.36 µM of (A) complex **1** (B) complex **2** and (C) complex **3** with 24 mM CF_3COOH in DMF.

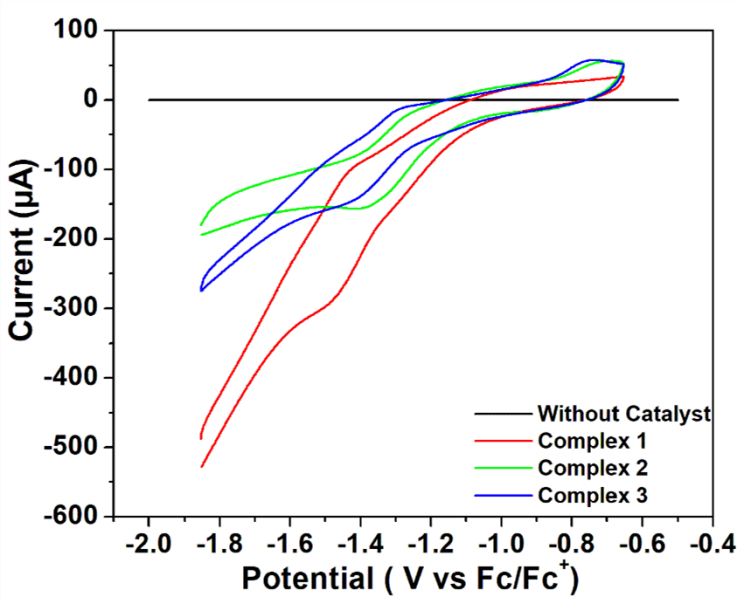


Fig. S28 CVs showing blank DMF with 24 mM CH_3COOH added (black) and with 24 mM CH_3COOH in the presence of 5.36 µM complex **1** (red), complex **2** (green), complex **3** (blue). Conditions: room temperature, 0.1 M [n-Bu_4N]Br as supporting electrolyte, scan rate = 50 mV/s, glassy carbon working electrode, Pt wire counter electrode and the potential is referenced against Fc/Fc^+.

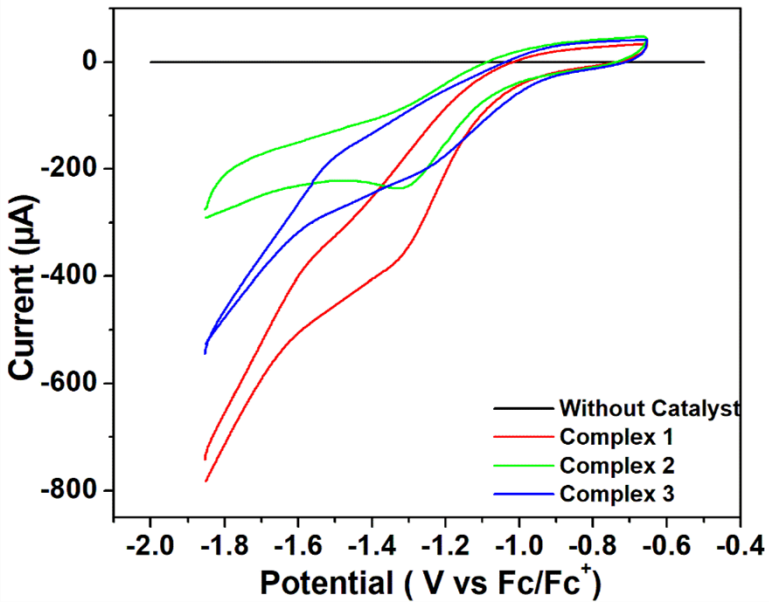


Fig. S29 CVs showing blank DMF with 24 mM CF_3COOH added (black) and with 24 mM CH_3COOH in the presence of 5.36 µM complex **1** (red), complex **2** (green), complex **3** (blue). Conditions: room temperature, 0.1 M [n-Bu_4N]Br as supporting electrolyte, scan rate = 50 mV/s, glassy carbon working electrode, Pt wire counter electrode and the potential is referenced against Fc/Fc^+.

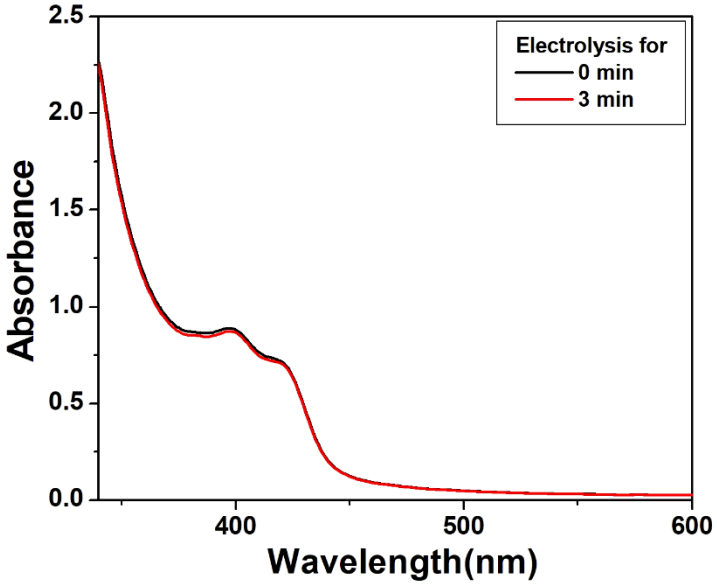


Fig. S30 UV-Vis spectra of complex **1** in DMF during electrolysis under –1.50 V versus Fc/Fc^{+}.

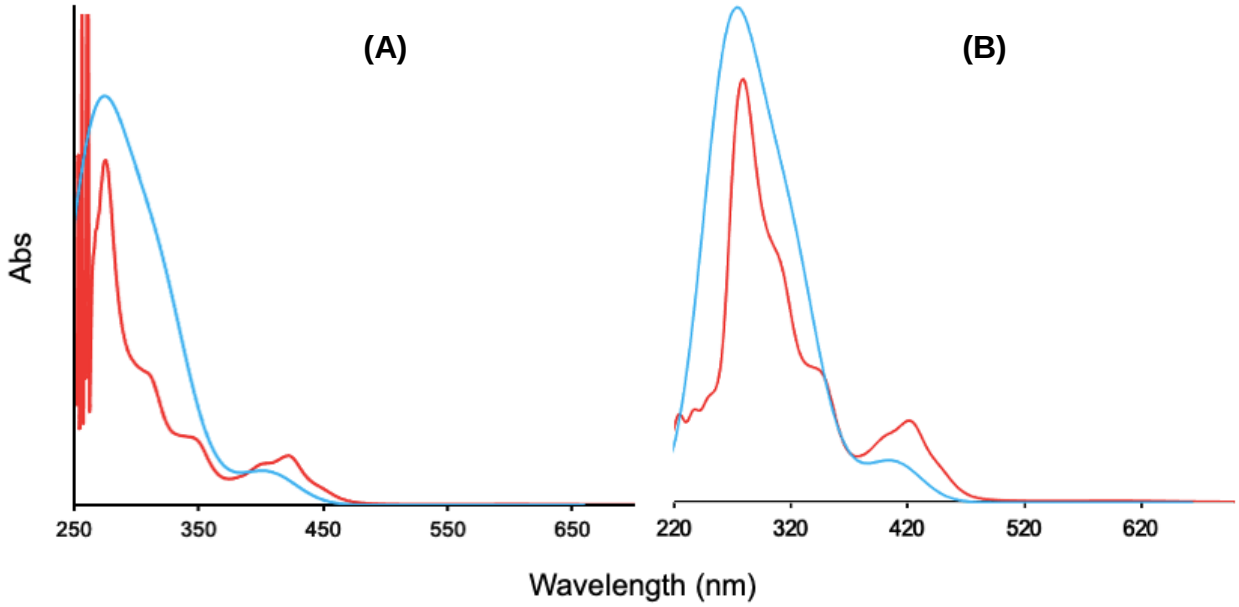


Fig. S31 TDDFTUV-Vis spectra of (A) complex 1 and (B) complex 2 (blue: calculated and red: experimental).

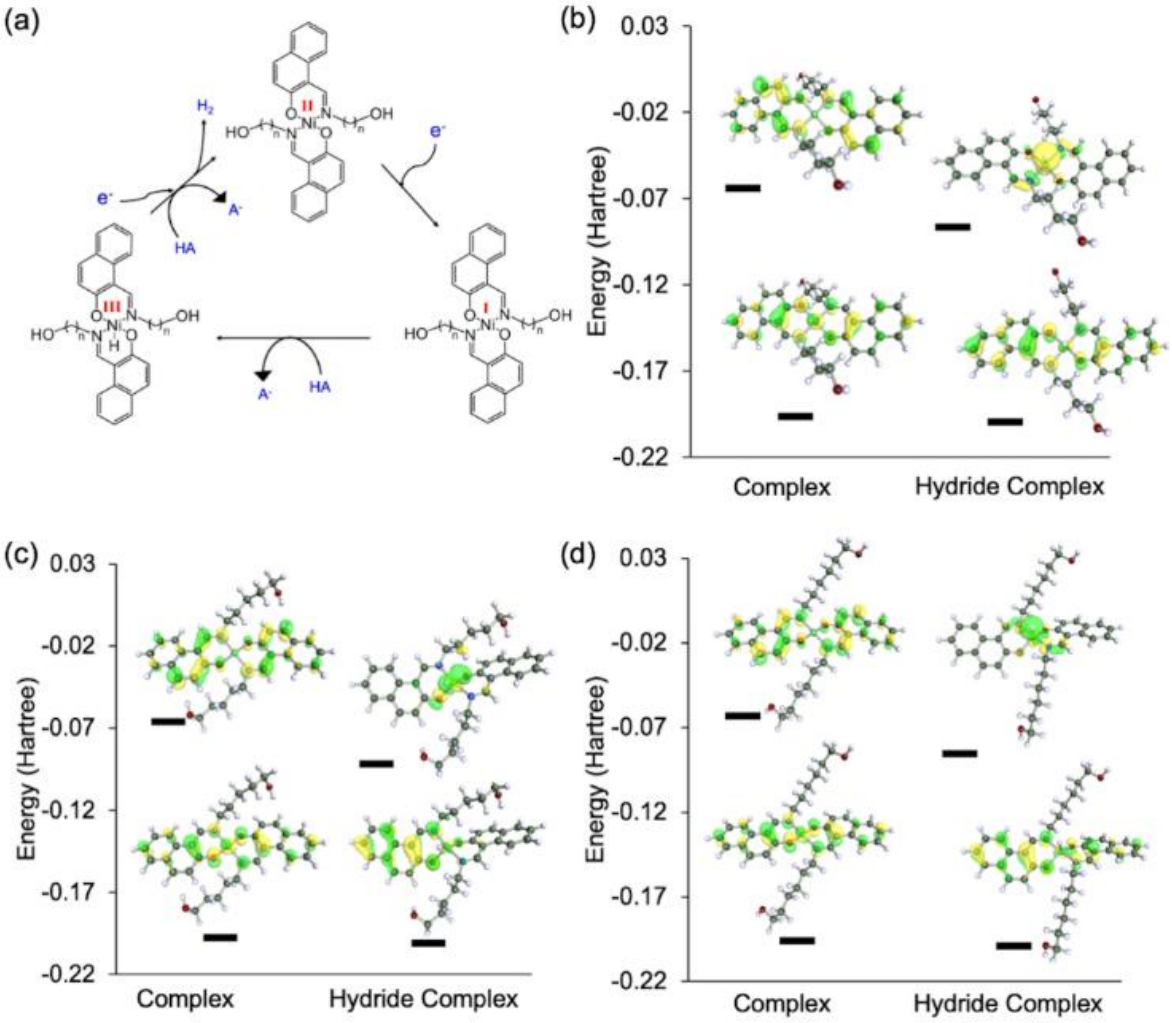


Fig. S32 (a) Plausible mechanistic pathway of HER by complexes **1**, **2** and **3** (n = 4, 5 and 6); (b-d) HOMO-LUMO electronic distribution for complexes **1**, **2** and **3** and their hydride complex derivative.

Table S1 Selected bond lengths (Å) and bond angles (°) of complexes **1**, **2** and **3.**

Complex 1

Ni1–O1	1.8261
Ni1–O1[a]	1.8261
Ni1–N1	1.9106
Ni1–N1[a]	1.9106
O1–Ni1–O1[a]	180.00
O1[a]–Ni1–N1[a]	92.14
O1[a]–Ni1–N1	87.86
O1–Ni1–N1[a]	87.86
O1–Ni1–N1	92.14
N1–Ni1–N1[a]	180.00

Complex 2

Ni1–O1	1.8226
Ni1–O1[a]	1.8226
Ni1–N1	1.9164
Ni1–N1[a]	1.9164
O1–Ni1–O1[a]	180.00
O1–Ni1–N1	92.13
O1–Ni1–N1[a]	87.87
O1[a]–Ni1–N1	87.87
O1[a]–Ni1–N1[a]	92.13
N1–Ni1–N1[a]	180.00

Complex 3

Ni1–O1[a]	1.8310
Ni1–O1	1.8310
Ni1–N1[a]	1.9162
Ni1–N1	1.9162
O1–Ni1–O1[a]	180.00
O1–Ni1–N1[a]	88.44
O1–Ni1–N1	91.56
O1[a]–Ni1–N1[a]	91.56
O1[a]–Ni1–N1	88.44
N1–Ni1–N1[a]	180.00

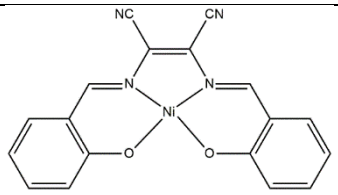
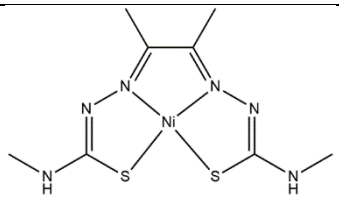
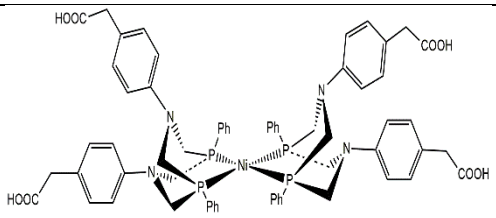
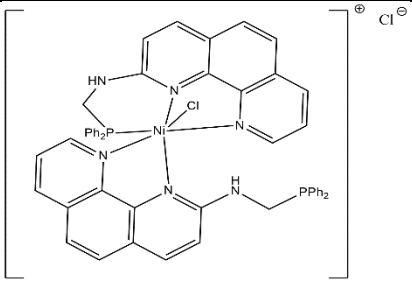
Table S2 Assignment of different IR spectral bands of Complexes **1**, **2** and **3**

Complex	**ν (cm^{-1})**	**Assigned for**
1	3536	O–H stretching
2	3316	
3	3272	
1	2939	aromatic C-H bond
2	2933	
3	2934	
1	2855	aliphatic C-H bond
2	2854	
3	2851	
1	1657	azomethine group
2	1658	
3	1642	
1	486	metal-nitrogen
2	485	
3	479	
1	562	metal-oxygen
2	534	
3	532	

Table S3 Assignment of different UV-vis spectral bands of Complexes **1**, **2** and **3**

Complex	π–π*(phenolic chromophore)	ε (M^{-1} cm^{-1})	π–π* (C=N and benzene ring)	ε (M^{-1} cm^{-1})	n –π* (C=N)	ε (M^{-1} cm^{-1})	LMCT	ε (M^{-1} cm^{-1})	*d–d*	ε (M^{-1} cm^{-1})
1	275	10500	312	4000	348	2000	424	1500	600	30
2	279	9500	310	5700	345	2500	420	1800	596	30
3	274	9600	307	4200	347	2000	421	1900	592	30

Table S4 Few parameters of recently published complexes used for hydrogen evolution reaction

Entry	Complex	Medium	Source	Overpotential (V)
1	 (*Int. J. Hydrogen Energy* **2014**, *39*, 10980)	DMF	CH_3COOH	0.320
2	 (*Inorg. Chem.* **2018**, *57*, 21, 13486)	DMF	CH_3COOH	0.85
			CF_3COOH	------
		ACN	CH_3COOH	0.53
			CF_3COOH	0.67
3	 (*Dalton Trans*., **2019**, *48*, 14653)	ACN	CF_3COOH	0.93
4	 (*Inorg. Chem.* **2020**, *59*, 1038)		H_2-saturated basic (1.0 M KOH)	0.364

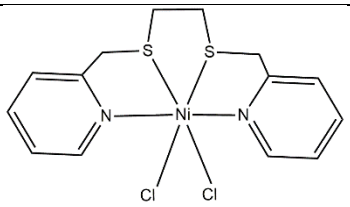
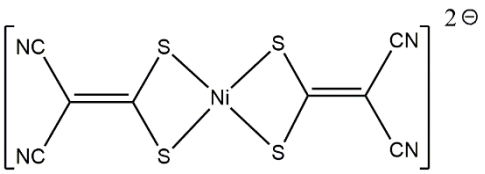
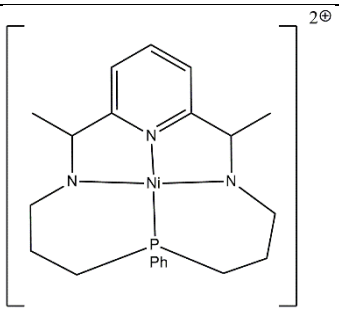
5	 (*Int. J. Hydrogen Energy* **2018**, *43*, 19047)		Neutral buffer	0.837
6	 (*Applied Catalysis B* **2017**, *219*, 353–361)		Neutral buffer	0.837.6
7	 (*ACS Catal*. **2015**, *5*, 356−364)	ACN	$HClO_4$	1.07
8	Complex **1** (Present study)	DMF	CH_3COOH	0.52
			CF_3COOH	0.22
9	Complex **2** (Present study)	DMF	CH_3COOH	0.55
			CF_3COOH	0.23
10	Complex **3** (Present study)	DMF	CH_3COOH	0.56
			CF_3COOH	0.24

Table S5 TON Calculations

Complex in DMF	Proton source	$q_{total}=q_{cat}-q_{blank}$	Theoretical moles of hydrogen produced = q_{total} (1 mol e^- / 96485 C) × (1 mol H_2 / 2 mol e^-)	Moles of catalyst used	TON = Theoretical moles of H_2 / Moles of catalyst used
1	Acetic acid	0.62	3.21×10^{-6}	1.34×10^{-7}	23.95
2	Acetic acid	0.40	2.07×10^{-6}		15.45
3	Acetic acid	0.33	1.71×10^{-6}		12.76
1	Trifluoroacetic acid	1.30	6.74×10^{-6}		50.30
2	Trifluoroacetic acid	0.50	2.59×10^{-6}		19.33
3	Trifluoroacetic acid	0.38	1.97×10^{-6}		14.70

Faradaic Efficiency

$$\text{Faradaic Efficiency} = \frac{\text{Quantified moles of } H_2}{\text{Theoretical moles of } H_2} \times 100\%$$

Table S6 Calculations of Faradaic Efficiency

Complex	Proton Source	Quantified moles of H_2	Theoretical moles of H_2 ($\times 10^{-6}$)	Faradaic Efficiency (%)
1	Acetic Acid	2.17	3.21	67.56
2		1.01	2.07	48.64
3		0.71	1.71	41.35
1	Trifluoroacetic acid	5.51	6.74	81.78
2		1.59	2.59	61.41
3		1.17	1.97	59.58

TOF Calculations:

For homogenous, diffusion controlled process the peak current can be given by Randle Sevcik equation

$$i_p = 0.4463FSC_p^0\sqrt{\frac{FvD}{RT}} \quad \text{.....(3)}$$

$$i_{cat} = \frac{2FSC_p^0\sqrt{\frac{FvD}{RT}}}{1+exp\left[\frac{F}{RT}(E-E_{\frac{1}{2}})\right]} \quad \text{.....(4)}$$

where, F is the Faraday's constant, S is the surface of electrode, C_p^0 is the concentration of the complex in solution, D is the diffusion coefficient, $E_{1/2}$ the half-wave potential of the redox couple triggering catalysis, R is the gas constant and T is the absolute temperature. Combining the equation (3) and (4) we get the equation (5). The plot of $i_{ca}t/i_p$ vs $1/(1+\exp[(F/RT)(E-E_{1/2})]$ gives access of the observed rate constant (k_{obs}).

$$\frac{i_{cat}}{i_p} = \frac{2}{0.4463}\sqrt{\frac{RT(K_{obs})}{Fv}}\frac{1}{1+exp\left[\frac{F}{RT}(E-E_{\frac{1}{2}})\right]} \quad \text{.....(5)}$$

$$Slope = \frac{2}{0.4463}\sqrt{\frac{RT(K_{obs})}{Fv}} \quad \text{.....(6)}$$

Table S7 TOF Calculations

Complex	Proton Source	Slope	$K_{obs}(s^{-1})$	C_H^0 (M)	$K_{cat}=(K_{obs}/C_H^0)$ $(M^{-1}s^{-1})$	TOF (s^{-1})
1	Acetic Acid	2.48	6.03	0.024	251.25	251.25
2		1.81	3.21		133.75	133.75
3		1.51	2.23		92.92	92.92
1	Trifluoroacetic acid	3.23	10.24		426.67	426.67
2		2.15	4.53		188.75	188.75
3		1.76	3.04		126.67	126.67

Table S8 Bond length comparison of complex **1**, **2** and **3** as obtained from X-ray analysis with DFT calculation.

Bond	X-ray	DFT
Complex 1		
Ni01-O002	1.83	1.85
Ni01-N004	1.91	1.92
Ni01-O002	1.83	1.85
Ni01-N004	1.91	1.92
Complex 2		
Ni01-O003	1.82	1.85
Ni01-N1	1.92	1.92
Ni01-O003	1.82	1.85
Ni01-N1	1.92	1.92
Complex 3		
Ni01-O005	1.83	1.85
Ni01-N004	1.92	1.92
Ni01-O005	1.83	1.85
Ni01-N004	1.92	1.92

Table S9 Geometry optimized coordinates of complex **1**.

total energy = -3079.28092039001 Hartree

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Ni	-0.1812007	2.4970776	11.9076476
O	-0.1749657	0.9775928	12.9577034
O	4.9815981	5.0736901	8.1282899
H	5.3534333	4.7096971	7.3081285
N	1.3862858	3.1624347	12.8003888
C	2.8962795	3.5539209	10.8696046
H	2.1166079	3.1085832	10.2297787
H	3.5699795	2.7322229	11.1736389
C	1.7708520	2.7666758	13.9777065
H	2.6618940	3.2574726	14.3851504
C	1.6080544	1.5219652	16.1463630
C	3.6722377	4.6039554	10.0729258
H	3.0031725	5.4421519	9.8058481
H	4.4872369	5.0296167	10.6869702
C	1.1862177	1.7310688	14.7760899
C	0.2658074	0.8411647	14.1686448
C	1.1175796	0.3811674	16.8592170
C	2.2330970	4.1455430	12.1162939

H	3.0068039	4.5068858	12.8153854
H	1.6059371	4.9975978	11.8244853
C	-0.1890558	-0.3028732	14.9110897
H	-0.8773667	-0.9872557	14.4110496
C	0.2198540	-0.5160514	16.1981676
H	-0.1460374	-1.3866080	16.7500841
C	2.4820072	2.4009654	16.8416029
H	2.8605607	3.3003030	16.3544382
C	1.5170697	0.1531166	18.2000571
H	1.1263285	-0.7269400	18.7186467
C	2.3802028	1.0214512	18.8444480
H	2.6835455	0.8384065	19.8782439
C	4.2702256	4.0400804	8.7925157
H	4.9408838	3.1905143	9.0354396
H	3.4581771	3.6416538	8.1498632
C	2.8602986	2.1551103	18.1522634
H	3.5338067	2.8537574	18.6560815
O	-0.1902210	4.0173296	10.8582303
O	-5.3498185	-0.0624068	15.6858335
H	-5.7295643	0.3065195	16.5001442
N	-1.7470957	1.8303848	11.0124663

C	-3.2623440	1.4476508	12.9406905
H	-2.4834184	1.8960306	13.5793451
H	-3.9362473	2.2676655	12.6325104
C	-2.1252851	2.2212012	9.8315378
H	-3.0146340	1.7295000	9.4213646
C	-1.9467572	3.4554095	7.6579756
C	-4.0381218	0.4004094	13.7412013
H	-3.3669425	-0.4331880	14.0173465
H	-4.8485455	-0.0328837	13.1264388
C	-1.5356560	3.2535785	9.0324509
C	-0.6221092	4.1481814	9.6433647
C	-1.4536135	4.5944195	6.9441067
C	-2.5976425	0.8510724	11.6971957
H	-3.3704544	0.4893968	10.9972873
H	-1.9730149	-0.0014961	11.9929661
C	-0.1650794	5.2907115	8.8999796
H	0.5171228	5.9792740	9.4026163
C	-0.5642246	5.4972546	7.6087075
H	-0.1965393	6.3666641	7.0561885
C	-2.8122209	2.5705601	6.9595506
H	-3.1920352	1.6723211	7.4478086

C	-1.8424729	4.8151075	5.5989074
H	-1.4500762	5.6939796	5.0795634
C	-2.6974489	3.9411291	4.9512764
H	-2.9924236	4.1183655	3.9140518
C	-4.6442884	0.9708672	15.0148371
H	-5.3205699	1.8131750	14.7625247
H	-3.8372640	1.3809656	15.6565002
C	-3.1800080	2.8091665	5.6445784
H	-3.8469351	2.1060688	5.1382044

Table S10 geometry optimized coordinates of complex **1-** hydride.

total energy = -3079.81651912751 Hartree

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Ni	0.1281212	1.6906863	11.0899346
O	0.2440406	0.0328020	12.1607019
O	5.8170364	5.2031510	8.5006166
N	1.5683283	2.4645438	12.0848730
C	3.4882352	3.2393094	10.7134221
C	1.9655396	2.0493760	13.2543230
C	2.0507501	0.6589466	15.3226817
C	4.0977977	4.4291359	9.9713255
C	1.5612350	0.8799794	13.9719368
C	0.7597647	-0.1130363	13.3319337
C	1.7720478	-0.5859449	15.9718513
C	2.2485265	3.6373375	11.5200452
C	0.5203910	-1.3556628	14.0210545
C	1.0043294	-1.5760101	15.2785635
C	2.7937106	1.6212486	16.0585970
C	2.2459079	-0.8299883	17.2846173
C	2.9801440	0.1235811	17.9675820
C	5.3181879	4.0425484	9.1487250

C	3.2492148	1.3595315	17.3417823
O	0.8415700	2.3300392	9.3496838
O	-4.9848889	-0.2535563	15.2038851
N	-1.5032624	1.1240193	10.2525524
C	-2.9084583	0.9695007	12.3115914
C	-1.8968535	1.4963518	9.0673885
C	-1.8712761	2.6585825	6.8624121
C	-3.7449613	0.0282364	13.1797019
C	-1.1954627	2.2738515	8.0915468
C	0.1831504	2.5980603	8.2787576
C	-1.1255646	3.3088535	5.8272381
C	-2.3964084	0.2759037	11.0472787
C	0.8919293	3.2439995	7.2011647
C	0.2655625	3.5786326	6.0356391
C	-3.2543713	2.4374263	6.6195569
C	-1.7577318	3.6850396	4.6164803
C	-3.1034761	3.4400797	4.4068542
C	-4.2329788	0.6925857	14.4587544
C	-3.8516207	2.8126695	5.4256481
H	6.5930643	4.9492850	7.9744671
H	3.1928475	2.4634264	9.9909168

H	4.2353681	2.7931192	11.3956903
H	2.7410309	2.6643856	13.7266601
H	3.3442871	4.8722175	9.2938258
H	4.3892233	5.2220916	10.6844252
H	2.5319506	4.3234877	12.3374010
H	1.5400667	4.1588510	10.8644992
H	-0.0744644	-2.1068913	13.4969909
H	0.8010926	-2.5236242	15.7859642
H	3.0083119	2.5998611	15.6288283
H	2.0168682	-1.7921583	17.7514556
H	3.3413242	-0.0724423	18.9801605
H	6.0887262	3.5963370	9.8106199
H	5.0354844	3.2657795	8.4087947
H	3.8176102	2.1265317	17.8748082
H	-5.2972929	0.1768061	16.0167078
H	-2.0473237	1.3364313	12.8947305
H	-3.5022991	1.8562137	12.0240940
H	-2.8847046	1.1273324	8.7707724
H	-3.1453206	-0.8596389	13.4533277
H	-4.6216018	-0.3405496	12.6159248
H	-3.2490754	-0.0353731	10.4192391

H	-1.8339281	-0.6236469	11.3358871
H	1.9503502	3.4592591	7.3646476
H	0.8239502	4.0730603	5.2353004
H	-3.8833917	1.9767863	7.3817540
H	-1.1575329	4.1780878	3.8466010
H	-3.5838043	3.7339390	3.4703189
H	-4.8496785	1.5796232	14.2069540
H	-3.3626742	1.0558954	15.0435131
H	-4.9187155	2.6244164	5.2791068
H	-0.6475886	2.8274268	11.5657552

Table S11 geometry optimized coordinates of complex **2**.

total energy = -3157.79871580081 Hartree

75

Ni	0.8165806	8.8677585	8.4053141
O	-0.6261819	8.0654392	7.5644028
O	3.9575507	14.4013472	9.6922124
H	3.3750181	13.9255175	10.3085343
N	1.5671993	9.3522104	6.7024184
C	0.3201433	7.7043135	5.3950781
C	-0.6478166	7.4833127	6.4059200
C	1.7846953	11.7956486	7.0589440
H	1.1844043	11.5898029	7.9603744
H	1.0735334	12.1067945	6.2722161
C	1.2882772	8.7443893	5.5892295
H	1.8196674	9.0965738	4.6974360
C	0.2461423	6.9854099	4.1402257
C	2.7761308	12.9175212	7.3761056
H	3.5618690	12.5179079	8.0382189
H	3.2876099	13.2547828	6.4550861
C	2.4817093	10.4963172	6.6410980
H	2.8882770	10.5861352	5.6193489

H	3.3145678	10.3017683	7.3290134
C	-1.7474844	6.5979168	6.1284864
H	-2.5072563	6.4785002	6.9019343
C	2.1284634	14.1152904	8.0788642
H	1.4983226	14.6911025	7.3765771
H	1.4467828	13.7483516	8.8719810
C	-0.8485170	6.0915531	3.9124734
C	3.1422220	15.0571279	8.7260253
H	3.8371380	15.4582609	7.9684167
H	2.6133216	15.9190709	9.1800116
C	-1.8376929	5.9361099	4.9341684
H	-2.6830964	5.2686048	4.7423357
C	1.2168509	7.1073761	3.1098289
H	2.0861108	7.7515533	3.2473274
C	-0.9449589	5.3799535	2.6903117
H	-1.7930957	4.7052226	2.5434014
C	0.0104379	5.5309170	1.7013697
H	-0.0704048	4.9789791	0.7617002
C	1.0995546	6.4029450	1.9220645
H	1.8656946	6.5208251	1.1509653
O	2.2607900	9.6669095	9.2471505

O	-2.3276432	3.3428523	7.1219887
H	-1.7426285	3.8178951	6.5074202
N	0.0640011	8.3870712	10.1086916
C	1.3077396	10.0410965	11.4111980
C	2.2800765	10.2544759	10.4029253
C	-0.1548395	5.9426890	9.7581463
H	0.4462980	6.1463486	8.8567940
H	0.5552735	5.6322673	10.5460798
C	0.3393333	9.0007531	11.2195345
H	-0.1946347	8.6532594	12.1116694
C	1.3778529	10.7672424	12.6619822
C	-1.1474097	4.8214778	9.4419986
H	-1.9328799	5.2215780	8.7798522
H	-1.6591304	4.4853220	10.3632832
C	-0.8509947	7.2435423	10.1726485
H	-1.2580540	7.1566614	11.1944571
H	-1.6834743	7.4366736	9.4838912
C	3.3817890	11.1371767	10.6808092
H	4.1454285	11.2497204	9.9101188
C	-0.5013817	3.6225375	8.7396374
H	0.1258411	3.0444705	9.4426756

H	0.1828773	3.9882668	7.9481663
C	2.4743138	11.6588562	12.8898105
C	-1.5163759	2.6840408	8.0895102
H	-2.2142694	2.2844317	8.8451913
H	-0.9889853	1.8208115	7.6362101
C	3.4689421	11.8049573	11.8720339
H	4.3160820	12.4701208	12.0643556
C	0.4014309	10.6547406	13.6880337
H	-0.4692802	10.0126243	13.5498467
C	2.5668976	12.3775367	14.1081267
H	3.4165692	13.0502694	14.2553867
C	1.6058299	12.2358830	15.0929524
H	1.6836183	12.7933825	16.0295929
C	0.5148490	11.3662464	14.8719419
H	-0.2557749	11.2558903	15.6396778

Table S12 geometry optimized coordinates of complex **2**-hydride.

total energy = -3158.33873725985 Hartree

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Ni	0.7532230	8.8267596	8.0910436
O	0.6791842	6.9723589	7.3820444
O	3.5963649	14.0832388	10.5173322
N	1.4701748	9.4805888	6.4491180
C	0.7387869	7.6103998	5.0571563
C	0.4596802	6.7130405	6.1371227
C	1.4362199	11.7148261	7.4992525
C	1.3537114	8.8856830	5.3042231
C	0.4699259	7.2048117	3.6883084
C	2.3107578	12.8094928	8.1126667
C	2.1992452	10.7399048	6.5930959
C	-0.0761303	5.4111211	5.8232242
C	1.5723421	13.6026693	9.1951707
C	-0.0507582	5.8960036	3.4304035
C	2.4404384	14.6407033	9.9040768
C	-0.3139525	5.0257230	4.5352174
C	0.6819511	8.0478880	2.5625790
C	-0.3141305	5.4774658	2.1024419

C	-0.0782104	6.3173138	1.0285755
C	0.4225210	7.6146328	1.2714936
O	2.5169192	8.9357453	8.9933134
O	-1.8627914	2.8388474	7.7155685
N	-0.1050914	8.6042589	9.7924357
C	1.5661338	9.9664550	10.9454555
C	2.6442809	9.6440927	10.0650688
C	-0.7172046	6.2388836	10.1341287
C	0.3292120	9.2414734	10.8370112
C	1.7721531	10.8874388	12.0403784
C	-1.7222363	5.1753916	9.6907778
C	-1.2264016	7.6737907	9.9214639
C	3.9608607	10.1236931	10.4033302
C	-1.2066157	3.7484214	9.9065665
C	3.0869320	11.3901029	12.3000295
C	-1.9902228	2.6930798	9.1282919
C	4.1680522	10.9558915	11.4661257
C	0.7146663	11.3593357	12.8625032
C	3.2995269	12.3108233	13.3580241
C	2.2479540	12.7450677	14.1469745
C	0.9469066	12.2609561	13.8899226

H	3.3133477	13.3981867	11.1467431
H	0.9854255	11.1442114	8.3352521
H	0.5849977	12.1509883	6.9481184
H	1.7933811	9.4094989	4.4464955
H	3.2060301	12.3494724	8.5644758
H	2.6719444	13.4957839	7.3237616
H	2.3932555	11.1799642	5.5996761
H	3.1718150	10.5061919	7.0575725
H	-0.3037184	4.7512827	6.6622307
H	0.6954028	14.1183839	8.7620200
H	1.1749156	12.8980875	9.9511310
H	2.8138460	15.3837084	9.1785787
H	1.8274747	15.1882700	10.6482610
H	-0.7280429	4.0342019	4.3291163
H	1.0451265	9.0672277	2.6958295
H	-0.7120417	4.4712902	1.9427948
H	-0.2830761	5.9870561	0.0072758
H	0.6025050	8.2936367	0.4335085
H	-0.9450574	2.6319834	7.4722034
H	0.1991024	6.1133859	9.5385404
H	-0.4432129	6.1027951	11.1967958

H	-0.2842889	9.1632588	11.7459248
H	-1.9315576	5.3211595	8.6162346
H	-2.6858145	5.3035271	10.2200966
H	-1.8768772	7.9871870	10.7573649
H	-1.8123113	7.7235252	8.9926700
H	4.7818135	9.8154494	9.7525964
H	-1.2297513	3.4920554	10.9818589
H	-0.1446465	3.6852316	9.5977969
H	-3.0687716	2.7843768	9.3427920
H	-1.6749177	1.6791544	9.4421959
H	5.1738689	11.3272826	11.6813081
H	-0.3099506	11.0356351	12.6731239
H	4.3136831	12.6789218	13.5364808
H	2.4200755	13.4589244	14.9559115
H	0.1082855	12.6085043	14.4990758
H	-0.5539050	9.1265765	7.5207964

Table S13 geometry optimized coordinates of complex **3**.

total energy = -3236.30986835935 Hartree

81

Ni	2.9592812	9.3157424	8.5153814
O	1.3247962	9.1326881	7.6754186
N	2.7242049	11.2208208	8.6360988
O	3.9847335	10.8407220	16.2812925
H	3.6563115	10.6394550	17.1730610
C	1.9030749	11.8978500	7.8891336
H	1.8960805	12.9834137	8.0408531
C	-1.0287187	10.3171287	5.2375378
H	-1.8093566	9.9131540	4.5866762
C	-0.7597998	11.7216992	5.1862438
C	3.4347912	11.9236195	13.5725719
H	2.3837252	12.2392407	13.7196528
H	3.4513815	10.8275594	13.7058054
C	4.3095063	12.5697393	14.6508154
H	5.3596929	12.2468728	14.5197787
H	4.2991459	13.6691036	14.5339574
C	3.8748581	12.2424927	16.0724021
H	4.5108575	12.7971612	16.7918213

H	2.8298049	12.5813921	16.2286792
C	0.5038797	13.6621197	5.9469678
H	1.2842356	14.1223671	6.5536901
C	3.0114155	11.6105437	11.0722512
H	1.9542007	11.9096270	11.1969481
H	3.0492374	10.5152278	11.1958646
C	0.9803186	11.3785599	6.9242887
C	3.4685404	11.9687424	9.6553762
H	3.3317216	13.0500969	9.4822637
H	4.5345288	11.7336726	9.5457797
C	0.7077924	9.9879608	6.9222526
C	3.8750722	12.2727634	12.1482682
H	3.8557125	13.3715267	12.0162089
H	4.9282485	11.9643527	12.0071465
C	0.2562242	12.2654560	6.0361109
C	-0.3328342	9.4835271	6.0681137
H	-0.5383501	8.4119887	6.1034449
C	-1.4829299	12.5682457	4.3087999
H	-2.2528687	12.1240886	3.6715635
C	-0.2195838	14.4701041	5.0838148
H	-0.0019511	15.5408510	5.0427585

C	-1.2251597	13.9264048	4.2543012
H	-1.7875628	14.5720699	3.5752865
O	4.5952881	9.4968729	9.3536084
N	3.1936623	7.4101027	8.3966962
O	1.9643932	7.8021848	0.7477133
H	2.2917286	8.0048260	-0.1441435
C	4.0077409	6.7333827	9.1513965
H	4.0145398	5.6474052	9.0023253
C	6.9283296	8.3162785	11.8134676
H	7.7071386	8.7204933	12.4663666
C	6.6515677	6.9135758	11.8725175
C	2.5049619	6.7141959	3.4560959
H	3.5565087	6.3984743	3.3127519
H	2.4892834	7.8104473	3.3242568
C	1.6343466	6.0698011	2.3734924
H	0.5835761	6.3920099	2.5014344
H	1.6447021	4.9702262	2.4883314
C	2.0737850	6.3999640	0.9540455
H	1.4402241	5.8467364	0.2314159
H	3.1194258	6.0615234	0.8005499
C	5.3818978	4.9749909	11.1166597

H	4.6024503	4.5153332	10.5082861
C	2.9180311	7.0237275	5.9586936
H	3.9759164	6.7256567	5.8373972
H	2.8797802	8.1192907	5.8372924
C	4.9244832	7.2543113	10.1212711
C	2.4555914	6.6622298	7.3729896
H	2.5937717	5.5808702	7.5450444
H	1.3886044	6.8949924	7.4781434
C	5.2036429	8.6435926	10.1162528
C	2.0588140	6.3631776	4.8781098
H	2.0774855	5.2642166	5.0086571
H	1.0051004	6.6715566	5.0154659
C	5.6380296	6.3696205	11.0198360
C	6.2419920	9.1480506	10.9730785
H	6.4536428	10.2181570	10.9318987
C	7.3644715	6.0688935	12.7600908
H	8.1327611	6.5130108	13.3993461
C	6.0954950	4.1688056	11.9896368
H	5.8716357	3.0995843	12.0365638
C	7.0989289	4.7125351	12.8217759
H	7.6534789	4.0683230	13.5085891

Table S14 geometry optimized coordinates of complex **3**-hydride.

total energy = -3236.84578928266 Hartree

82

Ni	3.0622614	9.7162009	8.3876950
O	2.3679192	9.8195747	6.5258323
N	2.7673679	11.5954709	8.6359946
O	3.8168998	10.2368398	16.2183368
C	1.9910885	12.3258060	7.8873266
C	0.1584712	11.3631719	4.1563785
C	-0.1884138	12.5969422	4.7955918
C	3.1816825	11.6276878	13.6692865
C	3.9199207	12.2190897	14.8738101
C	3.4961166	11.6219484	16.2081003
C	-0.0120744	14.1269594	6.6791138
C	2.8951891	11.6315921	11.1301208
C	1.3079112	11.9620572	6.6827555
C	3.3943116	12.2150291	9.8062342
C	1.5946970	10.7214263	6.0347284
C	3.6378207	12.2185410	12.3327095
C	0.3825069	12.9031928	6.0727640
C	1.0058469	10.4678070	4.7423108
C	-1.0890337	13.4994061	4.1777881

C	-0.8934093	14.9962308	6.0543007
C	-1.4404174	14.6896330	4.7900362
O	4.8572508	9.8076507	9.2047799
N	3.1312135	7.8054394	8.3758186
O	2.2790060	5.9751695	0.8775138
C	3.9408306	7.0908431	9.1043060
C	7.3400660	8.3504171	11.3496517
C	6.9065608	6.9907768	11.4657031
C	2.2906214	5.7692607	3.8404887
C	1.2409782	5.1860958	2.8900657
C	1.7922707	4.8059991	1.5234508
C	5.3323456	5.2173170	10.9177523
C	2.7691190	6.7307708	6.1602015
C	5.0259075	7.5303125	9.9273789
C	2.1740347	7.0836574	7.5264932
C	5.4645121	8.8874307	9.8723027
C	1.7217080	6.1444504	5.2113323
C	5.7367331	6.5701309	10.7555252
C	6.6575995	9.2569506	10.5901579
C	7.6205383	6.0734109	12.2759612
C	6.0485316	4.3366064	11.7139353

C	7.2061209	4.7592483	12.4018943
H	3.4927790	9.8549898	17.0504889
H	1.8815653	13.3674472	8.2101372
H	-0.2815648	11.1427467	3.1792879
H	2.0940768	11.7938148	13.7931421
H	3.3294183	10.5331767	13.6583774
H	5.0095420	12.0691272	14.7524101
H	3.7535552	13.3112691	14.9169512
H	4.0156910	12.1503630	17.0330523
H	2.4067947	11.7739726	16.3548233
H	0.3630001	14.4017008	7.6651573
H	1.8095084	11.8174406	11.2236931
H	3.0315373	10.5365363	11.1183690
H	3.2050904	13.3023714	9.7807864
H	4.4789694	12.0520867	9.7296025
H	3.5048336	13.3172469	12.3515065
H	4.7229988	12.0408734	12.2078489
H	1.2624433	9.5220629	4.2592609
H	-1.5054058	13.2336374	3.2019749
H	-1.1712893	15.9276665	6.5552435
H	-2.1364942	15.3801130	4.3074671

H	2.6738894	5.7124429	0.0299080
H	3.7831206	6.0070205	9.0467920
H	8.2367023	8.6576546	11.8958521
H	3.1089005	5.0352064	3.9715932
H	2.7448114	6.6601676	3.3717334
H	0.4214974	5.9157900	2.7482610
H	0.7876032	4.2838162	3.3402683
H	0.9931981	4.3288588	0.9205028
H	2.6032686	4.0583924	1.6451113
H	4.4337134	4.8463401	10.4247839
H	3.5974127	6.0114656	6.3005504
H	3.1952905	7.6459271	5.7206348
H	1.8485448	6.1647515	8.0459273
H	1.2951869	7.7251758	7.3855678
H	1.2584515	5.2514480	5.6733957
H	0.9058014	6.8803742	5.0780868
H	6.9824847	10.2965212	10.5099729
H	8.5101546	6.4273277	12.8045136
H	5.7044321	3.3034739	11.8125004
H	7.7616454	4.0581465	13.0295713
H	1.8295050	9.5477962	9.1443270

Table S15 Summary of Natural Population Analysis for complex **1**.

Natural Population

	Natural				
Atom No	Charge	Core	Valence	Rydberg	Total
1 ni	0.96584	17.99557	9.00160	0.03699	27.03416
2 o	-0.73757	1.99971	6.72504	0.01282	8.73757
3 o	-0.77419	1.99978	6.76384	0.01057	8.77419
4 h	0.46969	0.00000	0.52874	0.00157	0.53031
5 n	-0.55602	1.99920	5.53384	0.02297	7.55602
6 c	-0.42321	1.99912	4.40941	0.01468	6.42321
7 h	0.21476	0.00000	0.78132	0.00393	0.78524
8 h	0.21218	0.00000	0.78463	0.00319	0.78782
9 c	0.17229	1.99906	3.80414	0.02451	5.82771
10 h	0.20359	0.00000	0.79414	0.00227	0.79641
11 c	-0.02615	1.99888	4.01154	0.01573	6.02615
12 c	-0.43647	1.99914	4.42270	0.01463	6.43647
13 h	0.20740	0.00000	0.78829	0.00431	0.79260
14 h	0.21062	0.00000	0.78526	0.00412	0.78938
15 c	-0.21652	1.99882	4.20069	0.01701	6.21652
16 c	0.43659	1.99877	3.53154	0.03311	5.56341

17	c	-0.09750	1.99884	4.08294	0.01571	6.09750
18	c	-0.19353	1.99911	4.17537	0.01906	6.19353
19	h	0.20440	0.00000	0.79308	0.00252	0.79560
20	h	0.22958	0.00000	0.76666	0.00376	0.77042
21	c	-0.26538	1.99890	4.24854	0.01794	6.26538
22	h	0.23160	0.00000	0.76606	0.00234	0.76840
23	c	-0.15819	1.99893	4.14273	0.01653	6.15819
24	h	0.23213	0.00000	0.76590	0.00197	0.76787
25	c	-0.22303	1.99894	4.20850	0.01559	6.22303
26	h	0.22399	0.00000	0.77396	0.00205	0.77601
27	c	-0.18760	1.99893	4.17194	0.01673	6.18760
28	h	0.22761	0.00000	0.77048	0.00191	0.77239
29	c	-0.24139	1.99894	4.22584	0.01662	6.24139
30	h	0.22910	0.00000	0.76923	0.00167	0.77090
31	c	-0.01634	1.99914	3.99987	0.01733	6.01634
32	h	0.17156	0.00000	0.82568	0.00276	0.82844
33	h	0.17131	0.00000	0.82585	0.00284	0.82869
34	c	-0.20715	1.99895	4.19169	0.01651	6.20715
35	h	0.22884	0.00000	0.76945	0.00171	0.77116
36	o	-0.73757	1.99971	6.72507	0.01280	8.73757
37	o	-0.77422	1.99978	6.76388	0.01057	8.77422

38	h	0.46972	0.00000	0.52872	0.00157	0.53028
39	n	-0.55578	1.99920	5.53361	0.02297	7.55578
40	c	-0.42319	1.99912	4.40940	0.01467	6.42319
41	h	0.21480	0.00000	0.78126	0.00393	0.78520
42	h	0.21213	0.00000	0.78467	0.00320	0.78787
43	c	0.17240	1.99906	3.80404	0.02450	5.82760
44	h	0.20365	0.00000	0.79408	0.00227	0.79635
45	c	-0.02617	1.99888	4.01156	0.01573	6.02617
46	c	-0.43648	1.99914	4.42271	0.01464	6.43648
47	h	0.20741	0.00000	0.78826	0.00432	0.79259
48	h	0.21059	0.00000	0.78529	0.00412	0.78941
49	c	-0.21643	1.99882	4.20060	0.01702	6.21643
50	c	0.43627	1.99877	3.53185	0.03312	5.56373
51	c	-0.09746	1.99884	4.08291	0.01571	6.09746
52	c	-0.19348	1.99911	4.17532	0.01905	6.19348
53	h	0.20442	0.00000	0.79306	0.00252	0.79558
54	h	0.22947	0.00000	0.76676	0.00377	0.77053
55	c	-0.26553	1.99890	4.24867	0.01796	6.26553
56	h	0.23157	0.00000	0.76608	0.00234	0.76843
57	c	-0.15805	1.99893	4.14259	0.01653	6.15805
58	h	0.23213	0.00000	0.76590	0.00197	0.76787

59	c	-0.22305	1.99894	4.20851	0.01559	6.22305
60	h	0.22401	0.00000	0.77394	0.00205	0.77599
61	c	-0.18759	1.99893	4.17194	0.01673	6.18759
62	h	0.22762	0.00000	0.77047	0.00191	0.77238
63	c	-0.24140	1.99894	4.22585	0.01662	6.24140
64	h	0.22910	0.00000	0.76923	0.00167	0.77090
65	c	-0.01634	1.99914	3.99987	0.01732	6.01634
66	h	0.17165	0.00000	0.82559	0.00276	0.82835
67	h	0.17123	0.00000	0.82593	0.00284	0.82877
68	c	-0.20715	1.99895	4.19169	0.01651	6.20715
69	h	0.22884	0.00000	0.76945	0.00171	0.77116
* Total *		-0.00000	89.96186	195.27925	0.75889	286.00000

Table S16 Summary of Natural Population Analysis for complex **1**-hydride.

Natural Population

Atom No		Natural Charge	Core	Valence	Rydberg	Total
1	ni	1.06646	17.99438	8.89038	0.04878	26.93354
2	o	-0.79076	1.99973	6.77573	0.01530	8.79076
3	o	-0.77423	1.99978	6.76388	0.01057	8.77423
4	n	-0.55579	1.99920	5.53234	0.02425	7.55579
5	c	-0.42315	1.99912	4.41023	0.01381	6.42315
6	c	0.17486	1.99905	3.80108	0.02500	5.82514
7	c	-0.02562	1.99888	4.01094	0.01580	6.02562
8	c	-0.43823	1.99914	4.42428	0.01481	6.43823
9	c	-0.21373	1.99882	4.19794	0.01697	6.21373
10	c	0.45208	1.99881	3.51381	0.03530	5.54792
11	c	-0.09680	1.99884	4.08219	0.01577	6.09680
12	c	-0.19477	1.99912	4.17623	0.01943	6.19477
13	c	-0.26835	1.99890	4.25146	0.01799	6.26835
14	c	-0.15674	1.99893	4.14127	0.01654	6.15674
15	c	-0.22222	1.99894	4.20774	0.01554	6.22222
16	c	-0.18785	1.99893	4.17215	0.01677	6.18785

17	c	-0.23999	1.99894	4.22442	0.01664	6.23999
18	c	-0.01631	1.99914	3.99993	0.01724	6.01631
19	c	-0.20652	1.99895	4.19106	0.01651	6.20652
20	o	-0.77833	1.99973	6.76343	0.01517	8.77833
21	o	-0.77422	1.99978	6.76387	0.01057	8.77422
22	n	-0.55150	1.99919	5.52850	0.02380	7.55150
23	c	-0.42467	1.99912	4.41130	0.01426	6.42467
24	c	0.17825	1.99905	3.79795	0.02474	5.82175
25	c	-0.02550	1.99889	4.01085	0.01577	6.02550
26	c	-0.43701	1.99914	4.42318	0.01468	6.43701
27	c	-0.21992	1.99883	4.20408	0.01701	6.21992
28	c	0.45323	1.99882	3.51258	0.03537	5.54677
29	c	-0.09852	1.99884	4.08392	0.01576	6.09852
30	c	-0.19473	1.99911	4.17628	0.01935	6.19473
31	c	-0.26894	1.99890	4.25196	0.01808	6.26894
32	c	-0.15822	1.99893	4.14276	0.01654	6.15822
33	c	-0.22370	1.99894	4.20927	0.01549	6.22370
34	c	-0.18784	1.99893	4.17216	0.01676	6.18784
35	c	-0.24152	1.99894	4.22593	0.01666	6.24152
36	c	-0.01667	1.99915	4.00022	0.01730	6.01667
37	c	-0.20696	1.99895	4.19149	0.01651	6.20696

38	h	0.46969	0.00000	0.52874	0.00157	0.53031
39	h	0.22531	0.00000	0.77027	0.00442	0.77469
40	h	0.20860	0.00000	0.78863	0.00276	0.79140
41	h	0.20323	0.00000	0.79435	0.00242	0.79677
42	h	0.20769	0.00000	0.78778	0.00453	0.79231
43	h	0.20983	0.00000	0.78601	0.00416	0.79017
44	h	0.20882	0.00000	0.78858	0.00260	0.79118
45	h	0.22760	0.00000	0.76956	0.00284	0.77240
46	h	0.23237	0.00000	0.76504	0.00259	0.76763
47	h	0.23178	0.00000	0.76620	0.00202	0.76822
48	h	0.22306	0.00000	0.77482	0.00212	0.77694
49	h	0.22777	0.00000	0.77032	0.00191	0.77223
50	h	0.22924	0.00000	0.76910	0.00166	0.77076
51	h	0.17179	0.00000	0.82547	0.00274	0.82821
52	h	0.17092	0.00000	0.82636	0.00272	0.82908
53	h	0.22894	0.00000	0.76935	0.00171	0.77106
54	h	0.47003	0.00000	0.52841	0.00156	0.52997
55	h	0.21648	0.00000	0.78016	0.00336	0.78352
56	h	0.21358	0.00000	0.78326	0.00317	0.78642
57	h	0.20263	0.00000	0.79503	0.00233	0.79737
58	h	0.20933	0.00000	0.78633	0.00434	0.79067

59	h	0.21082	0.00000	0.78509	0.00410	0.78918
60	h	0.20868	0.00000	0.78879	0.00253	0.79132
61	h	0.23078	0.00000	0.76518	0.00405	0.76922
62	h	0.22832	0.00000	0.76900	0.00267	0.77168
63	h	0.23160	0.00000	0.76639	0.00201	0.76840
64	h	0.22283	0.00000	0.77505	0.00212	0.77717
65	h	0.22751	0.00000	0.77057	0.00192	0.77249
66	h	0.22898	0.00000	0.76936	0.00167	0.77102
67	h	0.17227	0.00000	0.82498	0.00275	0.82773
68	h	0.17112	0.00000	0.82611	0.00277	0.82888
69	h	0.22871	0.00000	0.76958	0.00172	0.77129
70	h	-0.05587	0.00000	1.05330	0.00257	1.05587
* Total *		-0.00000	89.96081	196.25395	0.78524	287.00000

Table S17 Summary of Natural Population Analysis for complex **2**.

Natural Population

	Natural				
Atom No	Charge	Core	Valence	Rydberg	Total
1 ni	0.96856	17.99558	8.99989	0.03596	27.03144
2 o	-0.73833	1.99971	6.72590	0.01272	8.73833
3 o	-0.77415	1.99979	6.76364	0.01073	8.77415
4 h	0.45912	0.00000	0.53889	0.00199	0.54088
5 n	-0.55235	1.99920	5.53011	0.02303	7.55235
6 c	-0.21323	1.99882	4.19739	0.01702	6.21323
7 c	0.43505	1.99876	3.53299	0.03320	5.56495
8 c	-0.41799	1.99912	4.40419	0.01468	6.41799
9 h	0.21096	0.00000	0.78528	0.00376	0.78904
10 h	0.21163	0.00000	0.78531	0.00306	0.78837
11 c	0.17278	1.99906	3.80371	0.02445	5.82722
12 h	0.20504	0.00000	0.79271	0.00225	0.79496
13 c	-0.02550	1.99888	4.01085	0.01577	6.02550
14 c	-0.41996	1.99913	4.40537	0.01546	6.41996
15 h	0.20739	0.00000	0.78753	0.00508	0.79261
16 h	0.21080	0.00000	0.78641	0.00279	0.78920

17	c	-0.19406	1.99911	4.17587	0.01908	6.19406
18	h	0.20533	0.00000	0.79222	0.00245	0.79467
19	h	0.22825	0.00000	0.76817	0.00358	0.77175
20	c	-0.26885	1.99890	4.25108	0.01888	6.26885
21	h	0.23541	0.00000	0.76200	0.00259	0.76459
22	c	-0.44439	1.99914	4.43290	0.01235	6.44439
23	h	0.22127	0.00000	0.77601	0.00272	0.77873
24	h	0.20283	0.00000	0.79377	0.00340	0.79717
25	c	-0.09556	1.99884	4.08084	0.01589	6.09556
26	c	-0.02363	1.99914	4.00544	0.01904	6.02363
27	h	0.18864	0.00000	0.80896	0.00240	0.81136
28	h	0.17868	0.00000	0.81881	0.00251	0.82132
29	c	-0.18009	1.99892	4.16421	0.01696	6.18009
30	h	0.23414	0.00000	0.76364	0.00222	0.76586
31	c	-0.22215	1.99894	4.20754	0.01567	6.22215
32	h	0.22445	0.00000	0.77352	0.00203	0.77555
33	c	-0.18743	1.99893	4.17178	0.01673	6.18743
34	h	0.22830	0.00000	0.76980	0.00191	0.77170
35	c	-0.23959	1.99894	4.22403	0.01662	6.23959
36	h	0.22948	0.00000	0.76885	0.00167	0.77052
37	c	-0.20597	1.99895	4.19053	0.01649	6.20597

38	h	0.22935	0.00000	0.76895	0.00171	0.77065
39	o	-0.73816	1.99971	6.72574	0.01271	8.73816
40	o	-0.77409	1.99979	6.76358	0.01073	8.77409
41	h	0.45914	0.00000	0.53887	0.00200	0.54086
42	n	-0.55233	1.99920	5.53010	0.02303	7.55233
43	c	-0.21316	1.99882	4.19731	0.01703	6.21316
44	c	0.43489	1.99876	3.53313	0.03322	5.56511
45	c	-0.41797	1.99912	4.40418	0.01467	6.41797
46	h	0.21104	0.00000	0.78519	0.00377	0.78896
47	h	0.21160	0.00000	0.78534	0.00306	0.78840
48	c	0.17273	1.99906	3.80377	0.02444	5.82727
49	h	0.20528	0.00000	0.79247	0.00224	0.79472
50	c	-0.02550	1.99888	4.01084	0.01578	6.02550
51	c	-0.41996	1.99913	4.40538	0.01545	6.41996
52	h	0.20731	0.00000	0.78761	0.00508	0.79269
53	h	0.21081	0.00000	0.78640	0.00279	0.78919
54	c	-0.19399	1.99911	4.17580	0.01908	6.19399
55	h	0.20533	0.00000	0.79222	0.00245	0.79467
56	h	0.22811	0.00000	0.76831	0.00358	0.77189
57	c	-0.26860	1.99890	4.25082	0.01889	6.26860
58	h	0.23533	0.00000	0.76210	0.00257	0.76467

59	c	-0.44444	1.99914	4.43295	0.01235	6.44444
60	h	0.22131	0.00000	0.77597	0.00272	0.77869
61	h	0.20286	0.00000	0.79375	0.00340	0.79714
62	c	-0.09554	1.99884	4.08082	0.01589	6.09554
63	c	-0.02364	1.99914	4.00546	0.01904	6.02364
64	h	0.18859	0.00000	0.80901	0.00240	0.81141
65	h	0.17868	0.00000	0.81880	0.00251	0.82132
66	c	-0.18041	1.99892	4.16450	0.01698	6.18041
67	h	0.23414	0.00000	0.76365	0.00221	0.76586
68	c	-0.22214	1.99894	4.20753	0.01568	6.22214
69	h	0.22448	0.00000	0.77349	0.00203	0.77552
70	c	-0.18751	1.99893	4.17185	0.01673	6.18751
71	h	0.22828	0.00000	0.76981	0.00191	0.77172
72	c	-0.23957	1.99894	4.22401	0.01662	6.23957
73	h	0.22949	0.00000	0.76884	0.00166	0.77051
74	c	-0.20596	1.99895	4.19051	0.01649	6.20596
75	h	0.22935	0.00000	0.76894	0.00171	0.77065

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* Total *	0.00000	93.96014	207.23812	0.80174	302.00000

Table S18 Summary of Natural Population Analysis for complex **2**-hydride.

Natural Population

	Natural				
Atom No	Charge	Core	Valence	Rydberg	Total
1 ni	1.08871	17.99447	8.86569	0.05113	26.91129
2 o	-0.75088	1.99973	6.73714	0.01401	8.75088
3 o	-0.77983	1.99978	6.76951	0.01055	8.77983
4 n	-0.54586	1.99917	5.52233	0.02436	7.54586
5 c	-0.22444	1.99883	4.20854	0.01707	6.22444
6 c	0.44421	1.99881	3.52138	0.03560	5.55579
7 c	-0.41160	1.99911	4.39796	0.01453	6.41160
8 c	0.18764	1.99904	3.78899	0.02433	5.81236
9 c	-0.02560	1.99888	4.01098	0.01574	6.02560
10 c	-0.41798	1.99913	4.40267	0.01618	6.41798
11 c	-0.19741	1.99913	4.17893	0.01936	6.19741
12 c	-0.26749	1.99889	4.25035	0.01826	6.26749
13 c	-0.44290	1.99913	4.43128	0.01250	6.44290
14 c	-0.09877	1.99884	4.08416	0.01577	6.09877
15 c	-0.02582	1.99913	4.00733	0.01936	6.02582
16 c	-0.15960	1.99892	4.14414	0.01653	6.15960

17	c	-0.22493	1.99894	4.21048	0.01551	6.22493
18	c	-0.18804	1.99893	4.17237	0.01675	6.18804
19	c	-0.24272	1.99894	4.22712	0.01667	6.24272
20	c	-0.20739	1.99895	4.19191	0.01653	6.20739
21	o	-0.78825	1.99974	6.77422	0.01430	8.78825
22	o	-0.77553	1.99979	6.76490	0.01085	8.77553
23	n	-0.56633	1.99920	5.54186	0.02527	7.56633
24	c	-0.22859	1.99879	4.21241	0.01739	6.22859
25	c	0.43775	1.99880	3.52650	0.03695	5.56225
26	c	-0.42125	1.99911	4.40861	0.01353	6.42125
27	c	0.17538	1.99904	3.80075	0.02483	5.82462
28	c	-0.02605	1.99885	4.01088	0.01631	6.02605
29	c	-0.41913	1.99914	4.40457	0.01542	6.41913
30	c	-0.19034	1.99913	4.17140	0.01981	6.19034
31	c	-0.26544	1.99887	4.24809	0.01848	6.26544
32	c	-0.44289	1.99914	4.43086	0.01289	6.44289
33	c	-0.12582	1.99884	4.11010	0.01688	6.12582
34	c	-0.02372	1.99914	4.00565	0.01893	6.02372
35	c	-0.16569	1.99892	4.14928	0.01749	6.16569
36	c	-0.22119	1.99893	4.20650	0.01576	6.22119
37	c	-0.20606	1.99892	4.18932	0.01781	6.20606

38	c	-0.23576	1.99893	4.21993	0.01690	6.23576
39	c	-0.20182	1.99895	4.18635	0.01651	6.20182
40	h	0.46667	0.00000	0.53103	0.00230	0.53333
41	h	0.18823	0.00000	0.80746	0.00430	0.81177
42	h	0.22268	0.00000	0.77422	0.00310	0.77732
43	h	0.20643	0.00000	0.79135	0.00222	0.79357
44	h	0.21195	0.00000	0.78312	0.00493	0.78805
45	h	0.21330	0.00000	0.78389	0.00281	0.78670
46	h	0.21718	0.00000	0.78050	0.00233	0.78282
47	h	0.22551	0.00000	0.77086	0.00364	0.77449
48	h	0.22388	0.00000	0.77087	0.00525	0.77612
49	h	0.22015	0.00000	0.77703	0.00282	0.77985
50	h	0.20310	0.00000	0.79294	0.00397	0.79690
51	h	0.18920	0.00000	0.80845	0.00235	0.81080
52	h	0.17804	0.00000	0.81940	0.00256	0.82196
53	h	0.22991	0.00000	0.76795	0.00213	0.77009
54	h	0.22274	0.00000	0.77516	0.00210	0.77726
55	h	0.22729	0.00000	0.77079	0.00192	0.77271
56	h	0.22873	0.00000	0.76960	0.00167	0.77127
57	h	0.22844	0.00000	0.76984	0.00172	0.77156
58	h	0.46486	0.00000	0.53338	0.00176	0.53514

59	h	0.22858	0.00000	0.76722	0.00420	0.77142
60	h	0.20776	0.00000	0.78942	0.00282	0.79224
61	h	0.21125	0.00000	0.78635	0.00240	0.78875
62	h	0.20971	0.00000	0.78527	0.00501	0.79029
63	h	0.20702	0.00000	0.79014	0.00284	0.79298
64	h	0.21114	0.00000	0.78635	0.00251	0.78886
65	h	0.21925	0.00000	0.77831	0.00244	0.78075
66	h	0.23587	0.00000	0.76147	0.00266	0.76413
67	h	0.21817	0.00000	0.77904	0.00278	0.78183
68	h	0.20426	0.00000	0.79218	0.00356	0.79574
69	h	0.18801	0.00000	0.80959	0.00241	0.81199
70	h	0.18133	0.00000	0.81638	0.00229	0.81867
71	h	0.23614	0.00000	0.76180	0.00206	0.76386
72	h	0.22762	0.00000	0.77042	0.00195	0.77238
73	h	0.23399	0.00000	0.76405	0.00196	0.76601
74	h	0.23164	0.00000	0.76671	0.00165	0.76836
75	h	0.23098	0.00000	0.76731	0.00170	0.76902
76	h	-0.06955	0.00000	1.06840	0.00115	1.06955
* Total *		0.00000	93.95900	208.20372	0.83728	303.00000

Table S19 Summary of Natural Population Analysis for complex **3**.

Natural Population

	Natural				
Atom No	Charge	Core	Valence	Rydberg	Total
1 ni	0.96653	17.99557	9.00081	0.03709	27.03347
2 o	-0.73758	1.99971	6.72507	0.01280	8.73758
3 n	-0.55498	1.99921	5.53276	0.02301	7.55498
4 o	-0.77697	1.99978	6.76646	0.01074	8.77697
5 h	0.46897	0.00000	0.52956	0.00146	0.53103
6 c	0.17126	1.99906	3.80511	0.02457	5.82874
7 h	0.20288	0.00000	0.79484	0.00228	0.79712
8 c	-0.15889	1.99893	4.14342	0.01654	6.15889
9 h	0.23183	0.00000	0.76620	0.00198	0.76817
10 c	-0.09765	1.99884	4.08308	0.01572	6.09765
11 c	-0.41313	1.99915	4.39852	0.01545	6.41313
12 h	0.20349	0.00000	0.79346	0.00305	0.79651
13 h	0.21013	0.00000	0.78568	0.00419	0.78987
14 c	-0.43448	1.99915	4.42154	0.01380	6.43448
15 h	0.20618	0.00000	0.78975	0.00407	0.79382
16 h	0.21557	0.00000	0.78205	0.00238	0.78443

17	c	-0.02107	1.99915	4.00414	0.01777	6.02107
18	h	0.17641	0.00000	0.82111	0.00248	0.82359
19	h	0.17047	0.00000	0.82660	0.00292	0.82953
20	c	-0.22250	1.99894	4.20795	0.01561	6.22250
21	h	0.22356	0.00000	0.77437	0.00207	0.77644
22	c	-0.41718	1.99912	4.40331	0.01474	6.41718
23	h	0.20912	0.00000	0.78781	0.00307	0.79088
24	h	0.21290	0.00000	0.78338	0.00373	0.78710
25	c	-0.21662	1.99882	4.20077	0.01704	6.21662
26	c	-0.19465	1.99911	4.17655	0.01899	6.19465
27	h	0.20318	0.00000	0.79429	0.00253	0.79682
28	h	0.22935	0.00000	0.76685	0.00380	0.77065
29	c	0.43597	1.99877	3.53212	0.03314	5.56403
30	c	-0.40866	1.99914	4.39580	0.01371	6.40866
31	h	0.20590	0.00000	0.79114	0.00296	0.79410
32	h	0.20454	0.00000	0.79230	0.00315	0.79546
33	c	-0.02626	1.99888	4.01166	0.01572	6.02626
34	c	-0.26469	1.99890	4.24792	0.01788	6.26469
35	h	0.23168	0.00000	0.76600	0.00232	0.76832
36	c	-0.18763	1.99893	4.17194	0.01676	6.18763
37	h	0.22746	0.00000	0.77063	0.00191	0.77254

38	c	-0.20739	1.99895	4.19196	0.01648	6.20739
39	h	0.22874	0.00000	0.76955	0.00171	0.77126
40	c	-0.24169	1.99894	4.22615	0.01660	6.24169
41	h	0.22903	0.00000	0.76930	0.00167	0.77097
42	o	-0.73761	1.99971	6.72513	0.01277	8.73761
43	n	-0.55468	1.99921	5.53247	0.02301	7.55468
44	o	-0.77711	1.99978	6.76660	0.01073	8.77711
45	h	0.46904	0.00000	0.52950	0.00146	0.53096
46	c	0.17140	1.99906	3.80499	0.02455	5.82860
47	h	0.20298	0.00000	0.79474	0.00228	0.79702
48	c	-0.15872	1.99893	4.14324	0.01654	6.15872
49	h	0.23180	0.00000	0.76623	0.00198	0.76820
50	c	-0.09764	1.99884	4.08308	0.01572	6.09764
51	c	-0.41313	1.99915	4.39853	0.01545	6.41313
52	h	0.20354	0.00000	0.79341	0.00305	0.79646
53	h	0.21006	0.00000	0.78575	0.00419	0.78994
54	c	-0.43449	1.99915	4.42155	0.01379	6.43449
55	h	0.20618	0.00000	0.78975	0.00407	0.79382
56	h	0.21561	0.00000	0.78201	0.00238	0.78439
57	c	-0.02108	1.99915	4.00417	0.01777	6.02108
58	h	0.17650	0.00000	0.82102	0.00248	0.82350

59	h	0.17046	0.00000	0.82662	0.00293	0.82954
60	c	-0.22256	1.99894	4.20801	0.01561	6.22256
61	h	0.22362	0.00000	0.77431	0.00206	0.77638
62	c	-0.41715	1.99912	4.40328	0.01474	6.41715
63	h	0.20910	0.00000	0.78782	0.00308	0.79090
64	h	0.21293	0.00000	0.78333	0.00374	0.78707
65	c	-0.21654	1.99882	4.20068	0.01704	6.21654
66	c	-0.19463	1.99911	4.17654	0.01898	6.19463
67	h	0.20323	0.00000	0.79424	0.00253	0.79677
68	h	0.22922	0.00000	0.76697	0.00381	0.77078
69	c	0.43568	1.99877	3.53240	0.03315	5.56432
70	c	-0.40866	1.99914	4.39581	0.01372	6.40866
71	h	0.20589	0.00000	0.79115	0.00296	0.79411
72	h	0.20455	0.00000	0.79230	0.00316	0.79545
73	c	-0.02631	1.99888	4.01170	0.01572	6.02631
74	c	-0.26473	1.99890	4.24794	0.01789	6.26473
75	h	0.23161	0.00000	0.76607	0.00232	0.76839
76	c	-0.18762	1.99893	4.17193	0.01676	6.18762
77	h	0.22746	0.00000	0.77063	0.00191	0.77254
78	c	-0.20739	1.99895	4.19195	0.01649	6.20739
79	h	0.22875	0.00000	0.76954	0.00171	0.77125

80	c	-0.24172	1.99894	4.22618	0.01661	6.24172
81	h	0.22903	0.00000	0.76930	0.00167	0.77097
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	* Total *	0.00000	97.95850	219.20283	0.83868	318.00000

Table S20 Summary of Natural Population Analysis for complex **3**-hydride.

Natural Population

Atom No		Natural Charge	Core	Valence	Rydberg	Total
1	ni	1.06583	17.99441	8.89065	0.04911	26.93417
2	o	-0.77567	1.99973	6.76089	0.01505	8.77567
3	n	-0.54932	1.99919	5.52623	0.02390	7.54932
4	o	-0.77783	1.99978	6.76734	0.01072	8.77783
5	c	0.17777	1.99905	3.79840	0.02478	5.82223
6	c	-0.15882	1.99892	4.14335	0.01655	6.15882
7	c	-0.09879	1.99884	4.08418	0.01577	6.09879
8	c	-0.41324	1.99915	4.39870	0.01539	6.41324
9	c	-0.43504	1.99915	4.42204	0.01386	6.43504
10	c	-0.02143	1.99915	4.00453	0.01775	6.02143
11	c	-0.22392	1.99894	4.20948	0.01550	6.22392
12	c	-0.41876	1.99912	4.40528	0.01436	6.41876
13	c	-0.22085	1.99883	4.20495	0.01707	6.22085
14	c	-0.19547	1.99911	4.17700	0.01937	6.19547
15	c	0.45223	1.99882	3.51347	0.03548	5.54777
16	c	-0.40895	1.99915	4.39593	0.01387	6.40895

17	c	-0.02567	1.99889	4.01100	0.01579	6.02567
18	c	-0.26945	1.99890	4.25242	0.01813	6.26945
19	c	-0.18805	1.99893	4.17239	0.01674	6.18805
20	c	-0.20735	1.99895	4.19185	0.01654	6.20735
21	c	-0.24201	1.99894	4.22639	0.01668	6.24201
22	o	-0.79300	1.99973	6.77784	0.01543	8.79300
23	n	-0.55487	1.99921	5.53128	0.02439	7.55487
24	o	-0.77715	1.99978	6.76665	0.01072	8.77715
25	c	0.17440	1.99905	3.80160	0.02495	5.82560
26	c	-0.15689	1.99893	4.14144	0.01652	6.15689
27	c	-0.09679	1.99884	4.08223	0.01572	6.09679
28	c	-0.41272	1.99915	4.39818	0.01538	6.41272
29	c	-0.43436	1.99915	4.42137	0.01385	6.43436
30	c	-0.02114	1.99915	4.00422	0.01777	6.02114
31	c	-0.22202	1.99894	4.20759	0.01549	6.22202
32	c	-0.41764	1.99912	4.40469	0.01383	6.41764
33	c	-0.21338	1.99883	4.19765	0.01691	6.21338
34	c	-0.19562	1.99912	4.17705	0.01946	6.19562
35	c	0.45129	1.99881	3.51465	0.03525	5.54871
36	c	-0.41027	1.99915	4.39722	0.01390	6.41027
37	c	-0.02588	1.99888	4.01125	0.01575	6.02588

38	c	-0.26730	1.99890	4.25042	0.01798	6.26730
39	c	-0.18784	1.99893	4.17217	0.01674	6.18784
40	c	-0.20674	1.99895	4.19128	0.01651	6.20674
41	c	-0.24001	1.99894	4.22445	0.01663	6.24001
42	h	0.46952	0.00000	0.52903	0.00145	0.53048
43	h	0.20255	0.00000	0.79511	0.00234	0.79745
44	h	0.23151	0.00000	0.76647	0.00202	0.76849
45	h	0.20414	0.00000	0.79281	0.00304	0.79586
46	h	0.20935	0.00000	0.78642	0.00423	0.79065
47	h	0.20633	0.00000	0.78959	0.00408	0.79367
48	h	0.21610	0.00000	0.78153	0.00237	0.78390
49	h	0.17675	0.00000	0.82078	0.00247	0.82325
50	h	0.17106	0.00000	0.82602	0.00291	0.82894
51	h	0.22291	0.00000	0.77499	0.00211	0.77709
52	h	0.21118	0.00000	0.78577	0.00305	0.78882
53	h	0.21394	0.00000	0.78284	0.00322	0.78606
54	h	0.20740	0.00000	0.79007	0.00253	0.79260
55	h	0.23018	0.00000	0.76582	0.00400	0.76982
56	h	0.20615	0.00000	0.79089	0.00296	0.79385
57	h	0.20663	0.00000	0.79023	0.00314	0.79337
58	h	0.22820	0.00000	0.76913	0.00266	0.77180

59	h	0.22735	0.00000	0.77073	0.00192	0.77265
60	h	0.22849	0.00000	0.76979	0.00172	0.77151
61	h	0.22878	0.00000	0.76956	0.00166	0.77122
62	h	0.46913	0.00000	0.52942	0.00146	0.53087
63	h	0.20329	0.00000	0.79430	0.00241	0.79671
64	h	0.23176	0.00000	0.76622	0.00202	0.76824
65	h	0.20370	0.00000	0.79326	0.00304	0.79630
66	h	0.20932	0.00000	0.78660	0.00408	0.79068
67	h	0.20600	0.00000	0.78994	0.00406	0.79400
68	h	0.21566	0.00000	0.78196	0.00237	0.78434
69	h	0.17663	0.00000	0.82090	0.00247	0.82337
70	h	0.17049	0.00000	0.82659	0.00292	0.82951
71	h	0.22299	0.00000	0.77488	0.00213	0.77701
72	h	0.20625	0.00000	0.79110	0.00265	0.79375
73	h	0.22333	0.00000	0.77241	0.00426	0.77667
74	h	0.20842	0.00000	0.78898	0.00261	0.79158
75	h	0.22580	0.00000	0.77144	0.00275	0.77420
76	h	0.20519	0.00000	0.79180	0.00301	0.79481
77	h	0.20478	0.00000	0.79187	0.00335	0.79522
78	h	0.23233	0.00000	0.76509	0.00258	0.76767
79	h	0.22779	0.00000	0.77030	0.00191	0.77221

80 h 0.22891 0.00000 0.76938 0.00171 0.77109

81 h 0.22928 0.00000 0.76905 0.00166 0.77072

82 h -0.05686 0.00000 1.05434 0.00252 1.05686

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* Total * -0.00000 97.95747 220.17710 0.86543 319.00000

Table S21. Dipole moment of complexes (**1**, **2** and **3**)

Complex **1**	$dipole from dscf x -0.00594651188212 y 0.00130130527805 z -0.01100192940339 a.u. | dipole | = 0.0319592898 debye
Complex **2**	$dipole from dscf x -0.00445480443091 y 0.00240391006082 z 0.00209883938714 a.u. | dipole | = 0.0139285960 debye
Complex **3**	$dipole from dscf x -0.00320946676061 y 0.00006161043984 z 0.00221978258378 a.u. | dipole | = 0.0099200225 debye