Supporting Information

Enhancing the Reactivity of Nickel(II) in Hydrogen Evolution Reactions (HERs) by β-Hydrogenation of Porphyrinoid Ligands

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Table of Contents

1. General

UV-vis spectra were recorded on an Agilent 8453 UV-vis spectrometer equipped with an Agilent 89090A thermostat (± 0.1 °C). ESI-MS were recorded on Bruker APEX IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer using electrospray ionization. ^{1}H , ^{19}F and ^{13}C NMR spectra were recorded on Bruker-400 MHz NMR. All ^{1}H NMR experiments were reported in δ units, parts per million (ppm), all coupling constants were in Hz and measured relative to the signal for residual chloroform (7.26 ppm) in the deuterated solvent $CDCl_3$. For ^{19}F NMR spectra, CF_3COOH was used as external reference at 0 ppm. Transmission electron microscopy were determined by JEM-2100F(JEOL). DLS measurements were performed by using a Laser Light Scattering Spectrometer (ALV/Laser Vertriebsgesellschaft m.b.H), which can detect particle sizes ranging from 1.0 nm-1.0 μm. SEM and EDX were performed by using Hitachi S-4800 field emission scanning electron microscope at an accelerating voltage of 5 and 15 kV, respectively. CH_3CN and dimethylformamide was distilled and degassed before use. Tetrabutylammonium hexafluorophosphate ($^{n}Bu_4NPF_6$) was recrystallized from absolute ethanol. Other commercially available reagents were used without further purification.

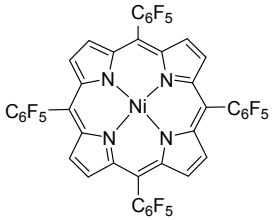
2. Synthesis

2.1 Porphyrin ligands

Meso-tetrakispentafluorophenylporphyrin (**1**), *meso*-tetrakispentafluorophenylchlorin (**2**), *meso*-tetrakispentafluorophenylporpholactone (**3**) and *adjacent*-hydroporpholactone (**4**) was synthesized according to the literature.[1]

2.2 Synthesis of Ni-1

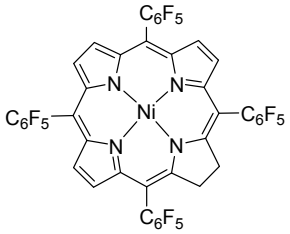
Nickel-*meso*-tetrakispentafluorophenylporphyrin (Ni-**1**)



1 (0.1 mmol) was refluxed with 30 equivalents of $Ni(OAc)_2$ (1.0 mmol, 180 mg) in acetonitrile under nitrogen for 6 hours. The solvent was removed by adding 100 equivalents of water and the residue was purified through silica column. Isolated yields were over 90%. Eluent: ethyl acetate: petroleum ether, 1:5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 8H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -136.47 (dd, *J* = 23.2, 7.7 Hz, 8F), -150.17 (m, 4H), -161.32 (dt, *J* = 22.5, 7.4 Hz, 8F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.98 (s), 132.52 (s), 103.09 (s). ESI-MS m/z: Calcd. For $C_{44}H_8F_{20}N_4Ni$ 1029.97831, found 1029.97854. Anal. Calcd for $C_{44}H_8F_{20}N_4Ni$: C, 51.25; H, 0.78; N, 5.43, found C, 51.29; H, 0.92; N, 5.38.

2.3 Synthesis of Ni-2

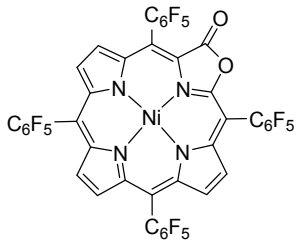
Nickel-*meso*-tetrakispentafluorophenylchlorin (Ni-**2**)



2 (0.1 mmol) was refluxed with 30 equivalents of $Ni(OAc)_2$ (1 mmol, 180 mg) in acetonitrile under nitrogen for 1 hours. The solvent was removed by adding 100 equivalents of water and the residue was purified through silica column. Isolated yields were 75%. Eluent: ethyl acetate: petroleum ether, 1: 4. ^{1}H NMR (400 MHz, $CDCl_3$) δ=8.29 (d, *J* = 4.9 Hz , 2H), 8.14 (s, 2H), 7.95 (d, *J* = 5.0 Hz, 2H), 3.93 (s, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ = -136.94 (dd, *J*=23.2, 7.7Hz, 4F), -137.89 (dd, *J*=23.8, 8.3Hz, 4F), -151.88 (t, *J*=20.9Hz, 2F), -152.10 (t, *J*=20.9Hz, 2F), -160.66 (dt, *J*=23.3, 8.0Hz, 4F), -161.57 (dt, *J*=22.6, 7.4Hz, 4F). ^{13}C NMR (101 MHz, CDC_{l3}) δ 169.03 (s), 152.66 (s), 140.39 (s), 135.31 (s), 132.27 (s), 128.22 (s), 123.62 (s), 106.31 (s), 96.83 (s), 35.31 (s, $-CH_2-$). ESI-MS m/z: Calcd. For $C_{44}H_{10}F_{20}N_4Ni$ 1031.99396, found 1031.98981. Anal. Calcd for $C_{44}H_{10}F_{20}N_4Ni$: C, 51.15; H, 0.98; N, 5.42, found C, 51.16; H, 1.14; N, 5.31.

2.4 Synthesis of Ni-3

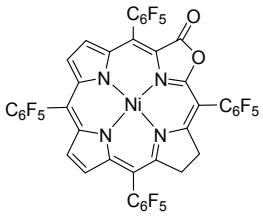
Nickel-*meso*-tetrakispentafluorophenylporpholactone (Ni-**3**)



3 (0.1 mmol) was refluxed with 30 equivalents of $Ni(OAc)_2$ (1.0 mmol, 180 mg) in acetonitrile under nitrogen for 6 hours. The solvent was removed by adding 100 equivalents of water and the residue was purified through silica column. Isolated yields were over 90%. Eluent: ethyl acetate: petroleum ether, 1:5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.1 Hz, 1H), 8.65 – 8.61 (m, 2H), 8.58 (d, *J* = 5.1 Hz, 1H), 8.55 (d, *J* = 4.9 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -136.69 – -136.96 (m), -138.17 – -138.39 (m), -150.28 – -150.62 (m), -151.20 (q, *J* = 20.9 Hz), -160.27 – -160.87 (m), -161.37 (qd, *J* = 22.1, 6.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.03 (s), 149.75 (s), 144.95 (s), 134.45 (s), 132.47 (d), 131.78 (s), 131.17 (s), 130.34 (s), 120.59 (s). ESI-MS m/z: Calcd. For $C_{43}H_6F_{20}N_4NiO_2$ M:1048.95556, found 1048.95959. Anal. Calcd for $C_{43}H_6F_{20}N_4NiO_2$: C, 49.23; H, 0.58; N, 5.34, found C, 48.66; H, 0.67; N, 5.26.

2.5 Synthesis of Ni-4

Nickel- *adjacent*-hydroporpholactone (Ni-**4**)



4 (0.1 mmol) was refluxed with 30 equivalents of $Ni(OAc)_2$ (1.0 mmol, 180 mg) in acetonitrile under nitrogen for 1 hours. The solvent was removed by adding 100 equivalents of water and the residue was purified through silica column. Isolated yields were over 90%. Eluent: ethyl acetate: petroleum ether, 1:5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 4.8 Hz, 1H), 7.77 (dd, J = 20.5, 4.5 Hz, 2H), 7.54 (d, J = 4.7 Hz, 1H), 3.76 (d, J = 8.4 Hz, 2H), 3.66 (d, J = 8.4 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -137.63 (d, J = 23.9 Hz), -137.89 (d, J = 15.5 Hz), -138.76 (d, J = 15.8 Hz), -151.16 (d, J = 34.0 Hz), -151.50 (s), -151.79 (s), -160.07 (d, J = 6.2 Hz), -160.31 (d, J = 5.9 Hz), -160.68 (d, J = 6.1 Hz), -161.42 (d, J = 5.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.72 (s, -C=O), 162.06 (s), 156.20 (s), 151.18 (s), 149.93 (s), 141.77 (s), 139.34 (s), 138.75 (s), 133.28 (s), 127.83 (s), 126.19 (s), 115.90 (s), 96.88 (s), 82.19 (s), 34.40 (s, $-CH_2-$), 32.29 (s, $-CH_2-$). Calcd. For $C_{43}H_8F_{20}N_4NiO_2$ $[M+H]^+$:1050.97586, found 1050.97686. Anal. Calcd for C43H8F20N4NiO2: C, 49.13; H, 0.77; N, 5.33, found C, 48.96; H, 0.93; N, 5.20.

2.6 Summary of Crystallographic Data

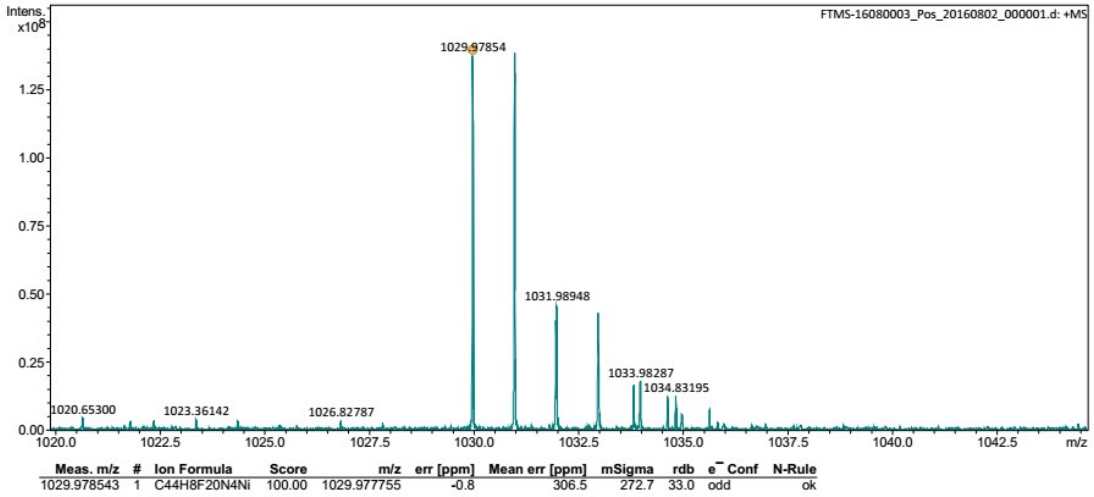
Table S1. Crystal data and structure refinement

Complex	Ni-**1**	Ni-**2**	Ni-**3**	Ni-**4**
molecular formula	$C_{44}H_8F_{20}N_4Ni$	$C_{44}H_{10}F_{20}N_4Ni$	$C_{43}H_6F_{20}N_4NiO_2$	$C_{43}H_8F_{20}N_4NiO_2$
formula wt. (g mol^{-1})	1031.25	1033.25	1049.21	1051.22
temperature (K)	200(2)	180.01(10)	180.01(10)	180.01(10)
radiation (λ, Å)	0.71073	0.71073	0.71073	0.71073
crystal system	tetragonal	tetragonal	trigonal	tetragonal
space group	$I\bar{4}2d$	$I\bar{4}2d$	$R\bar{3}$	$I41/a$
a (Å)	15.4077(6)	15.4001(2)	20.0377(5)	15.3093(2)
b (Å)	15.4077(6)	15.4001(2)	20.0377(5)	15.3093(2)
c (Å)	15.3877(7)	15.3253(4)	24.6135(9)	15.8346(4)
α (°)	90	90	90	90
β (°)	90	90	90	90
γ (°)	90	90	120	90
Volume ($Å^3$)	3653.0(3)	3634.59(15)	8558.5(5)	3711.23(13)
Z	4	4	9	4
ρ_{calcd} (g cm^{-3})	1.875	1.885	1.830	1.872
μ (mm^{-1})	0.678	0.681	0.656	0.673
F(000)	2032	2032	4635	2052
crystal size (mm^3)	0.20×0.20×0.15	0.32×0.28×0.15	0.32×0.25×0.15	0.25×0.20×0.18
Theta range	1.87, 27.41	3.243. 30.257	3.520, 27.478	3.702, 27.481
reflections collected	2076	2633	4340	2127
independent reflections	2007	2380	3677	2051
Completeness	97	99.67	99.70	99.68
goodness-of-fit on F^2	1.042	1.098	1.162	1.048
final R indices [R > 2σ (I)]	0.0278, 0.0689	0.0353, 0.0874	0.0634, 0.1342	0.0366, 0.0366
R indices (all data)	0.0291, 0.0698	0.0432, 0.0933	0.0756, 0.1418	0.0374, 0.1064
largest diff. peak and hole (e $Å^{-3}$)	0.223, -0.269	0.314, -0.240	0.360, -0.393	0.601, -0.436

Table S2. Selected bond length for nickel complexes.

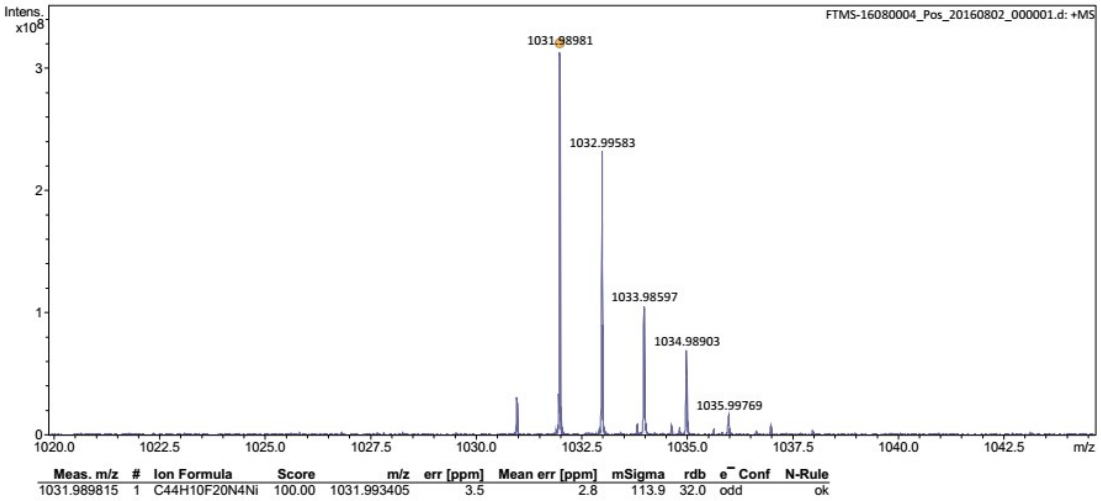
Complex	Ni-**1**	Ni-**2**	Ni-**3**	Ni-**4**
C-C / Å	1.346(4) 1.346(4) 1.346(4) 1.346(4)	1.383(5) 1.383(5) 1.383(5) 1.383(5)	1.341(5) 1.338(5) 1.341(5) 1.338(5)	1.404(3) 1.404(3) 1.404(3) 1.404(3)
Ni-N / Å	1.925(2) 1.925(2) 1.925(2) 1.925(2)	1.925(2) 1.925(2) 1.925(2) 1.925(2)	1.950(3) 1.950(3) 1.945(3) 1.945(3)	1.9210(15) 1.9210(15) 1.9210(15) 1.9210(15)
Ni-N4 plane / Å	0	0	0	0

2.7 ESI-MS spectra



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1029.978543	1	C44H8F20N4Ni	100.00	1029.977755	-0.8	306.5	272.7	33.0	odd	ok

Fig. S1 HR-MS(ESI) of Ni-**1**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1031.989815	1	C44H10F20N4Ni	100.00	1031.993405	3.5	2.8	113.9	32.0	odd	ok

Fig. S2 HR-MS(ESI) of Ni-**2**.

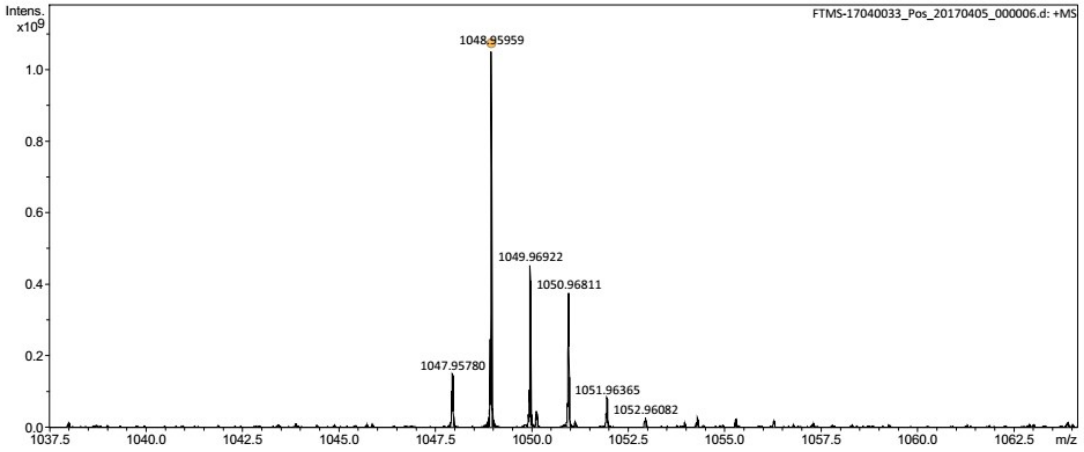


Fig. S3 HR-MS(ESI) of Ni-**3**.

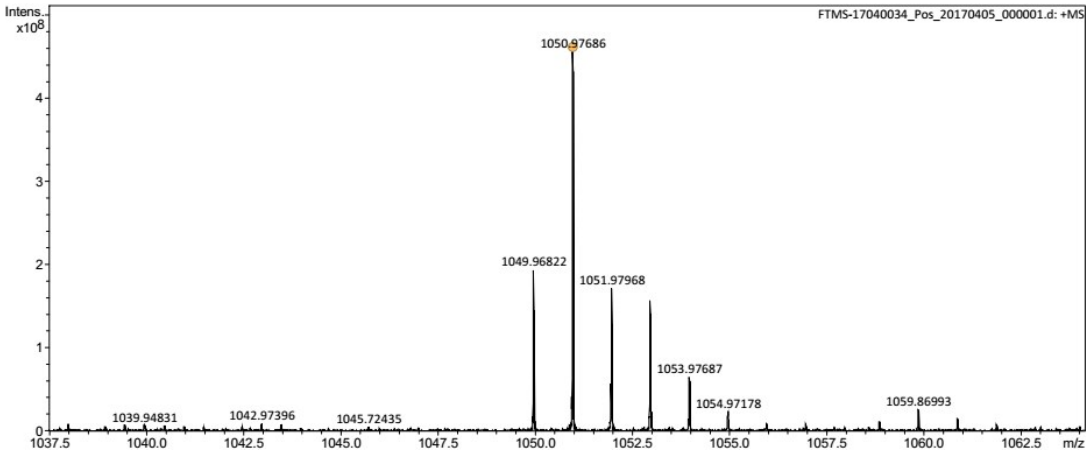


Fig. S4 HR-MS(ESI) of Ni-**4**.

2.8 ^{1}H, ^{19}F, ^{13}C and ^{2}D NMR spectra

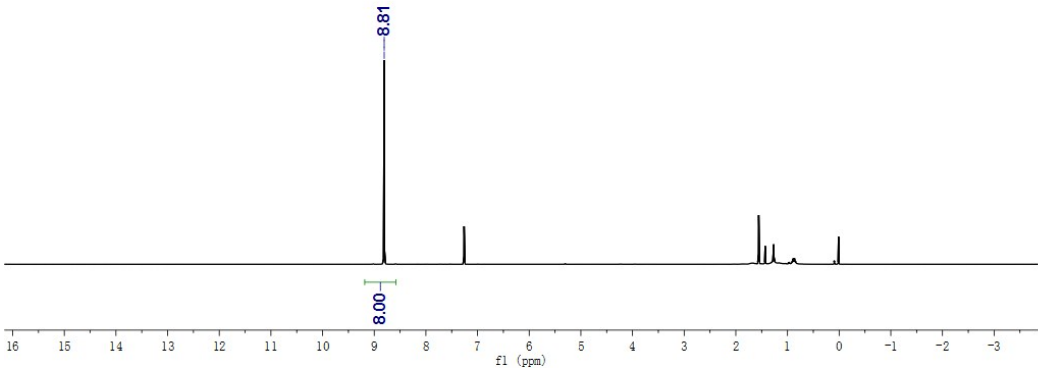


Fig. S5 ^{1}H NMR of Ni-**1** in $CDCl_3$.

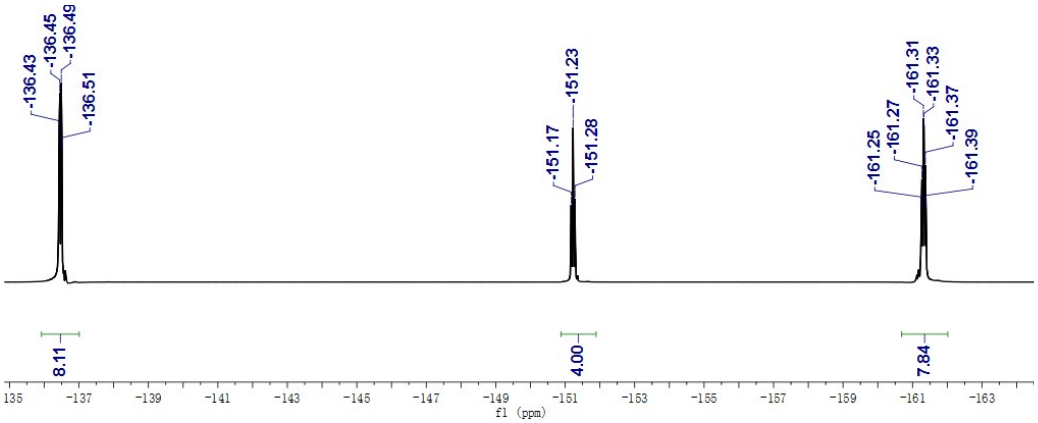


Fig. S6 ^{19}F NMR of Ni-**1** in $CDCl_3$.

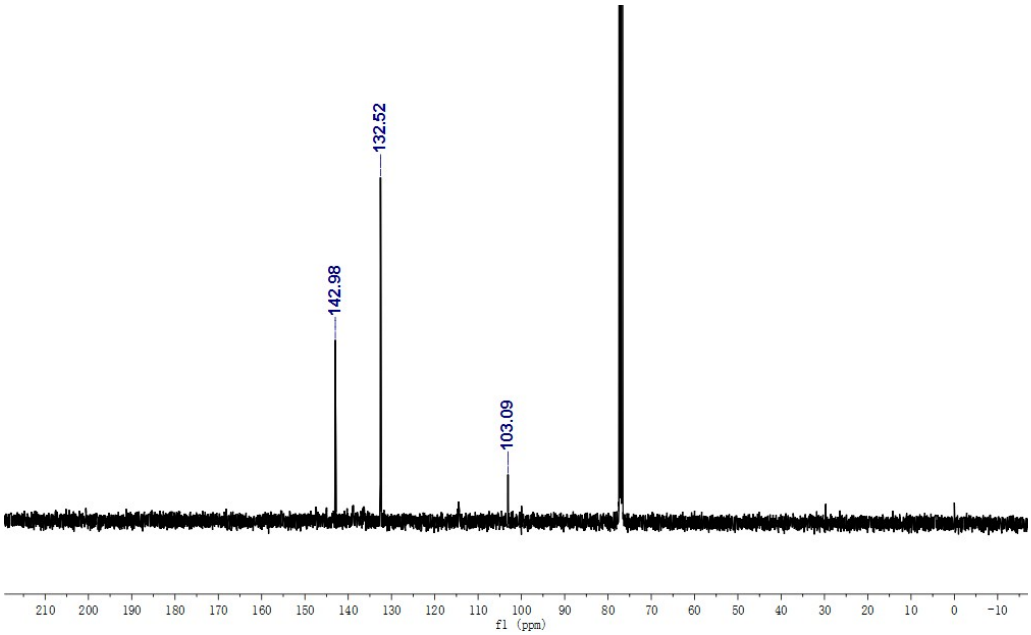


Fig. S7 ^{13}C NMR of Ni-**1** in $CDCl_3$.

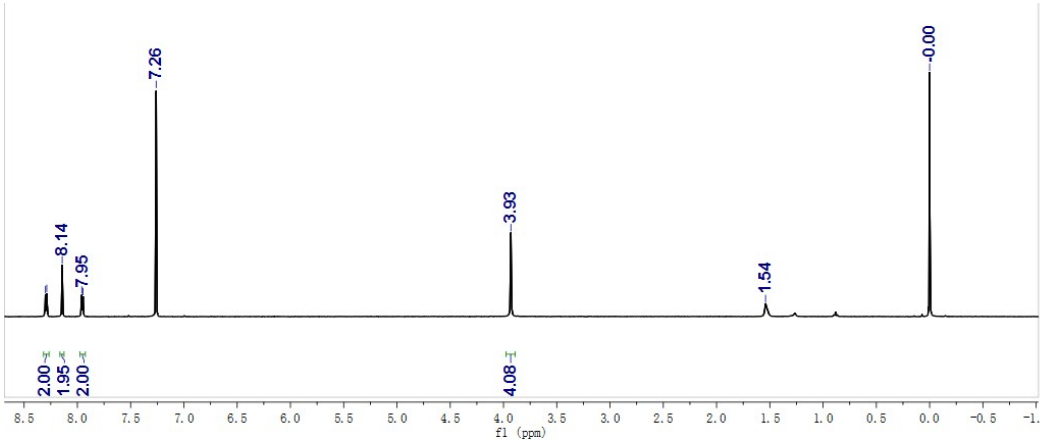


Fig. S8 ^{1}H NMR of Ni-**2** in $CDCl_3$.

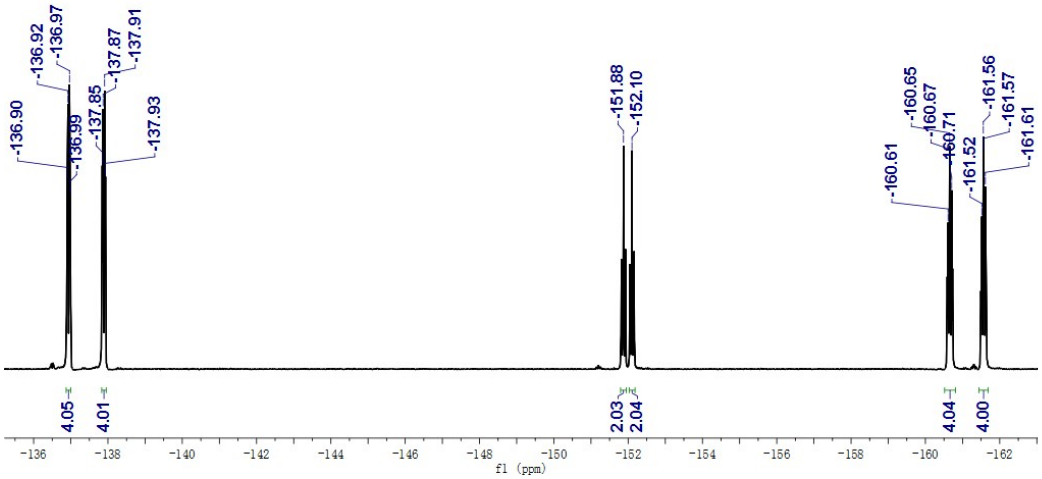


Fig. S9 ^{19}F NMR of Ni-**2** in $CDCl_3$.

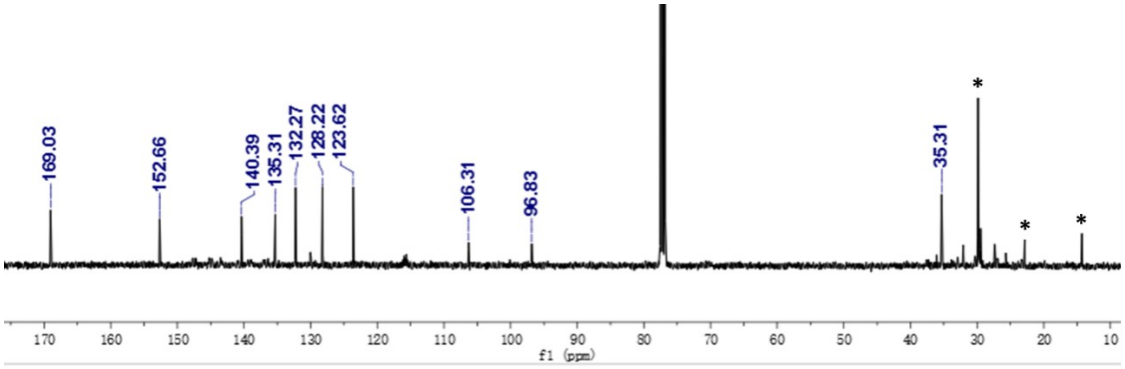


Fig. S10 ^{13}C NMR of Ni-**2** in $CDCl_3$. * refers to the residual n-hexane.

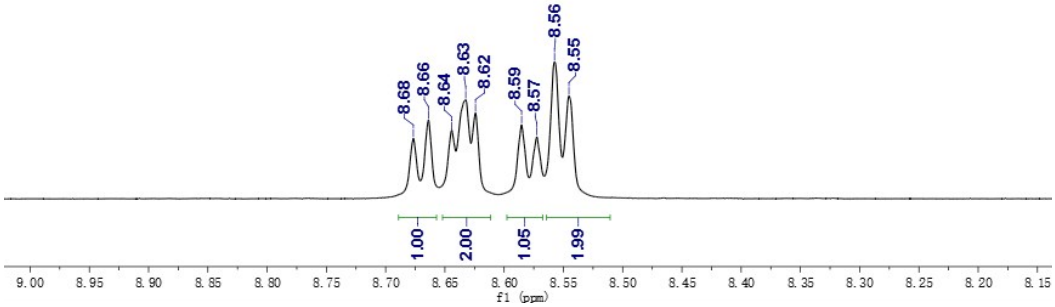


Fig. S11 ^{1}H NMR of Ni-**3** in $CDCl_3$.

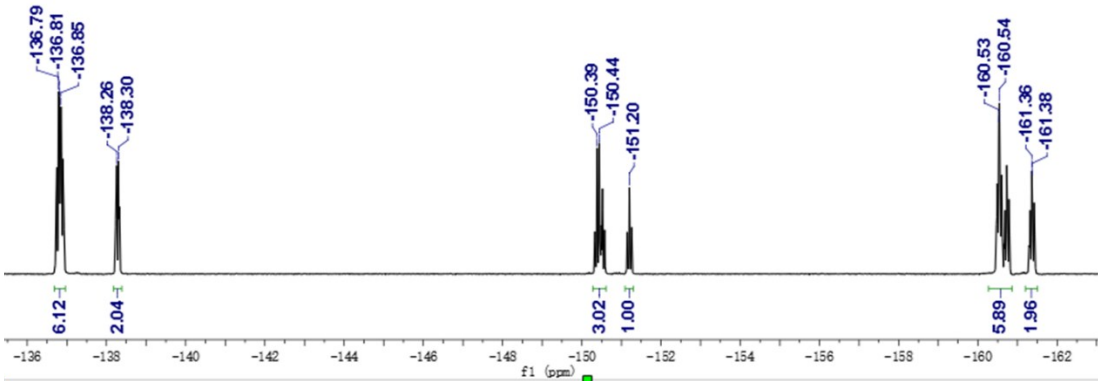


Fig. S12 ^{19}F NMR of Ni-**3** in $CDCl_3$.

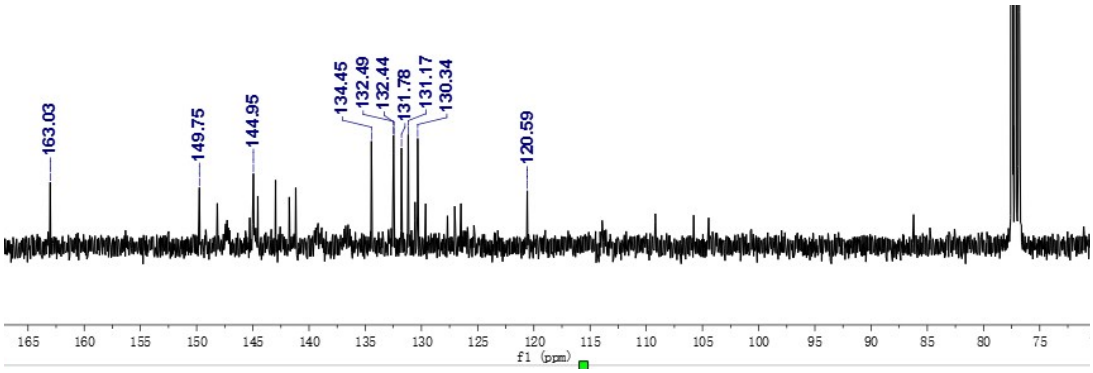


Fig. S13 ^{13}C NMR of Ni-**3** in $CDCl_3$.

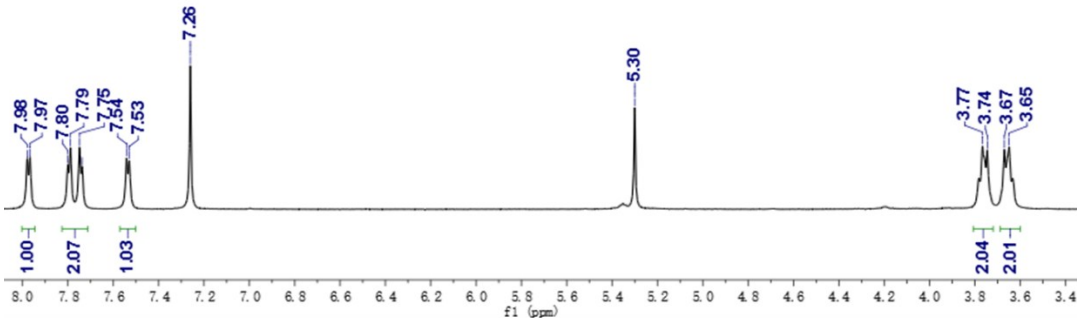


Fig. S14 ^{1}H NMR of Ni-**4** in $CDCl_3$.

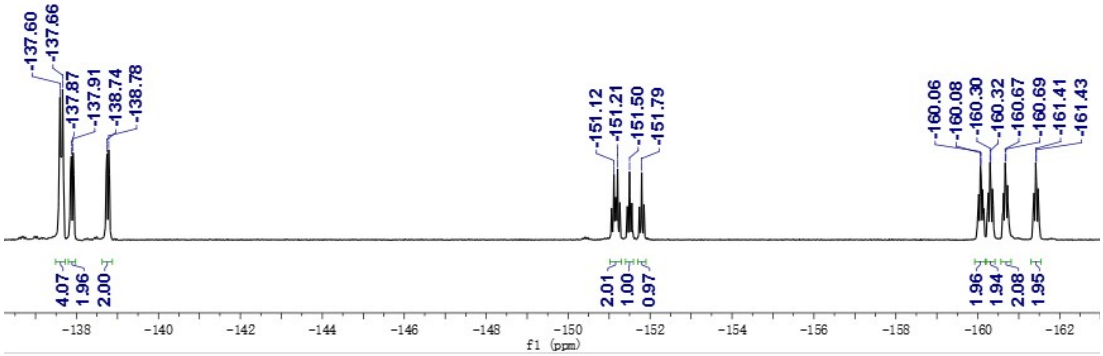


Fig. S15 ^{19}F NMR of Ni-**4** in $CDCl_3$.

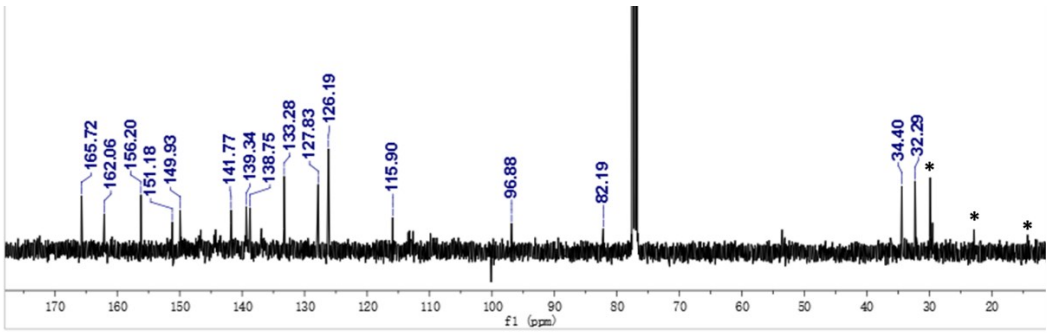


Fig. S16 ^{13}C NMR of Ni-**4** in $CDCl_3$. * refers to the residual n-hexane.

3. Electrochemistry

3.1 General

All the electrochemistry experimental procedures were conducted with a standard three-electrode configuration on Shanghai Chenhua CHI660C electrochemical workstation at room temperature, 25 ºC, under argon or a vacuum atmospheres.

Cyclic voltammetry experiments were recorded using glassy-carbon working electrode disks of 3mm diameter (Cypress Systems EE040). The working electrode was treated between scans by means of a sequence of polishing with diamond paste (Buehler) of decreasing sizes (3 to 0.05 μm) interspersed by washings with purified H_2O. Auxiliary electrode was platinum wire electrode and Ag/AgCl electrode was reference electrode. All glassware for electrochemical experiments was oven dried overnight and allowed to cool to room temperature before use. Ferrocene was used as an internal standard, and all potentials reported in this work are referenced to ferrocenium/ferrocene (Fc^+/Fc) couple at 0 V.

Spectroelectrochemical measurements were carried out in a quartz cell with an optical path length of 1 mm. A platinum net, a platinum filament and an Ag/AgCl were used as working electrode, counter electrode, and reference electrode, respectively. The sample solutions were deaerated with acetonitrile-saturated argon. The spectra were recorded on an Agilent 8453 UV-vis spectrophotometer during electrolysis on a CHI 660C instrument.

Controlled potential electrolyses were performed using a CHI 760D electrochemistry workstation, the working electrode is the GCE plate (1 cm × 1 cm). A clean platinum foil is used as counter electrode. A saturated Ag/AgCl electrode is used as reference electrode. The electrolyte was deoxygenized in which the solved air had been removed under vaccum. During the test, the evolved hydrogen was introduced into the gas chromatograph (GC, GC3420, Beifen Instrument), then quantified by the integrated areas of the peaks corresponding to hydrogen.

3.2 HER process

Typical Experimental Conditions: 1.0 mmol of Ni-**1**, Ni-**2**, Ni-**3** or Ni-**4** was weighed into an electrochemical cell and dissolved in 14 mL of a supporting electrolyte solution (0.10 M $^nBu_4PF_6$ / CH_3CN). Purity of the electrolyte medium was confirmed over the available electrochemical window through background scans taken prior to addition of analyte.

3.3 Catalytic hydrogen production using TFA as acid

Typical Experimental Conditions: 1.0 mmol of Ni-**1**, Ni-**2**, Ni-**3 or** Ni-**4** (1.0 mmol of ferrocene was added before and after the reaction) was added into an electrochemical cell and dissolved in 14 mL of a supporting electrolyte solution (0.10 M $^nBu_4PF_6$ / CH_3CN). Purity of the electrolyte medium was confirmed over the available electrochemical window through background scans taken prior to addition of analyte. In each trail, Additional of TFA was added and stired evenly before test.

Turnover frequencies (TOFs) were introduced (determined by eq 1).

$$\frac{i_{cat}}{i_p} = \frac{n}{0.4463}\sqrt{\frac{RT\kappa_{obs}}{Fv}} \quad (eq.\,1)$$

In equation 1, i_{cat} is the catalytic current in presence of acid, i_p is the peak current for the second reduction wave ($Ni^{II/I}$) measured in the absence of acid, n is the number of electrons involved in the catalytic reaction and we believed a two-electron transfer reaction in this process, κ_{obs} is the observed first-order rate constant, R is the universal gas constant, T is the temperature in Kelvin, F is Faraday's constant, υ is the scan rate, and the 0.4463 is a constant determined by numerical solution of the diffusion equations. The maximum TOF was obtained when the peak current do not increase when adding more TFA.

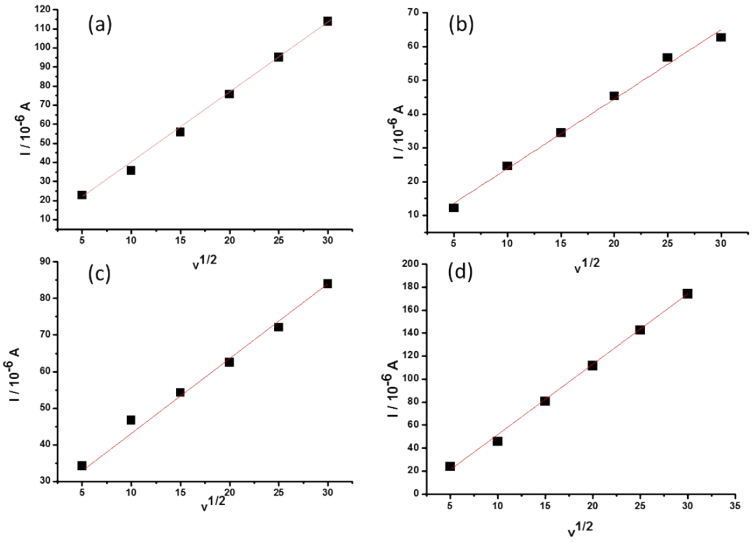


Fig. S17 Plot of i_{cat} (μA) vs. scan rate$^{1/2}$ (V/s) for 1 mM Ni-**1**, Ni-**2**, Ni-**3** and Ni-**4**.

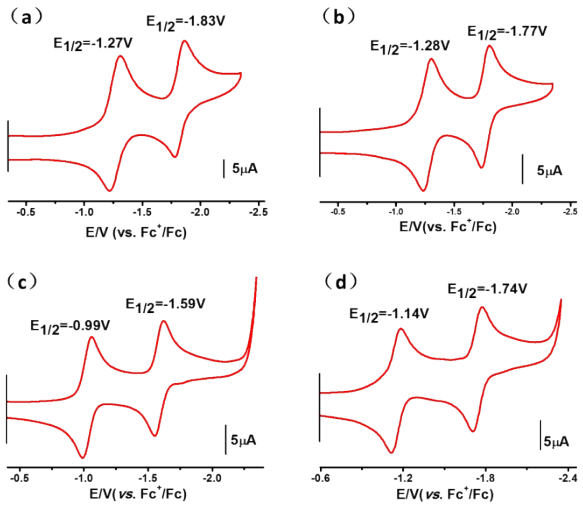


Fig. S18 Cyclic voltammograms of complexes of Ni-**1** (a), Ni-**2** (b), Ni-**3** (c) and Ni-**4** (d).

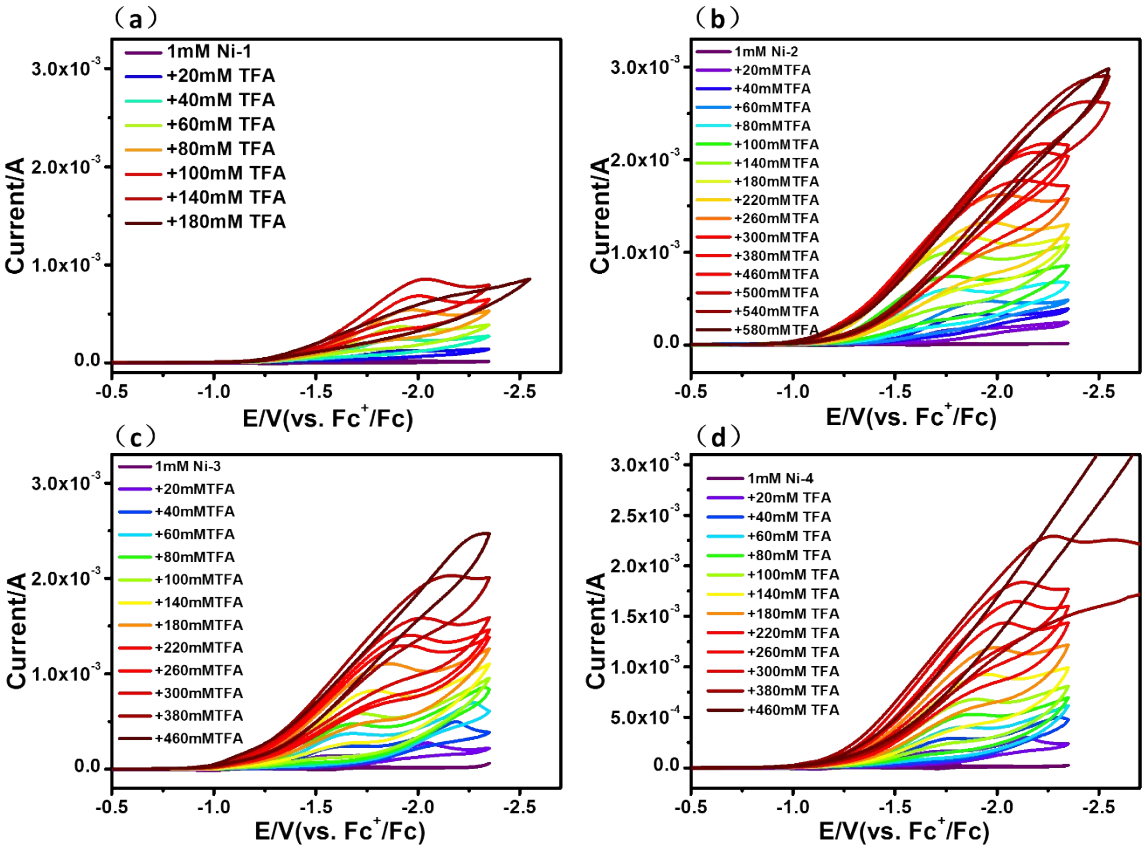


Fig. S19 Successive cyclic voltammograms of 1.0 mM Ni-**1** (a) Ni-**2** (b) Ni-**3** (c) and Ni-**4** (d) in CH_3CN (0.10 M $^nBu4NPF_6$) at increasing concentrations of TFA. Conditions: 3 mm glassy-carbon working electrode; 25 °C; scan rate 100 mV/s.

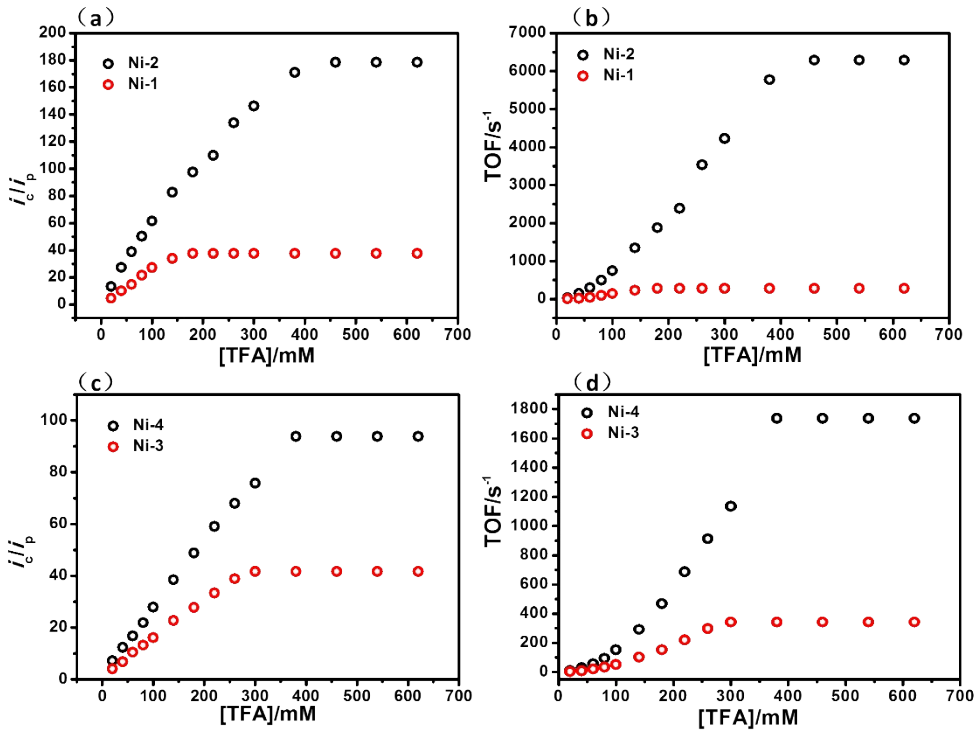


Fig. S20 Plot of i_c/i_p *vs*. concentration of TFA for a typical acid titration of 1.0 mM Ni-**1**, Ni-**2** (a) and Ni-**3**, Ni-**4** (c). Plot of TOF *vs*. concentration of TFA for a typical acid titration of 1.0 mM Ni-**1**, Ni-**2** (b) and Ni-**3**, Ni-**4** (d).

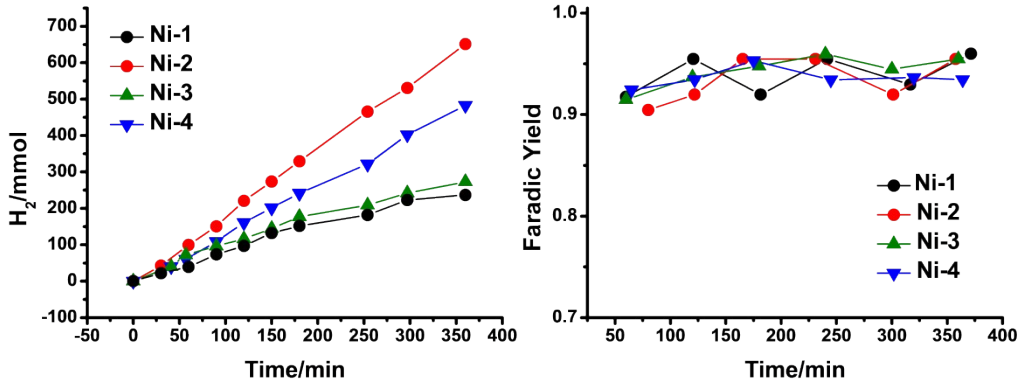


Fig. S21 (left) Plot of the amount of hydrogen *vs*. reaction time during the controlled-potential coulometry experiment of 1.0 mM Ni-**1** to Ni-**4**. (right) Faradic yield *vs*. Reaction time during the controlled-potential coulometry experiment of 1.0 mM Ni-**1** to Ni-**4**. Conditions: GCE plate(1 cm × 1 cm) as working electrode; 25 °C; scan rate 100 mV/s.

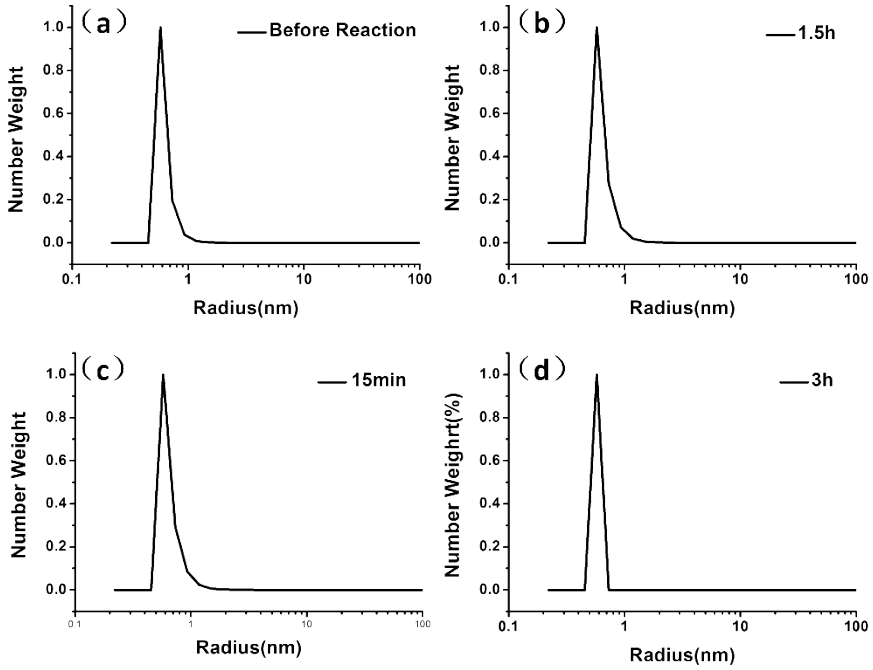


Fig. S22 Particle distribution determined by DLS experiments during the bulk electrolysis experiments. Electrolysis conditions: 1.0 mM Ni-**2** in acetonitrile with 0.1 M $^{n}Bu_4NPF_6$ supporting electrolyte and 100 mM of TFA.

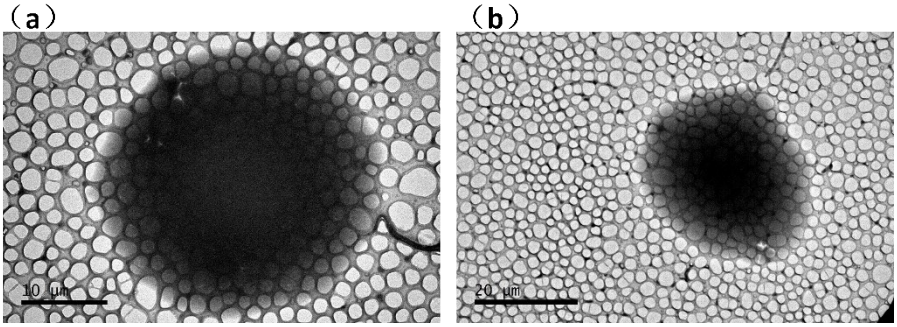


Fig. S23 TEM experiments before (a) and after (b) the bulk electrolysis experiments. Electrolysis conditions: 1.0 mM Ni-**2** in acetonitrile with 0.1 M $^{n}Bu_4NPF_6$ supporting electrolyte and 100 mM of TFA.

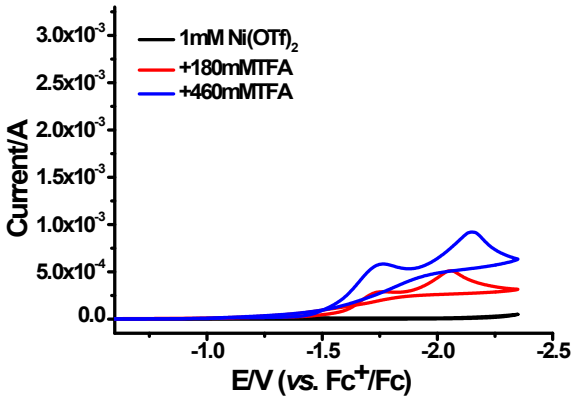


Fig. S24 Successive cyclic voltammograms of 1.0 mM $Ni(OTf)_2$ in CH_3CN (0.10 M $^nBu_4NPF_6$) at increasing concentrations of TFA. Conditions: 3 mm glassy-carbon working electrode; 25 °C; scan rate 100 mV/s.

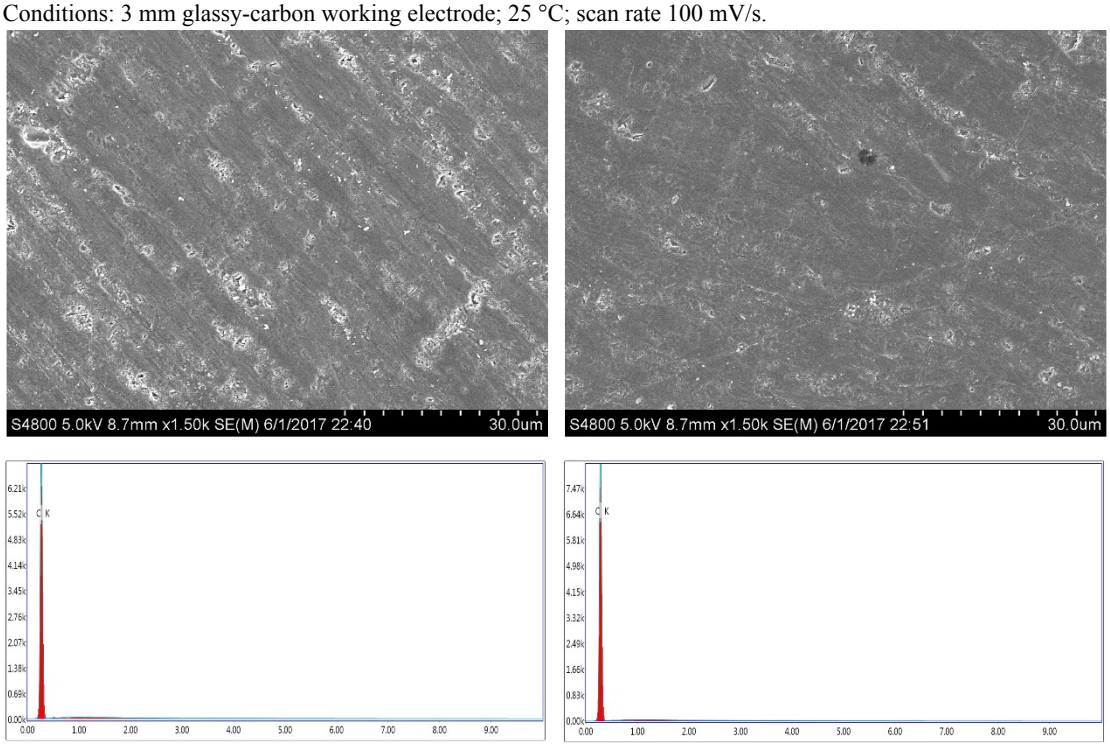


Fig. S25 SEM images and EDX data for GC electrodes before (left) and after (right) the bulk electrolysis experiments. Electrolysis conditions: 1.0 mM Ni-**2** in acetonitrile with 0.10 M $^nBu_4NPF_6$ supporting electrolyte and 100 mM of TFA.

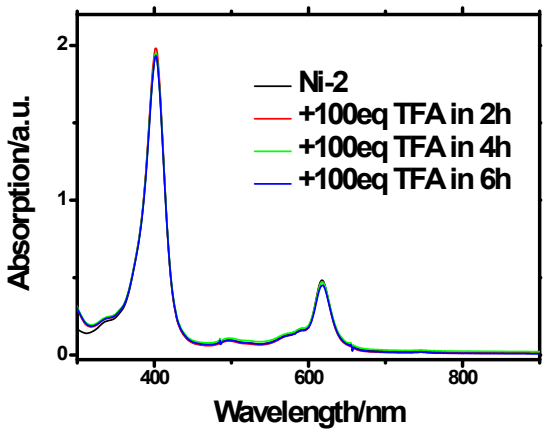


Fig. S26 Stability studies of Ni-**2**.

Table S3 Cyclic and differential pulse voltammetry data of Ni-**1** to Ni-**4**

	Ni-**1**	Ni-**2**	Ni-**3**	Ni-**4**	Fc^+/Fc
Cyclic Voltammetry ΔEp (mV) of the first reduction wave	65	59	60	58	57
Cyclic Voltammetry ΔEp (mV) of the second reduction wave	65	59	60	58	57

Table S4 Experimental results from a typical acid titration of Ni-**1**

[Ni-**1**](mM)	[TFA](mM)	i_{cat}(A)	i_p(A,corrected)	i_{cat}/i_p	TOFs(s^{-1})
1.0	20	1.21×10^{-4}	2.33×10^{-5}	5	5
1.0	40	2.42×10^{-4}	2.33×10^{-5}	10	21
1.0	60	3.71×10^{-4}	2.33×10^{-5}	15	50
1.0	80	5.01×10^{-4}	2.33×10^{-5}	21	91
1.0	100	6.11×10^{-4}	2.33×10^{-5}	26	135
1.0	140	6.82×10^{-4}	2.33×10^{-5}	29	168
1.0	180	8.56×10^{-4}	2.33×10^{-5}	36	265

Table S5 Experimental results from a typical acid titration of Ni-**2**

[Ni-**2**](mM)	[TFA](mM)	i_{cat}(A)	i_p(A,corrected)	i_{cat}/i_p	TOFs(s^{-1})
1.0	20	2.82×10^{-4}	1.21×10^{-5}	13	34
1.0	40	4.19×10^{-4}	1.21×10^{-5}	27	147
1.0	60	5.68×10^{-4}	1.21×10^{-5}	39	298
1.0	80	6.99×10^{-4}	1.21×10^{-5}	50	497
1.0	100	8.11×10^{-4}	1.21×10^{-5}	61	745
1.0	140	1.13×10^{-3}	1.21×10^{-5}	83	1348
1.0	180	1.18×10^{-3}	1.21×10^{-5}	97	2566
1.0	220	1.33×10^{-3}	1.21×10^{-5}	109	2384
1.0	260	1.62×10^{-3}	1.21×10^{-5}	133	3537
1.0	300	1.77×10^{-3}	1.21×10^{-5}	146	4222
1.0	380	2.07×10^{-3}	1.21×10^{-5}	171	5774
1.0	460	2.16×10^{-3}	1.21×10^{-5}	179	6287
1.0	540	2.16×10^{-3}	1.21×10^{-5}	179	6287
1.0	620	2.16×10^{-3}	1.21×10^{-5}	179	6287

Table S6 Experimental results from a typical acid titration of Ni-**3**

[Ni-**3**](mM)	[TFA](mM)	i_{cat}(A)	i_p(A,corrected)	i_{cat}/i_p	TOFs(s^{-1})
1.0	20	1.47×10^{-4}	3.60×10^{-5}	4	3
1.0	40	2.44×10^{-4}	3.60×10^{-5}	7	9
1.0	60	3.77×10^{-4}	3.60×10^{-5}	10	22
1.0	80	4.75×10^{-4}	3.60×10^{-5}	13	34
1.0	100	5.85×10^{-4}	3.60×10^{-5}	16	51
1.0	140	8.19×10^{-4}	3.60×10^{-5}	23	102
1.0	180	1.00×10^{-3}	3.60×10^{-5}	28	152
1.0	220	1.20×10^{-3}	3.60×10^{-5}	33	219
1.0	260	1.40×10^{-3}	3.60×10^{-5}	38	298
1.0	300	1.50×10^{-3}	3.60×10^{-5}	42	342
1.0	380	1.50×10^{-3}	3.60×10^{-5}	42	342
1.0	460	1.50×10^{-3}	3.60×10^{-5}	42	342
1.0	540	1.50×10^{-3}	3.60×10^{-5}	42	342
1.0	620	1.50×10^{-3}	3.60×10^{-5}	42	342

Table S7 Experimental results from a typical acid titration of Ni-**4**

[Ni-**4**](mM)	[TFA](mM)	i_{cat}(A)	i_p(A,corrected)	i_{cat}/i_p	TOFs(s^{-1})
1.0	20	1.76×10^{-4}	2.44×10^{-5}	7	10
1.0	40	3.01×10^{-4}	2.44×10^{-5}	12	30
1.0	60	4.10×10^{-4}	2.44×10^{-5}	16	56
1.0	80	5.35×10^{-4}	2.44×10^{-5}	21	95
1.0	100	6.82×10^{-4}	2.44×10^{-5}	27	154
1.0	140	9.40×10^{-4}	2.44×10^{-5}	38	293
1.0	180	1.19×10^{-3}	2.44×10^{-5}	48	469
1.0	220	1.44×10^{-3}	2.44×10^{-5}	59	687
1.0	260	1.66×10^{-3}	2.44×10^{-5}	68	913
1.0	300	1.85×10^{-3}	2.44×10^{-5}	75	1134
1.0	380	2.29×10^{-3}	2.44×10^{-5}	94	1737

1.0	460	2.29×10^{-3}	2.44×10^{-5}	94	1737
1.0	540	2.29×10^{-3}	2.44×10^{-5}	94	1737
1.0	620	2.29×10^{-3}	2.44×10^{-5}	94	1737

FOWA begins with eq. 2, which describes a catalytic response current for a typical EECC reaction. For normalization of eq. 2 by i_p, the peak current in the absence of a substrate, as defined by eq. 3, yields eq. 4.

$$i = \frac{nFAC_p^0\sqrt{Dn'k_{obs}}}{1 + exp[\frac{nF}{RT}(E - E_{redox})]} \quad (\text{eq. 2})$$

$$i_p = 0.1463nFAC_p^0(\frac{nFvD}{RT})^{1/2} \quad (\text{eq. 3})$$

$$\frac{i}{i_p} = \frac{2.24\sqrt{\frac{RT}{nFv}}\sqrt{n'k_{obs}}}{1 + exp[\frac{nF}{RT}(E - E_{redox})]} \quad (\text{eq. 4})$$

Figure S27(a) presents data in the format of i/i_p versus E - Eredox, where the $E_{cat/2} = E_{redox}$. The influence of substrate consumption caused the response current to deviate from an ideal S shape. In figure S27(b), we observed a deviation from the predicted linear relationship according to eq. 4, but at the foot of the wave, the plot holds to the linear expectation. Thus, a linear extrapolation can be performed to retrieve the expected linear relationship. From eq. 4, k_{obs} can be determined from the slope of the foot of the wave (eq. 5). In eq. 5, m is slope of the tangent line, n is the number of unique electron-transfer processes that occur at the electrode per catalyst and n′ is the catalyst equivalents used per turnover. R is the universal gas constant, T is the temperature in Kelvin, F is Faraday's constant, υ is the scan rate.

$$m = 2.24\sqrt{\frac{RT}{nFv}}\sqrt{n'k_{obs}} \quad (\text{eq. 5})$$

In the presence of 100 mM TFA, we can get a slop of 16, 43, 23 and 36 for Ni-**1** to Ni-**4** respectively from Fig. S25b. Thus we can get the k_{obs} of 384, 2773.5, 793.5, 1944 for Ni-**1** to Ni-**4** respectively by eq. 5. Compared to k_{obs} of 135, 745, 51, 154 for Ni-**1** to Ni-**4** calculated by eq. 1 in this work, the k_{obs} calculated form the FOWA is larger. However, the results from the two calculation methods show the same trend that the β- hydrogenation of the pyrrole ring enhance the reactivities of nickel porphyrinoids with the k_{obs} of Ni-**2** > Ni-**1**, and Ni-**4** > Ni-**3**.

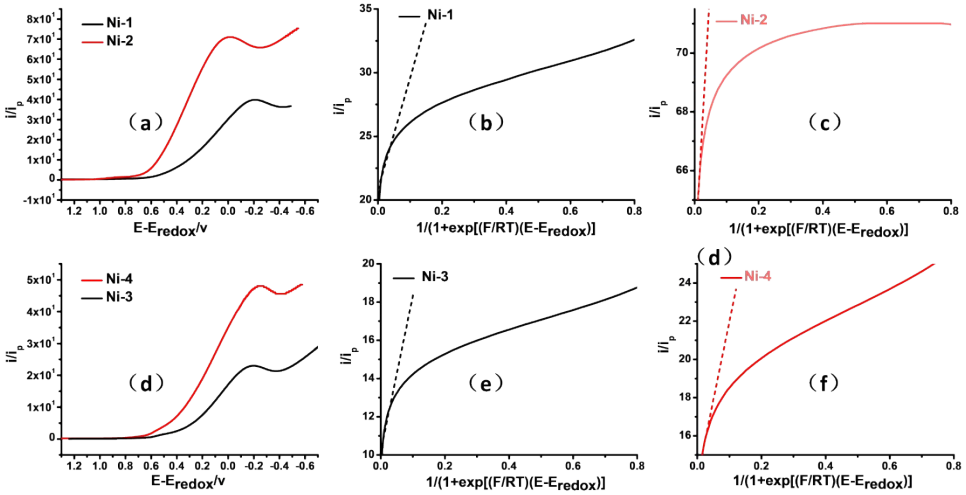


Fig. S27 Segment of the cyclic voltammogram of Ni-**1**, Ni-**2** (a) and Ni-**3**, Ni-**4** (b) with TFA. Conditions: MeCN, 0.1 M $^nBu_4NPF_6$, 0.1 Vs^{-1}, [Ni-P] = 1 mM, [TFA] = 100 mM. FOWA plot for the same CV responses showing the linear fits obtained for Ni-**1**(b), Ni-**2**(c), Ni-**3**(e) and Ni-**4**(f).

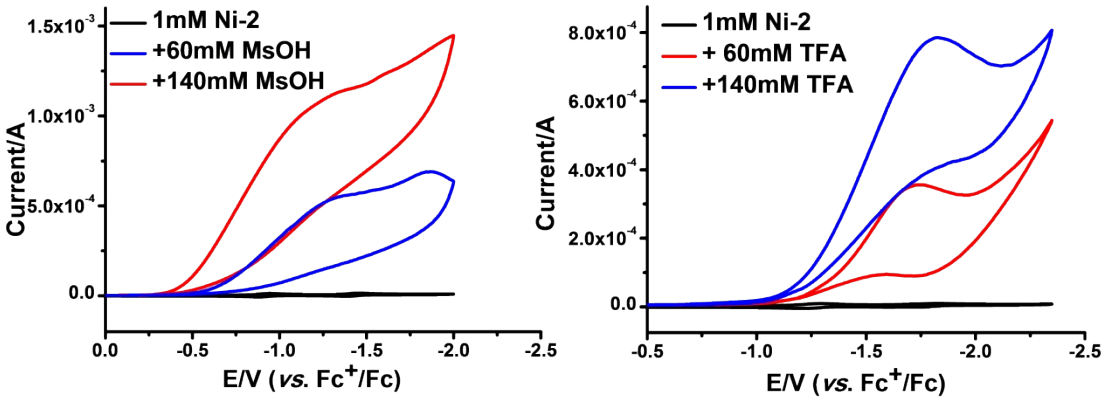


Fig. S28 Successive cyclic voltammograms of 1.0 mM Ni-**2** in CH_3CN (0.10 M $^nBu_4NPF_6$) at increasing concentrations of TFA. Conditions: 3 mm glassy-carbon working electrode; 25 °C; scan rate 100 mV/s.

4. Chemistry titration.

Typical Experimental Conditions: Acetonitrile solutions of Ni-**1** or Ni-**2** (1.6×10^{-5} M) and $Co(Cp^*)_2$ (9.3×10^{-4} M) were prepared in the glove box and stored in airtight cuvettes and vial respectively. The solution of Ni-**1** or Ni-**2** and 25μL $Co(Cp^*)_2$ were mixed and the UV-vis spectra were recorded immediately after the mixing.

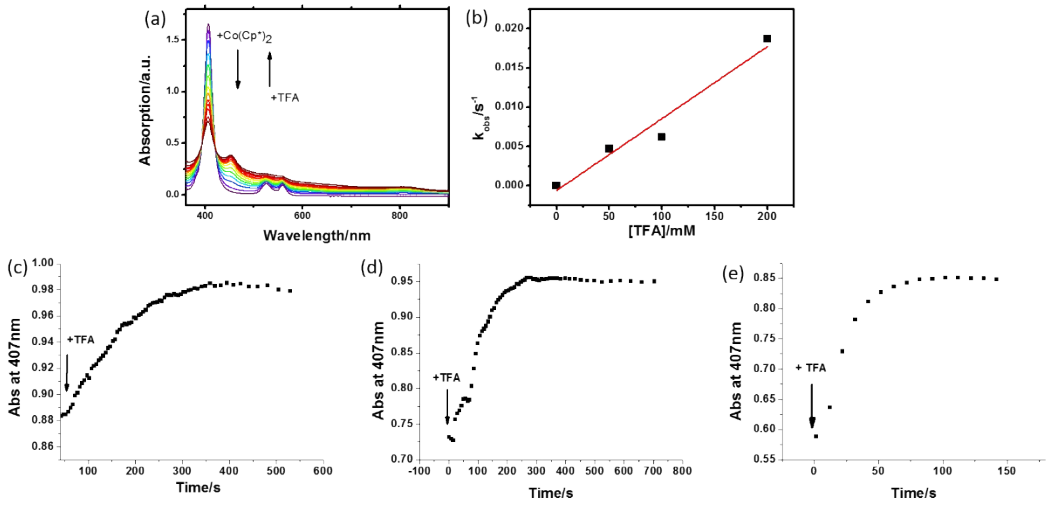


Fig. S29 (a) UV-*vis* spectral changes due to the reaction of Ni-**1** with excessive amount of $Co(Cp^*)_2$ to generate $[Ni\text{-}\mathbf{1}]^{2-}$ and the subsequent reaction with TFA in deaerated CH_3CN ([Ni-**1**] = 1.6×10^{-5} M; [Co(Cp*)2] = 1.6×10^{-5} M; T=10 °C). Time profiles of absorbance at 407 nm band due to the reaction of $[Ni\text{-}\mathbf{1}]^{2-}$ with various amounts of TFA: (c) 8.0×10^{-4} M (50eq), (d) 1.6×10^{-3} M (100eq), (e) 3.2×10^{-3} M (200eq). k_{obs} obtained by First-order plots of the reaction of $[Ni\text{-}\mathbf{1}]^{2-}$ with various amounts of TFA are summarized as plot of k_{obs} *vs.* the concentration of TFA (b).

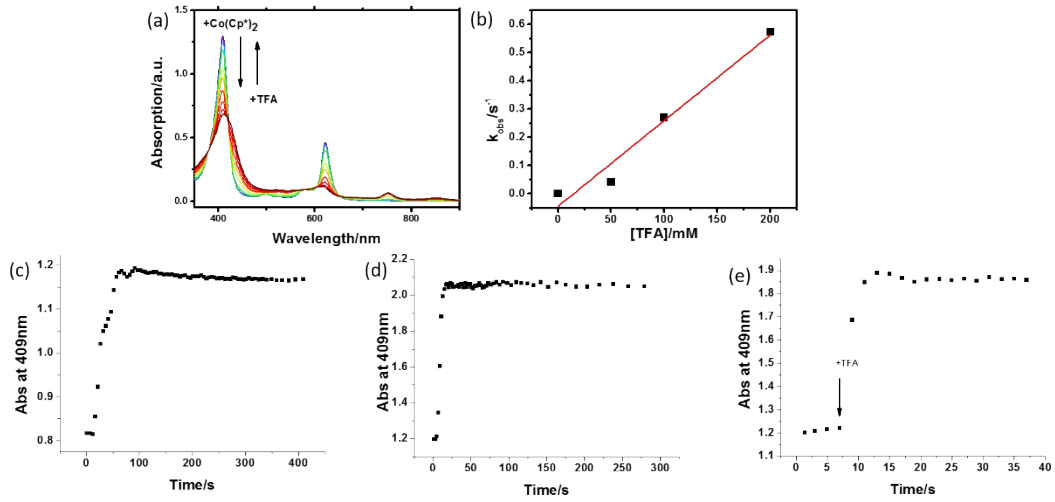


Fig. S30 (a) UV-*vis* spectral changes due to the reaction of Ni-**2** with excessive amount of $Co(Cp^*)_2$ to generate $[Ni\text{-}\mathbf{2}]^{2-}$ and the subsequent reaction with TFA in deaerated CH_3CN ($[Ni\text{-}\mathbf{2}] = 1.6\times10^{-5}$ M; $[Co(Cp^*)_2] = 1.6\times10^{-5}$ M; T=10 °C). Time profiles of absorbance at 409 nm band due to the reaction of $[Ni\text{-}\mathbf{2}]^{2-}$ with various amounts of TFA: (c) 8.0×10^{-4} M (50eq), (d) 1.6×10^{-3} M (100eq), (e) 3.2×10^{-3} M (200eq). K_{obs} obtained by first-order plots of the reaction of $[Ni\text{-}\mathbf{2}]^{2-}$ with various amounts of TFA are summarized as plot of k_{obs} *vs.* the concentration of TFA (b).

5. Computational details

5.1. General

All geometry optimizations calculations were performed using the density functional theory (DFT) functional B3LYP/6-31+G(d) as basis set and LAN2DZ as pseudopotential as implemented in the Gaussian 09 software.[2] Solvent effect was considered in all geometry optimizations and property calculations using the conductor-like polarizable continuum model (CPCM). The energies were corrected by single point calculations using B3LYP/6-31+G(d,p) as basis set. The frequency calculations at the same level were carried out to confirm each stationary point to be either a minimum or transition state. Intrinsic reaction coordinate (IRC) paths were calculated to connect each TS to corresponding reactant and product.[3]

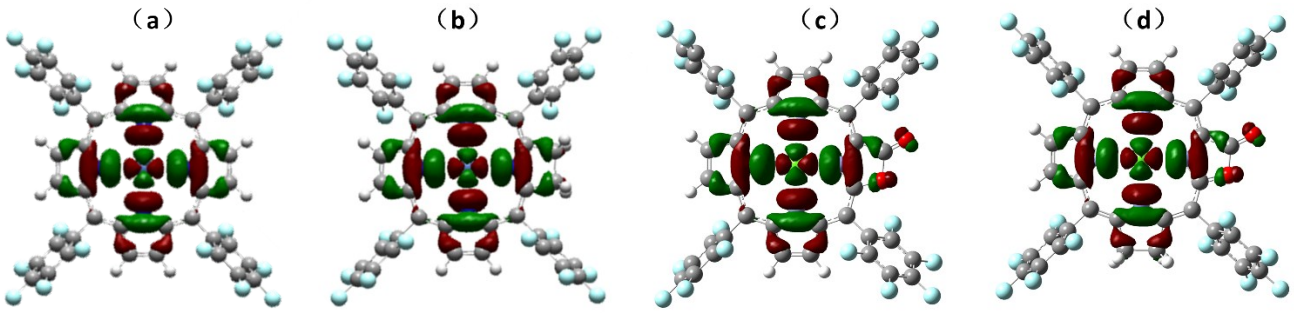


Fig. S31 Calculated SOMO of [Ni-**1**]$^{-}$ (a), [Ni-**2**]$^{-}$ (b), [Ni-**3**]$^{-}$ (c), [Ni-**4**]$^{-}$ (d) showing electron density localized on the nickel center.

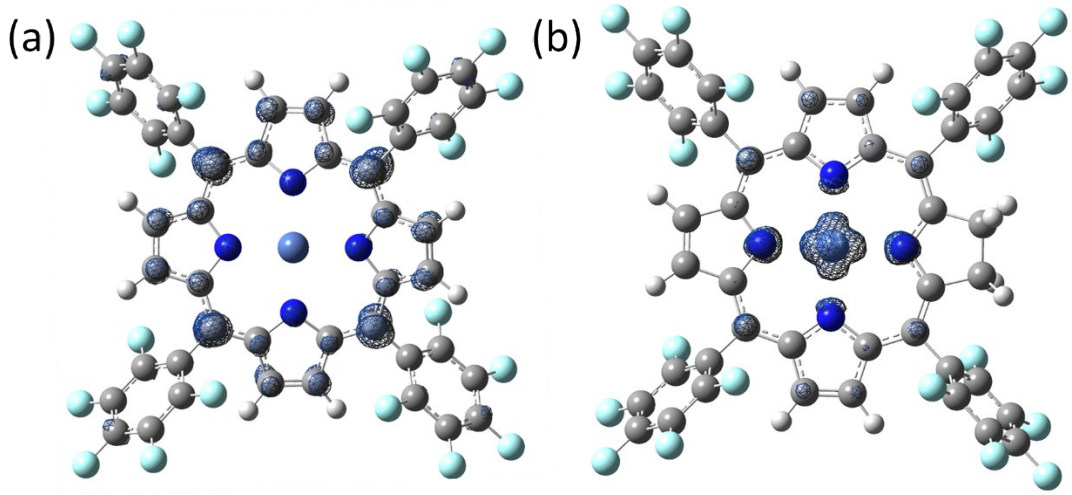


Fig. S32 Computed Mulliken atomic spin density (B3LYP with geometry optimized in solution, IsoValue: 0.005) plots of [Ni-**1**]$^{2-}$ (a) and [Ni-**2**]$^{2-}$ (b).

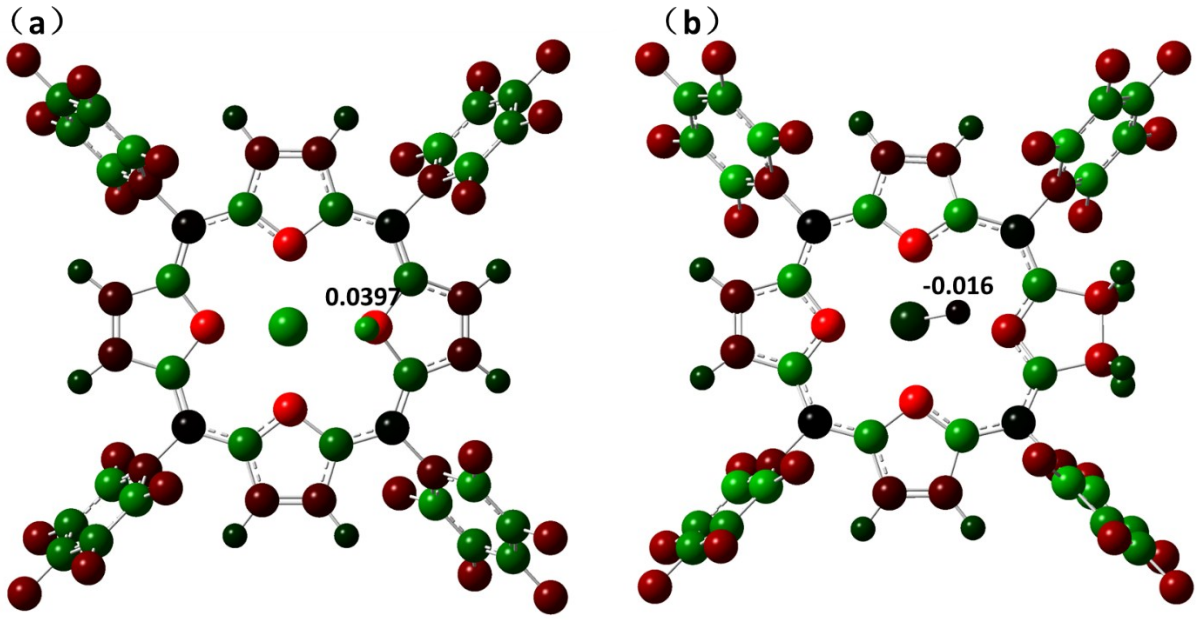


Fig. S33 Computed Mulliken charge distribution plots of [Ni-**1**-H]$^{2-}$ (a) and [H-Ni-**2**]$^{2-}$ (b).

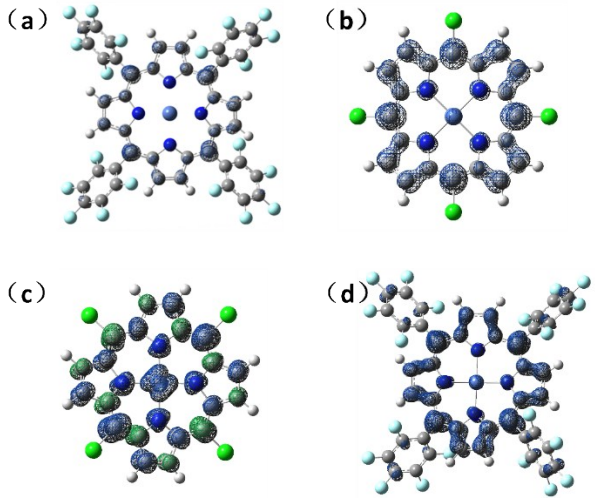


Fig. S34 Computed Mulliken atomic spin density (geometry optimized in solution, IsoValue: 0.005 for (a) and 0.03 for (b), (c) and (d)) plots of [Ni-**1**]$^{2-}$. The computed spin density is found to be almost entirely on the ligand for (a), (b) and (d) (SD on Ni=0.0026, 0.0021 and 0.0048 for (a), (b) and (d) respectively). Computational Details: Optimizations were performed with B3LYP as functional, 6-31+G(d) as basis set and LAN2DZ as pseudopotential for (a) and (b). Optimizations were performed with B3P86 as functional and the 6-31+G(d,p) as basis set for (c) and (d). Chlorine atoms to truncate pentafluorophenyl meso-substituents of the porphyrin ring for (b) and (c).

Table S8. Calculated Mulliken atomic spin densities of [Ni-**1**]$^{2-}$

Functional	B3LYP	B3P86	BLYP	BP86	M06L
[Ni-**1**]$^{2-}$	0.017	0.0032	0.032	0.037	0.020

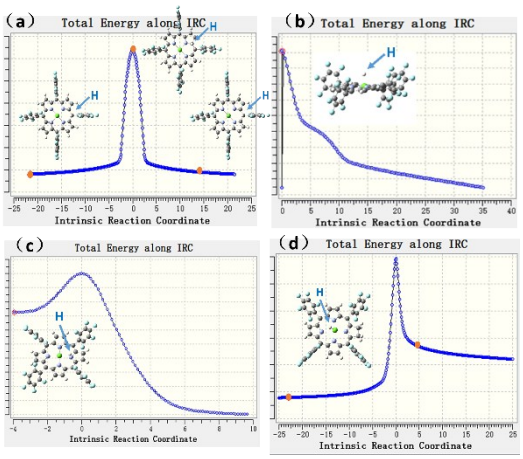


Fig. S35 IRC path for the transition state of H-atom added to the meso-carbon (a), nickel center (b) and the pyrrolic nitrogen (c) for Ni-1. IRC path for the transition state of H-atom added to nickel center (d) for Ni-**2**.

Table S9 Mulliken atomic spin densities of triplet [Ni-**1**]$^{2-}$

Mulliken atomic spin densities:1

1	C	0.165520
2	C	0.165477
3	C	0.046756
4	C	0.046546
5	N	0.039237
6	N	0.039234
7	C	0.043133
8	C	0.043111
9	C	0.165659
10	C	0.165352
11	C	0.046606
12	C	0.046689
13	C	0.043154
14	C	0.043099
15	C	0.000577
16	C	0.000540
17	C	0.027394
18	C	0.022753
19	C	-0.011412
20	C	-0.007924
21	C	0.042178
22	C	0.042019
23	C	-0.007926
24	C	-0.011323
25	C	0.022775
26	C	0.027248
27	C	0.000570
28	C	0.000544
29	C	0.027395
30	C	0.022703
31	C	-0.011410
32	C	-0.007892
33	C	0.042218
34	C	0.041969
35	C	-0.007957
36	C	-0.011320
37	C	0.022822
38	C	0.027239
39	F	0.000904
40	F	0.000803
41	F	0.000805
42	F	0.000899
43	F	-0.000395
44	F	-0.000237
45	F	0.002097
46	F	0.002089
47	F	-0.000237
48	F	-0.000390

49	F	0.000804
50	F	0.000899
51	F	0.000904
52	F	0.000801
53	F	-0.000394
54	F	-0.000235
55	F	0.002099
56	F	0.002087
57	F	-0.000239
58	F	-0.000390
59	N	0.039285
60	N	0.039183
61	C	0.070802
62	C	0.065404
63	H	-0.003855
64	H	-0.004104
65	C	0.070944
66	C	0.065343
67	H	-0.004110
68	H	-0.003853
69	Ni	0.002623
70	C	0.070868
71	C	0.065282
72	C	0.070730
73	C	0.065336
74	H	-0.003850
75	H	-0.004101
76	H	-0.003849
77	H	-0.004106

Sum of Mulliken atomic spin densities = 2.00000

Table S10 Mulliken atomic spin densities of triplet [Ni-**2**]$^{2-}$

Mulliken atomic spin densities:

		1
1	C	0.074918
2	C	0.051145
3	C	-0.043439
4	C	-0.037727
5	N	0.036239
6	N	0.037375
7	C	-0.042013
8	C	-0.039743
9	C	0.071546
10	C	0.054375
11	C	0.022346
12	C	0.032131
13	C	0.032119
14	C	0.020905
15	C	-0.000336
16	C	0.000391
17	C	0.004082
18	C	0.010928
19	C	-0.000175
20	C	-0.003869
21	C	0.014392
22	C	0.009040
23	C	-0.005410
24	C	0.002118
25	C	0.013550
26	C	0.001024
27	C	0.000109
28	C	0.001158
29	C	0.013507
30	C	0.002897
31	C	-0.005427
32	C	0.001195
33	C	0.014288
34	C	0.014093
35	C	0.000016
36	C	-0.005726

37	C	0.003745
38	C	0.013727
39	F	-0.000024
40	F	0.000510
41	F	-0.000030
42	F	0.000629
43	F	0.000006
44	F	-0.000084
45	F	0.000696
46	F	0.000435
47	F	-0.000141
48	F	0.000096
49	F	0.000613
50	F	-0.000039
51	F	0.000623
52	F	-0.000011
53	F	-0.000147
54	F	0.000071
55	F	0.000689
56	F	0.000679
57	F	0.000014
58	F	-0.000205
59	N	0.109593
60	N	0.126573
61	C	0.041773
62	C	0.051247
63	H	-0.002054
64	H	-0.001623
65	C	-0.008401
66	C	-0.007138
67	H	0.001447
68	H	0.001369
69	Ni	1.218029
70	C	0.052464
71	C	0.040978
72	C	0.005881
73	C	0.005449
74	H	-0.001864
75	H	-0.001151
76	H	-0.001587
77	H	-0.002145
78	H	-0.001908
79	H	-0.000809

Sum of Mulliken atomic spin densities = 2.00000

Table S11 Mulliken atomic spin densities of triplet [Ni-**3**]$^{2-}$

Mulliken atomic spin densities: 1

1	C	-0.062735
2	C	-0.108728
3	C	0.271139
4	C	0.268664
5	N	-0.620713
6	N	-0.635201
7	C	-0.156721
8	C	-0.131128
9	C	0.252454
10	C	0.246197
11	C	-0.022747
12	C	-0.030656
13	C	0.168533
14	C	0.262029
15	C	0.517091
16	C	0.282303

17 C -0.188204
18 C -0.141870
19 C 0.332207
20 C 0.320379
21 C 0.271092
22 C 0.268620
23 C 0.280313
24 C 0.275013
25 C 0.272558
26 C 0.268099
27 C 0.325196
28 C 0.330164
29 C -0.191290
30 C -0.206002
31 C 0.362295
32 C 0.339184
33 C 0.271870
34 C 0.275073
35 C 0.288584
36 C 0.287865
37 C 0.274724
38 C 0.273658
39 C 0.344130
40 C 0.345212
41 F -0.306076
42 F -0.305889
43 F -0.300735
44 F -0.301372
45 F -0.304324
46 F -0.306376
47 F -0.300208
48 F -0.302498
49 F -0.304229
50 F -0.306502
51 F -0.305412
52 F -0.308547
53 F -0.301687
54 F -0.301240
55 F -0.301751
56 F -0.301383
57 F -0.297213
58 F -0.297142
59 F -0.301311
60 F -0.301575
63 N -0.604280
64 N -0.605716
65 C -0.108016
66 C -0.130083
69 C -0.051515
70 C -0.072699

73	Ni	0.356712
74	C	0.493260
75	O	-0.501559
76	O	-0.499285

Sum of Mulliken atomic spin densities = 2.00000

Table S12 Mulliken atomic spin densities of triplet [Ni-**4**]$^{2-}$

Mulliken atomic spin densities: 1

1	C	0.073495
2	C	0.018154
3	C	0.085184
4	C	0.073195
5	N	0.113414
6	N	0.165968
7	C	0.043737
8	C	0.092067
9	C	0.004950
10	C	0.010518
11	C	0.073343
12	C	0.202410
13	C	-0.043283
14	C	-0.076899
15	C	0.008097
16	C	-0.022786
17	C	-0.006750
18	C	-0.001014
19	C	0.003569
20	C	-0.000211
21	C	-0.001712
22	C	0.001026
23	C	0.005032
24	C	0.000245
25	C	-0.002146
26	C	0.000268
27	C	0.007505
28	C	0.001754
29	C	-0.004749
30	C	-0.014811
31	C	0.006588
32	C	0.012677
33	C	-0.002352
34	C	-0.004175
35	C	0.005236
36	C	0.008847
37	C	-0.001793
38	C	-0.002605
39	C	0.004356
40	C	0.007742
41	F	-0.000005
42	F	0.000098
43	F	0.000054

44	F	-0.000005
45	F	-0.000030
46	F	0.000060
47	F	0.000319
48	F	0.000017
49	F	-0.000037
50	F	0.000060
51	F	0.000406
52	F	0.000129
53	F	0.000254
54	F	0.000355
55	F	-0.000037
56	F	-0.000044
57	F	0.000342
58	F	0.000575
59	F	-0.000037
60	F	-0.000011
61	H	-0.002033
62	H	-0.004034
63	N	0.036685
64	N	0.039957
65	C	0.070876
66	C	0.012418
67	C	-0.031411
68	H	0.000507
69	H	0.002405
70	Ni	0.949478
71	C	0.001432
72	H	-0.000176
73	H	0.000285
74	C	0.005691
75	H	-0.001754
76	H	-0.001177
77	O	0.082737
78	O	-0.008441

Sum of Mulliken atomic spin densities = 2.0000

5.2. Energy plot

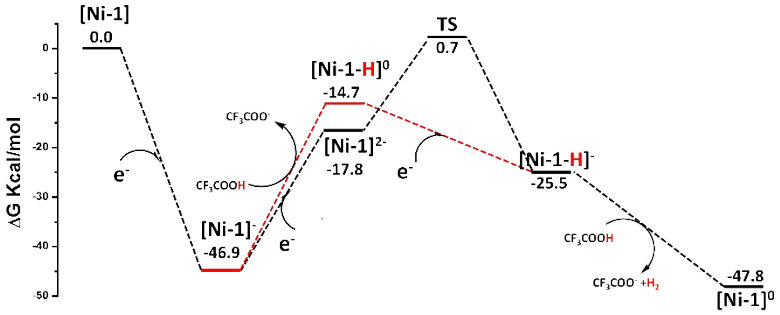


Fig. S36 Energy diagram for HER catalyzed by Ni-**1**. Free-energy values are given in kcal/mol.

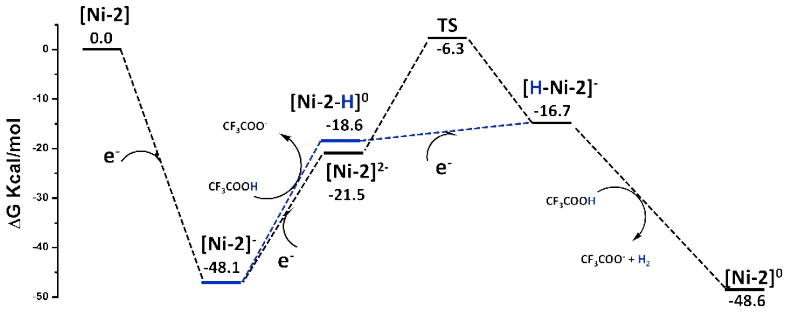


Fig. S37 Energy diagram for HER catalyzed by Ni-**2**. Free-energy values are given in kcal/mol.

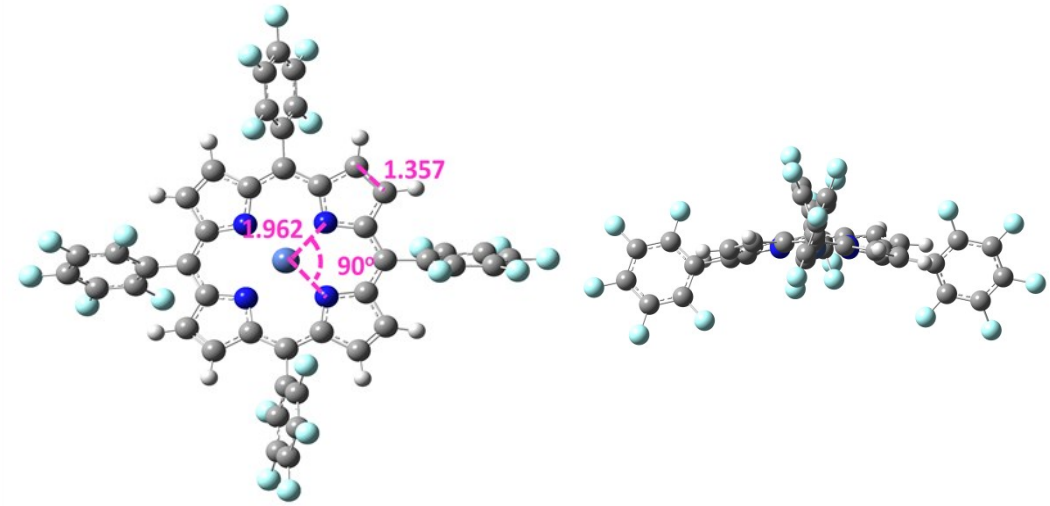
The energies of hydrogen evolution are calculated by a thermodynamic cycle as follow.

$[Ni\text{-}P]^-$	⟶	$[Ni\text{-}P] + e^-$	FE^o
$[Ni\text{-}P]^{2-}$	⟶	$[Ni\text{-}P]^- + e^-$	FE^o
$2AH$	⟶	$2A^- + 2H^+$	$\ln(10)RTpK_a$
$2H^+ + 2e^-$	⟶	H_2	$-2FE^o(H^+/H_2)$
$[Ni\text{-}P]^{2-} + 2AH$	⟶	$[Ni\text{-}P]^0 + 2A^- + H_2$	ΔG^o

Scheme S1. Thermodynamic analysis of HER. $E^o(H^+/H_2)$ is the experimental potential for the normal hydrogen electrode in acetonitrile, determined to be -0.14 V *vs*. Fc^+/Fc. The $pK_a$was the experimental value of TFA (p*K*a = 12.7).

5.3. Cartesian Coordinates for Key Species

Ni-1

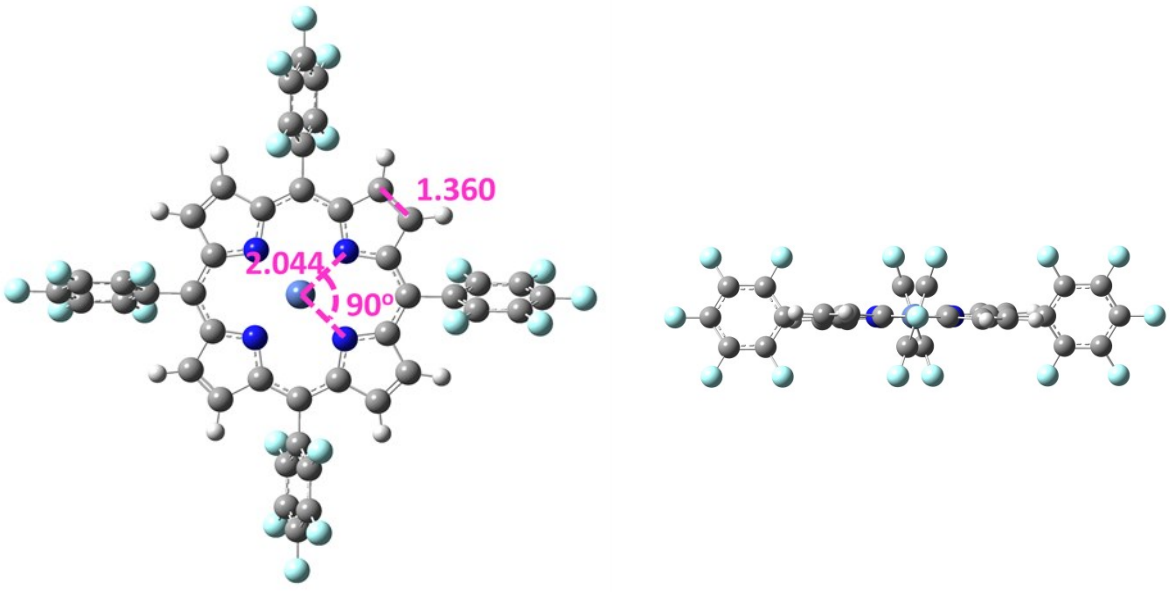


Charge = 0 Multiplicity = 1

C	-3.0806	1.25475	-0.3579
C	3.33011	-0.87534	-0.32652
C	-2.85549	-0.09859	-0.11005
C	3.10449	0.48342	-0.11118
N	1.00167	-1.55776	0.08768
N	-0.75296	1.94647	0.04492
C	-1.89661	-2.0021	0.39483
C	2.14465	2.39792	0.34818
C	-0.94133	-3.00582	0.53802
C	1.18902	3.40456	0.46652
C	0.41513	-2.78309	0.30564
C	-0.16684	3.17651	0.23584
C	2.3248	-1.82928	-0.18533
C	-2.07541	2.21163	-0.2375
C	-4.4704	1.69447	-0.68102
C	4.72045	-1.32262	-0.63668
C	-5.27547	2.36208	0.24797
C	5.27886	-1.09674	-1.89958
C	-6.57359	2.76529	-0.05729
C	6.57593	-1.49537	-2.21508
C	-7.09868	2.4946	-1.31924
C	7.34918	-2.13929	-1.25158
C	-6.32408	1.82697	-2.26538
C	6.82261	-2.37786	0.01624
C	-5.02726	1.43681	-1.93851
C	5.52424	-1.96684	0.30977
C	-1.38538	-4.39237	0.86911
C	1.63205	4.79807	0.76837
C	-2.0405	-5.2065	-0.06089
C	1.38827	5.36943	2.02214
C	-2.4481	-6.50153	0.25159
C	1.78205	6.66984	2.32981
C	-2.19477	-7.01416	1.52224
C	2.43928	7.43337	1.36753
C	-1.5398	-6.23038	2.46965
C	2.69601	6.89375	0.10879
C	-1.14492	-4.93687	2.13538
C	2.28943	5.59227	-0.17711
F	-4.80305	2.63222	1.47213

F	4.56003	-0.48249	-2.84736
F	-0.51978	-4.20783	3.06811
F	2.54637	5.10579	-1.3986
F	-7.31871	3.40245	0.85188
F	7.07956	-1.268	-3.43225
F	-8.3415	2.87505	-1.62087
F	8.5922	-2.52766	-1.54208
F	-6.8262	1.56903	-3.47706
F	7.56658	-2.99207	0.94197
F	-4.30716	0.79934	-2.86983
F	5.05027	-2.2063	1.53969
F	-2.29393	-4.7461	-1.29318
F	0.76105	4.66009	2.96857
F	-3.07301	-7.25549	-0.65878
F	1.53738	7.18598	3.53834
F	-2.57965	-8.2539	1.83086
F	2.82311	8.6795	1.65065
F	-1.29838	-6.72056	3.6896
F	3.32316	7.62829	-0.81581
N	1.87655	1.07201	0.08552
N	-1.62794	-0.68257	0.10217
C	2.55857	-3.25159	-0.17938
C	1.38483	-3.83986	0.16243
H	1.1768	-4.89399	0.27514
H	3.50445	-3.72912	-0.38872
C	-3.31892	-2.23549	0.40763
C	-3.91078	-1.06607	0.05732
H	-3.79425	-3.17842	0.63454
H	-4.96608	-0.85921	-0.04629
Ni	0.12432	0.19453	0.08004
C	-2.3089	3.63371	-0.2658
C	-1.13601	4.22975	0.06529
C	3.56695	2.63173	0.35775
C	4.15942	1.45466	0.0352
H	5.21486	1.24562	-0.06229
H	4.04183	3.57972	0.56356
H	-0.92816	5.28622	0.15373
H	-3.2541	4.10626	-0.48905

[Ni-1]$^{-}$

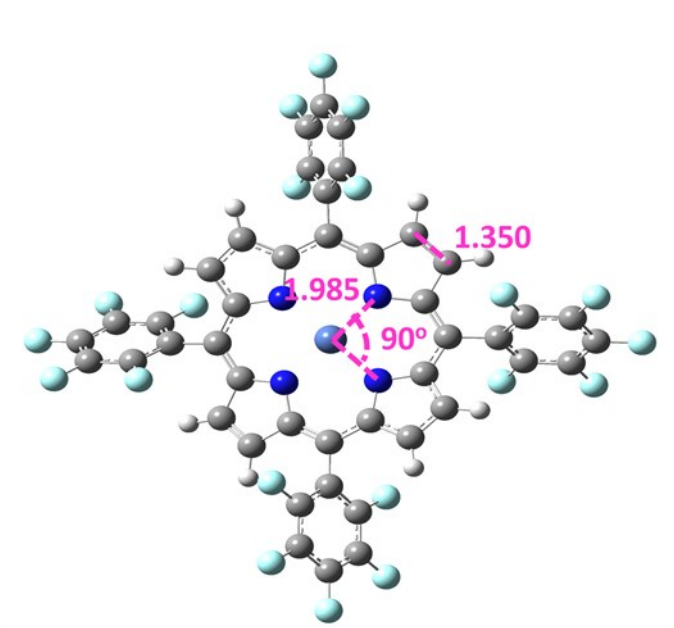


Charge = -1 Multiplicity = 2

C	-3.15227	1.24913	0.06287
C	3.40055	-0.86109	0.09517
C	-2.92688	-0.13767	0.10182
C	3.17502	0.52627	0.10154
N	1.05745	-1.62532	0.10397
N	-0.80917	2.01346	0.05912
C	-1.92626	-2.08961	0.12656
C	2.17443	2.47829	0.0787
C	-0.93111	-3.0821	0.11762
C	1.17935	3.47032	0.04416
C	0.45607	-2.85693	0.09419
C	-0.20781	3.24454	0.02228
C	2.40822	-1.85641	0.08393
C	-2.15991	2.24392	0.03064
C	-4.57584	1.70753	0.05552
C	4.82417	-1.31926	0.10016
C	-5.16073	2.3086	1.17608
C	5.64234	-1.19208	-1.02833
C	-6.48452	2.74386	1.18028
C	6.97107	-1.61227	-1.03481
C	-7.26782	2.57626	0.04228
C	7.51663	-2.18667	0.10933
C	-6.72027	1.97913	-1.0892
C	6.73112	-2.33225	1.24882
C	-5.39177	1.55847	-1.07185
C	5.40715	-1.89776	1.23355
C	-1.38951	-4.5056	0.13408
C	1.63757	4.89386	0.02995
C	-1.97632	-5.10248	-0.98771
C	1.49576	5.72411	1.14781
C	-2.41125	-6.42638	-0.98343
C	1.9161	7.0528	1.14551
C	-2.25776	-7.19764	0.16474
C	2.50551	7.58599	0.00318
C	-1.67498	-6.638	1.29779
C	2.66585	6.78829	-1.12582
C	-1.25447	-5.3096	1.27176
C	2.231	5.46457	-1.10198
F	-4.44877	2.48143	2.29743
F	5.15782	-0.65445	-2.15548
F	-0.70868	-4.81127	2.38894
F	2.39662	4.73845	-2.21533
F	-7.01345	3.31472	2.274
F	7.72598	-1.47627	-2.13635
F	-8.54369	2.98847	0.0364
F	8.79273	-2.59821	0.1142
F	-7.47305	1.82187	-2.18936
F	7.25823	-2.88122	2.35458
F	-4.90534	0.99856	-2.18727
F	4.69322	-2.04873	2.35682
F	-2.1351	-4.40256	-2.11867
F	0.94336	5.25177	2.27298
F	-2.9682	-6.96692	-2.07865
F	1.76599	7.81947	2.23706
F	-2.66966	-8.47355	0.17888
F	2.91738	8.86192	-0.01001
F	-1.53124	-7.37916	2.40764
F	3.22935	7.30351	-2.22986
N	1.94365	1.12733	0.06971
N	-1.69542	-0.73923	0.08706
C	2.6705	-3.28345	0.0435
C	1.4611	-3.90322	0.05001

H	1.26776	-4.96695	0.01583
H	3.64668	-3.74767	0.00352
C	-3.3528	-2.35123	0.18482
C	-3.97264	-1.14193	0.16952
H	-3.81661	-3.32677	0.24183
H	-5.03596	-0.94806	0.21228
Ni	0.12413	0.19405	0.07997
C	-2.42215	3.66961	-0.04334
C	-1.21277	4.28944	-0.04853
C	3.60082	2.74118	0.13484
C	4.22063	1.53188	0.14879
H	5.28383	1.33911	0.19877
H	4.06451	3.71777	0.17065
H	-1.01943	5.3521	-0.10714
H	-3.39822	4.1328	-0.09617

[Ni-1]$^{2-}$

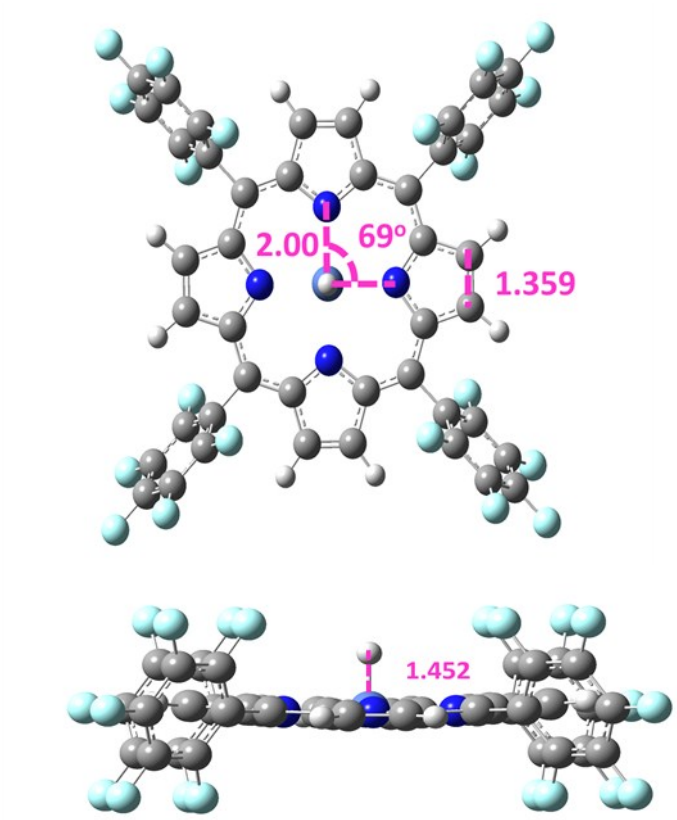


Charge = -2 Multiplicity = 3

C	-3.14291	1.2369	-0.32321
C	3.39227	-0.85761	-0.29145
C	-2.89778	-0.09587	-0.07414
C	3.14653	0.48047	-0.07297
N	1.02493	-1.58334	-0.05267
N	-0.77623	1.96799	-0.0955
C	-1.9042	-2.04292	0.26381
C	2.15207	2.43472	0.21757
C	-0.96558	-3.05224	0.28022
C	1.21345	3.44409	0.20865
C	0.4133	-2.82198	-0.04411
C	-0.16472	3.20662	-0.1131
C	2.35347	-1.83782	-0.3634
C	-2.10414	2.21544	-0.41421
C	-4.54618	1.69769	-0.41773
C	4.79569	-1.32019	-0.37246
C	-5.10364	2.62577	0.48239
C	5.66547	-0.88455	-1.3896
C	-6.41923	3.06781	0.38616
C	6.99087	-1.30311	-1.47985
C	-7.24726	2.5811	-0.62373

C	7.49766	-2.20695	-0.55324
C	-6.738	1.65916	-1.53094
C	6.66668	-2.67392	0.46353
C	-5.41295	1.24215	-1.42853
C	5.35075	-2.23033	0.5473
C	-1.36617	-4.43538	0.60363
C	1.61342	4.83431	0.50127
C	-2.31185	-5.16274	-0.14604
C	1.02882	5.56473	1.55718
C	-2.68632	-6.4666	0.16915
C	1.37235	6.88038	1.84463
C	-2.09082	-7.12217	1.2404
C	2.336	7.53509	1.07776
C	-1.12743	-6.45078	1.99304
C	2.93291	6.85581	0.02218
C	-0.78288	-5.14217	1.67625
C	2.5595	5.54489	-0.26373
F	-4.38144	3.09459	1.50842
F	5.23047	-0.04256	-2.3417
F	0.11689	-4.54302	2.46817
F	3.1337	4.97558	-1.33911
F	-6.91862	3.93833	1.28763
F	7.78331	-0.8611	-2.47802
F	-8.52871	2.99271	-0.71257
F	8.77947	-2.61985	-0.63009
F	-7.52761	1.19768	-2.52248
F	7.16359	-3.52626	1.38357
F	-4.97539	0.38132	-2.3624
F	4.62584	-2.67904	1.58043
F	-2.88468	-4.61771	-1.2347
F	0.1286	4.98304	2.36149
F	-3.59812	-7.11782	-0.58369
F	0.80992	7.52543	2.888
F	-2.4447	-8.38631	1.55453
F	2.68878	8.80629	1.36329
F	-0.56632	-7.07223	3.05137
F	3.84513	7.49035	-0.74423
N	1.90273	1.09447	-0.03992
N	-1.65409	-0.70891	-0.02361
C	2.55051	-3.2076	-0.61375
C	1.32542	-3.83256	-0.40008
H	1.09158	-4.88445	-0.50471
H	3.48665	-3.66998	-0.89973
C	-3.32588	-2.23996	0.48712
C	-3.93458	-1.05892	0.24641
H	-3.78805	-3.17421	0.77454
H	-4.99113	-0.83463	0.30855
Ni	0.12433	0.19271	-0.03819
C	-2.30095	3.57941	-0.69482
C	-1.07633	4.20906	-0.49271
C	3.5731	2.63696	0.44011
C	4.18241	1.45064	0.22857
H	5.23874	1.22785	0.29916
H	4.03449	3.57756	0.70742
H	-0.84242	5.25841	-0.62017
H	-3.23667	4.03519	-0.9925

[H-Ni-1]^{0}

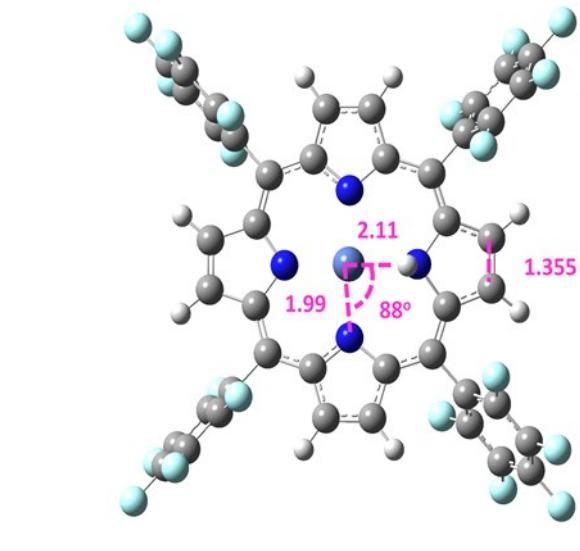


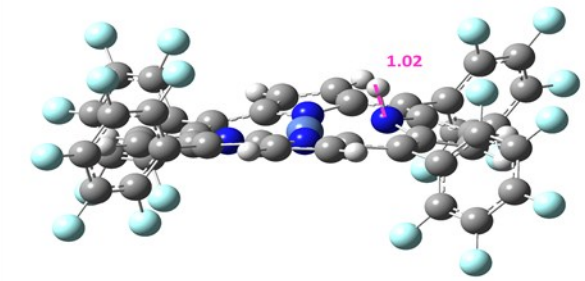
Charge = 0 Multiplicity = 2

C	-3.15227	1.24913	0.06287
C	3.40055	-0.86109	0.09517
C	-2.92688	-0.13767	0.10182
C	3.17502	0.52627	0.10154
N	1.05745	-1.62532	0.10397
N	-0.80917	2.01346	0.05912
C	-1.92626	-2.08961	0.12656
C	2.17443	2.47829	0.0787
C	-0.93111	-3.0821	0.11762
C	1.17935	3.47032	0.04416
C	0.45607	-2.85693	0.09419
C	-0.20781	3.24454	0.02228
C	2.40822	-1.85641	0.08393
C	-2.15991	2.24392	0.03064
C	-4.57584	1.70753	0.05552
C	4.82417	-1.31926	0.10016
C	-5.16073	2.3086	1.17608
C	5.64234	-1.19208	-1.02833
C	-6.48452	2.74386	1.18028
C	6.97107	-1.61227	-1.03481
C	-7.26782	2.57626	0.04228
C	7.51663	-2.18667	0.10933
C	-6.72027	1.97913	-1.0892
C	6.73112	-2.33225	1.24882
C	-5.39177	1.55847	-1.07185
C	5.40715	-1.89776	1.23355
C	-1.38951	-4.5056	0.13408
C	1.63757	4.89386	0.02995
C	-1.97632	-5.10248	-0.98771
C	1.49576	5.72411	1.14781
C	-2.41125	-6.42638	-0.98343
C	1.9161	7.0528	1.14551
C	-2.25776	-7.19764	0.16474
C	2.50551	7.58599	0.00318

C	-1.67498	-6.638	1.29779
C	2.66585	6.78829	-1.12582
C	-1.25447	-5.3096	1.27176
C	2.231	5.46457	-1.10198
F	-4.44877	2.48143	2.29743
F	5.15782	-0.65445	-2.15548
F	-0.70868	-4.81127	2.38894
F	2.39662	4.73845	-2.21533
F	-7.01345	3.31472	2.274
F	7.72598	-1.47627	-2.13635
F	-8.54369	2.98847	0.0364
F	8.79273	-2.59821	0.1142
F	-7.47305	1.82187	-2.18936
F	7.25823	-2.88122	2.35458
F	-4.90534	0.99856	-2.18727
F	4.69322	-2.04873	2.35682
F	-2.1351	-4.40256	-2.11867
F	0.94336	5.25177	2.27298
F	-2.9682	-6.96692	-2.07865
F	1.76599	7.81947	2.23706
F	-2.66966	-8.47355	0.17888
F	2.91738	8.86192	-0.01001
F	-1.53124	-7.37916	2.40764
F	3.22935	7.30351	-2.22986
N	1.94365	1.12733	0.06971
N	-1.69542	-0.73923	0.08706
C	2.6705	-3.28345	0.0435
C	1.4611	-3.90322	0.05001
H	1.26776	-4.96695	0.01583
H	3.64668	-3.74767	0.00352
C	-3.3528	-2.35123	0.18482
C	-3.97264	-1.14193	0.16952
H	-3.81661	-3.32677	0.24183
H	-5.03596	-0.94806	0.21228
Ni	0.12413	0.19405	0.07997
C	-2.42215	3.66961	-0.04334
C	-1.21277	4.28944	-0.04853
C	3.60082	2.74118	0.13484
C	4.22063	1.53188	0.14879
H	5.28383	1.33911	0.19877
H	4.06451	3.71777	0.17065
H	-1.01943	5.3521	-0.10714
H	-3.39822	4.1328	-0.09617
H	0.14135	0.17195	1.7505

[H-Ni-1]$^{-}$



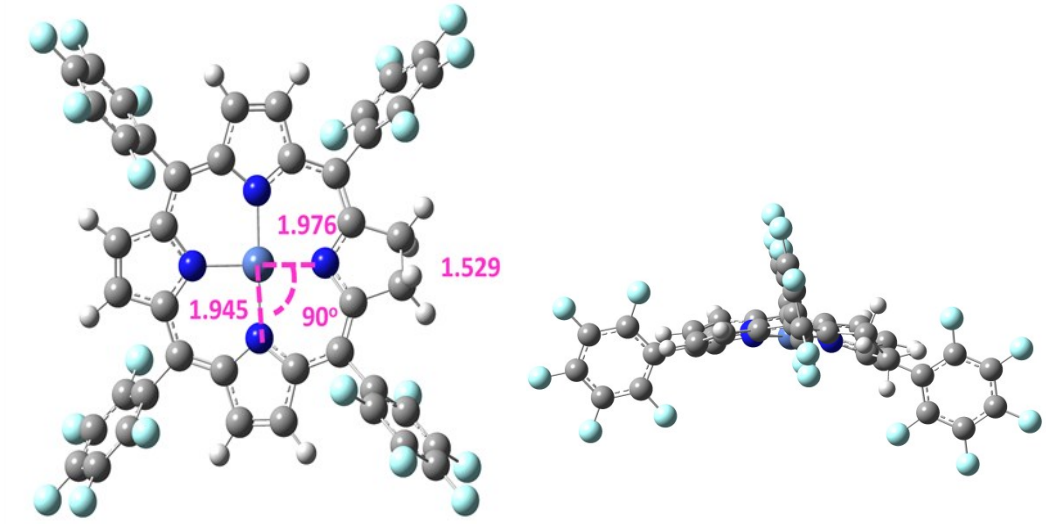


Charge = -1 Multiplicity = 1

C	-3.14329	1.24064	-0.09413
C	3.43231	-0.8555	0.26817
C	-2.88024	-0.10131	-0.22341
C	3.24309	0.49101	0.26383
N	1.03253	-1.58197	0.24715
N	-0.78427	1.96991	0.2132
C	-1.88041	-2.07625	-0.13667
C	2.19416	2.54474	0.32607
C	-0.95451	-3.06934	0.06749
C	1.21004	3.48392	0.34975
C	0.44252	-2.8267	0.25714
C	-0.18828	3.22259	0.36256
C	2.40037	-1.83418	0.34549
C	-2.13491	2.22835	0.13739
C	-4.55707	1.69929	-0.1486
C	4.83483	-1.34566	0.12514
C	-5.21434	2.21834	0.97615
C	5.27996	-1.97929	-1.04157
C	-6.53271	2.66452	0.93159
C	6.58396	-2.45141	-1.1744
C	-7.24728	2.58903	-0.2609
C	7.48581	-2.29335	-0.12515
C	-6.63209	2.07347	-1.39701
C	7.07714	-1.66526	1.04698
C	-5.30683	1.64708	-1.33173
C	5.76693	-1.20376	1.15891
C	-1.41607	-4.48242	0.11297
C	1.64075	4.91232	0.27409
C	-1.90743	-5.14025	-1.02288
C	2.22295	5.55516	1.37137
C	-2.33664	-6.46584	-0.99247
C	2.62536	6.88869	1.32354
C	-2.266	-7.18638	0.19527
C	2.44646	7.6179	0.15235
C	-1.77473	-6.57032	1.34315
C	1.87014	7.00862	-0.95927
C	-1.36564	-5.24025	1.29183
C	1.47759	5.67358	-0.88919
F	-4.58028	2.2877	2.15476
F	4.45437	-2.13645	-2.08183
F	-0.92229	-4.68723	2.42926
F	0.94422	5.12515	-1.98626

F	-7.12891	3.14793	2.03437
F	6.98298	-3.04663	-2.30864
F	-8.52176	3.00647	-0.31201
F	8.74354	-2.74057	-0.24613
F	-7.3162	2.00508	-2.55119
F	7.9437	-1.51444	2.06081
F	-4.75726	1.17366	-2.45951
F	5.4156	-0.61128	2.30967
F	-1.97906	-4.49826	-2.19791
F	2.40808	4.89348	2.5229
F	-2.80336	-7.05887	-2.10398
F	3.17828	7.47448	2.39697
F	-2.67253	-8.46474	0.23622
F	2.83068	8.90054	0.09251
F	-1.71859	-7.25935	2.49517
F	1.70762	7.70997	-2.09137
N	1.94724	1.11699	0.53209
N	-1.63325	-0.71063	-0.20107
C	2.64313	-3.21804	0.45013
C	1.41216	-3.84601	0.4007
H	1.21719	-4.90902	0.40581
H	3.61321	-3.68126	0.57147
C	-3.31317	-2.31848	-0.22484
C	-3.92073	-1.11801	-0.28456
H	-3.77819	-3.29415	-0.19878
H	-4.98214	-0.91481	-0.31571
Ni	0.08816	0.17618	0.10926
C	-2.39452	3.6128	0.27004
C	-1.1684	4.23445	0.41149
C	3.58622	2.73058	0.02793
C	4.2014	1.52277	-0.01683
H	5.23064	1.3284	-0.28593
H	4.0274	3.69148	-0.19974
H	-0.97876	5.29017	0.5516
H	-3.36599	4.0829	0.21464
H	1.72029	0.96925	1.52146

Ni-2



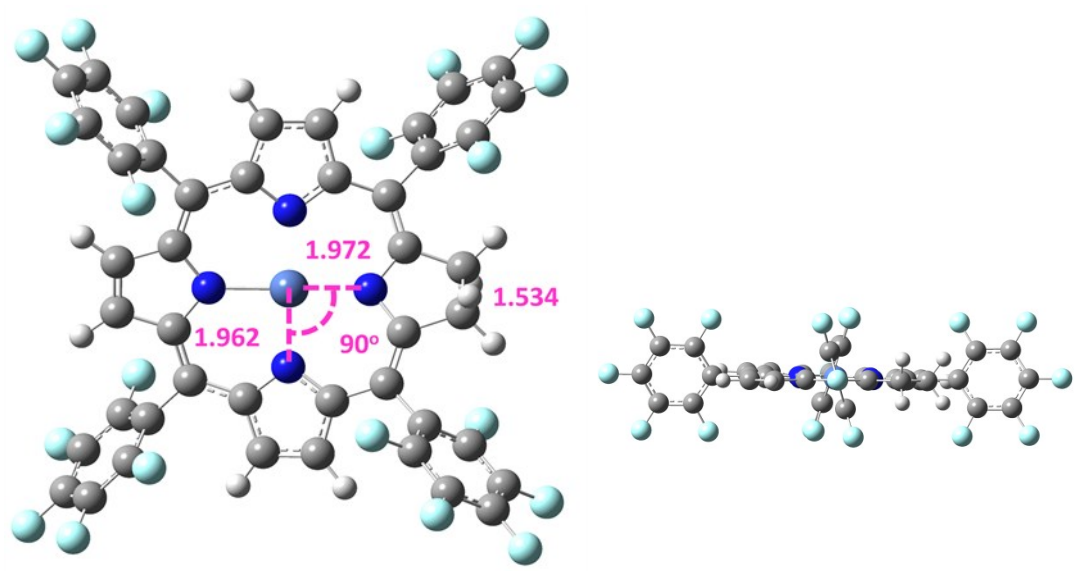
Charge = 0 Multiplicity = 1

C	2.36472	2.35516	0.57526
C	-2.3635	-2.37061	0.50418
C	2.7824	1.0481	0.39057
C	-2.78273	-1.05533	0.21197
N	-0.00221	-1.98848	0.00004
N	0.0021	1.94603	0.00009

C	-4.1613	-0.66638	0.04538
C	-4.15576	0.63019	-0.36934
C	2.78032	-1.06146	-0.21204
C	-2.78011	1.05422	-0.39066
C	2.3582	-2.37582	-0.50419
C	-2.35956	2.36039	-0.57518
C	1.05706	-2.79212	-0.33463
C	-1.04639	2.78029	-0.31623
C	-1.06326	-2.78976	0.33475
C	1.05243	2.77795	0.31648
C	3.37568	3.38534	0.97068
C	-3.40161	-3.36675	0.91416
C	4.15807	4.05939	0.02716
C	-3.71	-3.5787	2.2626
C	5.09577	5.02314	0.39373
C	-4.68101	-4.49195	2.6709
C	5.26813	5.3358	1.74104
C	-5.37711	-5.22676	1.71314
C	4.50433	4.68383	2.70739
C	-5.09569	-5.04365	0.36012
C	3.57376	3.72375	2.31353
C	-4.12008	-4.12375	-0.01808
C	3.39417	-3.37415	-0.91424
C	-3.36827	3.39278	-0.9706
C	4.11037	-4.13342	0.0179
C	-3.56611	3.73113	-2.3135
C	5.08411	-5.05527	-0.36036
C	-4.49465	4.69318	-2.70736
C	5.36595	-5.23806	-1.71333
C	-5.25658	5.34725	-1.74096
C	4.67209	-4.501	-2.671
C	-5.08439	5.03471	-0.39359
C	3.70289	-3.58585	-2.26265
C	-4.14875	4.06897	-0.02703
F	4.01604	3.78502	-1.28015
F	-3.05727	-2.88947	3.21332
F	3.05227	-2.8945	-3.21327
F	-4.00684	3.79474	1.28032
F	5.82999	5.64918	-0.53637
F	-4.94857	-4.66797	3.97187
F	6.16454	6.25895	2.10522
F	-6.31094	-6.10653	2.0901
F	4.66954	4.9827	4.00298
F	-5.76166	-5.75195	-0.56261
F	2.85483	3.11405	3.26965
F	-3.869	-3.97832	-1.33188
F	3.85887	-3.98829	1.33165
F	-2.84892	3.11946	-3.26967
F	5.74792	-5.76573	0.56228
F	-4.65969	4.99194	-4.003
F	6.29802	-6.11967	-2.09035
F	-6.15104	6.27229	-2.10513
F	4.94005	-4.67672	-3.97193
F	-5.81682	5.66277	0.53657
H	-5.0166	-1.30967	0.19798
H	-5.00642	1.25455	-0.60502
N	-1.95194	-0.00719	-0.04862
N	1.95187	-0.01148	0.0486
C	4.15976	-0.67554	-0.04554
C	4.1571	0.62103	0.3692
H	5.01362	-1.32074	-0.19814
H	5.00916	1.24349	0.60486
C	-0.64361	4.15304	-0.21472

C	0.65267	4.15159	0.2151
H	-1.27422	5.00838	-0.41354
H	1.28516	5.00553	0.41398
Ni	-0.00004	-0.0098	0.00002
C	-0.63759	-4.23937	0.42951
H	-0.40197	-4.49038	1.47385
H	-1.40377	-4.93524	0.0836
C	0.62821	-4.2408	-0.42928
H	1.39286	-4.93831	-0.0833
H	0.39205	-4.49137	-1.4736

[Ni-2]$^-$



Charge = -1 Multiplicity = 2

C	-2.64807	1.41569	0.21141
C	3.66002	-0.71226	0.22415
C	-2.32901	0.11612	0.2783
C	3.46521	0.6501	0.22268
N	1.39217	-1.44432	0.92566
N	-0.4673	2.17787	0.87659
C	-1.36296	-1.76822	0.30578
C	2.45482	2.62748	0.20181
C	-0.49301	-2.78658	0.27232
C	1.46175	3.58059	0.17465
C	0.81187	-2.61727	0.46369
C	0.07233	3.35374	0.37662
C	2.66527	-1.70465	0.44109
C	-1.75203	2.3809	0.39415
C	-4.05698	1.79654	-0.11509
C	5.03464	-1.21324	-0.08847
C	-4.92279	2.31568	0.85365
C	5.57387	-1.16576	-1.37869
C	-6.23571	2.67837	0.55864
C	6.84796	-1.6435	-1.67785
C	-6.71935	2.51957	-0.73643
C	7.62444	-2.20476	-0.66882
C	-5.88645	2.0034	-1.72462
C	7.12266	-2.2732	0.62749
C	-4.57538	1.65358	-1.40703
C	5.84909	-1.77813	0.90122
C	-1.002	-4.16058	-0.02731
C	1.85888	4.98686	-0.14738
C	-1.40518	-4.52896	-1.31568

C	1.85095	5.98933	0.83078
C	-1.88143	-5.80546	-1.60857
C	2.19098	7.31116	0.54897
C	-1.95892	-6.75964	-0.59851
C	2.56246	7.66572	-0.74448
C	-1.56316	-6.42868	0.69386
C	2.5878	6.69649	-1.74246
C	-1.096	-5.14361	0.96385
C	2.23306	5.38466	-1.43575
F	-4.50547	2.47636	2.11629
F	4.86575	-0.62745	-2.38517
F	-0.73582	-4.86828	2.22434
F	2.27702	4.48583	-2.43285
F	-7.04027	3.17187	1.51359
F	7.32949	-1.57378	-2.92929
F	-7.98194	2.86316	-1.03055
F	8.85094	-2.67274	-0.94239
F	-6.3504	1.85477	-2.97566
F	7.87396	-2.80709	1.60346
F	-3.80786	1.16972	-2.39239
F	5.41525	-1.85604	2.16637
F	-1.33863	-3.6473	-2.32179
F	1.50929	5.69546	2.09242
F	-2.25799	-6.12562	-2.85687
F	2.1714	8.24357	1.51443
F	-2.41256	-7.99224	-0.86972
F	2.89579	8.93346	-1.02726
F	-1.64178	-7.34716	1.67004
F	2.9453	7.03523	-2.99155
N	2.2748	1.29079	0.3995
N	-1.03208	-0.40732	0.39391
C	2.94364	-3.0976	0.24525
C	1.74872	-3.68776	0.27795
H	1.51035	-4.70979	0.01554
H	3.89167	-3.53541	-0.03729
C	-2.76512	-2.04226	0.17336
C	-3.36836	-0.86544	0.15618
H	-3.21946	-3.02061	0.09256
H	-4.42692	-0.66538	0.0585
Ni	0.88242	0.5776	0.57731
C	-2.07171	3.76303	0.17968
C	-0.8943	4.38872	0.15125
C	3.91499	2.98269	-0.06585
C	4.60817	1.6188	-0.06588
H	5.40912	1.51693	0.67688
H	4.29358	3.68368	0.68932
H	-0.69308	5.4091	-0.14657
H	-3.03741	4.16095	-0.10185
H	5.04727	1.42373	-1.04955
H	4.03159	3.4617	-1.04359

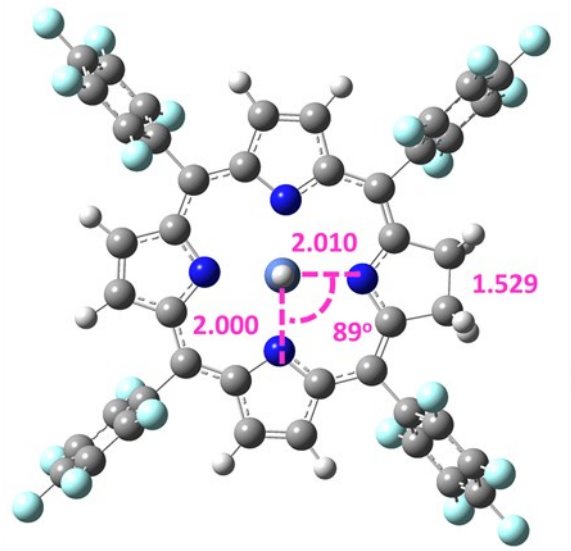
[Ni-2]$^{2-}$

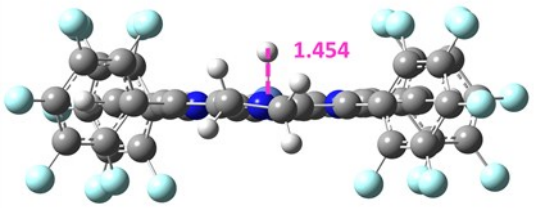
Charge = -2 Multiplicity = 3

C	2.36472	2.35516	0.57526
C	-2.3635	-2.37061	0.50418
C	2.7824	1.0481	0.39057
C	-2.78273	-1.05533	0.21197
N	-0.00221	-1.98848	0.00004
N	0.0021	1.94603	0.00009
C	-4.1613	-0.66638	0.04538
C	-4.15576	0.63019	-0.36934
C	2.78032	-1.06146	-0.21204
C	-2.78011	1.05422	-0.39066
C	2.3582	-2.37582	-0.50419
C	-2.35956	2.36039	-0.57518
C	1.05706	-2.79212	-0.33463
C	-1.04639	2.78029	-0.31623
C	-1.06326	-2.78976	0.33475
C	1.05243	2.77795	0.31648
C	3.37568	3.38534	0.97068
C	-3.40161	-3.36675	0.91416
C	4.15807	4.05939	0.02716
C	-3.71	-3.5787	2.2626
C	5.09577	5.02314	0.39373
C	-4.68101	-4.49195	2.6709
C	5.26813	5.3358	1.74104
C	-5.37711	-5.22676	1.71314
C	4.50433	4.68383	2.70739
C	-5.09569	-5.04365	0.36012
C	3.57376	3.72375	2.31353
C	-4.12008	-4.12375	-0.01808
C	3.39417	-3.37415	-0.91424
C	-3.36827	3.39278	-0.9706
C	4.11037	-4.13342	0.0179
C	-3.56611	3.73113	-2.3135
C	5.08411	-5.05527	-0.36036
C	-4.49465	4.69318	-2.70736
C	5.36595	-5.23806	-1.71333
C	-5.25658	5.34725	-1.74096
C	4.67209	-4.501	-2.671
C	-5.08439	5.03471	-0.39359
C	3.70289	-3.58585	-2.26265
C	-4.14875	4.06897	-0.02703
F	4.01604	3.78502	-1.28015
F	-3.05727	-2.88947	3.21332

F	3.05227	-2.8945	-3.21327
F	-4.00684	3.79474	1.28032
F	5.82999	5.64918	-0.53637
F	-4.94857	-4.66797	3.97187
F	6.16454	6.25895	2.10522
F	-6.31094	-6.10653	2.0901
F	4.66954	4.9827	4.00298
F	-5.76166	-5.75195	-0.56261
F	2.85483	3.11405	3.26965
F	-3.869	-3.97832	-1.33188
F	3.85887	-3.98829	1.33165
F	-2.84892	3.11946	-3.26967
F	5.74792	-5.76573	0.56228
F	-4.65969	4.99194	-4.003
F	6.29802	-6.11967	-2.09035
F	-6.15104	6.27229	-2.10513
F	4.94005	-4.67672	-3.97193
F	-5.81682	5.66277	0.53657
H	-5.0166	-1.30967	0.19798
H	-5.00642	1.25455	-0.60502
N	-1.95194	-0.00719	-0.04862
N	1.95187	-0.01148	0.0486
C	4.15976	-0.67554	-0.04554
C	4.1571	0.62103	0.3692
H	5.01362	-1.32074	-0.19814
H	5.00916	1.24349	0.60486
C	-0.64361	4.15304	-0.21472
C	0.65267	4.15159	0.2151
H	-1.27422	5.00838	-0.41354
H	1.28516	5.00553	0.41398
Ni	-0.00004	-0.0098	0.00002
C	-0.63759	-4.23937	0.42951
H	-0.40197	-4.49038	1.47385
H	-1.40377	-4.93524	0.0836
C	0.62821	-4.2408	-0.42928
H	1.39286	-4.93831	-0.0833
H	0.39205	-4.49137	-1.4736

[H-Ni-2]^{0}



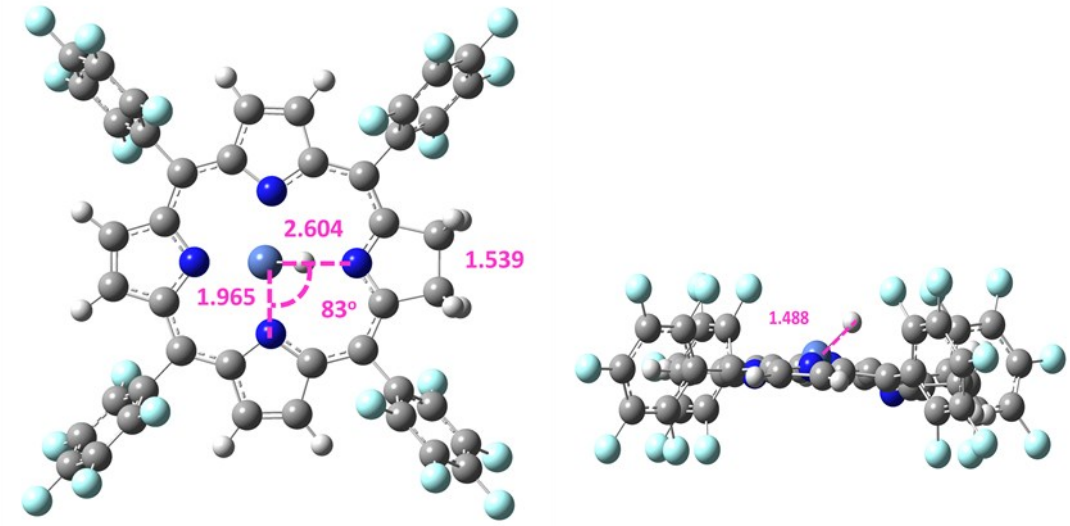


Charge = 0 Multiplicity = 2

C	2.43792	2.44254	0.07124
C	-2.43264	-2.42688	0.01948
C	2.87878	1.11226	0.06397
C	-2.87452	-1.0728	-0.02555
N	-0.00219	-2.06668	-0.00002
N	0.00214	2.04512	0.00008
C	-4.25861	-0.6601	-0.05242
C	-4.25816	0.70485	-0.08237
C	2.87222	-1.07886	0.02561
C	-2.87646	1.11833	-0.0638
C	2.42749	-2.432	-0.01954
C	-2.43281	2.44767	-0.07105
C	1.11193	-2.86185	-0.04046
C	-1.09459	2.87427	-0.0371
C	-1.11799	-2.8595	0.04034
C	1.10061	2.87195	0.03729
C	3.49078	3.50518	0.11229
C	-3.50113	-3.47327	0.04744
C	4.23597	3.84652	-1.02117
C	-3.7953	-4.20739	1.20183
C	5.22234	4.83076	-0.99247
C	-4.7909	-5.18127	1.23809
C	5.48244	5.50973	0.19409
C	-5.54164	-5.43839	0.09519
C	4.7573	5.19786	1.34022
C	-5.28232	-4.7262	-1.07212
C	3.78	4.20568	1.2881
C	-4.27291	-3.76557	-1.08426
C	3.49375	-3.48066	-0.04758
C	-3.48339	3.51256	-0.11212
C	4.26482	-3.77477	1.08413
C	-3.77124	4.21351	-1.288
C	5.27214	-4.7376	1.07194
C	-4.74634	5.20785	-1.34014
C	5.52998	-5.45022	-0.09542
C	-5.47059	5.52153	-0.19394
C	4.77987	-5.19134	-1.23835
C	-5.2118	4.84218	0.9927
C	3.78639	-4.2153	-1.20204
C	-4.22763	3.85575	1.0214
F	4.01354	3.22606	-2.18729
F	-3.09816	-3.99664	2.33039
F	3.08977	-4.00292	-2.33062

F	-4.00638	3.23499	2.18758
F	5.91849	5.13448	-2.09957
F	-5.03786	-5.86651	2.36592
F	6.42764	6.46039	0.23282
F	-6.50649	-6.36945	0.11696
F	5.0106	5.84983	2.48619
F	-5.99967	-4.97869	-2.17834
F	3.11279	3.93282	2.41709
F	-4.05219	-3.11661	-2.23566
F	4.04542	-3.12548	2.23559
F	-3.10481	3.93898	-2.41705
F	5.98885	-4.99179	2.17819
F	-4.99836	5.86021	-2.48617
F	6.49279	-6.38338	-0.11723
F	-6.41366	6.4743	-0.23266
F	5.0254	-5.877	-2.36624
F	-5.90708	5.14765	2.09986
H	-5.11978	-1.31443	-0.04051
H	-5.11752	1.36109	-0.11569
N	-2.05577	0.01033	-0.03216
N	2.05576	0.00599	0.03224
C	4.25718	-0.66907	0.05259
C	4.2596	0.69587	0.08258
H	5.11698	-1.3252	0.0407
H	5.12032	1.35032	0.11599
C	-0.67579	4.25851	-0.02244
C	0.68472	4.25707	0.02265
H	-1.33176	5.11857	-0.03684
H	1.34248	5.11577	0.03707
Ni	-0.00002	-0.00154	0.00003
C	-0.75665	-4.33678	0.13493
H	-0.98503	-4.71204	1.14037
H	-1.32008	-4.95196	-0.57359
C	0.74746	-4.33836	-0.13517
H	1.30958	-4.9548	0.57329
H	0.97504	-4.71401	-1.14064
H	0.14408	0.08781	1.39162

[H-Ni-2]$^{-}$



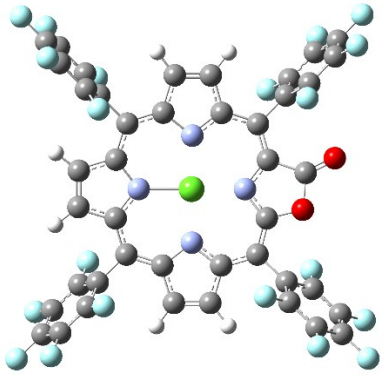
Charge = -1 Multiplicity = 1

C	-2.9712	1.16287	0.23611
C	3.60118	-0.84257	0.0726
C	-2.79094	-0.23503	0.17065

C	3.49706	0.53157	-0.16429
N	1.19356	-1.59907	0.36094
N	-0.58271	1.85535	0.33569
C	-1.79108	-2.18003	0.18213
C	2.49392	2.48124	-0.18154
C	-0.75948	-3.13918	0.26253
C	1.43549	3.36863	0.03673
C	0.61	-2.85499	0.30807
C	0.04648	3.06354	0.17935
C	2.54313	-1.79272	0.21684
C	-1.94325	2.11165	0.27509
C	-4.37718	1.6655	0.2411
C	4.98818	-1.37916	0.22268
C	-4.93592	2.2765	1.37063
C	5.91639	-1.3588	-0.82636
C	-6.24875	2.74342	1.38962
C	7.21635	-1.83963	-0.68997
C	-7.04805	2.59941	0.2596
C	7.62659	-2.37594	0.52646
C	-6.52676	1.99389	-0.87987
C	6.7341	-2.41757	1.59381
C	-5.2091	1.541	-0.87849
C	5.44219	-1.92077	1.43484
C	-1.16894	-4.57502	0.27753
C	1.80601	4.81142	0.16324
C	-1.74321	-5.18917	-0.84232
C	1.62996	5.51677	1.36328
C	-2.14127	-6.52434	-0.83551
C	1.97902	6.85874	1.4991
C	-1.96333	-7.29046	0.31262
C	2.53409	7.54143	0.42052
C	-1.39242	-6.71403	1.44325
C	2.73152	6.87458	-0.78441
C	-1.00817	-5.37476	1.41584
C	2.36408	5.53596	-0.89788
F	-4.21162	2.42399	2.48708
F	5.57058	-0.85888	-2.025
F	-0.47728	-4.86155	2.53284
F	2.56938	4.94364	-2.08659
F	-6.75277	3.32096	2.49137
F	8.07178	-1.80229	-1.72468
F	-8.31341	3.04267	0.26855
F	8.87416	-2.84643	0.67051
F	-7.29348	1.86204	-1.97381
F	7.13142	-2.92418	2.77159
F	-4.7472	0.98004	-2.00394
F	4.63008	-1.96927	2.49788
F	-1.91917	-4.49758	-1.97602
F	1.11735	4.90384	2.43725
F	-2.68354	-7.08136	-1.92988
F	1.79763	7.49717	2.6658
F	-2.33964	-8.57725	0.32866
F	2.8784	8.83182	0.54316
F	-1.22657	-7.44967	2.5535
F	3.26103	7.52936	-1.83059
N	2.33224	1.16373	-0.34325
N	-1.56983	-0.83708	0.13793
C	2.8217	-3.21532	0.13284
C	1.63287	-3.86704	0.18871
H	1.46007	-4.93086	0.10227
H	3.79921	-3.65366	-0.01044
C	-3.20942	-2.44778	0.21018
C	-3.83416	-1.23252	0.20315

H	-3.67235	-3.42459	0.25155
H	-4.89825	-1.04085	0.2376
Ni	0.1738	0.0625	0.61055
C	-2.16989	3.53108	0.13834
C	-0.94758	4.11725	0.07918
C	3.97296	2.87564	-0.1071
C	4.67708	1.50679	-0.09063
H	5.34984	1.3748	-0.94443
H	4.261	3.48081	-0.9732
H	-0.73447	5.16539	-0.07645
H	-3.13491	4.00923	0.0428
H	4.19214	3.468	0.78887
H	5.27269	1.35584	0.81727
H	1.16634	0.5803	1.59172

Ni-**3**

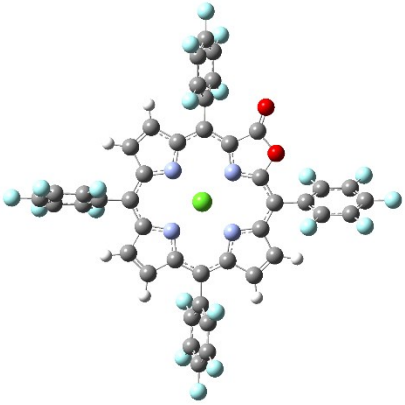


Charge = 0 Multiplicity = 1

C	2.36577	2.32511	0.58199
C	-2.35154	-2.38792	0.55994
C	2.77998	1.01858	0.38552
C	-2.77122	-1.07582	0.25501
N	-0.00214	-2.01169	-0.00004
N	0.0021	1.91461	-0.00002
C	-4.15026	-0.69791	0.06945
C	-4.14948	0.5892	-0.37155
C	2.76894	-1.08183	-0.25493
C	-2.77773	1.02461	-0.38543
C	2.34643	-2.393	-0.55999
C	-2.36069	2.33023	-0.58197
C	1.05116	-2.81577	-0.35586
C	-1.04657	2.74954	-0.31925
C	-1.0572	-2.81349	0.35567
C	1.05258	2.74726	0.31918
C	3.36665	3.35585	0.98809
C	-3.38919	-3.35615	1.02582
C	4.32532	3.85235	0.1006
C	-3.85809	-3.31415	2.34262
C	5.24957	4.82129	0.48053
C	-4.8428	-4.18148	2.80699
C	5.22374	5.32353	1.77851
C	-5.38739	-5.1262	1.94208
C	4.27773	4.85357	2.68524
C	-4.94406	-5.19591	0.62424
C	3.36594	3.8823	2.28297
C	-3.96224	-4.31349	0.18432
C	3.38198	-3.36349	-1.02584
C	-3.35936	3.36314	-0.98799
C	3.95259	-4.32239	-0.18445

C	-3.35773	3.88949	-2.28291
C	4.93235	-5.20707	-0.6244
C	-4.26745	4.86275	-2.68507
C	5.37612	-5.13812	-1.94214
C	-5.21224	5.33486	-1.7782
C	4.83397	-4.19188	-2.80692
C	-5.23893	4.83278	-0.48017
C	3.85125	-3.32231	-2.34253
C	-4.31676	3.86182	-0.10035
F	4.37301	3.39621	-1.16042
F	-3.35587	-2.41466	3.20257
F	3.35134	-2.42143	-3.20239
F	-4.36522	3.40587	1.16071
F	6.15617	5.27565	-0.39348
F	-5.26684	-4.11346	4.07524
F	6.10587	6.25404	2.15357
F	-6.33226	-5.96585	2.37552
F	4.25304	5.33404	3.93443
F	-5.46754	-6.10388	-0.20915
F	2.46848	3.44844	3.18099
F	-3.55377	-4.4114	-1.09197
F	3.54365	-4.41962	1.09174
F	-2.46141	3.45357	-3.18107
F	5.45345	-6.11652	0.20887
F	-4.24194	5.34306	-3.93431
F	6.31903	-5.97996	-2.37559
F	-6.09237	6.26731	-2.15315
F	5.25841	-4.12456	-4.07508
F	-6.14433	5.28924	0.39399
H	-5.00056	-1.34766	0.21939
H	-5.00132	1.19801	-0.63868
N	-1.94473	-0.02782	-0.0204
N	1.94471	-0.03204	0.02044
C	4.14878	-0.70694	-0.06927
C	4.15078	0.58017	0.37171
H	4.99767	-1.35857	-0.21915
H	5.00393	1.18714	0.63888
C	-0.64381	4.12055	-0.21501
C	0.65283	4.11914	0.21486
H	-1.27651	4.97497	-0.40887
H	1.28741	4.97217	0.4087
Ni	-0.00001	-0.03577	0.00001
C	0.62567	-4.265	-0.43321
O	1.25336	-5.60822	-0.38384
O	-0.63497	-4.26368	0.43272

[Ni-**3**]$^{2-}$

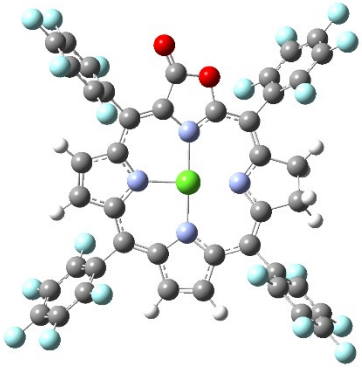


Charge = -2 Multiplicity = 3

C	2.38223	2.35924	0.55145
C	-2.37649	-2.38161	0.57786
C	2.79519	1.03639	0.35566
C	-2.81357	-1.06093	0.28941
N	-0.01522	-1.95843	0.06623
N	-0.00456	1.965	0.01015
C	-4.17247	-0.68429	0.11228
C	-4.17156	0.62636	-0.32545
C	2.76747	-1.09533	-0.25607
C	-2.81452	1.06212	-0.34289
C	2.34035	-2.41265	-0.52262
C	-2.38254	2.38364	-0.5478
C	1.02572	-2.81236	-0.27177
C	-1.06387	2.803	-0.29749
C	-1.0669	-2.74757	0.38594
C	1.07005	2.79507	0.30974
C	3.39845	3.38171	0.92957
C	-3.36615	-3.4088	0.99319
C	4.36139	3.85041	0.02913
C	-3.88873	-3.43231	2.29102
C	5.30407	4.81311	0.38065
C	-4.83634	-4.36824	2.69642
C	5.29647	5.34539	1.66609
C	-5.29016	-5.32148	1.78989
C	4.34929	4.90885	2.58715
C	-4.79485	-5.32787	0.48952
C	3.42098	3.94154	2.21182
C	-3.85414	-4.37522	0.10794
C	3.3576	-3.40426	-0.96479
C	-3.38099	3.41386	-0.94436
C	3.88478	-4.37468	-0.10703
C	-3.38479	3.96621	-2.23091
C	4.85412	-5.28348	-0.51809
C	-4.29789	4.94104	-2.62359
C	5.34218	-5.22804	-1.82045
C	-5.25065	5.39449	-1.71662
C	4.84735	-4.27198	-2.70093
C	-5.27837	4.87087	-0.42783
C	3.86893	-3.38137	-2.26631
C	-4.35041	3.90041	-0.05924
F	4.40105	3.37186	-1.22578
F	-3.47769	-2.53014	3.1983
F	3.41869	-2.47384	-3.15137
F	-4.40994	3.43222	1.19904
F	6.21387	5.23606	-0.5106
F	-5.31223	-4.36108	3.95158
F	6.19762	6.27264	2.0157
F	-6.19917	-6.23035	2.16764
F	4.34233	5.41814	3.82863
F	-5.23372	-6.24583	-0.38606
F	2.52745	3.54658	3.13435
F	-3.39926	-4.41986	-1.15518
F	3.42038	-4.48647	1.14684
F	-2.48591	3.55539	-3.14185
F	5.3281	-6.21066	0.331
F	-4.27166	5.4419	-3.86883
F	6.28026	-6.09621	-2.22539
F	-6.13776	6.32974	-2.08272
F	5.31205	-4.21818	-3.96025
F	-6.19356	5.31085	0.45039
H	-5.02427	-1.33594	0.25699
H	-5.02634	1.23569	-0.58727

N	-1.97865	0.0067	0.01757
N	1.94561	-0.01776	0.02081
C	4.13994	-0.71386	-0.11141
C	4.15198	0.59023	0.32041
H	4.98742	-1.36772	-0.26826
H	5.01482	1.19673	0.56152
C	-0.64575	4.16801	-0.19839
C	0.66972	4.16097	0.20378
H	-1.27754	5.02733	-0.38018
H	1.31197	5.01388	0.37966
Ni	-0.01507	0.01118	0.02703
C	0.57876	-4.16745	-0.18722
O	1.0336	-5.28948	-0.44531
O	-0.73333	-4.06375	0.40602

Ni-**4**



Charge = 0 Multiplicity = 1

C	2.4013	2.35038	0.59312
C	-2.31601	-2.36264	0.57107
C	2.81551	1.04385	0.39664
C	-2.73569	-1.05054	0.26613
N	0.03339	-1.98642	0.01109
N	0.03762	1.93989	0.0111
C	-4.11474	-0.67263	0.08057
C	-4.11395	0.61447	-0.36042
C	2.80446	-1.05656	-0.24381
C	-2.7422	1.04989	-0.3743
C	2.38196	-2.36773	-0.54886
C	-2.32516	2.35551	-0.57084
C	1.08669	-2.79049	-0.34473
C	-1.01104	2.77481	-0.30813
C	-1.02167	-2.78821	0.3668
C	1.08811	2.77253	0.3303
C	3.40218	3.38112	0.99922
C	-3.35366	-3.33088	1.03695
C	4.36085	3.87762	0.11172
C	-3.82256	-3.28888	2.35374
C	5.2851	4.84657	0.49166
C	-4.80727	-4.15621	2.81811
C	5.25927	5.34881	1.78964
C	-5.35187	-5.10093	1.95321
C	4.31326	4.87885	2.69636
C	-4.90853	-5.17064	0.63536
C	3.40146	3.90758	2.2941
C	-3.92671	-4.28821	0.19544
C	3.41751	-3.33821	-1.01471
C	-3.32383	3.38842	-0.97687
C	3.98811	-4.29711	-0.17332

C	-3.3222	3.91477	-2.27179
C	4.96788	-5.1818	-0.61327
C	-4.23192	4.88802	-2.67395
C	5.41165	-5.11284	-1.93101
C	-5.17671	5.36013	-1.76707
C	4.8695	-4.1666	-2.79579
C	-5.2034	4.85806	-0.46904
C	3.88678	-3.29703	-2.3314
C	-4.28123	3.88709	-0.08922
F	4.40854	3.42148	-1.14929
F	-3.32034	-2.38938	3.2137
F	3.38686	-2.39615	-3.19126
F	-4.32969	3.43114	1.17183
F	6.1917	5.30093	-0.38235
F	-5.23132	-4.08818	4.08637
F	6.1414	6.27932	2.1647
F	-6.29673	-5.94058	2.38664
F	4.28857	5.35932	3.94556
F	-5.43201	-6.0786	-0.19802
F	2.50401	3.47371	3.19212
F	-3.51824	-4.38612	-1.08085
F	3.57918	-4.39434	1.10287
F	-2.42588	3.47885	-3.16995
F	5.48898	-6.09124	0.21999
F	-4.20642	5.36834	-3.92319
F	6.35456	-5.95468	-2.36446
F	-6.05684	6.29259	-2.14202
F	5.29394	-4.09929	-4.06395
F	-6.1088	5.31452	0.40511
H	-4.96504	-1.32239	0.23051
H	-4.96579	1.22329	-0.62756
N	-1.9092	-0.00254	-0.00927
N	1.98024	-0.00676	0.03156
C	4.18631	0.60545	0.38284
C	-0.60828	4.14583	-0.20389
C	0.68836	4.14442	0.22599
H	-1.24099	5.00025	-0.39774
H	1.32294	4.99745	0.41982
Ni	0.03552	-0.01049	0.01113
C	-0.59944	-4.2384	0.44384
H	-0.36298	-4.50276	1.48332
H	-1.36609	-4.92562	0.0888
C	0.66119	-4.23972	-0.42209
H	1.42627	-4.92878	-0.06724
H	0.42413	-4.50326	-1.46163
O	5.24428	1.35813	0.71414
O	4.18431	-0.68166	-0.05815

[Ni-**4**]$^{2-}$

Charge = -2 Multiplicity = 3

C	2.4013	2.35038	0.59312
C	-2.31601	-2.36264	0.57107
C	2.81551	1.04385	0.39664
C	-2.73569	-1.05054	0.26613
N	0.03339	-1.98642	0.01109
N	0.03762	1.93989	0.0111
C	-4.11474	-0.67263	0.08057
C	-4.11395	0.61447	-0.36042
C	2.80446	-1.05656	-0.24381
C	-2.7422	1.04989	-0.3743
C	2.38196	-2.36773	-0.54886
C	-2.32516	2.35551	-0.57084
C	1.08669	-2.79049	-0.34473
C	-1.01104	2.77481	-0.30813
C	-1.02167	-2.78821	0.3668
C	1.08811	2.77253	0.3303
C	3.40218	3.38112	0.99922
C	-3.35366	-3.33088	1.03695
C	4.36085	3.87762	0.11172
C	-3.82256	-3.28888	2.35374
C	5.2851	4.84657	0.49166
C	-4.80727	-4.15621	2.81811
C	5.25927	5.34881	1.78964
C	-5.35187	-5.10093	1.95321
C	4.31326	4.87885	2.69636
C	-4.90853	-5.17064	0.63536
C	3.40146	3.90758	2.2941
C	-3.92671	-4.28821	0.19544
C	3.41751	-3.33821	-1.01471
C	-3.32383	3.38842	-0.97687
C	3.98811	-4.29711	-0.17332
C	-3.3222	3.91477	-2.27179
C	4.96788	-5.1818	-0.61327
C	-4.23192	4.88802	-2.67395
C	5.41165	-5.11284	-1.93101
C	-5.17671	5.36013	-1.76707
C	4.8695	-4.1666	-2.79579
C	-5.2034	4.85806	-0.46904
C	3.88678	-3.29703	-2.3314
C	-4.28123	3.88709	-0.08922
F	4.40854	3.42148	-1.14929
F	-3.32034	-2.38938	3.2137
F	3.38686	-2.39615	-3.19126
F	-4.32969	3.43114	1.17183
F	6.1917	5.30093	-0.38235
F	-5.23132	-4.08818	4.08637
F	6.1414	6.27932	2.1647
F	-6.29673	-5.94058	2.38664
F	4.28857	5.35932	3.94556
F	-5.43201	-6.0786	-0.19802
F	2.50401	3.47371	3.19212
F	-3.51824	-4.38612	-1.08085
F	3.57918	-4.39434	1.10287
F	-2.42588	3.47885	-3.16995
F	5.48898	-6.09124	0.21999
F	-4.20642	5.36834	-3.92319
F	6.35456	-5.95468	-2.36446
F	-6.05684	6.29259	-2.14202
F	5.29394	-4.09929	-4.06395

F	-6.1088	5.31452	0.40511
H	-4.96504	-1.32239	0.23051
H	-4.96579	1.22329	-0.62756
N	-1.9092	-0.00254	-0.00927
N	1.98024	-0.00676	0.03156
C	4.18631	0.60545	0.38284
C	-0.60828	4.14583	-0.20389
C	0.68836	4.14442	0.22599
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C	-0.59944	-4.2384	0.44384
H	-0.36298	-4.50276	1.48332
H	-1.36609	-4.92562	0.0888
C	0.66119	-4.23972	-0.42209
H	1.42627	-4.92878	-0.06724
H	0.42413	-4.50326	-1.46163
O	5.24428	1.35813	0.71414
O	4.18431	-0.68166	-0.05815

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