SUPPORTING INFORMATION FOR

Ligand-Based Electronic Effects on the Electrocatalytic Hydrogen Production by Thiosemicarbazone Nickel Complexes

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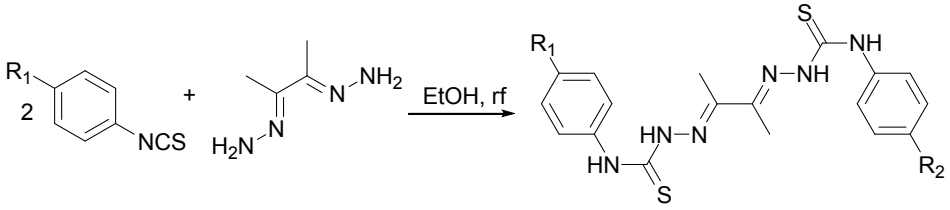
1. Synthesis



$R_1 = R_2 = SCH_3$; $R_1 = R_2 = N(CH_3)_2$; $R_1 = R_2 = CN$

A - General procedure for the synthesis of symmetric ligands

To a solution of butan-2,3-dihydrazone (1 eq.) in ethanol is added a solution of isothiocyanate (2 eq) in ethanol. After addition, the mixture was heated at reflux. After 2 hours, the heater was removed and the mixture was allowed to cool down to room temperature, then a water bath is used to cool the mixture down to 0°C. A precipitate formed. The solid obtained after filtration is washed with two portions of ethanol and used without any further purification.

1) (R_1= R_2= SCH_3): 2,3-di(4-(methylmercaptophenylthiosemicarbazone) butane

From butan-2,3-dione dihydrazone (0.148 g; 1.3 mmol), 4-methylthiophenyl isothiocyanate (2,6 mmol; 0.480 g), (**1**) is obtained as a yellow solid (0,352 g, 56 %)
^{1}H NMR (400 MHz, [D_6] DMSO, TMS): δ = 10.64 (s, 1H; NH), 9.95 (s, 1H; NH), 7.53 (d, *J* = 8,4 Hz, 2H; *o*-CH), 7.28 (d, *J* = 8,4 Hz, 2H; *m*-CH), 2.49 (s, 6H; S-CH_3), 2.30 (s, 6H; CH_3);
FT-IR: $\tilde{\nu}$ = 3218 cm^{-1} (N-H), 1582 cm^{-1} (C=N), 1486 cm^{-1} (C-N), 817 cm^{-1} (C=S).

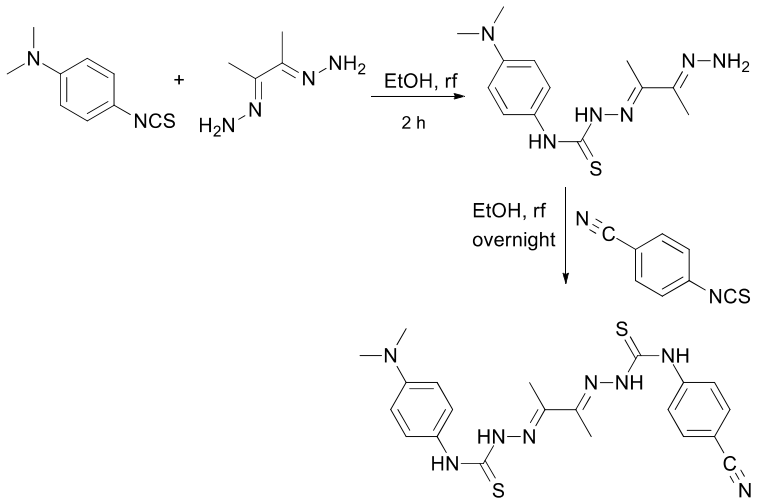
2) (R_1= R_2= $N(CH_3)_2$): 2,3-di(4-dimethylaminophenylthiosemicarbazone) butane

From butan-2,3-dione, dihydrazone (0,300 g, 2.6 mmol), 4-dimethylaminophenyl isothiocyanate (5.2 mmol; 0.916 g), (**2**) is obtained as a yellow solid (0,984g, 81 %)
^{1}H NMR (400 MHz, [D_6] DMSO, TMS): δ = 10.41 (s, 2H; NH), 9.78 (s, 2H; NH), 7,3 (d, *J* = 8.9 Hz, 4H; *o*-CH), 6.72 (d, *J* = 8,9 Hz, 4H; *m*-CH), 2.91 (s, 12H; N-$(CH_3)_2$), 2.31 (s, 6H; CH_3);
^{13}C NMR (100 MHz, [D_6] DMSO and [D_6] Acetone (5:1), TMS): δ = 12.2 (C-C=), 40.67 (N-CH_3), 112.2 (*o*-C=C), 126.9 (*m*-C=C), 128.5 (N-C=C), 149.0 (C=N), 149.0 (C=C-N), 177.3 (N-C=S);
FT-IR: $\tilde{\nu}$ = 3200 cm^{-1} (N-H), 1550 cm^{-1} (C=N), 1500 cm^{-1} (C-N), 800 cm^{-1} (C=S).

3) (R1 = R2 = CN): 2,3-di(4-cyanophenylthiosemicarbazone) butane

From butan-2,3-dione, dihydrazone (0.300 g, 2.6 mmol), 4-cyanophenyl isothiocyanate (5.2 mmol; 0.830 g), (**3**) was obtained as a yellow solid (0.930g, 82 %)

^{1}H NMR (300 MHz, [D_6] DMSO, TMS): δ = 10.98 (s, 1H; NH), 10.2 (s, 1H; NH), 7.95 (d, *J* = 8.6 Hz, 2H; *o*-CH), 7.83 (d, *J* = 8.6 Hz, 2H; *m*-CH) 2.34 (s, 3H; CH_3);
^{13}C NMR (75 MHz, [D_6] DMSO, TMS): δ = 12,82 (C-C=), 119.35 (CN), 132.84 (*o*-C=C), 125.25 (*m*-C=C), 143.80 (N-C=C), 150.3 (C=N), 107.41 (C=C-CN), 177 (N-C=S);
FT-IR: $\tilde{\nu}$ = 3299 cm^{-1} (N-H), 2219 cm^{-1} (CN), 1585 cm^{-1} (C=N), 1532 cm^{-1} (C-N), 816 cm^{-1} (C=S).



B- General procedure for the synthesis of the asymmetric ligand

General procedure for the preparation of symmetric ligand was employed for the preparation of the asymmetric ligands except that the mono-hydrazone intermediate was prepared by using 1 eq. instead of 2 eq. of isothiocyanate. From butan-2,3-dione, dihydrazone (0.300 g, 2.6 mmol) and 4-dimethylaminophenyl isothiocyanate (2.6 mmol; 0.463 g), the intermediate was obtained as a white solid (0.610 g, 80%). A 4-cyanophenyl isothiocyanate (0.200g, 1.2 mmol) solution in 20 ml of ethanol (1 eq.) was added dropwise to a solution of the mono-hydrazone intermediate (0.350 g, 1.2 mmol) in ethanol (15 ml). The mixture was heated at reflux. After one night, the reaction mixture was cooled to 0°C. The golden yellow solid compound precipitated and was filtered, washed with two portions of ethanol to give 0.517 g (94 % yield) of crude compound that was used for the complexation step (see below) without further purification.
^{1}H NMR (300 MHz, [D_6] DMSO, TMS): δ = 10.5 (s, 1H; NH), 9.8 (s, 1H; NH), 7.3 (d, J = 8,9 Hz, 2H; o-CH), 6.72 (d, J = 8,9 Hz, 2H; m-CH), 2.91 (s, 6H; N-$(CH_3)_2$), 2.31 (s, 3H; CH_3) for dimethylaminophenyl substitution, and δ = 10.94 (s, 1H; NH), 10.2 (s, 1H; NH), 7.96 (d, J = 8,6 Hz, 2H; o-CH), 7.84 (d, J = 8,6 Hz, 2H; m-CH) 2.34 (s, 3H; CH_3) for cyanophenyl substitution.
^{13}C NMR(75 MHz, [D_6] DMSO, TMS): δ = 12.47 (C-C=), 40.9 (N-CH_3), 112.28 (o-C=C), 127.21 (m-C=C), 128.6 (N-C=C), 149.04 (C=N), 148.6 (C=C-N-CH_3), 177.53 (N-C=S) for dimethylaminophenyl substitution, and δ = 12.77 (C-C=), 119.37 (CN), 132.83 (o-C=C), 125.17 (m-C=C), 143.8 (N-C=C), 150.7 (C=N), 107.35 (C=C-CN), 176.9 (N-C=S) for cyanophenyl substitution.;

FT-IR: $\tilde{\nu}$ = 3300 cm^{-1} (N-H), 2219 cm^{-1} (CN), 1585 cm^{-1} (C=N), 1500 cm^{-1} (C-N), 817 cm^{-1} (C=S).

C- General procedure for the synthesis of nickel complexes

On a solution of H_2L (1 eq) in methanol was added dropwise to a methanolic solution of $Ni(NO_3)_2(H_2O)_6$ (1 eq). The slurry mixture was heated at reflux. After 6 hours, the reaction mixture was cooled to 0°C. a precipitate formed that was washed with two portion of methanol and did not require further purification.

1) $NiSCH_3$

From 2,3-di(4-(methylmercaptophenylthiosemicarbazone) butane (**1**) (0.085 mmol, 40 mg) in 3 ml methanol and $Ni(NO_3)_2(H_2O)_6$ (0.082 mmol, 24 mg) in solution in 2 ml methanol. A dark brown solid (32 mg, 80 %) was obtained after filtration and washing with two portions of methanol.

^{1}H NMR (300 MHz, [D_6] DMSO, TMS): δ = 10.00 (s, 2H; NH), 7.60 (d, J = 8.9 Hz, 2H; o-CH), 7.23 (d, J = 8.4 Hz, 2H; m-CH), 2.46 (s, 6H; S-CH_3), 2.09 (s, 6H; CH_3).

^{13}C NMR (75 MHz, [D_6] DMSO, TMS):: δ = 14.8 (C-C=), 14.8 (S-CH_3), 120.9 (*m*-C=C), 127.3 (*o*-C=C), 132.1 (C=C-N), 138.2 (N-C=C), 159.1 (N=C-S), 206.9 (C=N);

FT-IR: $\tilde{\nu}$ = 3300 cm^{-1} (N-H), 1550 cm^{-1} (C=N), 1436 cm^{-1} (C-N), 812 cm^{-1} (C-S).

HR ESI-MS: $[M+H]^+$ calculated for $C_{20}H_{23}N_6S_4Ni$: 533.0215, observed: 533.0211.

2) $NiN(CH_3)_2$

From 2,3-di(4-dimethylaminophenylthiosemicarbazone) butane (**2**) (0.17 mmol, 80 mg) in 5 ml methanol and $Ni(NO_3)_2(H_2O)_6$ (0.082 mmol, 24 mg) solution in 2 ml methanol. 32 mg of dark purple solid solid (80 %) was obtained after filtration and washing with two portions of methanol.

^{1}H NMR (300 MHz, [D_6] DMSO, TMS): δ = 10.09 (s, 2H; NH), 7.68 (d, *J* = 8.3 Hz, 4H; *o*-CH), 7.33 (d, *J* = 8 Hz, 4H; *m*-CH), 3.09 (s, 12H; N-$(CH_3)_2$), 2.10 (s, 6H; CH_3).

^{13}C NMR (75 MHz, [D_6] DMSO, TMS): δ = 14.9 (C-C=), 44.7 (N-CH_3), 118.9 (*o*-C=C), 121.3 (*m*-C=C), 159.5 (N=C-S), 206.9 (C=N);

FT-IR: $\tilde{\nu}$ = 3289 cm^{-1} (N-H), 1615 cm^{-1} (C=N), 1462 cm^{-1} (C-N), 846 cm^{-1} (C-S).

HR ESI-MS: $[M+H]^+$ calculated for $C_{22}H_{29}N_8S_2Ni$: 527.1305, observed: 527.1297.

3) NiCN

From (**3**) (0.115 mmol, 50 mg) in 5 ml methanol and $Ni(NO_3)_2(H_2O)_6$ (0.115 mmol, 34 mg) solution in 2 ml methanol. Dark green solid (48 mg, 95.6 %)

^{1}H NMR (300 MHz, [D_6] DMSO, TMS): δ = 10.39 (s, 2H; NH), 7.80 (d, *J* = 8.5 Hz, 2H; *o*-CH), 7.70 (d, *J* = 8.6 Hz, 2H; *m*-CH) 2.09 (s, 6H; CH_3).

FT-IR: $\tilde{\nu}$ = 3304 cm^{-1} (N-H), 2225 cm^{-1} (CN), 1595 cm^{-1} (C=N), 1474 cm^{-1} (C-N), 834 cm-1 (C-S).

HR ESI-MS: $[M+H]^+$ calculated for $C_{20}H_{217}N_8S_2Ni$: 491.0366, observed: 491.0358.

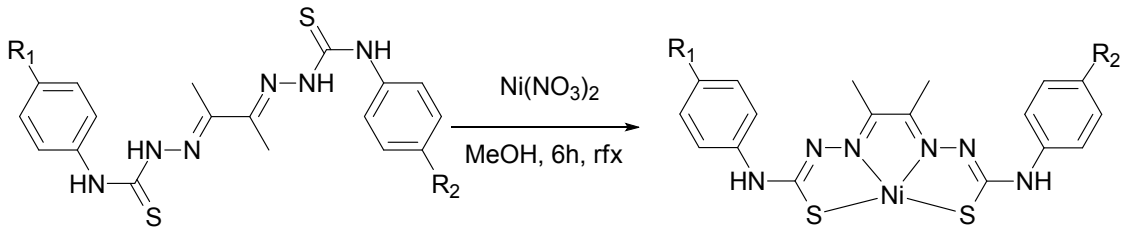
4) Ni(N(CH$_3$)$_2$,CN)

From (**4**) (0.1106 mmol, 40 mg) in 5 ml methanol and Ni(NO$_3$)$_2$(H$_2$O)$_6$ (0.1106 mmol, 26 mg) solution in 2 ml methanol. Army green solid (38 mg, 95 %).

^{1}H NMR (300 MHz, [D$_6$] DMSO, TMS): δ = 10.09 (s, 1H; NH), 7.62 (d, J = 9.6 Hz, 2H; o-CH), 7.23 (d, J = 9.6 Hz, 2H; m-CH), 3.06 (s, 6H; N-(CH$_3$)$_2$), 2.10 (s, 3H; CH$_3$) for dimethylaminophenyl substitution, and δ = 10.32 (s, 1H; NH), 7.79 (d, J = 9.2 Hz, 2H; o-CH), 7.69 (d, J = 9.2 Hz, 2H; m-CH) 2.15 (s, 3H; CH$_3$) for cyanophenyl substitution

FT-IR: ṽ = 3311 cm^{-1} (N-H), 2221 cm^{-1} (CN), 1605 cm^{-1} (C=N), 1483 cm^{-1} (C-N), 833 cm^{-1} (C-S).

HR ESI-MS: [M+H]$^+$ calculated for C$_{21}$H$_{23}$N$_8$S$_2$Ni: 509.0835, observed: 509.0833.

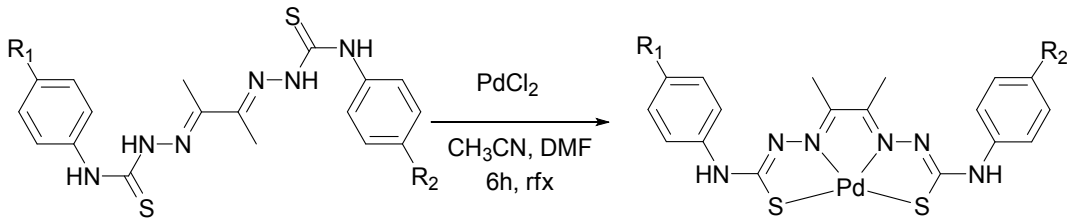


H$_2$L : R$_1$ = R$_2$ = SCH$_3$; R$_1$ = R$_2$ = N(CH$_3$)$_2$; R$_1$ = R$_2$ = CN

H$_2$L$_{diss}$: R$_1$ = N(CH$_3$)$_2$, R$_2$ = CN

D- General procedure for the synthesis of palladium complexes

On a solution of H$_2$L(1 eq) in DMF was added dropwise a solution of PdCl$_2$ (1eq) in acetonitrile. The slurry mixture was heated at reflux. After 6 hours, the reaction mixture was allowed to cool down to room temperature and acetonitrile was evaporated. The crude compound was left at room temperature to crystallized upon standing.



H$_2$L : R$_1$ = R$_2$ = SCH$_3$; R$_1$ = R$_2$ = N(CH$_3$)$_2$; R$_1$ = R$_2$ = CN

H$_2$L : R$_1$ = N(CH$_3$)$_2$, R$_2$ = CN

1) PdSCH$_3$ complex

From (**1**) (0.077 mmol, 37 mg) in 3 ml DMF and PdCl$_2$ (0.077 mmol, 14 mg) dissolved in 3ml CH$_3$CN. Single crystal suitable for crystallographic analysis obtained.

2) PdN(CH$_3$)$_2$ complex

From (**2**) (0.11 mmol, 80 mg) in 3 ml DMF and PdCl$_2$ (0.11 mmol, 20 mg) dissolved in 3ml CH$_3$CN. No single crystal suitable for crystallographic analysis obtained.

3) PdCN complex

From (**3**) (0.115 mmol, 50 mg) in 5 ml DMF and $PdCl_2$ (0.115 mmol, 20 mg) dissolved in 3ml CH_3CN. No single crystal suitable for crystallographic analysis obtained.

4) Pd(N(CH$_3$)$_2$,CN) complex

From (**4**) (0.1106 mmol, 50 mg) in 5 ml DMF and $PdCl_2$ (0.1106 mmol, 20 mg) dissolved in 3ml CH_3CN. No single crystal suitable for crystallographic analysis obtained.

2. Single crystal X-Ray diffraction

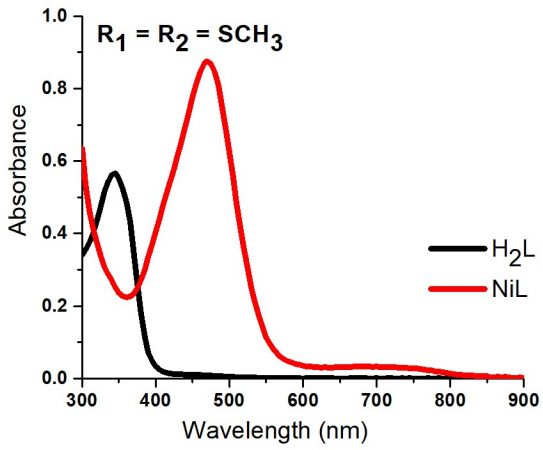
Table SI-1. Crystallographic data, details of data collection and structure refinement parameters for [PdSCH$_3$].2DMF.

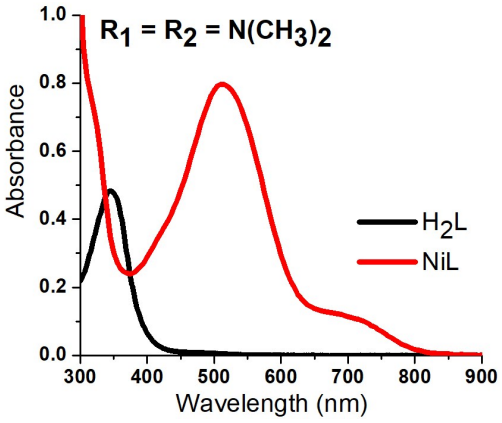
Identification code	ap22pdl2
Empirical formula	$C_{26}H_{33}N_8O_2PdS_4$
Formula weight	724.24
Temperature/K	293
Crystal system	triclinic
Space group	P-1
a/Å	11.3380(3)
b/Å	12.5181(3)
c/Å	12.8599(3)
α/°	70.595(2)
β/°	70.544(2)
γ/°	82.812(2)
Volume/Å^3	1623.01(7)
Z	2
ρ_{calc}g/cm^3	1.482
μ/mm^{-1}	7.324
F(000)	742.0
Crystal size/mm^3	0.36 × 0.14 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.488 to 137.686
Index ranges	-13 ≤ h ≤ 13, -15 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	21621
Independent reflections	5954 [R_{int} = 0.0847, R_{sigma} = 0.0530]
Data/restraints/parameters	5954/0/377
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0416, wR_2 = 0.1147
Final R indexes [all data]	R_1 = 0.0434, wR_2 = 0.1171
Largest diff. peak/hole / e Å^{-3}	1.02/-0.85

3. UV-vis spectroscopic data

Table SI-2. Selected spectral features from the electronic absorption spectra of 0.5 mM solutions of each **H_2L** ligand and **NiL** complex in DMF.

	Compound	λ (nm)	ε (M-1cm-1)
Ligand	$R_1 = R_2 = OCH_3$	350	50222
	$R_1 = R_2 = SCH_3$	350	38555
	$R_1 = R_2 = N(CH3)_2$	350	50449
	$R_1 = N(CH3)_2$, $R_2 = CN$	356	59396
	$R_1 = R_2 = CN$	351	31104
Complex	NiCN	445	23086
		750	2123
	$NiSCH_3$	471	20715
		703	784
	$NiOCH_3$	471	16925
		744	1349
	$Ni(N(CH_3)_2,CN)$	400, 490	13816, 9184
		735,734	771
	$NiN(CH_3)_2$	514	16775
		716	2187





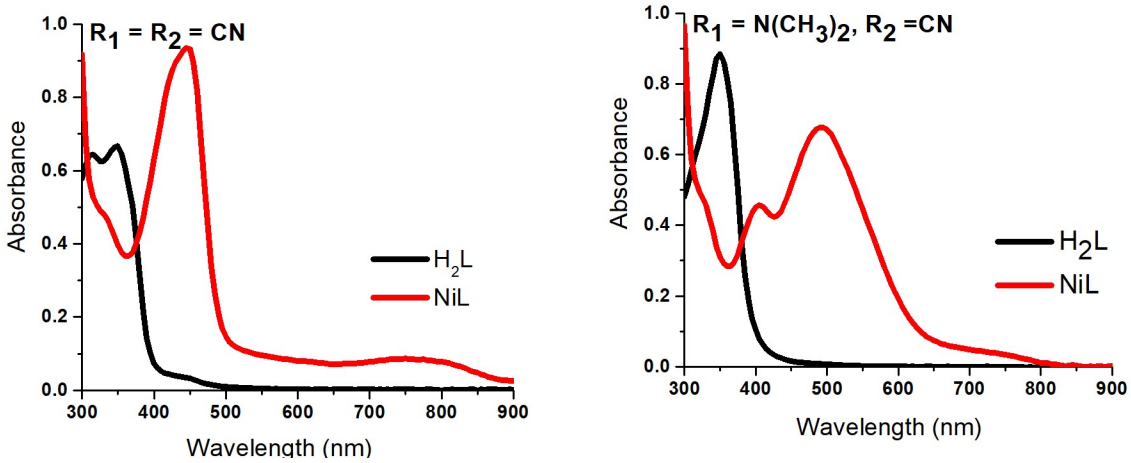


Figure SI-1. Electronic absorption spectra of 0.5 mM solutions of each **H_2L** ligand and **NiL** complex in DMF.

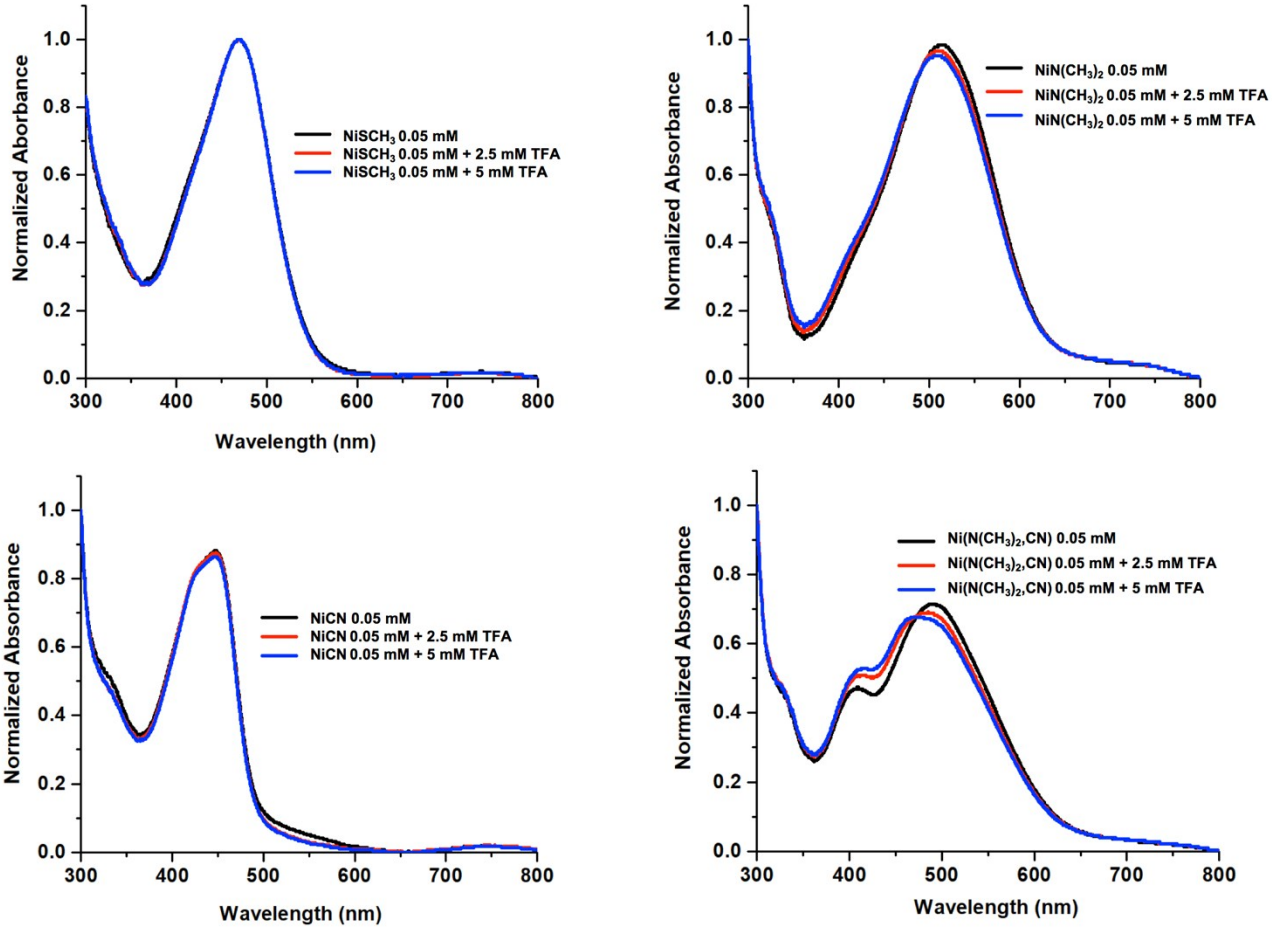


Figure SI-2. Electronic absorption spectra of 0.5 mM solutions of **NiL** complexes in DMF in the absence (black line) and in the presence (blue and red lines) of TFA.

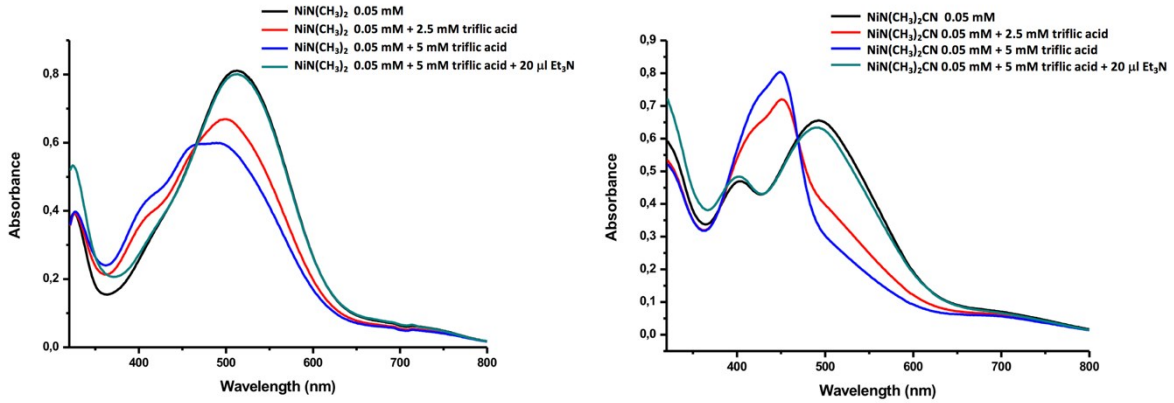


Figure SI-3. Electronic absorption spectra of 0.5 mM solutions of **NiL** complexes in DMF in the absence (black line) or in the presence (blue and red lines) of triflic acid and in the presence of base (green lines).

4. Electrochemical Studies

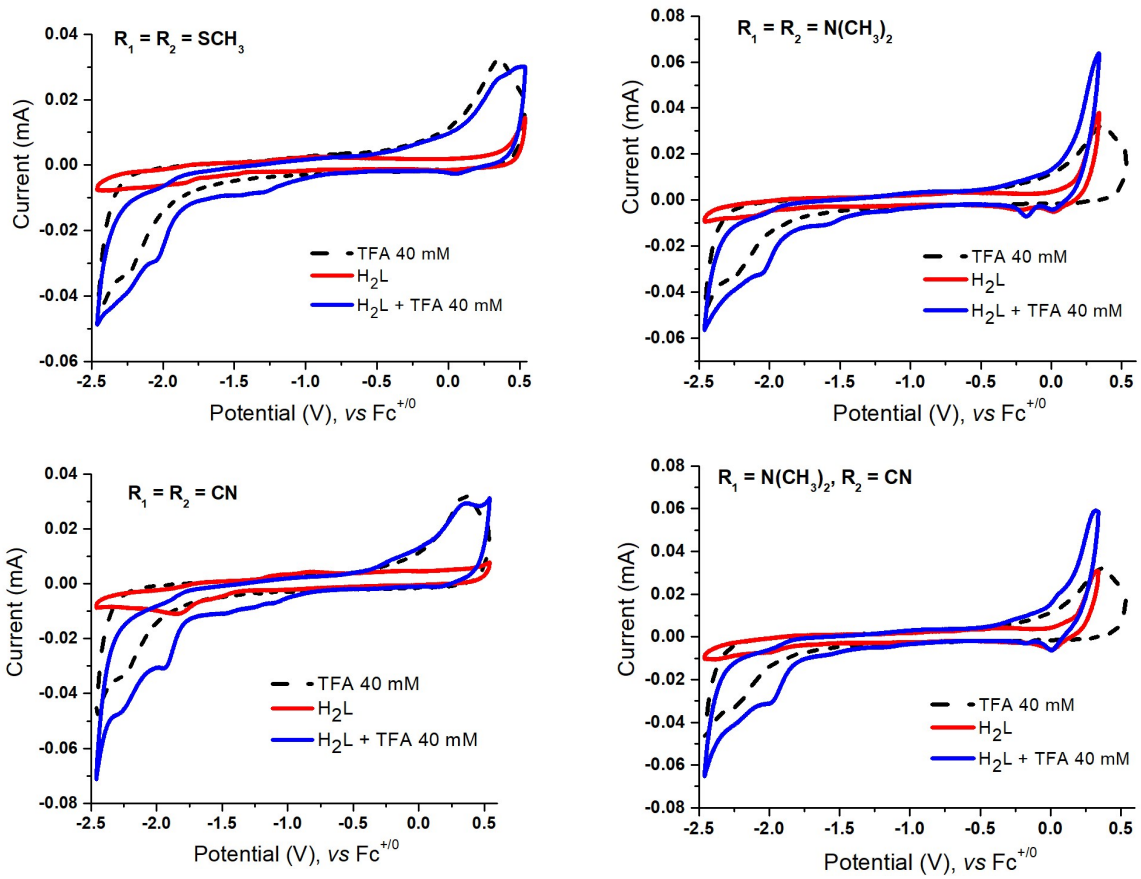
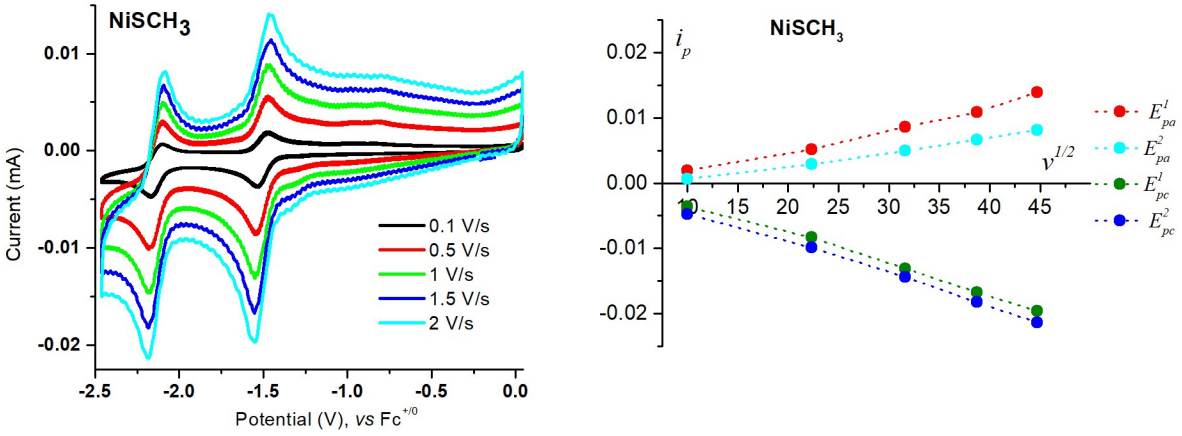


Figure SI-4. Cyclic voltammograms of 1 mM **H_2L** (red line) recorded at a stationary glassy carbon elctrode in DMF with 0.1 M NBu_4PF_6 as supporting electrolyte. The cyclic voltammograms of a 40 mM of TFA solution in the absence (dotted black line) and in the presence of 1 mM **H_2L** (blue line) are also shown. Scan rate: 500mV/s.



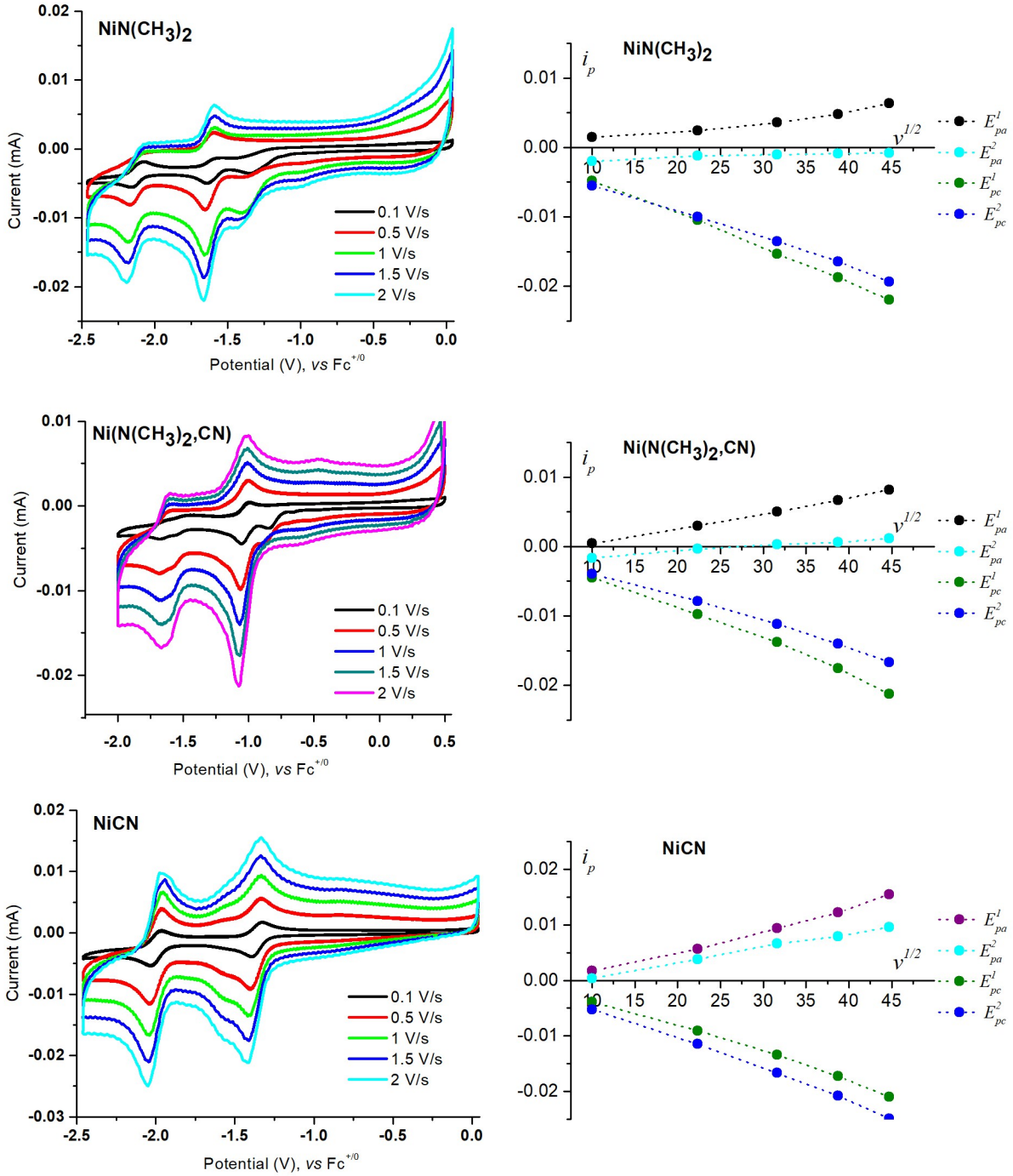


Figure SI-5. Cyclic voltammograms of **NiL** at a stationary glassy carbon electrode at different scan rates (v) in DMF with 0.1 M NBu_4PF_6 as supporting electrolyte (left) and linear plot of ip vs. $v^{1/2}$ for anodic and cathodic waves of both processes (right).

5. Electrocatalysis

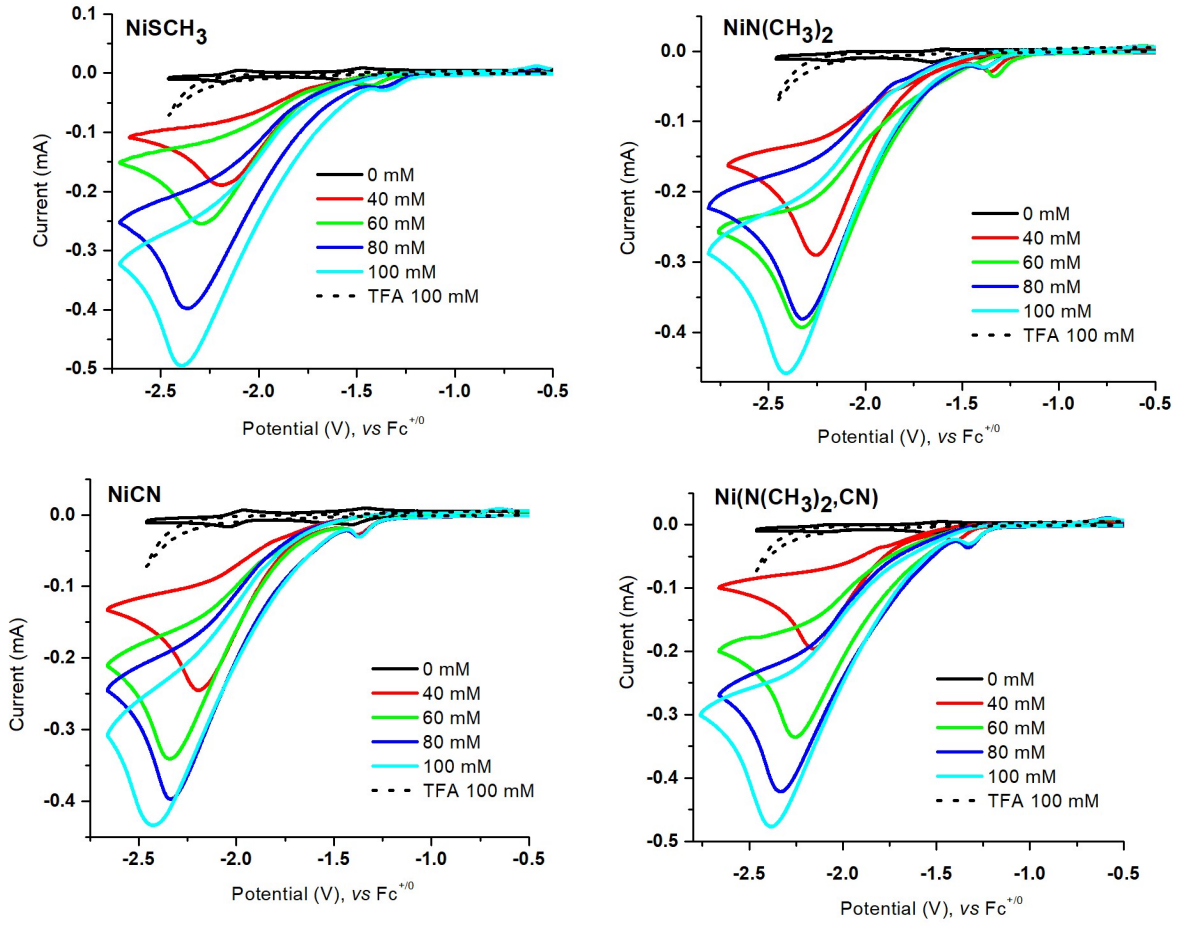


Figure SI-6: Successive cyclic voltammograms recorded at a glassy carbon as working electrode of a 1mM solution of **NiL** complex in DMF (0.1M NBu_4PF_6) in the presence of increasing amounts of TFA. The black dotted curve shows the CV of 100 mM TFA in the absence of catalysts under the same conditions. Scan rate: 500mV/s.

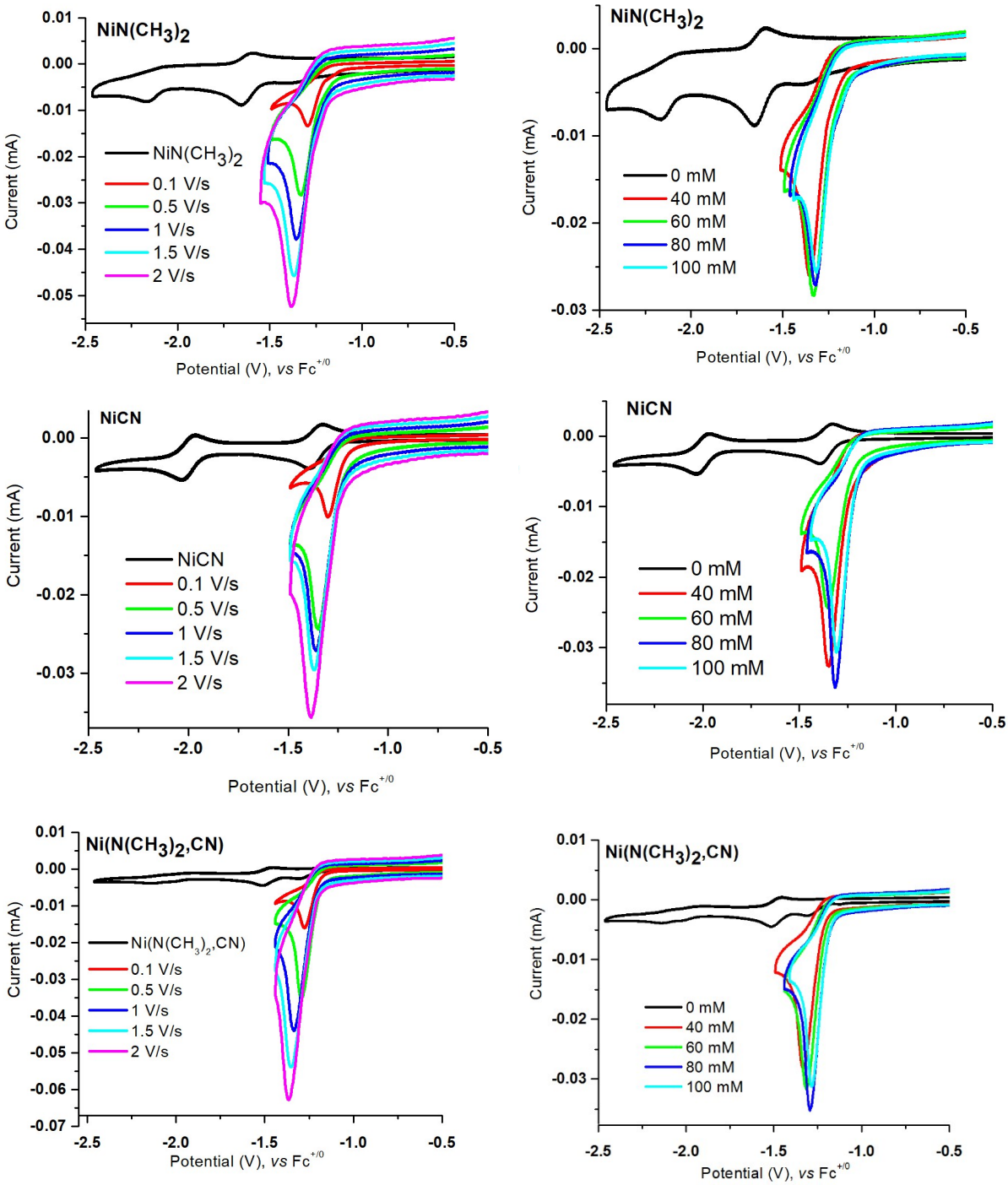


Figure SI-7: Successive cyclic voltammograms recorded at a glassy carbon as working electrode of a 1mM solution of **NiL** complex in DMF (0.1M NBu_4PF_6) with 60 mM TFA at five different scan rates (left) and increasing concentration of TFA at 500 mV/s scan rates **(**right**)**.

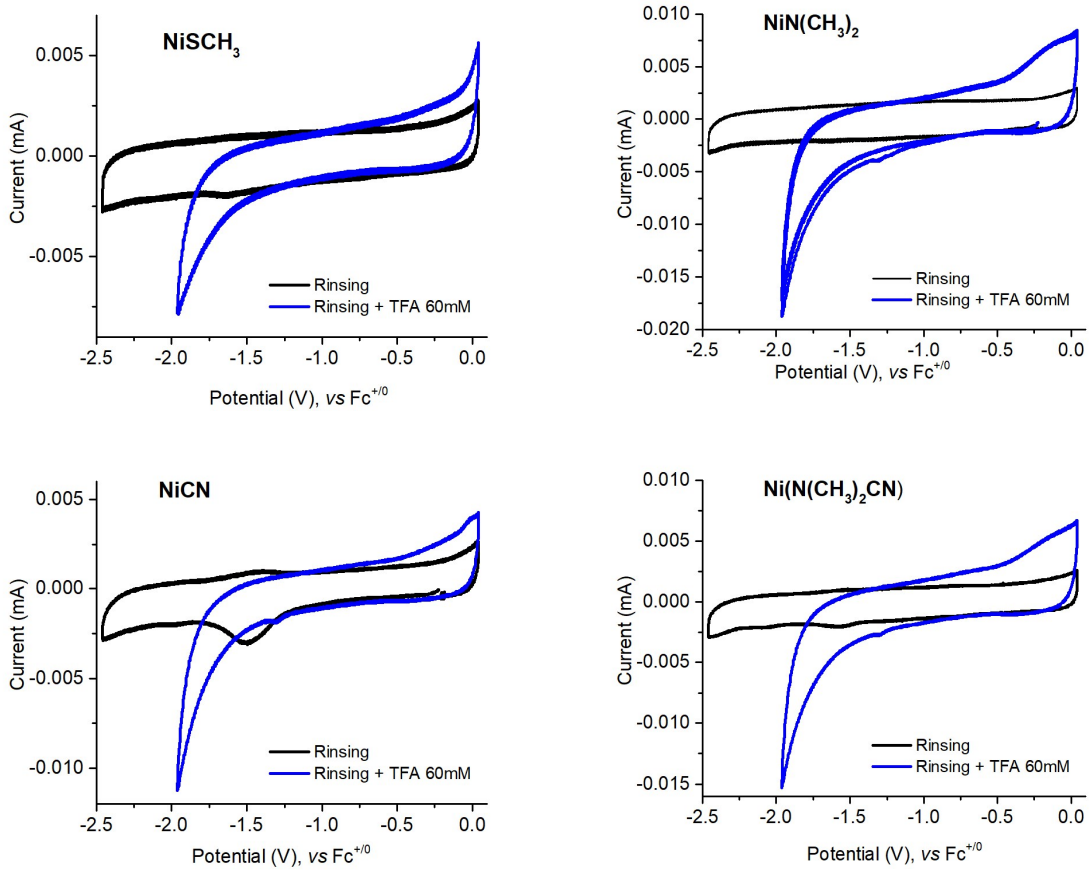
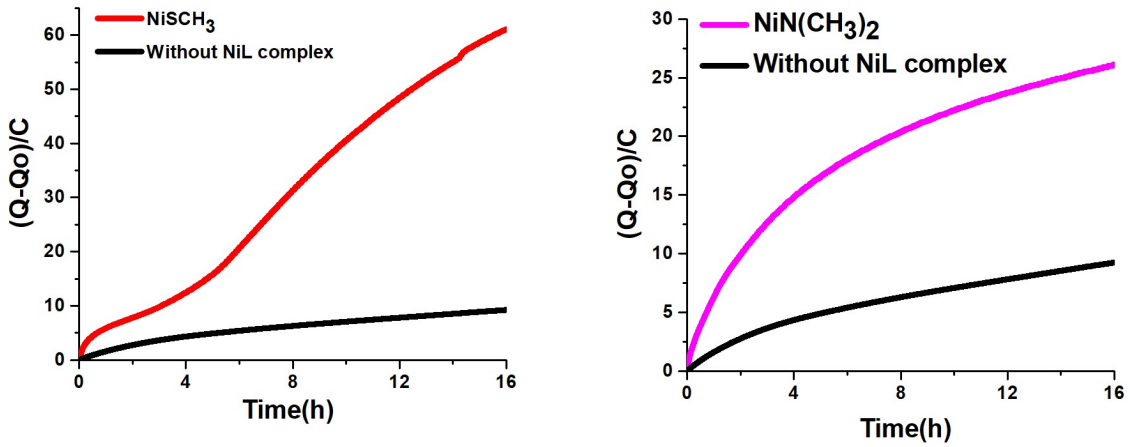


Figure SI-8: Successive cyclic voltammograms recorded after electrocatalysis upon washing the glassy carbon electrode and immersion into a fresh solution of DMF (0.1 M $NBu4PF_6$, black line) and in the presence of 60 mM of TFA (blue line).

6. Gas analysis



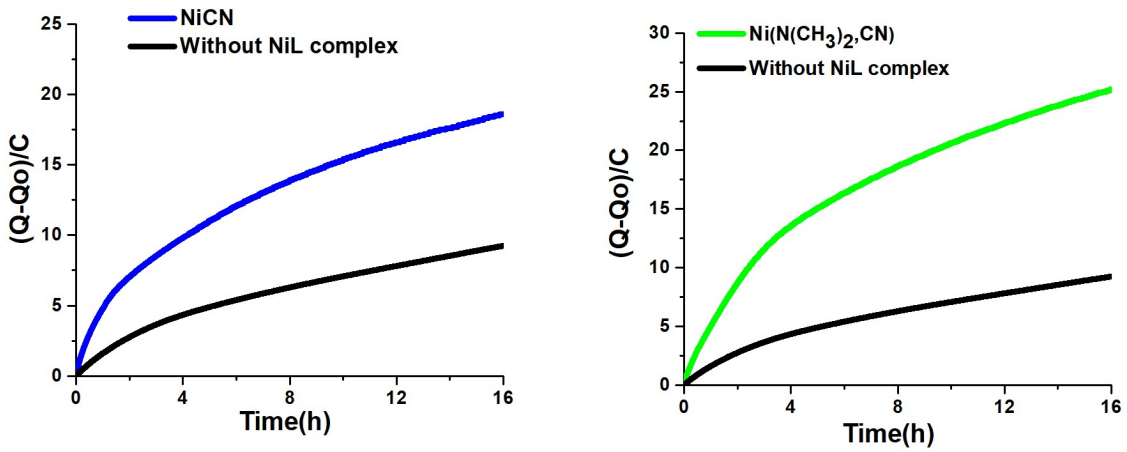


Figure SI-9: Coulometry during bulk electrolysis experiment at -1.70 V vs. versus $Fc^{+/0}$ using a pool mercury working electrode. The electrolytic solution contains 0.1 M NBu_4PF_6 in DMF, 100 mM TFA and no (black line) or 1 mM of **$NiSCH_3$,** (red line), **$NiN(CH_3)_2$** (pink line), **NiCN** (blue line) and **$NiN(CH_3)_2$,CN** (green line).

7. Kinetic analysis and determination of rate constants

7.1 Foot-of-the-wave analysis (FOWA):

As stated in the main text, an ECEC mechanism – with the second electron transfer easier than the first one – was considered. For such multi-electron, multi-proton process, the expression of the current is given by equations (1-2):

$$i = \frac{i_{pl}}{1 + e^{[\frac{RT}{F}(E - E_c^0)]}} \quad (1)$$

$$i_{pl} = 2FS[Cat]\sqrt{D_{cat}}\frac{1}{\frac{1}{\sqrt{k_1[H^+]}} + \frac{1}{\sqrt{k_2[H^+]}}} \quad (2)$$

where i_{pl} the catalytic plateau current, R the gas constant, T the temperature, F the Faraday constant, E_c^0 standard potential of the catalytic process, S the active surface of the electrode, [Cat] the concentration of the catalyst, D_{cat} the diffusion coefficient of catalyst; $[H^+]$ the concentration of acid; k_1 the first protonation rate constant and k_2 the second protonation rate constant.

Dividing *i* by the current i_p^0 associated with a reversible one-electron transfer under diffusion control (Randles-Sevcik equation (3)) allows simplification of redundant constants.

$$i_p^0 = 0.446FS[Cat]\sqrt{\frac{FvD_{cat}}{RT}} \quad (3)$$

$$\frac{i}{i_p^0} = \frac{i_{pl}}{i_p^0} \times \frac{1}{1 + e^{\left[\frac{F}{RT}\left(E - E_c^0\right)\right]}} \quad (4)$$

Plotting the catalytic enhancement ($i_{cat}/i_p{}^0$) as a function of $\frac{1}{1 + e^{\left[\frac{F}{RT}\left(E - E_c^0\right)\right]}}$ near the foot of the catalytic wave, gives a linear curve the slope of which allows further determination of relevant rate constants. From this point, two situations must be considered :

- $k_1 << k_2$, *ie* the first protonation step is the rate-determining one,
- $k_2 << k_1$, *ie* the second protonation step is the rate-determining one.

In the case where $k_1 << k_2$, E_c^0 is equaling the potential of the redox couple which triggers the catalytic process (equation (5)). In addition, the expression of the plateau current is also simplified as shown by equation (6). Unambiguous putative k_1 values were thus extracted from the slopes of the linearization plots. Multiple scan rates have been investigated (spanning from 50 to 2000 mV.s^{-1}) and revealed a clear independence of the rate constant determined (Table SI-3), thus ensuring the reliability of the calculated catalytic rate constant (Figure SI-10).

$$E_c^0 = E^0_{\left(Ni^{II}{}_{L/Ni^{II}{}_{L^{\cdot-}}}\right)} \quad (5)$$

$$i_{pl} = 2FS[Cat]\sqrt{D_{cat}}\sqrt{k_1[H^+]} \quad (6)$$

When $k_1 >> k_2$, the value of the catalytic potential must be comprised between $E^0_{\left(Ni^{II}{}_{L/Ni^{II}{}_{L^{\cdot-}}}\right)}$ (lower limit) and the graphically-determined $E_{1/2}$ (higher limit). In principle, only the minimum value that can be reached by k_2 can be calculated thanks to equation (7), using the previously determined k_1 and considering the graphically-determined value of the catalytic potential $E_{1/2}$ as equalling E_c^0, respectively.

$$E_c^0 = E^0_{\left(Ni^{II}{}_{L/Ni^{II}{}_{L^{\cdot-}}}\right)} + \frac{RT}{F} ln\left(\sqrt{\frac{k_1}{k_2}}\right) \quad (7)$$

Consequently, the value of the catalytic potential cannot be unambiguously determined preventing direct extraction of the k_2 value from FOWA and no accurate evaluation of the TOF values can be performed.

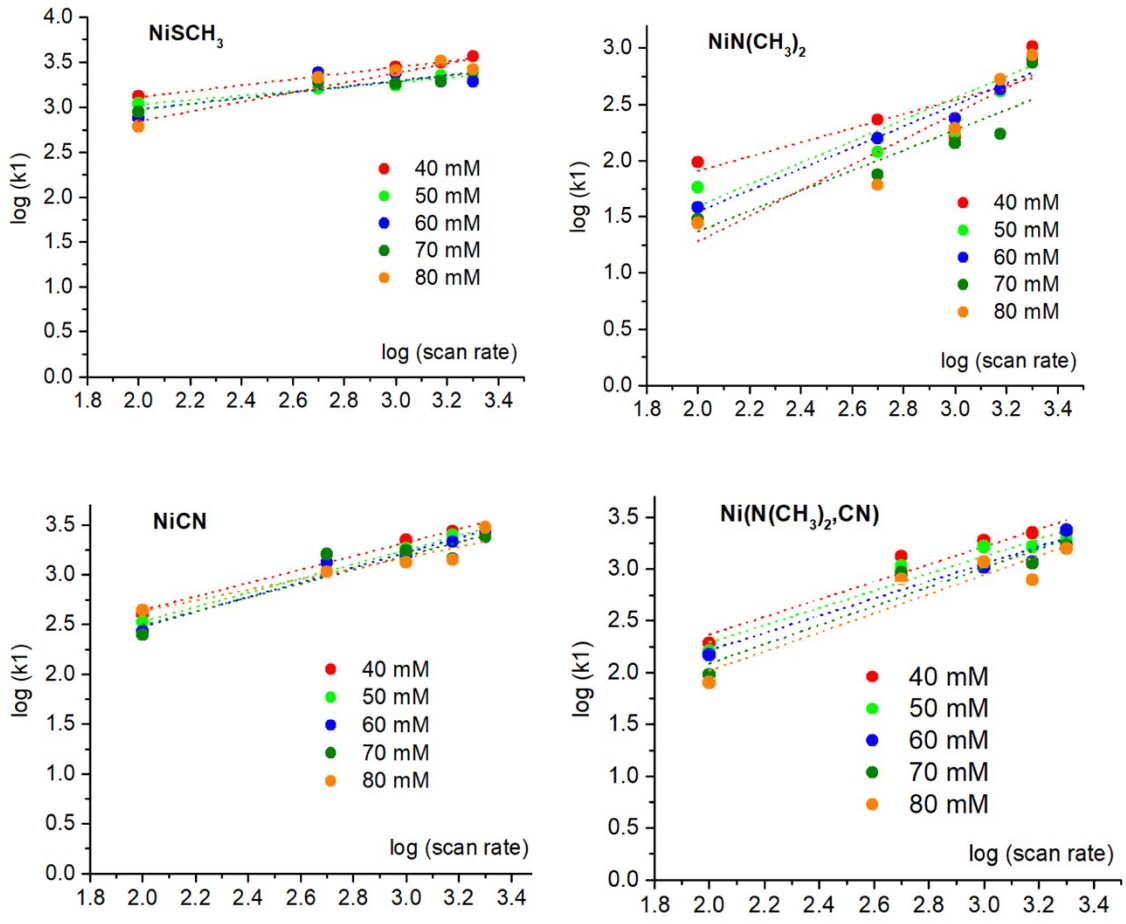


Figure SI-10: Log(k_1) values obtained through *FOWA* for **NiL** complexes.

Table SI-3. k_1 calculations using different concentrations of TFA at 4 different scan rates.

$NiSCH_3$	k_1				
v (V/s)	40 mM	50 mM	60 mM	70 mM	80 mM
0.5	2052.67	1581.35	2412.18	1874.32	2126.08
1	2829.57	1719.88	2381.55	1834.45	2561.88
1.5	3115.97	2261.95	1906.86	1920.63	3287.39
2	3662.72	2264.61	1933.42	2552.03	2611.35

$NiN(CH_3)_2$	k_1

v (V/s)	40 mM	50 mM	60 mM	70 mM	80 mM
0.5	231.27	119.67	158.57	75.06	60.6
1	161.11	179.56	238.75	142.72	191.9
1.5	414.34	413.28	430.19	173.12	523.43
2	1039.92	1900.56	805.87	743.80	865

Ni(N(CH$_3$)$_2$,CN)	k_1				
v (V/s)	40 mM	50 mM	60 mM	70 mM	80 mM
0.5	1320.41	1063.73	870.14	931.86	795.46
1	1887.08	1632.08	1041.31	1153.50	1166.01
1.5	2218.10	1630.74	1162.93	1139.21	779.45
2	2289.52	1897.87	2362.53	1708.15	1576.31

NiCN	k_1				
v (V/s)	40 mM	50 mM	60 mM	70 mM	80 mM
0.5	1615.57	1101.11	1336.36	1620.57	1071.96
1	2226.91	1829.16	1573.89	1732.60	1325.10
1.5	2734.09	2496.50	2131.68	1451.80	1413.13
2	2944.09	2702.22	2630.99	2397.19	2976.48

As described above, the *FOWA* affords a direct measurement of k_1 but does not provide information about k_2 or the rate constant for the rate determining step (RDS). Cyclic voltammograms are often used to estimate k_{cat} through comparison between catalytic plateau current (i) and the peak current in the absence of substrate (i_p^0). In both situations considered in the previous section ($k_1 << k_2$ or $k_2 << k_1$), the ratio is given by the following equation:

$$\frac{i}{i_p^0} = \frac{2}{0.4465}\frac{\sqrt{RT}}{\sqrt{Fv}} \times \sqrt{[H^+} \times \sqrt{k_{cat}} \quad \textbf{(8)}$$

Following an approach previously developed by Elgrishi *et al.*, we estimate the maximum value of k_2 as approximately $k_1/10$ to conform to a regime where catalysis is kinetically-controlled by the second protonation step. Under such condition, theoretical values of the catalytic enhancement ratio i/i^0_p can be estimated in regard to the nature of the rate determining step. These estimates were made for the **NiL** series and are reported in Figures SI-11-14 at various scan rates. The i/i^0_p values for $k_{cat} = k_1$ are shown in red and the maximum i/i^0_p values for $k_{cat} = k_2 = k_1/10$ are shown in green. Such theoretical boundaries allow us to define three different kinetic zones: (i) above the red trace, $i/i_p{}^0$ values are theoretically impossible to reach since they exceed the maximum possible values based on $k_{cat} = k_1$, (ii) in between the red and green traces $i/i_p{}^0$ values belongs to a regime kinetically-controlled by the first protonation step as they are below maximum theoretical values for $k_{cat} = k_1$ but above the maximum theoretical values for $k_{cat} = k_2$ and (iii) below the green trace, no conclusive statement can be made for the $i/i_p{}^0$ values of this area, as they are both below the maximum theoretical values for $k_{cat} = k_1$ and $k_{cat} = k_2$. Upon comparing the experimental data to the theoretical boundaries established for $k_1 = k_{cat}$ and $k_2 = k_{cat}$, it is clearly observed that the experimental values for all complexes fall in the last region, precluding any insight regarding the nature of the rate determining step.

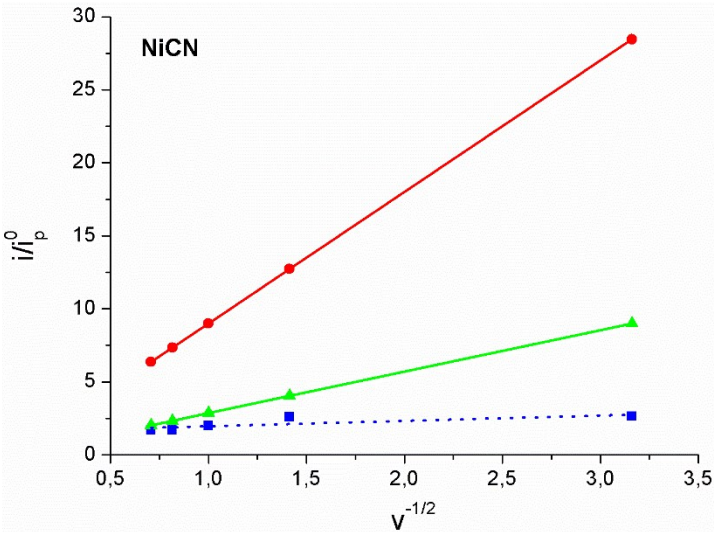


Figure SI-11: Theoretical values for i_c/i^0_p for **NiCN** in the presence of 60 mM TFA and various scan rates plotted using equation (8). Red circles represent values were $k_{cat} = k_1 = 2617$ $M^{-1}s^{-1}$. Green triangles represent values were $k_{cat} = k_2 = k_1/10 = 262$ $M^{-1}s^{-1}$

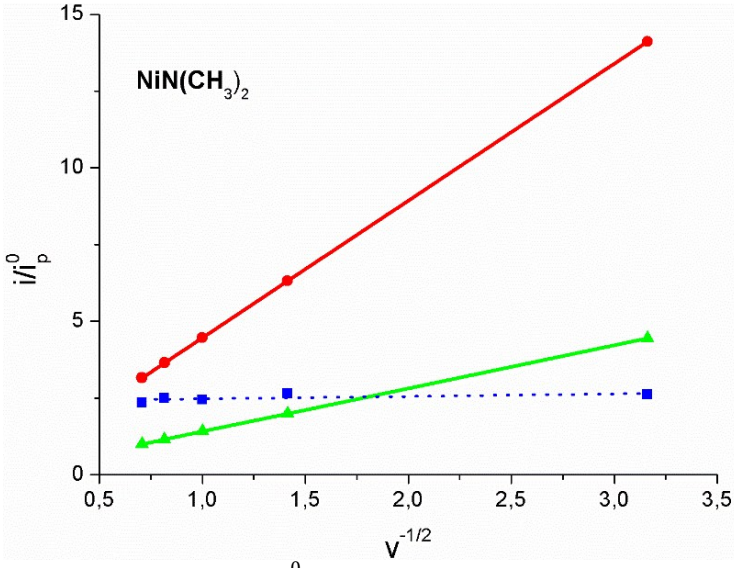


Figure SI-12: Theoretical values for i_c/i_p^0 for **$NiN(CH_3)_2$** in the presence of 60 mM TFA and various scan rates plotted using equation (8). Red circles represent values were $k_{cat} = k_1 = 644$ $M^{-1}s^{-1}$. Green triangles represent values were $k_{cat} = k_2 = k_1/10 = 64$ $M^{-1}s^{-1}$

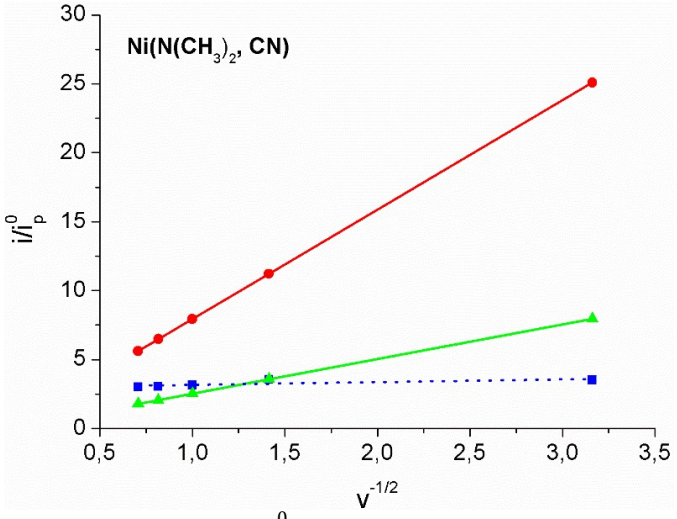


Figure SI-13: Theoretical values for i_c/i_p^0 for **$Ni((NCH_3)_2,CN)$** in the presence of 60 mM TFA and various scan rates plotted using equation (8). Red circles represent values were $k_{cat} = k_1 = 2035$ $M^{-1}s^{-1}$. Green triangles represent values were $k_{cat} = k_2 = k_1/10 = 204$ $M^{-1}s^{-1}$

7.2 TOF calculations and Tafel plots from controlled potential electrolysis experiments

The TOF values were determined from the electrolyses data as previously reported by Saveant and co-workers. Equations 1–4 were used for the calculation under the assumption that the electron transfer to the catalyst is fast and the Nernst law is obeyed. In these equations, i_{el} is the current during electrolysis, TOF_{max} is the maximum turnover frequency obtained from CVs, F is Faraday's constant (F = 96500 C.mol^{-1}), A is the surface area of the mercury-pool working electrode (A ~1.23 cm^2), D is the diffusion coefficient (8.66 × 10^{-9} cm^2.s^{-1}), [Cat] is the concentration of the catalyst ([Cat] = 1 mM), E_{appl} is the applied potential during electrolyses (E_{appl} = -1.70 V vs. Fc$^{+/0}$), $E_{1/2}$ is the half-wave potential for the catalytic wave, Q_{el} is the charge passed during the electrolysis, FY. is the Faradaic yield, and t is the electrolysis time. The passed charge increased linearly in the early stage of electrolysis and became non-linear after about 20-30 min due to catalyst degradation or substrate consumption. Therefore, the *TOF* values were calculated using the amount of charge passed during the initial twenty minutes of electrolyses.

$$TOF = \frac{i_{el}^2\left(1 + exp\left[\frac{F}{RT}\left(E_{appl} - E_{1/2}\right)\right]\right)}{F^2 A^2 D_{cat}[Cat]^2} \quad (9)$$

$$i_{el} = \frac{Q_{el}.FY}{t} \quad (10)$$

$$i_p = 0.446FA[Cat]\sqrt{\frac{FvD_{cat}}{RT}} \quad (11)$$

$$TOF = \frac{TOF_{max}}{1 + exp\left[\frac{F}{RT}\left(E_{appl} - E_{1/2}\right)\right]} \quad (12)$$

Table SI-4. Calculated TOF values for the **NiL** series.

Complex	D (cm^2.s^{-1})	i_{el} (A)	*FY (%)*	$E_{1/2}$ (V vs. Fc$^{+/0)}$	*TOF*
NiSCH$_3$	4.50.10^{-6}	2.71.10^{-3}	94	-1.32	115.9
NiOCH$_3$	5.82.10^{-6}	2.71.10^{-3}	80	-1.33	89.7
Ni(N(CH$_3$)$_2$,CN)	4.50.10^{-6}	1.44.10^{-3}	86	-1.28	18.8
NiN(CH$_3$)$_2$	7.80.10^{-6}	1.29.10^{-3}	56	-1.31	14.3

NiCN	$8.43.10^{-6}$	$1.10.10^{-3}$	63	-1.27	10.2

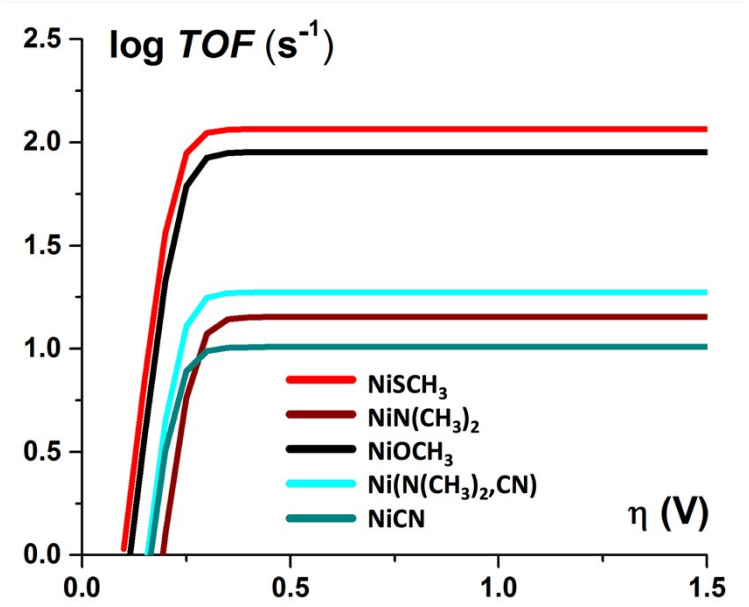


Figure SI-14: Catalytic Tafel plots: comparison of performances for HER catalyzed by the series of **NiL** complexes in DMF in presence of 1 M TFA.

8. DFT Calculations

The results shown below correspond to two sets of calculations using different functionals: BP86 and B3LYP. The idea here is to compare their performances in reproducing redox potential changes for different substituents. As we shall see from comparisons of absolute and relative redox potentials, BP86 seems to be a more suitable functional to study the electrochemistry of these **NiL** complexes. We will show additional orbitals and bond lengths from BP86 calculations, corresponding to the first and second reductions, as well as comparison between reduction potentials for the two functionals. Finally, we include Cartesian coordinates of optimized structures for all complexes in the many possible states associated with the two reduction processes.

8.1 Optimized structures

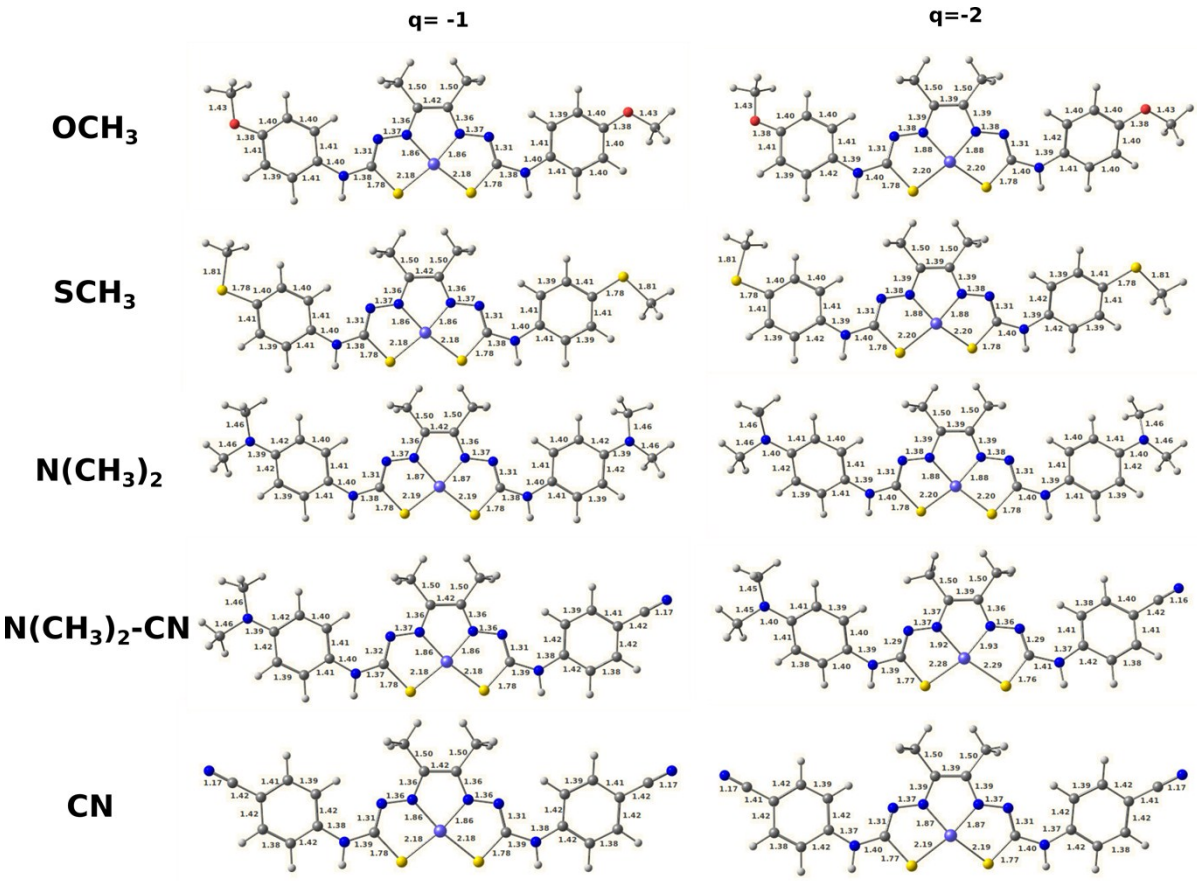


Figure SI-15. DFT-optimized structures of all the complexes in their first and second reduced states. Optimization performed with BP86/def2-TZVP.

8.2 Electronic structures

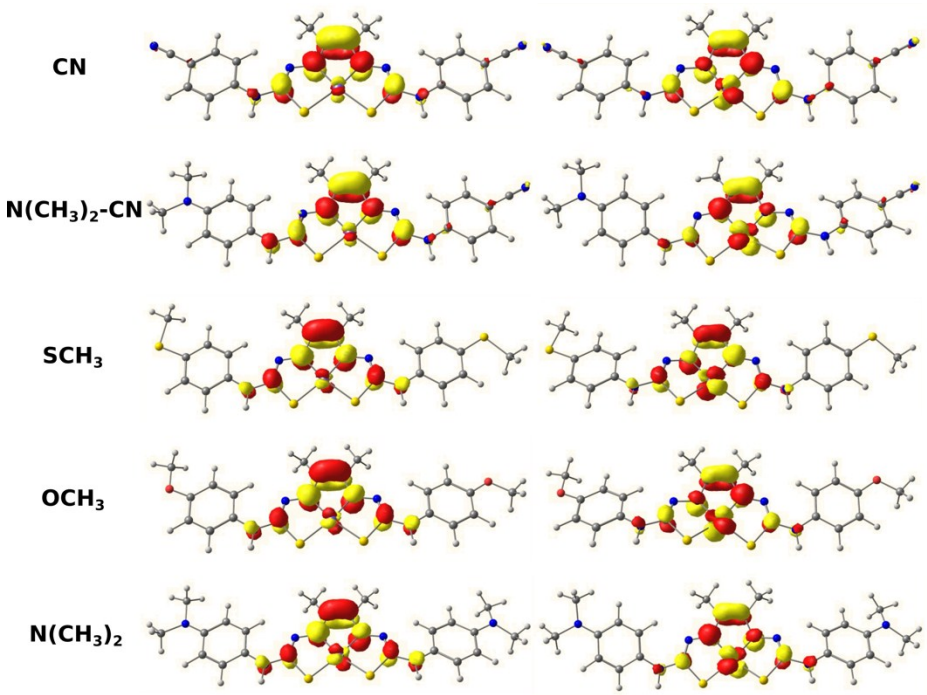


Figure SI-16. Frontier orbitals for the 2-electron reduced species of the **NiL** series.

8.3 Optical properties

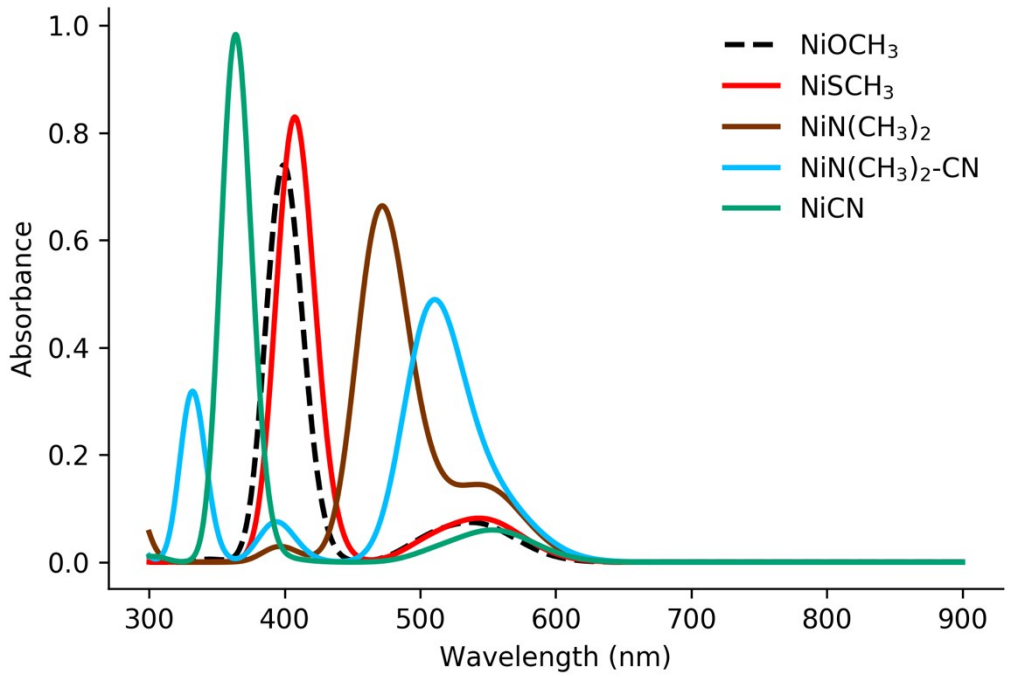


Figure SI-17. Theoretical fit of the UV-vis spectra of the **NiL** series of complexes.

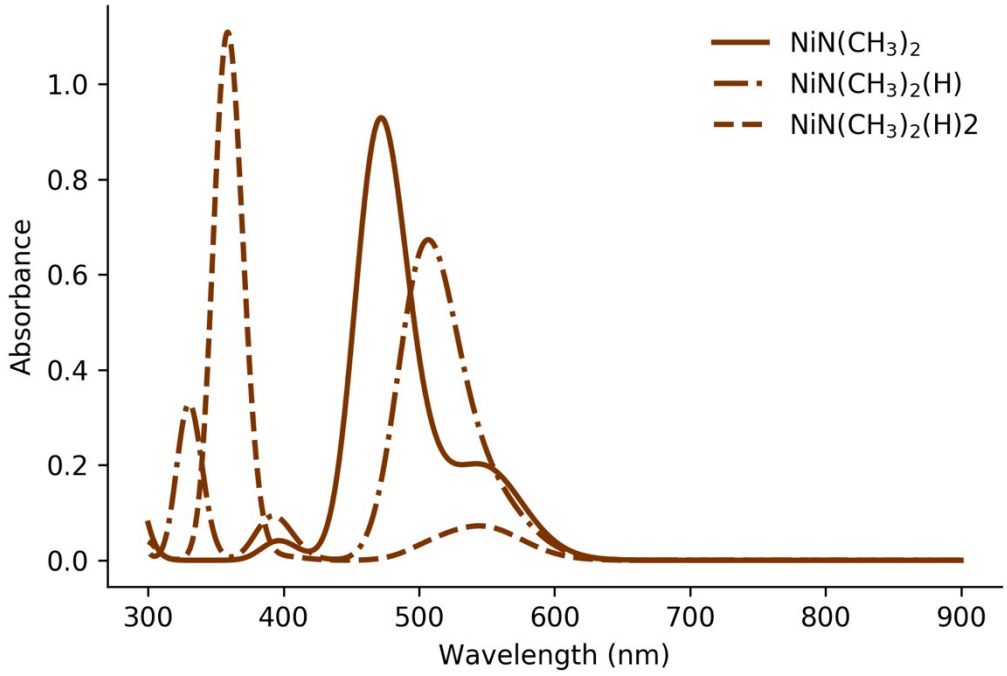


Figure SI-18. Theoretical fit of the UV-vis spectra of the **NiN(CH3)$_2$** complex in the unprotonated, mono- and diprotonated form with protonation involving the phenyl ring substituent.

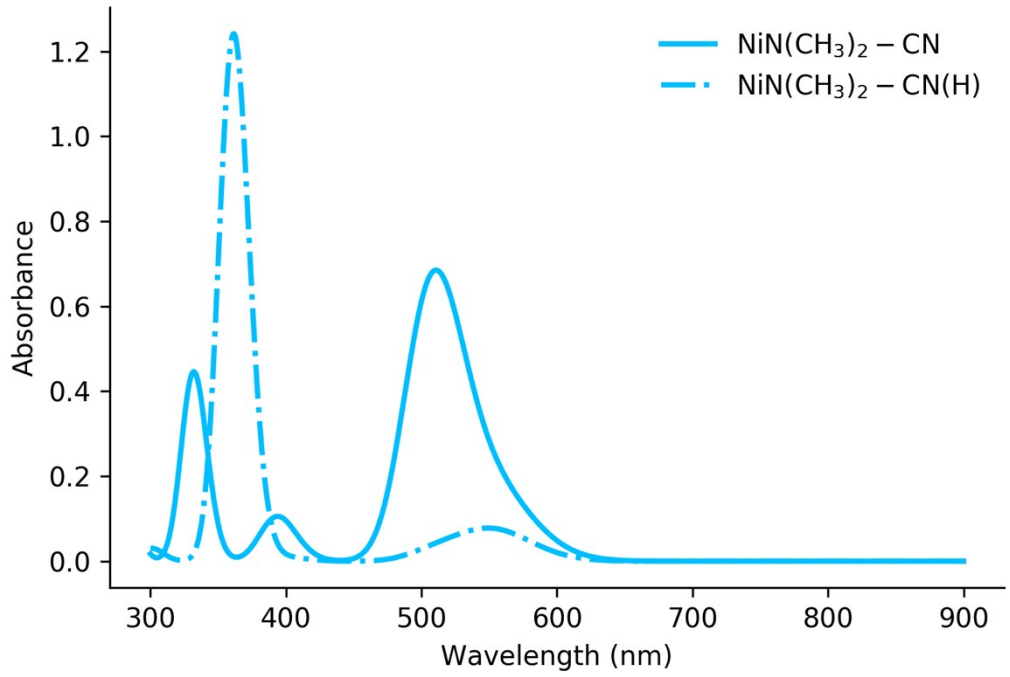


Figure SI-19. Theoretical fit of the UV-vis spectra of the **NiN(CH3)$_2$CN** complex in the unprotonated and protonated form with protonation involving the phenyl ring substituent.

8.4 Redox potentials

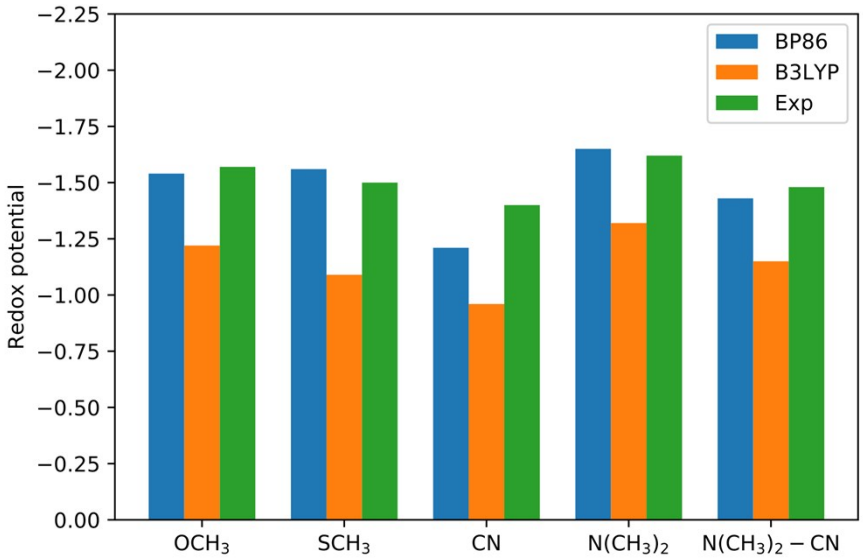


Figure SI-20. Absolute redox potentials for the first reduction of all substituents compared with experiments.

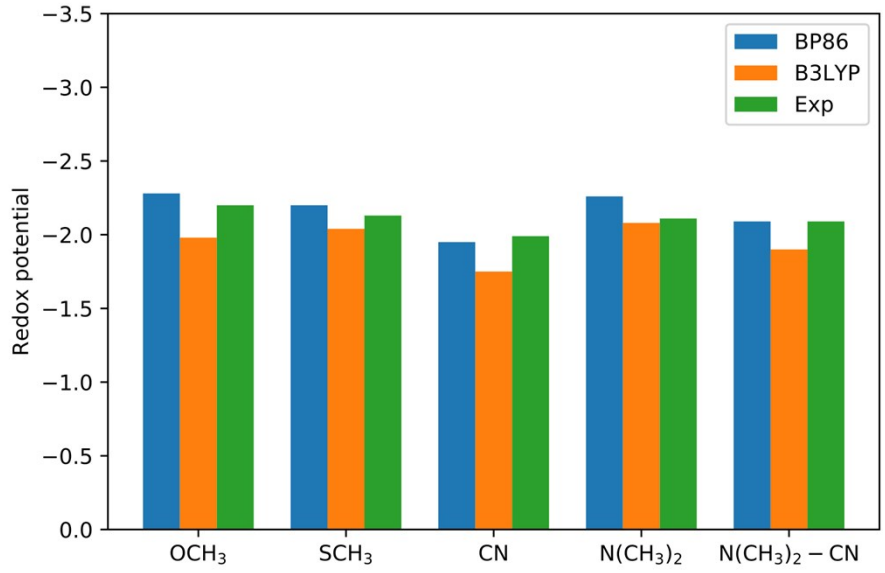


Figure SI-21. Absolute redox potentials for the second reduction of all substituents compared with experiments.

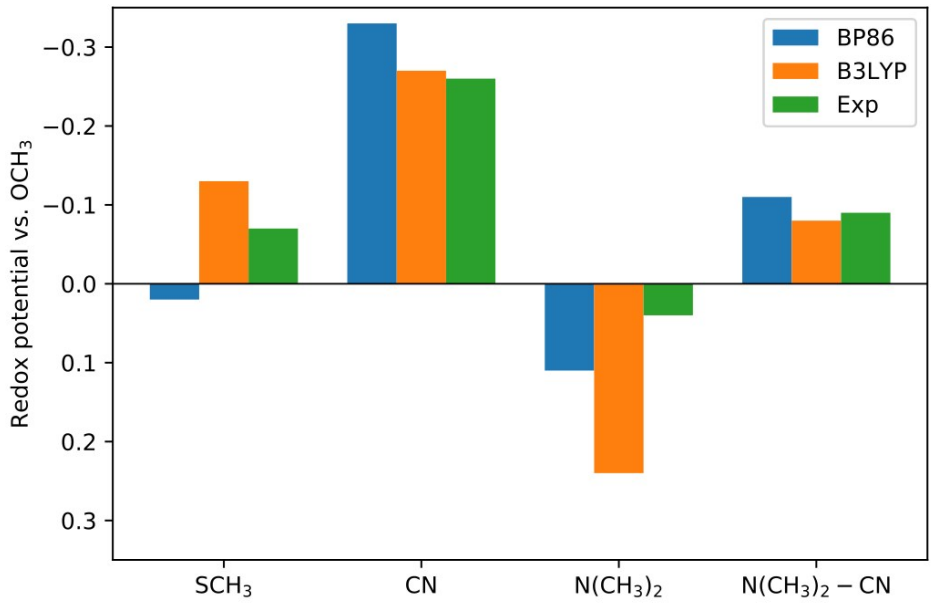


Figure SI-22. Relative redox potentials *vs.* OCH_3 for the first reduction of all substituents compared with experiments.

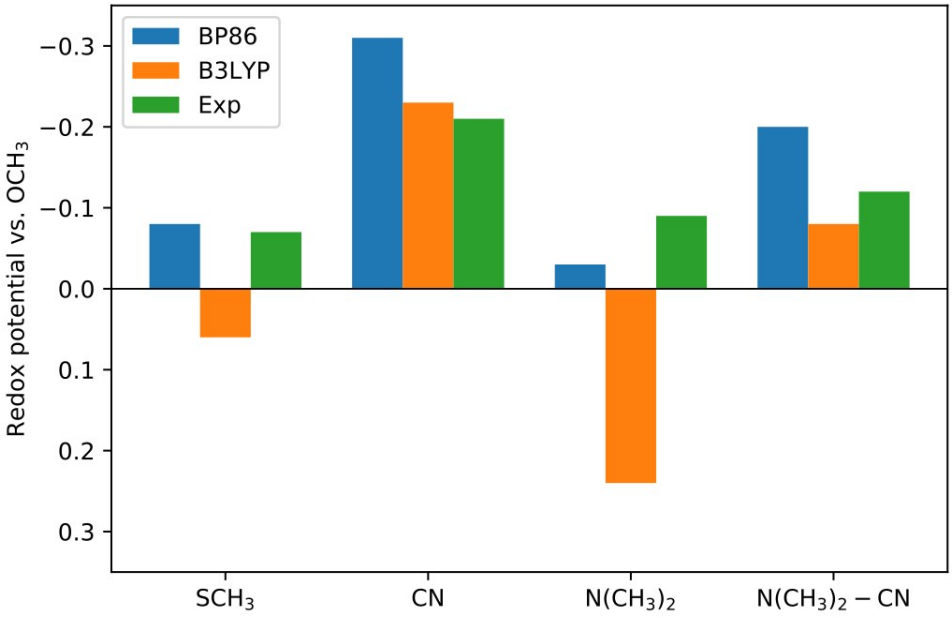


Figure SI-23. Relative redox potentials *vs.* OCH_3 for the second reduction of all substituents compared with experiments.

Table SI-5: Gibbs free energies associated with each state for all the complexes. All values are shifted to the free energy of the neutral complex, and shown in eVs. Results obtained using BP86/def2-TZVP.

	Gibbs free energy *vs.* neutral state, in eV (BP86/def2-TZVP)				
	OCH_3	SCH_3	$N(CH_3)_2$	$N(CH_3)_2$,CN	CN
$Ni^{II}L$	0	0	0	0	0
$Ni^{II}L^{\bullet-}$	-3.33	-3.31	-3.66	-3.22	-3.44
$Ni^{I}L^{\bullet-}$(S=0)	-5.77	-5.68	-6.58	-5.81	-6.21
$Ni^{I}L^{\bullet-}$(S=1)	-5.44	-5.47	-6.05	-5.39	-5.67
$Ni^{I}L^{\bullet-}$ (M_s=0)	-5.92	-5.98	-6.56	-5.83	-6.23

Table SI-6: Gibbs free energies associated with each state for all the complexes. All values are shifted to the free energy of the neutral complex, and shown in eVs. Results obtained using B3LYP/def2-TZVP.

	Gibbs free energy *vs.* neutral state, in eV (B3LYP/def2-TZVP)				
	OCH_3	SCH_3	$N(CH_3)_2$	$N(CH_3)_2$,CN	CN
$Ni^{II}L$	0	0	0	0	0
$Ni^{II}L^{\bullet-}$	-3.14	-3.27	-3.40	-3.04	-3.21
$Ni^{I}L^{\bullet-}$(S=0)	-5.45	-5.59	-6.02	-5.32	-5.67
$Ni^{I}L^{\bullet-}$(S=1)	-5.35	-5.50	-5.84	-5.29	-5.58
$Ni^{I}L^{\bullet-}$(M_s=0)	-5.52	-5.39	-5.97	-5.33	-5.68

Table SI-7: Redox potentials for the two reduction processes of each complex. All values *vs.* Fc (4.87 V). Values and reference calculated with BP86/def2-TZVP.

	ΔE (V) vs. Fc (BP86/def2-TZVP)									
	OCH_3		SCH_3		$N(CH_3)_2$		$N(CH_3)_2$,CN		CN	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
$Ni^{II}L/Ni^{II}L^{\bullet-}$	-1.54	-1.57	-1.56	-1.50	-1.65	-1.62	-1.43	-1.48	-1.21	-1.40
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (S=0)	-2.43	-2.20	-2.50	-2.13	-2.28	-2.11	-2.11	-2.09	-1.95	-1.99
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (S=1)	-2.76	-2.20	-2.71	-2.13	-2.70	-2.11	-2.64	-2.09	-2.49	-1.99
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (M_s=0)	-2.28	-2.20	-2.20	-2.13	-2.26	-2.11	-2.09	-2.09	-1.98	-1.99

Table SI-8: Redox potentials for the two reduction processes of each complex. All values *vs.* Fc (4.38 V). Values and reference calculated with B3LYP/def2-TZVP.

	ΔE (V) vs. Fc (B3LYP/def2-TZVP)									
	OCH_3		SCH_3		$N(CH_3)_2$		$N(CH_3)_2$,CN		CN	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
$Ni^{II}L/Ni^{II}L^{\bullet-}$	-1.22	-1.57	-1.09	-1.50	-1.32	-1.62	-1.15	-1.48	-0.96	-1.40
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (S=0)	-2.05	-2.20	-2.04	-2.13	-2.09	-2.11	-1.90	-2.09	-1.75	-1.99
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (S=1)	-2.15	-2.20	-2.13	-2.13	-2.18	-2.11	-2.00	-2.09	-1.92	-1.99
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$ (M_s=0)	-1.98	-2.20	-2.24	-2.13	-2.08	-2.11	-1.90	-2.09	-1.79	-1.99

Table SI-9: Comparison of calculated and experimental shifts of redox potentials compared to $NiOCH_3$ substituent for B3LYP/def2-TZVP calculations.

	ΔE (V) vs. $NiOCH_3$ (B3LYP/def2-TZVP)							
	SCH_3		$N(CH_3)_2$		$N(CH_3)_2$,CN		CN	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
$Ni^{II}L/N_i^{II}L^{\bullet-}$	-0.13	-0.07	0.24	0.04	-0.08	-0.09	-0.27	-0.26
$Ni^{II}L^{\bullet-}/Ni^{I}L^{2-}$	0.06	-0.07	0.24	-0.09	-0.08	-0.12	-0.23	-0.21

8.5 Cartesian coordinates

1) $NiOCH_3$: starting complex (q=0)

C	8.07952998951881	15.46451597425837	9.53758548484799
C	9.41753673764106	15.88330692165889	9.63033623927366
C	9.81728939967725	17.05292892876954	8.96428753196294
C	8.88512012840650	17.77912320247435	8.22353303451121
C	7.54594891129964	17.36350651660581	8.12879938161750
C	7.14995388919828	16.19004761033935	8.79841430311337
N	6.68736226178176	18.16900887692485	7.35352014407180
C	5.36813287906021	18.06214052713858	7.04983185333387
N	4.62587941995472	17.06888639922015	7.51118003072562
N	3.34005999377534	17.16881380503444	7.07316082065177
C	2.42870844413798	16.27230873857813	7.42545624223533
C	2.71288578024545	15.11085232978770	8.31859427067080
O	10.24717157883449	15.09656985239523	10.3820191850154
C	11.62304743650247	15.49632127917381	10.4944188058948
Ni	2.71762406651408	18.53176878490616	5.95315259132749
N	1.09518466164885	17.62189565907837	6.09041305136663
C	1.12097240478708	16.53196689075692	6.84333896607427
C	-0.08138773606231	15.67416567544224	7.05585310783263
S	4.72815247919096	19.34558936538897	5.99264256678649

S	1.68925066464795	19.95172977131488	4.67317319611015
C	0.12259065715495	19.11037495786723	4.77199663583225
N	-0.89005392362192	19.67659662482808	4.06827431944277
C	-2.24056365419402	19.30766242552468	3.90257748732295
C	-3.01141761408354	20.11384181293873	3.03840079536259
C	-4.35126007131363	19.83537836075266	2.81317439066922
C	-4.96364663037950	18.73830950645358	3.44723069830924
C	-4.20370033608440	17.93291699984740	4.30693126770054
C	-2.85164877547458	18.21448763520156	4.53392229690209
O	-6.28788749132865	18.54270762595818	3.16455736115344
C	-6.94679012955811	17.43294500842251	3.79673041556531
N	-0.05790927709871	18.00564219937336	5.48006713709206
H	-0.62188140419552	20.51907523401790	3.56187798915297
H	7.14114395955103	18.98078831629621	6.93780015507290
H	10.84570837223051	17.40676718780138	9.01361558267221
H	-2.54608454604614	20.96686928174377	2.53972820245504
H	-4.94183222253128	20.46185947860778	2.14313814093775
H	-4.65028013668658	17.07787822204200	4.81211657666760
H	9.20399397656129	18.68762089094735	7.70760596487260
H	-2.27027898249402	17.58498519449378	5.20292284514906
H	-0.81966881172360	16.18936776587608	7.69148285698973
H	0.18648119701806	14.72676924899124	7.53558452469603
H	-0.57574909088642	15.46538081934486	6.09663930765671
H	6.11840412663571	15.85398383350528	8.73308026018635
H	2.76875059833268	14.17598016999260	7.73702108685318
H	1.91259300086010	14.98603026170371	9.06112109498961
H	3.66724694392297	15.25101462230521	8.83583452214734
H	7.77388110300401	14.55450058304191	10.0564771143520
H	-7.98068780279402	17.45978278600997	3.43696985070255
H	-6.93245339962487	17.53629292518956	4.89268735789608
H	-6.47891709804030	16.47871311289494	3.50944485494961
H	12.11148179571025	15.51598608413409	9.50795171454770
H	12.09940162378549	14.73970009643864	11.1266271825642
H	11.71053865263217	16.48532661820694	10.9701132017123

2) $NiOCH_3$: 1 electron reduced complex (q=-1)

C	8.03588315477137	15.51161918174270	9.60233034473833
C	9.38678481494373	15.88033810021216	9.68765266882708
C	9.83829709784669	16.98798125772298	8.95215565476215
C	8.94502507893878	17.70142587029608	8.15178081156182
C	7.58716805066414	17.33782535845505	8.06041036765738
C	7.14232235456894	16.22362926172256	8.80325300270876
N	6.76552038667421	18.11100359266051	7.23063919044533
C	5.42112000081278	18.01909242755320	6.93590260815343
N	4.65083146654492	17.07972602451398	7.43608479723183
N	3.34730562134162	17.22114760300587	7.04244555580753
C	2.42731135735715	16.28232059169812	7.38961766426264
C	2.80721587367057	15.11300484117348	8.24368429600239
O	10.18108212492537	15.10911447250113	10.5039976809452

C	11.56658849205312	15.46656909101593	10.6043378323014
Ni	2.73913072329140	18.54764510295862	5.88693412742399
N	1.12635109487402	17.62942717618699	6.03058603790268
C	1.14222264761250	16.54647289590509	6.85256002254797
C	-0.10789010574347	15.76846194809975	7.12231739506490
S	4.79746141054304	19.26441028851241	5.82247360083973
S	1.65879915802518	20.00928822972901	4.68325733363042
C	0.09539514756000	19.15820944899314	4.78662044034630
N	-0.94381261909528	19.74511185208767	4.09523441920358
C	-2.27892622042879	19.35745811618999	3.92794405068812
C	-3.09956416257749	20.19142062181836	3.13347749503200
C	-4.43482463581148	19.88354775685010	2.91405686559559
C	-5.00167854796340	18.72750892271256	3.48214345561718
C	-4.19988566074647	17.89496874649645	4.27177570760673
C	-2.85036922568531	18.20499435427788	4.49446236726150
O	-6.33098353223606	18.50752988544393	3.20593051340188
C	-6.93513090125920	17.33672315529003	3.77288313456863
N	-0.05252759407254	18.04962058207077	5.47585229784669
H	-0.68661243046389	20.60932341657184	3.62525260242604
H	7.23610221769660	18.87902733313471	6.75853514897375
H	10.87930269691343	17.30507803894152	8.99316238667866
H	-2.67438893887439	21.09244851735051	2.68485633015399
H	-5.05730721437208	20.53496972093193	2.29834847611483
H	-4.60868149559652	16.99357763800963	4.72676328446053
H	9.30892655954241	18.56112778385049	7.58407170571876
H	-2.23347713529226	17.55400579666087	5.10983099690273
H	-0.87179149406189	16.39815988163851	7.60679536137817
H	0.08995307693075	14.90898929604963	7.77318444872041
H	-0.55741028150445	15.39864337227189	6.18691003918968
H	6.09727215800125	15.92805400084059	8.74317966054993
H	3.58427704057117	14.50135776363740	7.75722328760281
H	1.94275828970539	14.47036199712999	8.44630883488428
H	3.22774276661979	15.44198964844590	9.20744185854003
H	7.68663748232224	14.65003496781059	10.1745637242766
H	-7.97719102316473	17.34549510320204	3.43536627636734
H	-6.90309226995927	17.36519454384963	4.87359140581520
H	-6.43928478000195	16.41991572740493	3.41644589863066
H	12.06605781410894	15.40717570133184	9.62427691884923
H	12.01383834731337	14.73736358541406	11.28851723225902
H	11.68807376216607	16.48109240762493	11.01598638152398

3) $NiOCH_3$: 2-electron reduced complex (q=-2, S = 0)

C	7.98912192629950	15.67757206329693	9.76952055039545
C	9.36456037102930	15.94935331682361	9.77852650649483
C	9.88180055699884	16.85951929143551	8.84238022889617
C	9.02949514163945	17.47824001025408	7.92598052211294
C	7.64169807525436	17.21560086981927	7.90868795703726

C	7.13471560844759	16.29232445577049	8.85359202304154
N	6.86086998654167	17.87223718550080	6.96258277488130
C	5.48031576698571	17.86097000744893	6.73170295935119
N	4.67064098263520	17.04059698350810	7.35406451363550
N	3.33667329824112	17.32481711953580	7.12826135896994
C	2.41456030022587	16.31735266034547	7.39861678838023
C	2.82277359599209	15.10523205446606	8.18423202100515
O	10.11851886376309	15.28469536010587	10.7262398037899
C	11.52525633348010	15.55293173120285	10.7482199634073
Ni	2.76085924248947	18.57209589701301	5.84109857140775
N	1.16205244733793	17.57882973301697	5.89936386845265
C	1.15891808234445	16.56000554477140	6.84919573424009
C	-0.12107986367978	15.86630447255645	7.21378258947754
S	4.89041448095117	19.04135820470909	5.54140894830612
S	1.56883838193689	20.17747541845794	4.91879842041805
C	0.03598821536539	19.28017515162397	4.96265497106408
N	-1.05092606357116	19.90886617401952	4.34510289546515
C	-2.34244169196685	19.46411344041605	4.08288224814868
C	-3.20883779678843	20.33120475709731	3.37003814155585
C	-4.51402897741185	19.96326284637297	3.07357554564641
C	-5.01254878776178	18.71035135780839	3.47748200926945
C	-4.17158765044892	17.84359344248566	4.18350644258777
C	-2.85155033718914	18.21291865361514	4.48630786791411
O	-6.32252265630493	18.43846294459771	3.13433142493026
C	-6.85272371624660	17.17172146821947	3.54087995436993
N	-0.06249020577489	18.10324019909473	5.52940910652373
H	-0.83039358499191	20.83722617845845	3.99540770293072
H	7.36272982020734	18.51176639597194	6.35265066662748
H	10.94477763514106	17.09666444579699	8.81645511479334
H	-2.83961207427765	21.30772314166046	3.04628156469037
H	-5.16617795463867	20.64333315370524	2.52209272884304
H	-4.52696583769768	16.86747637187073	4.51312577202002
H	9.44822546165667	18.18577591639966	7.20573059156764
H	-2.20143536847709	17.53804563892209	5.03992291856182
H	-0.82777164265121	16.54733064351477	7.71969778148174
H	0.06661196322795	15.02064694534621	7.88862399527965
H	-0.65103983148133	15.48438285473252	6.32471181127565
H	6.06888135879145	16.07157253956437	8.84899657918456
H	3.56971473597615	14.49832996689983	7.64320597759008
H	1.95843816592008	14.46116027756000	8.39339683691714
H	3.29005533744833	15.37539940784586	9.14653646784135
H	7.58718762403924	14.96756144104056	10.4957430015199
H	-7.88601247007075	17.14774695799914	3.17697499002028
H	-6.84602954410497	17.06864394861728	4.63820952351307
H	-6.28589719886386	16.33832036070779	3.09495291960017
H	12.00229228488483	15.27113034257653	9.79543629698167
H	11.93537105340717	14.93890823277240	11.5578277777311
H	11.72764415573999	16.61641502264759	10.9550062698527

4) $NiOCH_3$: 2-electron reduced complex (q=-2, S = 1)

C	7.97710910951263	15.41703993356491	9.55727938711197
C	9.33428894321825	15.73279405407785	9.71436071786167
C	9.84110858600612	16.88186167177570	9.08592898824492
C	8.99626845690368	17.68607069564013	8.31910300849620
C	7.62868473732027	17.37782031507116	8.15166751972517
C	7.13025772190055	16.21914026830221	8.79190171449212
N	6.86151259988584	18.23652289667594	7.36500212339645
C	5.52097610282855	18.21083703802836	6.98588246553360
N	4.71512015430349	17.26282146789070	7.41749516993267
N	3.43608464628155	17.39862749037536	6.93273202976564
C	2.49727522679998	16.48946095425405	7.30724765857704
C	2.83717496781566	15.35884529572184	8.23628604514492
O	10.08081814144142	14.87074049176519	10.4913108044253
C	11.47122155472555	15.17452671207540	10.6566865222296
Ni	2.85259105907162	18.81690561026764	5.71547478383998
N	1.18002784186837	17.81889667991405	5.92169682283928
C	1.21424363054331	16.73030222348872	6.73551611760251
C	-0.01456499887160	15.89983631685577	6.97541799160014
S	5.02978165124902	19.53709770390758	5.90168467157758
S	1.59879480693812	20.15530095087614	4.32659454656427
C	0.09714215072114	19.22339812222822	4.55659291392934
N	-1.00474186651941	19.71451044334777	3.86019704188782
C	-2.33318939258011	19.29552623265099	3.79771616681837
C	-3.21553408339885	20.04440558290584	2.97975018192293
C	-4.55507051603415	19.70144999368766	2.86021293471786
C	-5.07205233800927	18.59174378560598	3.55505613969367
C	-4.21421023101877	17.84133790231891	4.36631202236024
C	-2.85900619755361	18.18563115519265	4.48877633826603
O	-6.41461419355085	18.33253959762346	3.37093084171742
C	-6.96513855719511	17.20987044124878	4.07038885012549
N	-0.00726173899479	18.15106517654053	5.31429561022861
H	-0.78102113225751	20.54133243406435	3.31106382917581
H	7.36391704741315	19.02385179608215	6.96130947490080
H	10.88934781691307	17.16164378275127	9.18440467967766
H	-2.83226390299143	20.90977869017054	2.43305198357597
H	-5.22041287381706	20.28993462599192	2.22552511803053
H	-4.58267294197226	16.97635618483862	4.91730807135081
H	9.40603995765245	18.57657463867772	7.83553921123365
H	-2.19360911507416	17.60005807320052	5.11992951275121
H	-0.83300604220060	16.50582992496784	7.40024202745239
H	0.18201071138323	15.06739355794742	7.66211136764529
H	-0.40800814136341	15.47861615323961	6.03436770914495
H	6.07788232603794	15.96888011849061	8.67373144186231
H	3.64288674275755	14.72727154579204	7.82446734243043
H	1.97029071520339	14.71611664713367	8.43233480921807
H	3.21115315975724	15.73103846091318	9.20549845246593
H	7.58367694639800	14.52351044400275	10.0468615637024
H	-8.02517125561064	17.17602678320150	3.79528064107046

H	-6.87118951212035	17.33300748056867	5.16149284629239
H	-6.47563815015549	16.27016427294797	3.76729197448127
H	11.99883701661673	15.17571943123512	9.689110785762631
H	11.87721813457889	14.38083520088028	11.29364505412577
H	11.61256251724267	16.15011554902268	11.14934797302024

5) $NiOCH_3$: 2-electron reduced complex (q=-2, M_s = 0)

C	8.11984768898092	15.34427160229637	9.30393566977726
C	9.42619405162659	15.78682298730703	9.55495733439778
C	9.78770137463433	17.08754744978125	9.16834185239890
C	8.85281204336220	17.91489116314170	8.54335899098230
C	7.53435056148182	17.48017308330095	8.28225805086293
C	7.18224469998472	16.16898202285781	8.68133577556850
N	6.66263847443142	18.36569293051291	7.65656558553107
C	5.33662890400030	18.21707314909698	7.23413503852077
N	4.62525080790611	17.15321551573699	7.51320841563661
N	3.41894637630925	17.11878344205287	6.83889923526361
C	2.43102737375369	16.27604428978885	7.34059772924017
C	2.76904309400286	15.23807663057972	8.37084979833653
O	10.27198727105876	14.88943488304746	10.1783488441098
C	11.60995977738833	15.32732080033404	10.4422191003250
Ni	2.75999487423885	18.57855701608325	5.84697339152606
N	1.09219743175456	17.75470711202193	6.14583453418713
C	1.16890915336726	16.53485850491775	6.81241057856705
C	-0.02648107726822	15.62964310372519	6.87868191255102
S	4.67821819243259	19.56476964991483	6.28078539648680
S	1.77263154614927	19.67699647591546	4.21671337990266
C	0.18305598958373	18.91923560506726	4.45538357694413
N	-0.85231850112295	19.42016515030770	3.65873526660182
C	-2.21917439862867	19.16203194494412	3.65837528279052
C	-3.02686964240993	19.87692180048922	2.73800247949118
C	-4.39891229971629	19.67605642145027	2.67435853894969
C	-5.02566818190183	18.74983544811976	3.52908439734175
C	-4.24329365945031	18.03409452321833	4.44125638004328
C	-2.85524713782768	18.23326184532184	4.50718459328274
O	-6.39414840494647	18.62298034367240	3.38823555304594
C	-7.05257300254463	17.68408104337357	4.24628646336938
N	-0.00426240325521	17.96176112443088	5.32964193450105
H	-0.53935101666041	20.11258638957318	2.98401981841112
H	7.05641583501475	19.27361987428547	7.42551575613062
H	10.79266359047096	17.46865848726037	9.34658428611455
H	-2.55870464554834	20.60173144355643	2.06691821611704
H	-5.00505223543728	20.23656915407341	1.95990607848167
H	-4.69706989380278	17.30731586604722	5.11483329207874
H	9.15107894000808	18.92388214256497	8.24708648641867
H	-2.24861876066563	17.67051777507946	5.21422462425191
H	-0.91968705508595	16.15396725494143	7.25867527866597
H	0.16665365196410	14.76776357427724	7.53111326316398
H	-0.30245478912470	15.24009317439684	5.88300001443115

H	6.16785653725605	15.82085644471232	8.49516472552524
H	3.61736991846002	14.60715210388616	8.05582303075845
H	1.91020433242814	14.58257998889493	8.56710636844391
H	3.06821821022266	15.69364013691886	9.33129361243815
H	7.83800050078407	14.33344378493759	9.60712308122743
H	-8.11521539135432	17.73114024215194	3.98308814900835
H	-6.92342908888345	17.95218487784085	5.30753367694956
H	-6.67740186557668	16.66072228672264	4.08249004504047
H	12.14172927132362	15.57623202702549	9.50947717157583
H	12.10919492230220	14.48499018028242	10.9341163213681
H	11.62084305452956	16.20305072776189	11.1113646228655

$NiSCH_3$: starting complex (q=0)

C	7.99138968119926	15.41234828133432	9.59044934264652
C	9.34330441045560	15.79433951937814	9.68531841552436
C	9.76187229639381	16.95153807033527	9.00655376689592
C	8.85154725704458	17.69609466760442	8.26041103425178
C	7.50146219718243	17.31202043679728	8.16807248018419
C	7.07772419152715	16.15318673801266	8.84587581104191
N	6.66361641650758	18.13297221958352	7.39154090089052
C	5.34451134575158	18.04482255984516	7.07357213079576
N	4.58714362777351	17.05639976811803	7.51815298760548
N	3.30687557341903	17.17541614417488	7.06819054169769
C	2.38191410807203	16.28612534303329	7.40172802761602
C	2.64270249659362	15.11118434875320	8.28380431406068
S	10.40147552509019	14.76636745270248	10.6622864420959
C	12.01866303035334	15.57824635348710	10.5609337221226
Ni	2.71337524786769	18.55595145553736	5.95398431154880
N	1.07858733698698	17.66511140299108	6.06716097090662
C	1.08277116197526	16.56816044177416	6.80981419789089
C	-0.13241150948301	15.72455869337376	7.00342703460099
S	4.73177889511122	19.34615682372794	6.02378199820844
S	1.71696537775508	19.99712308991715	4.67227642567752
C	0.13964709896711	19.17638999632436	4.75162057717564
N	-0.85979230637425	19.76220759012746	4.04154656568349
C	-2.21003823333487	19.41193764123466	3.85847867462599
C	-2.96633415711719	20.24407648940648	3.00601785435545
C	-4.30609499795671	19.97969838353637	2.76261643827638
C	-4.94212553993606	18.87437653492920	3.36520985486568
C	-4.18834914608556	18.04960199388711	4.21377642136873
C	-2.83725476427113	18.30972026715920	4.46031970861024
S	-6.65488342483036	18.63647556656634	2.99128038556286
C	-7.08894485386380	17.11284348913248	3.87164051030156
N	-0.06336717232708	18.06939886711755	5.44871800631909
H	-0.57557570136678	20.60620669188095	3.54691733509035
H	7.13244710429287	18.93947220555916	6.98256334155444
H	10.79809741612831	17.28288602106954	9.05137696651535
H	-2.49005621535318	21.10339256784228	2.53003492961849
H	-4.86842939463786	20.63672921396447	2.09669176662856

H	-4.64491203468507	17.18803148745213	4.69879648553651
H	9.19264512187060	18.59205419108138	7.73766080014682
H	-2.26835507163344	17.66040415096102	5.12053087472387
H	-0.86987328567023	16.24422093250200	7.63583297024939
H	0.11741932759239	14.76980666574143	7.47757687390821
H	-0.62041467358553	15.53052518679322	6.03819882284592
H	6.03910053059275	15.84063092735016	8.78381565577732
H	2.68592338380576	14.18203042374305	7.69263628560999
H	1.83666227078538	14.99151810559038	9.02050297717017
H	3.59619749594421	15.22948393693931	8.80739942151903
H	7.64459766166285	14.51692013963670	10.1099138800488
H	-8.13928205214900	16.92618823944975	3.61666379901571
H	-6.99870913126653	17.23639357799226	4.95778305263926
H	-6.47927668034495	16.26798326031549	3.52859690916623
H	12.39264494281134	15.59900613700174	9.53000895019127
H	12.68624452561586	14.96007757817382	11.17357708794876
H	11.98310128914321	16.59217072905720	10.97777496068774

$NiSCH_3$: 1-electron reduced complex (q=-1)

C	7.95254211243379	15.43977188324671	9.62289324177900
C	9.30844871661626	15.79339943561282	9.74224840955706
C	9.77014305561037	16.91338301801839	9.02812437347079
C	8.89897281912568	17.64766387289808	8.22673178555931
C	7.53827826313374	17.29471708791752	8.10685155808820
C	7.07516483762799	16.17010504797537	8.82244718185774
N	6.73707711968926	18.08760187131426	7.28242132973564
C	5.39578652682650	18.00894319737685	6.96265596542082
N	4.61337943771674	17.06467498211671	7.43272783454827
N	3.32083404358369	17.21216126720862	7.01050877048701
C	2.38512198785645	16.28474747782331	7.34582167771312
C	2.73868953541632	15.11398853536082	8.20881237735165
S	10.32047379282581	14.78302332439437	10.7940800724322
C	11.95972218111767	15.55175717144500	10.6929712548180
Ni	2.73886939269442	18.56191817444988	5.87110958126319
N	1.11427999607257	17.66492359645650	5.99264362501810
C	1.11066392155944	16.56546811625407	6.79225644245054
C	-0.14719693339341	15.78781236857314	7.02324073124313
S	4.79728879959241	19.27878526602941	5.86459755539764
S	1.69800170358171	20.03290178002587	4.64637422358163
C	0.12326331387779	19.20246549852702	4.72949933843934
N	-0.90178570552397	19.80577549552039	4.02774484846461
C	-2.23994336769244	19.44517046943350	3.85642643453418
C	-3.04375182802812	20.29502275778027	3.06137905078026
C	-4.38404374770944	20.01195853209265	2.83984778245688
C	-4.98215201764853	18.86502556239557	3.40354485745603
C	-4.18804294113990	18.02134723982627	4.19228594367052
C	-2.83555555685162	18.30116981136766	4.42009907980931
S	-6.70217153063519	18.60054796730956	3.05294165542919
C	-7.09591358835390	17.06728549817095	3.93728591863353

N	-0.04779219168758	18.09399826442676	5.41273096210475
H	-0.62594788421832	20.66501170083062	3.55832093644956
H	7.21984446454629	18.86205723771146	6.83312245517251
H	10.81245441199228	17.22569048549259	9.08881865820467
H	-2.60139501273513	21.18896209261789	2.61490449581885
H	-4.97668840953592	20.68914556376156	2.22067113878311
H	-4.61180194473655	17.12573737973632	4.64649736560376
H	9.27782996482170	18.51509341014391	7.68043465730191
H	-2.23323995198420	17.63670429215551	5.03585796760557
H	-0.91836080238787	16.41234520883630	7.50296744284060
H	0.03491815579374	14.91651437317470	7.66293057036013
H	-0.57785462871071	15.43570499357842	6.07221117627310
H	6.02944732738863	15.88144040169461	8.74175988590593
H	3.52573624948976	14.49993110119665	7.74183500209238
H	1.86660152681562	14.47514981792118	8.38958095514467
H	3.13556317181555	15.44208894362218	9.18299076475495
H	7.56911306458818	14.57325950139467	10.1671207894606
H	-8.15807476230758	16.88253113827361	3.73372316682255
H	-6.95051427813973	17.18148602438412	5.01903459813586
H	-6.50426714523409	16.22420510018656	3.55840912671540
H	12.35317385440618	15.52217304417587	9.66897814819542
H	12.60197219998402	14.94483327353475	11.3433696970663
H	11.94076628005361	16.58340334422822	11.0665711377403

$NiSCH_3$: 2-electron reduced complex (q=-2, S = 0)

C	7.90497773583326	15.62205717340319	9.81376151151697
C	9.28911647771367	15.86809634937362	9.84147139729986
C	9.81798726622781	16.78574720708963	8.91526861686377
C	8.98669320487756	17.42968127982927	8.00195076000524
C	7.59262583022069	17.18788682086615	7.97084350464921
C	7.06532504407537	16.25983398644831	8.90104900121178
N	6.83137803244799	17.86804105535666	7.03264988450117
C	5.45605264985851	17.85969064499945	6.76857119508268
N	4.62995000255890	17.04381510583027	7.37500379775383
N	3.30487977934057	17.33008185715098	7.11577890384224
C	2.36998294196764	16.33208923827072	7.37142232485032
C	2.75153994829947	15.11967058195285	8.16960362892040
S	10.25213034441779	14.98480499615184	11.0507027062745
C	11.94033793798326	15.59336094108812	10.7922895716531
Ni	2.76284268985036	18.58561688135512	5.82319861037033
N	1.15517638519127	17.60806026187612	5.85562712048154
C	1.12620411605644	16.58652972043935	6.79977079917976
C	-0.16431216089234	15.89757600579353	7.13492695724819
S	4.89825294633113	19.04043739471824	5.56460799970437
S	1.60608564261818	20.19853017754197	4.87783207532404
C	0.06615324077372	19.31354557150227	4.88799552528271
N	-1.00025406917750	19.94891941559588	4.23997633131352
C	-2.30401495538812	19.54388333631634	3.99859344925800
C	-3.15117079758216	20.42856361957986	3.28295887746876

C	-4.46912689156700	20.09693136979411	3.00402438586961
C	-5.01129785605752	18.86373762623576	3.42754063407705
C	-4.18089939259402	17.98571030446371	4.13672825609140
C	-2.84921843686173	18.31158704607576	4.42193457570842
S	-6.71507993378009	18.54871664101334	3.01977352759428
C	-7.01154130389353	16.87949584811224	3.66132728238963
N	-0.05426202225244	18.13714195159355	5.45243796393134
H	-0.76102783917227	20.87420623694159	3.89354378974925
H	7.34865777739157	18.50328365900046	6.43069758925338
H	10.88486323938282	17.00872572352600	8.89658081344874
H	-2.75550331446523	21.38924633465891	2.94290438973636
H	-5.09005863096247	20.80330624142873	2.44776425997043
H	-4.56049937839772	17.02429789924675	4.48444426981135
H	9.42142045094946	18.13949134538732	7.29314628746700
H	-2.21504208251504	17.62159342295419	4.97554335026081
H	-0.87513521275312	16.57837576515425	7.63530202491756
H	0.00666528015155	15.04394144279761	7.80390902135560
H	-0.67959845315994	15.52855299721155	6.23211160869687
H	5.99638012224486	16.05465794926388	8.88701141154695
H	3.50516979285843	14.50541115676924	7.64664035831908
H	1.87776197624869	14.48372578267757	8.36297180160273
H	3.19990394751357	15.39082158919626	9.14052784199233
H	7.46844918706445	14.91236925722487	10.5215037963097
H	-8.05290478437611	16.64982739950220	3.40349005837671
H	-6.89411261735089	16.84226037808860	4.75193843986804
H	-6.35077420299387	16.14530917221062	3.18270235022048
H	12.30523619313780	15.34969516866187	9.78629641285465
H	12.55392737491411	15.06772203555330	11.5345836935764
H	12.00763477769220	16.67432163272612	10.9701792549472

$NiSCH_3$: 2-electron reduced complex (q=-2, S = 1)

C	7.88817110782323	15.36858619690986	9.60104494723646
C	9.25231104063132	15.66037160911458	9.77582280570970
C	9.77630644124432	16.79563037269045	9.13037561076977
C	8.95850210284534	17.60192818342252	8.34256162420796
C	7.58571877074693	17.31291462363641	8.16317375183290
C	7.06231211494489	16.17062192381451	8.81344714717406
N	6.84391062888576	18.17131101987325	7.35949552563854
C	5.50431109216408	18.17015091725544	6.97175077912952
N	4.68309956196985	17.22976306276465	7.39146962358965
N	3.40966167129328	17.38831721470464	6.90263297605708
C	2.45620023637134	16.49026203136310	7.26322458260117
C	2.77354618192620	15.34735090330177	8.18499469474016
S	10.19738385375276	14.55955732996630	10.8037415026566
C	11.86269889988833	15.27633537466799	10.7950187005490
Ni	2.85405128878297	18.82749608662704	5.69668060729960
N	1.16591044571197	17.85173029940887	5.88391008556499
C	1.17946976179083	16.75572992241779	6.68675393747895
C	-0.06242503324062	15.94070460186061	6.91115134638356

S	5.04093650960570	19.51166008341457	5.89643224380122
S	1.62903776836391	20.19921669111278	4.31640681750305
C	0.11449478753447	19.28695632693680	4.52838862503407
N	-0.97766200461356	19.80270814137407	3.83192184133061
C	-2.30647014502990	19.40233377539932	3.74978304574321
C	-3.17364357302599	20.17660265590774	2.93864363710561
C	-4.51557456790137	19.85071339572978	2.80175901982240
C	-5.05987640553613	18.73260520137412	3.46940681255969
C	-4.20762625961059	17.96204722902142	4.27249872114556
C	-2.85249071015028	18.28390112204013	4.41576245200451
S	-6.79083049043364	18.40986577709561	3.22369549002364
C	-7.09497846855840	16.91380166455193	4.20073989553178
N	-0.01148975873190	18.20792962375526	5.27336450741588
H	-0.73752653717322	20.63356364128175	3.29532615006857
H	7.36166612153451	18.95100154068075	6.95943652895070
H	10.82775403498663	17.06229705381106	9.23462104680073
H	-2.77618808110933	21.04761020163599	2.41162258894527
H	-5.15241480334367	20.47189675751377	2.16761668182940
H	-4.58805180256986	17.09022671802631	4.80502482626701
H	9.38850351838293	18.47831154678866	7.85086639733535
H	-2.20062907751227	17.67812065997737	5.04196573444931
H	-0.87784583882090	16.55856349660302	7.32377539728478
H	0.11405986293267	15.10684769770392	7.60144294496577
H	-0.44830236937697	15.52293356297227	5.96549237695667
H	6.00796311802310	15.93366170958616	8.68651626545769
H	3.57754538491088	14.71224215638579	7.77585950528368
H	1.89826864742592	14.71152640380169	8.36491727568855
H	3.13975475347651	15.70686285303427	9.16185560177991
H	7.45534220687372	14.49274749260182	10.0911616960003
H	-8.15814283910747	16.68467252119644	4.05583542978720
H	-6.90593570694081	17.08674674667103	5.26791932605771
H	-6.49202146292051	16.07131530500104	3.83861222369607
H	12.29034660725867	15.28512547628428	9.78435877702985
H	12.46358192437185	14.61706333929814	11.4339308410055
H	11.86523348925247	16.28854275763100	11.2192030267188

$NiSCH_3$: 2-electron reduced complex (q=-2, M_s = 0)

C	8.04678848695060	15.28606963135614	9.33321164574808
C	9.35174200194094	15.72016824063764	9.62582704662845
C	9.70726462820330	17.03511754149908	9.27327518922142
C	8.78791344499405	17.87506282701328	8.64956488400504
C	7.47398821062565	17.44299686338471	8.35060962087521
C	7.11829065345271	16.12123549778557	8.71230893306680
N	6.61695450565725	18.33784614698687	7.72815080312570
C	5.29634804813899	18.20240031255680	7.28129877787498
N	4.58270213263771	17.12945684007089	7.51698104881450
N	3.38893835909610	17.11519165738736	6.82452136214228
C	2.39505422613573	16.25190506654972	7.27502459693506
C	2.71478985106799	15.18345722521586	8.27927151117946

S	10.43852766112401	14.56106732252127	10.42818205861446
C	12.00916297046842	15.45744518784901	10.56062366722887
Ni	2.74788211900900	18.59637424123677	5.85737590585746
N	1.07981150683853	17.75679282800222	6.08835608120757
C	1.14471398968498	16.52066965564634	6.72418146259152
C	-0.04845889867947	15.61069432679007	6.73744862524654
S	4.65321652699723	19.57691294089993	6.35897151099531
S	1.79468018669102	19.74466987921404	4.24060044768477
C	0.20384585363856	18.97677882449451	4.42286254032841
N	-0.81807549657184	19.50321943227416	3.62325172883157
C	-2.18168310916867	19.25400793455559	3.59228277828057
C	-2.97078729301842	19.99685208117979	2.67698738167758
C	-4.34245334885966	19.80762732976674	2.58878751615238
C	-4.99815458655032	18.86408330771932	3.40937424659761
C	-4.22393567066860	18.12290369982914	4.31234181598863
C	-2.83903457190096	18.30685062602252	4.40795569303921
S	-6.75917616412257	18.70614989928583	3.20831074043281
C	-7.22599402503829	17.46175704833805	4.44112997925531
N	0.00038561376527	17.99019108998839	5.26060812629810
H	-0.49070500074615	20.21321570834827	2.97354787054784
H	7.01321743181099	19.25276696712936	7.52957056329311
H	10.70648647744427	17.41797161278294	9.48095416440031
H	-2.48760164916151	20.73538191104625	2.03195664692177
H	-4.91684290492858	20.40164766449249	1.87382038938022
H	-4.69017024762345	17.38070606557265	4.96112814762821
H	9.08929923290248	18.89145907504458	8.38274878091541
H	-2.24864233996530	17.72075406153367	5.10992235936587
H	-0.95202246474351	16.12261101842389	7.10946544772112
H	0.13136350710736	14.73208045950900	7.37092428115419
H	-0.29903814600310	15.24748462758438	5.72530950743316
H	6.10979316386517	15.77284784150933	8.49693493395353
H	3.57223313267675	14.56572620941542	7.96296204643053
H	1.85485822086822	14.51916087224349	8.43662946300289
H	2.99180759075912	15.61003840107420	9.25935557212510
H	7.74348766813211	14.26949906990528	9.59718889415494
H	-8.31410925797665	17.35591825893142	4.34807226037265
H	-6.98162373996682	17.79524555385196	5.45792054331366
H	-6.75113785223273	16.49414020058840	4.23414035123295
H	12.39803687504441	15.73079053241218	9.57129059910740
H	12.70317261131870	14.75502643103907	11.03898669625111
H	11.91081787887895	16.35055495150392	11.19090675536827

NiCN: starting complex (q=0)

C	8.20252926515684	15.29816730053248	8.83769040032547
C	9.17593041325715	15.99950896376816	9.57660008259836
C	9.49251384495140	17.32987149991184	9.22304500497835
C	8.85776299476729	17.94876647444037	8.15901636018330
C	7.88311641805245	17.24714149091182	7.41761507708022
C	7.56579280030606	15.92074092933127	7.77035600140525

N	9.87005789620073	15.46645438918250	10.6659121730515
C	9.82554846246468	14.23753733342689	11.2600856964511
N	9.02853724042621	13.28506837916564	10.8100395085518
N	9.15599305435714	12.15299269281921	11.5560378708320
C	8.44547167573324	11.07849928598383	11.2602007004551
C	7.48781189289899	11.02783003047014	10.1190602968035
C	7.22506165116735	17.87472254418415	6.32122922216143
Ni	10.29597825635508	11.98181791144855	13.0226603486488
S	10.90329098130399	14.03488021076971	12.6542557021629
N	9.59474421162905	10.24946875480380	13.0978795651372
C	8.69724410780181	9.96315022080312	12.1695694055198
C	8.01541064374561	8.64384173331616	12.0463563786501
N	9.96277321668156	9.31905471426376	14.0252445664958
C	10.86322157974508	9.80942796885619	14.8553198033783
S	11.49808996972881	11.46380682143464	14.7534768238452
N	11.38037345008876	9.05722836868612	15.8726599880445
C	11.14444016546542	7.73991034339139	16.2729097369568
C	11.86296552670245	7.29060109478621	17.4031764437398
C	11.69894498470313	5.99983622346221	17.8777164765218
C	10.80617082478066	5.12020097792413	17.2285951373078
C	10.09020824718459	5.56683733477736	16.1006374898697
C	10.25393990576053	6.86210296814721	15.6237204111391
C	10.63114491681257	3.79129487710922	17.7103545422926
H	10.53146270656804	16.10932902414270	11.0999436807296
H	12.06129149842248	9.55495455028557	16.4448240496325
H	12.25746401625143	5.66360920135501	18.7507879953532
H	10.24610449095300	17.87359687463439	9.79566605807515
H	9.11022252723356	18.97510725243094	7.89413685934987
H	6.81286927956987	15.37587338306599	7.20111049599324
H	12.55346267819263	7.96984593551750	17.9064186366628
H	7.95489948354768	14.27529454063284	9.10725854628768
H	6.57941826389898	11.60696124495259	10.3516632917159
H	7.19110864693732	9.99769551729716	9.89557554935296
H	7.93660625893660	11.47857118193044	9.22359623547079
H	9.70078567424964	7.20242728119692	14.7530846061714
H	8.40398741467429	8.08945992520245	11.1764526981637
H	6.93617512069302	8.77926858216590	11.8895444684536
H	8.17880966988792	8.03971402923170	12.9436065648765
H	9.40045049887335	4.89045700083515	15.5960951022086
N	10.48677209832347	2.70138990896654	18.1044244712902
N	6.68608907455806	18.38986072804821	5.42233147562317

NiCN: 1-electron reduced complex (q=-1)

C	8.20770341650958	15.30605997812808	8.82768851535248
C	9.17567828975819	16.02396025172411	9.57047104962104
C	9.46078268517541	17.36509499589801	9.20642226721560
C	8.81015976784775	17.96865789950185	8.14668644164561
C	7.84176259673178	17.25001919114793	7.40411372141874
C	7.55586308872359	15.91515233380426	7.76431396487385

N	9.87261061279546	15.50019954275200	10.6437217208629
C	9.83470966321529	14.25407487888120	11.2484221186201
N	9.04813466506378	13.29347092657104	10.8210117720448
N	9.17549780141721	12.16235047256752	11.5714675062086
C	8.44513173455347	11.05896024541635	11.2722899875828
C	7.48958412126737	11.05847896363865	10.1215264194449
C	7.16905220570367	17.86235763215952	6.31389248560521
Ni	10.32384245917423	11.99575746667837	13.0234188366764
S	10.92336311623272	14.05135388026927	12.6387990230594
N	9.62973572615453	10.27318367394162	13.0964190216366
C	8.70329899765669	9.97403457831484	12.1516992815679
C	8.06461143701188	8.62227457928390	12.1019564270338
N	9.98892852352408	9.34127739805686	14.0247468670338
C	10.88568259159136	9.80757447341807	14.8628924433524
S	11.51962753781086	11.46524608796779	14.7617485997915
N	11.40411647421523	9.03778286856676	15.89174016607987
C	11.15916300623035	7.73313061389481	16.27887244766831
C	11.88113271055144	7.24384380678386	17.39769226636212
C	11.69727135422926	5.95189620444363	17.85350876898382
C	10.77788694812896	5.09243944705623	17.20403656869748
C	10.05822769362097	5.57674643662544	16.09008494074329
C	10.24058208360962	6.87347666304387	15.62985510662667
C	10.58318476674157	3.76417250312647	17.66633705210987
H	10.53544690748308	16.13988562729509	11.07748680551784
H	12.09138857363327	9.53084875126038	16.45837912397710
H	12.26053152457576	5.59255754074278	18.71477163175076
H	10.20594758560877	17.92552842855902	9.77465385855426
H	9.04201034715865	19.00001883562852	7.88072475856874
H	6.81170606616242	15.35390252978212	7.19844369100452
H	12.59162426645632	7.90091857150056	17.90341205574120
H	7.98479372731525	14.27770307459658	9.10100180911829
H	6.73378774634553	11.85149873348669	10.23546662765257
H	6.97140516153318	10.09712266647663	10.03389560558261
H	8.01301691773839	11.25738298318597	9.17272260559607
H	9.68484233644426	7.24262407091198	14.77143614151749
H	8.81966350683131	7.83254350121138	11.96132637855546
H	7.33831683036098	8.55365467721600	11.28443123480521
H	7.54576989525289	8.39598509158107	13.04686406322914
H	9.34797364187842	4.92219564997088	15.58400538486766
N	10.42280632073709	2.66967813967971	18.04766995878004
N	6.61469056923821	18.36710113325232	5.41541447726034

NiCN: 2-electron reduced complex (q=-2, S = 0)

C	8.28444565010077	15.28703094823051	8.75926120945110
C	9.08671424970210	16.07476643803960	9.63084972808628
C	9.29356967940688	17.44548551047287	9.30246774598614
C	8.73763236483861	18.00199266276026	8.16897521121573
C	7.93828737502059	17.21260024463485	7.29701768907515
C	7.72837036740170	15.84986290987099	7.62212348538966

N	9.67251270787034	15.59564191368590	10.77524192516166
C	9.66906885235229	14.33163474100126	11.37574616587519
N	9.01368595578181	13.31577668462801	10.86546098481645
N	9.28077827705110	12.13905569955148	11.50724943453668
C	8.44412624027285	11.05674402727110	11.29076556945347
C	7.39714579493599	11.11061015142027	10.21905170224712
C	7.36579190951744	17.77554648881272	6.13277601217803
Ni	10.33597454723483	12.02162884241299	13.05235167431610
S	10.62815298129860	14.18499011199646	12.86130791464696
N	9.53195839201617	10.33688179485288	13.20713499510612
C	8.68481396018119	9.99751940290810	12.16545969771533
C	8.14181817278502	8.60441700933079	12.05256624640086
N	10.01535568875847	9.34350090687391	14.01245828663448
C	11.02550088828892	9.73747954245639	14.75165652840072
S	11.77755079458104	11.33216995014788	14.55000861099373
N	11.56911513489539	8.93604181123995	15.76161888513651
C	11.24864367125589	7.68249479482288	16.21748629563402
C	12.02580307814298	7.14474970189651	17.28377008810782
C	11.76639077855890	5.89061821601659	17.79701260533089
C	10.70886456559599	5.10082731770937	17.26761910318162
C	9.93603444268688	5.63138907370993	16.20555474709483
C	10.19330048612691	6.88987297065198	15.68669325624889
C	10.43483962668727	3.81518786590738	17.78937745666445
H	10.20546923544507	16.28071213578371	11.30763976120421
H	12.36252207842236	9.37467562601818	16.22523030803211
H	12.37404987702739	5.50098056636419	18.61459897467116
H	9.90600339023099	18.06298016999926	9.96372620216328
H	8.91212113487194	19.05345441669465	7.93769985009021
H	7.11608792803129	15.23241398274668	6.96295312425905
H	12.84062504407229	7.74176288622350	17.70004780740873
H	8.11884324624528	14.24024852732771	9.00551181269700
H	6.63518764385091	11.87935572707471	10.43439935224688
H	6.88227052527701	10.14667742983549	10.12073048946760
H	7.82954091647663	11.37137918951214	9.23887661257584
H	9.59713957991112	7.29243247664174	14.87033614315300
H	8.94508760984880	7.86978297302663	11.87126050653455
H	7.42271628669316	8.52486961537741	11.22752122982183
H	7.63768723082316	8.28721132047218	12.98038762556689
H	9.12256394005540	5.03572166330912	15.78836937905759
N	10.20728478421620	2.74866431509985	18.22211891014515
N	6.89160091515409	18.24433724517902	5.16747065581900

NiCN: 2-electron reduced complex (q=-2, S = 1)

C	8.15856185249301	15.28491930643669	8.81739465830849
C	9.14503739025626	16.05288307105982	9.49211268451317
C	9.39291685621545	17.37951636793318	9.04174441934666
C	8.69734038110617	17.91677669254394	7.97691602887512
C	7.71099233501597	17.14779905623752	7.30375411676589
C	7.46111202114432	15.82748862891009	7.74918982940675

N	9.88283247744087	15.60107048980495	10.56413938953143
C	9.90386631617668	14.39082072406975	11.25787627684663
N	9.14185844883430	13.38808604526226	10.86587510821183
N	9.29188683933400	12.28319237900454	11.65845597639296
C	8.57432272193759	11.17389744568863	11.36889455232936
C	7.61658428332107	11.14315856262962	10.21317695566890
C	6.99336516892058	17.69035537862756	6.21051995457674
Ni	10.50937909573044	12.17695947584964	13.19336048651049
S	11.01222099982873	14.35049076313528	12.64255534598492
N	9.74777802808409	10.37051070715005	13.21038261769323
C	8.83084857206610	10.08310115083696	12.25847803519981
C	8.17422065030575	8.73470979369172	12.18935269240412
N	10.07306510877383	9.40369457946338	14.12208012590879
C	10.95951430246915	9.82595544275141	15.00272703413160
S	11.66433713492540	11.45398007229074	15.04247219228372
N	11.41620844588190	8.96924453387175	16.00471596616607
C	11.13379932033031	7.65713200150040	16.31486286436994
C	11.80354796242092	7.09203021423318	17.43582720975453
C	11.58180976596186	5.78399940088888	17.81829555290166
C	10.67180631083119	4.96957024970165	17.09317365540996
C	10.00326134135461	5.52838228590491	15.97761962766352
C	10.22357238995197	6.84129672474442	15.59112607507428
C	10.43800899104587	3.62726256418238	17.47841052060671
H	10.53800485974241	16.27619657797796	10.95653869698083
H	12.09118000686800	9.42516942565475	16.61737975418896
H	12.10648231262021	5.37243709508333	18.68107348648089
H	10.14922203722742	17.98064481031030	9.55136075989458
H	8.90484300599945	18.93603348986179	7.64967448147321
H	6.70567729743241	15.22627821117443	7.24133077352998
H	12.50541109071720	7.70899502899681	18.00150045122697
H	7.96717655403543	14.26891569805858	9.15527116970224
H	6.84310674346936	11.92214868456275	10.31582311159807
H	7.11340784681843	10.17342379695659	10.12354684586702
H	8.13413373212588	11.34932320989538	9.26162144887807
H	9.70847182517524	7.26926039554967	14.73406158175633
H	8.91993147385801	7.93455427488414	12.04960877855898
H	7.45030188921182	8.67178674830248	11.36857216429441
H	7.64726986978604	8.50082023823543	13.12914200026811
H	9.30145833428217	4.91365031034276	15.41223800248502
N	10.24436179928748	2.51598788640814	17.79788653361956
N	6.39855180918455	18.14026800933943	5.30582200635953

NiCN: 2-electron reduced complex (q=-2, M_s = 0)

C	8.15437584665011	15.34329152327066	8.86638837226643
C	9.24438000311027	16.00512931501566	9.49724360674214
C	9.57250871445100	17.32340307302268	9.06842896727619
C	8.85568352449416	17.95082814584825	8.07051535372414
C	7.76482464446932	17.28917405392886	7.44219306495572
C	7.43743075682450	15.97724670762212	7.86492362644169

N	10.00579821393924	15.44844295832353	10.49351157327891
C	9.95473227457873	14.20523742660833	11.13356124866599
N	9.06263478928954	13.29386319881356	10.82347163552043
N	9.07619329148311	12.22971736364644	11.68131179213803
C	8.42285224454635	11.06615766744666	11.30982834096522
C	7.55075910993401	11.04169344670205	10.09062451944695
C	7.02499065153910	17.92568471249636	6.41870598926229
Ni	10.34157223546058	12.02009799302784	13.04799551396192
S	11.16089923072695	13.94834250261385	12.40911633160353
N	9.73520109149937	10.24705782422727	13.03687045860456
C	8.69580209323370	9.99261661256060	12.15756039669322
C	7.97512743684466	8.67837123776281	12.19568858598990
N	9.96678473551673	9.36472388998432	14.05475772217852
C	10.75768128543612	9.85600503970237	14.97987259695254
S	11.28023996020595	11.55157890895658	14.97015411620824
N	11.25792735623444	9.07376667414932	16.02658262323017
C	11.10169835788280	7.74789713742595	16.34292161690572
C	11.76264176937153	7.25994959590338	17.50667939926920
C	11.65348409487154	5.93938817966041	17.89101742687057
C	10.87145373052180	5.02921882560644	17.12777477916215
C	10.21096053969142	5.51213085095436	15.97122858412669
C	10.31738537792968	6.83717573173117	15.58175037978822
C	10.75549827206213	3.67395177374035	17.51490203464698
H	10.76670015408405	16.03325682930948	10.83386422756616
H	11.83344298718954	9.60785005342503	16.67480168257502
H	12.17015740388455	5.58868765972339	18.78510962494422
H	10.40790138749164	17.84335080713822	9.54296511121281
H	9.12471485717472	18.96122684598630	7.76048887395198
H	6.60369479394343	15.45665857989719	7.391245135565453
H	12.36734860669059	7.94831042940620	18.10161427178983
H	7.89976569187791	14.33507825722732	9.18640652190854
H	6.78048856737561	11.83000742247825	10.12289124356757
H	7.04565115871803	10.07333067690817	9.98542819265130
H	8.13462231748756	11.21921570286434	9.17116056664298
H	9.80741428072266	7.20388045287255	14.69338671546430
H	8.67070940283758	7.82819535283311	12.09927676553084
H	7.23528982603235	8.60861860547070	11.38842042711377
H	7.44506878188462	8.53492931444983	13.15277186472207
H	9.60655859769168	4.82555468835567	15.37640097724973
N	10.65981952750018	2.54990858533182	17.83699166103020
N	6.41218102461441	18.45397236557024	5.56913847963699

Ni(N(CH$_3$)$_2$: starting complex (q=0)

C	-2.89268005735066	18.31091473843240	4.58795260147884
C	-2.27037999656696	19.41955282578190	3.98746978335290
C	-3.04631174603102	20.24974293925254	3.15519873728751
C	-4.39096491259165	19.99284918689341	2.92644639276714
C	-5.03744826671172	18.87879064086091	3.52863935225549
C	-4.24163144301956	18.04895589385669	4.36212244174859

N	-0.91626959027356	19.77178170053943	4.15553445108687
C	0.09544175313451	19.18450992848640	4.84107702232936
N	-0.08556398955680	18.06282315436816	5.52408999706753
N	1.06609382833323	17.65997618854869	6.12177967110531
C	1.09014226932446	16.54848614558217	6.84895810662316
C	-0.11901024285166	15.69342834625920	7.03811425193714
N	-6.37063461994934	18.61927421328890	3.31483028631453
C	-6.99499217479646	17.45116021432670	3.91911449427268
Ni	2.69238751262228	18.56452752455701	6.00426167137532
S	1.66939595186109	20.01852614251903	4.75950695113902
N	3.31155277067071	17.17141963793691	7.08765443765274
C	2.39359836528624	16.26826648255715	7.41814972835974
C	2.68114376843057	15.08279410105278	8.28026087053959
N	4.59718398699121	17.05255932729458	7.51788706532922
C	5.34567373284438	18.05437745654408	7.08327632586430
S	4.70482133225006	19.36947355884702	6.06228824682994
N	6.66488639239109	18.14554120249721	7.38691829013586
C	7.52178672157433	17.31888453316547	8.14032571848153
C	8.86750190548088	17.72261741778907	8.24257253644458
C	9.79417734729033	16.97980043068667	8.96086930238539
C	9.41727004650726	15.77904741398342	9.62252223936833
C	8.05793040866644	15.38406444257448	9.50980314584467
C	7.13232645639741	16.13343833757892	8.78760256822454
N	10.32774754403203	15.03656219649710	10.3369481288978
C	11.71340303676391	15.47227132606536	10.4341192432695
H	-0.64415985502022	20.62388875940924	3.66773880187932
H	7.12203571285242	18.96443010400926	6.98929648864685
H	10.82200540407955	17.33535246927838	9.00813854114317
H	-2.58030384854542	21.11436847403607	2.67635874503297
H	-4.94529191660527	20.66348732811519	2.27219978375219
H	-4.68279926161276	17.17965685388182	4.84706982064103
H	9.19092765096631	18.64051696530844	7.74555091022044
H	-2.31330212164157	17.65448500492552	5.23286672874075
H	-0.87018337725433	16.20945736085318	7.65753092766645
H	0.13626598343304	14.74477588045740	7.52205777570551
H	-0.59535728966905	15.48464665266449	6.06943564220547
H	6.09959807495917	15.79991539944829	8.72082802685332
H	2.76884791372875	14.16678267306622	7.67308612508480
H	1.87079465189002	14.91937284988297	9.00363037612882
H	3.62293374322228	15.22450328648122	8.82021466013900
H	7.71319073016308	14.47258154770406	9.99555934158608
H	-8.05074091369125	17.42567683156981	3.63185594811203
H	-6.93907949090800	17.48387827260612	5.02018786720486
H	-6.52265308104630	16.51175764721108	3.58330740792040
H	12.19605899911705	15.52699339304852	9.44336466829048
H	12.26848808520468	14.75388398944421	11.0453574522323
H	11.79801346370907	16.46513214197248	10.9080055423843
C	9.91184965784929	13.80959163541780	11.0008931169526
H	10.77730656132723	13.36837243248035	11.5054648652606
H	9.13090550163809	13.99791360858992	11.7574789831024

H	9.51749050720546	13.06975466420142	10.2834247321906
C	-7.14961911002917	19.47139947331647	2.42768342256588
H	-8.18213213405314	19.10846744946438	2.40352792093149
H	-7.16175202277782	20.51767048735444	2.77659264953885
H	-6.75557730964419	19.46183971517754	1.39650766811747

$Ni(N(CH_3)_2$: 1-electron reduced complex (q=-1)

C	-2.89336123096450	18.33556844950390	4.59170697619448
C	-2.32558901412025	19.52821377524807	4.10796706589552
C	-3.16008110684313	20.40355002693678	3.38316557775524
C	-4.50036545866227	20.11213406292427	3.15550053646384
C	-5.09233976875781	18.92302511931470	3.65561530059508
C	-4.23981774727508	18.04165555199734	4.36257182936412
N	-0.98597487476332	19.90635977444428	4.28550493816602
C	0.06185673070463	19.27876502245788	4.92165471833655
N	-0.07822057688161	18.12878636337360	5.54371980157576
N	1.11369267091808	17.65954620515704	6.03119307929938
C	1.12870382762157	16.55559537293948	6.82352693679503
C	-0.12952002127084	15.79629324317123	7.11023048437447
N	-6.44655933181903	18.65136903150837	3.47567927116091
C	-6.93592074989391	17.30767762685929	3.75504574586107
Ni	2.73277122792774	18.57836090215660	5.90832885713644
S	1.62470489631387	20.13544713741101	4.84884569497512
N	3.34152473319284	17.20530862685363	7.01527853051496
C	2.42201880015588	16.25231211839808	7.32082113406286
C	2.80822444240470	15.02872453907881	8.09281360690922
N	4.65511477612564	17.01508743491512	7.35653067998948
C	5.43447443796765	17.95004402488693	6.85918640144689
S	4.81542981105267	19.22747352371747	5.77910311727471
N	6.78310960265212	18.00909794850999	7.13188467896942
C	7.60074173676113	17.21402732683186	7.94953036994630
C	8.96748978127207	17.55058814794424	8.02961261571323
C	9.85334888431014	16.82227813012898	8.81574774156225
C	9.42157991284794	15.69618713145781	9.56406372614706
C	8.04350972511703	15.38073332671459	9.49282111356528
C	7.15414007740097	16.11277261763231	8.70227953919164
N	10.31386177826291	14.93163245272588	10.3120310387388
C	11.63830585736100	15.47085885594367	10.5937492790604
H	-0.73772597283142	20.80343523365481	3.87603920110029
H	7.26443293847720	18.76717264165778	6.65466113569947
H	10.89553649931634	17.13651307518495	8.84306932027784
H	-2.74332160603456	21.33160534442191	2.98273222376520
H	-5.09188851701052	20.82398892494563	2.58193336391057
H	-4.62725583894793	17.10109242177268	4.75172030137813
H	9.34090569183414	18.41006121870242	7.46657235447358
H	-2.26868211991261	17.63669777892759	5.14427155173409
H	-0.85999398694943	16.42468982385006	7.64568791989586
H	0.07082693165951	14.90911621108007	7.72222624704144
H	-0.62163428798173	15.47213050177702	6.17934204896982

H	6.10170009081559	15.83864855820732	8.66751852177881
H	3.56770837764694	14.44151522375991	7.55129479213447
H	1.94177060917237	14.38232339733571	8.27489228477864
H	3.25449294683719	15.29265846550099	9.06508531830291
H	7.64458013727591	14.54199378832213	10.0617394110871
H	-8.02331150624810	17.29339594520415	3.61736695503667
H	-6.72612212602580	17.02230503214799	4.79602639564521
H	-6.48869457935538	16.54028491429524	3.09311450053196
H	12.17960697822626	15.69167580492170	9.66255051123104
H	12.21457926448193	14.71784866049246	11.1435882413544
H	11.60583787912427	16.39752804964471	11.1995702743867
C	9.78263210272955	13.97410487228569	11.2732755871579
H	10.61909964140673	13.42868615958555	11.7253113151951
H	9.19954683892494	14.45532344616355	12.0828938105275
H	9.13235596250265	13.23936520768471	10.7769826523259
C	-7.19556555712607	19.42740508594942	2.49533042851154
H	-8.24435631928066	19.11033014928801	2.52348522457173
H	-7.16380788792995	20.50009629624892	2.73494136350935
H	-6.81776741391616	19.29550489584363	1.46257535664495

$Ni(N(CH_3)_2$: 2-electron reduced complex (q=-2, S = 0)

C	-2.88376819264538	18.37968940412309	4.59714249092418
C	-2.35060675684458	19.51527516236603	3.95367748503117
C	-3.24085651964514	20.30002031133154	3.18717207958118
C	-4.59012451242438	19.98153314200960	3.07477928065507
C	-5.14218869116552	18.85531551871954	3.73763346545839
C	-4.24080017204316	18.06109859659876	4.48256702496216
N	-1.01321821715617	19.91485753966910	4.01128714798920
C	0.09609308007779	19.37217717409595	4.65227281207690
N	-0.00413989028770	18.26294292455252	5.35582537601972
N	1.19449696214542	17.88300138101867	5.91268978233934
C	1.23388943017911	16.75279702732499	6.66793338734520
C	0.00004098924586	15.92596933953628	6.89466570793052
N	-6.51132017734722	18.56610604673012	3.67720376789402
C	-6.95491244589043	17.24543271120940	4.10490520681041
Ni	2.88030516229756	18.86164265817515	5.70450239601828
S	1.60775525185661	20.29360986056720	4.43386378717602
N	3.47121029211871	17.37809085062518	6.83672207790782
C	2.52706786305891	16.46577429926823	7.19268096768853
C	2.87237295440034	15.28855156096581	8.06004636692644
N	4.75889174843827	17.20212638042517	7.28641530365292
C	5.57192220421201	18.15361019205810	6.87527392362783
S	5.07921190130234	19.52738142350930	5.84966604119838
N	6.91742487980101	18.14512022085765	7.22978758400100
C	7.67228917743653	17.27497618362435	8.02026627331168
C	9.04428109209636	17.56354622043567	8.19408095774566
C	9.87244030413118	16.75584412107609	8.96648983006162
C	9.37955136250380	15.59133452983923	9.60981328764199
C	8.00107461522901	15.32164814583722	9.44986482293445

C	7.16705654420655	16.13160170157146	8.67238171762595
N	10.22216522021011	14.74364734192211	10.3398003532094
C	11.52107024759048	15.25511933833715	10.7600228848266
H	-0.78960723660841	20.76421308212394	3.49785643792326
H	7.42907912277169	18.93162334903026	6.83664420528365
H	10.91955767851995	17.03917688627192	9.06460909422243
H	-2.85905226866102	21.17947025094228	2.66117819944437
H	-5.22051818664174	20.62563007611055	2.46310516612801
H	-4.59596593836692	17.16815599514453	4.99606085658296
H	9.46749041657653	18.45119464673883	7.71563786855454
H	-2.21634990688934	17.74849035790078	5.18093267745641
H	-0.79296208724192	16.51058964305168	7.39200303162353
H	0.20678408381631	15.04343290264699	7.51246727036073
H	-0.43417761345041	15.58002730634020	5.94106308752791
H	6.11013445763155	15.89452979650019	8.56581505343291
H	3.67220516918579	14.67701353498702	7.60883993265165
H	2.00531964525124	14.63920088710146	8.23274823878196
H	3.25752130873308	15.60935355291322	9.04342220227042
H	7.55405825589240	14.45513899806982	9.93617684751066
H	-8.04815385609146	17.20203391381623	4.03377585144527
H	-6.68022620903662	17.06003314679133	5.15311356121881
H	-6.53054893502697	16.42610191528478	3.49044771429451
H	12.12670999172545	15.55193090415120	9.89210134306645
H	12.05985785826160	14.45651720783907	11.2836233288011
H	11.44347400263754	16.12834151573059	11.4384534497626
C	9.60996659395185	13.76648289191149	11.2309646990247
H	10.40247823336831	13.16046777584817	11.6858568228777
H	9.01586581784287	14.23307327132057	12.0424705843007
H	8.94834056936437	13.08831657455143	10.6736901391266
C	-7.30314635182837	19.18804645274335	2.62263045529389
H	-8.34970777316110	18.88435999909312	2.74431672779736
H	-7.26372265749244	20.28411333840076	2.69506803486593
H	-6.97104089212208	18.90006951826342	1.60500252779674

Ni(N(CH$_3$)$_2$: 2-electron reduced complex (q=-2, S = 1)

C	-2.88376819264538	18.37968940412309	4.59714249092418
C	-2.35060675684458	19.51527516236603	3.95367748503117
C	-3.24085651964514	20.30002031133154	3.18717207958118
C	-4.59012451242438	19.98153314200960	3.07477928065507
C	-5.14218869116552	18.85531551871954	3.73763346545839
C	-4.24080017204316	18.06109859659876	4.48256702496216
N	-1.01321821715617	19.91485753966910	4.01128714798920
C	0.09609308007779	19.37217717409595	4.65227281207690
N	-0.00413989028770	18.26294292455252	5.35582537601972
N	1.19449696214542	17.88300138101867	5.91268978233934
C	1.23388943017911	16.75279702732499	6.66793338734520
C	0.00004098924586	15.92596933953628	6.89466570793052
N	-6.51132017734722	18.56610604673012	3.67720376789402
C	-6.95491244589043	17.24543271120940	4.10490520681041

Ni	2.88030516229756	18.86164265817515	5.70450239601828
S	1.60775525185661	20.29360986056720	4.43386378717602
N	3.47121029211871	17.37809085062518	6.83672207790782
C	2.52706786305891	16.46577429926823	7.19268096768853
C	2.87237295440034	15.28855156096581	8.06004636692644
N	4.75889174843827	17.20212638042517	7.28641530365292
C	5.57192220421201	18.15361019205810	6.87527392362783
S	5.07921190130234	19.52738142350930	5.84966604119838
N	6.91742487980101	18.14512022085765	7.22978758400100
C	7.67228917743653	17.27497618362435	8.02026627331168
C	9.04428109209636	17.56354622043567	8.19408095774566
C	9.87244030413118	16.75584412107609	8.96648983006162
C	9.37955136250380	15.59133452983923	9.60981328764199
C	8.00107461522901	15.32164814583722	9.44986482293445
C	7.16705654420655	16.13160170157146	8.67238171762595
N	10.22216522021011	14.74364734192211	10.3398003532094
C	11.52107024759048	15.25511933833715	10.7600228848266
H	-0.78960723660841	20.76421308212394	3.49785643792326
H	7.42907912277169	18.93162334903026	6.83664420528365
H	10.91955767851995	17.03917688627192	9.06460909422243
H	-2.85905226866102	21.17947025094228	2.66117819944437
H	-5.22051818664174	20.62563007611055	2.46310516612801
H	-4.59596593836692	17.16815599514453	4.99606085658296
H	9.46749041657653	18.45119464673883	7.71563786855454
H	-2.21634990688934	17.74849035790078	5.18093267745641
H	-0.79296208724192	16.51058964305168	7.39200303162353
H	0.20678408381631	15.04343290264699	7.51246727036073
H	-0.43417761345041	15.58002730634020	5.94106308752791
H	6.11013445763155	15.89452979650019	8.56581505343291
H	3.67220516918579	14.67701353498702	7.60883993265165
H	2.00531964525124	14.63920088710146	8.23274823878196
H	3.25752130873308	15.60935355291322	9.04342220227042
H	7.55405825589240	14.45513899806982	9.93617684751066
H	-8.04815385609146	17.20203391381623	4.03377585144527
H	-6.68022620903662	17.06003314679133	5.15311356121881
H	-6.53054893502697	16.42610191528478	3.49044771429451
H	12.12670999172545	15.55193090415120	9.89210134306645
H	12.05985785826160	14.45651720783907	11.2836233288011
H	11.44347400263754	16.12834151573059	11.4384534497626
C	9.60996659395185	13.76648289191149	11.2309646990247
H	10.40247823336831	13.16046777584817	11.6858568228777
H	9.01586581784287	14.23307327132057	12.0424705843007
H	8.94834056936437	13.08831657455143	10.6736901391266
C	-7.30314635182837	19.18804645274335	2.62263045529389
H	-8.34970777316110	18.88435999909312	2.74431672779736
H	-7.26372265749244	20.28411333840076	2.69506803486593
H	-6.97104089212208	18.90006951826342	1.60500252779674

$Ni(N(CH_3)_2$: 1-electron reduced complex (q=-2, M_s = 0)

C	-2.88535327891455	18.33876334010120	4.57162674850061
C	-2.36960536922986	19.61371940027297	4.26009324101176
C	-3.25577892112359	20.53805458580130	3.66209145104441
C	-4.58269046249876	20.21585568072136	3.39512726471589
C	-5.11692542160702	18.94332257707313	3.72248527490406
C	-4.21936065675103	18.01664167669886	4.29925956406521
N	-1.05619735750366	20.01740142977092	4.49543462905299
C	0.03499002095628	19.33805071462255	5.04423340137130
N	-0.06136881108247	18.12280427216156	5.52402159503034
N	1.16716873357343	17.56582029891397	5.83620745435049
C	1.16825874488802	16.48348921368862	6.71282958916592
C	-0.11111421490072	15.76876594891395	7.03708237946493
N	-6.47054195239758	18.63713225904769	3.51345767883792
C	-6.86600231431745	17.23483596892303	3.54969948051205
Ni	2.76837826167821	18.55689089248962	5.83574732926894
S	1.57564499823311	20.22734818067688	5.04009886986296
N	3.35066957026986	17.22188794224776	7.03073791503415
C	2.42731878570674	16.19896964481136	7.23441605879657
C	2.83846284656781	14.93144787139954	7.92537837438681
N	4.68632584230955	16.91289209568563	7.21848529134348
C	5.49502937807574	17.76946844911611	6.64488485925484
S	4.89758238787132	19.03292651364435	5.54492348432947
N	6.87681646272543	17.75422767063655	6.85578531679968
C	7.65898708757872	17.05845813491105	7.77689166670114
C	9.05053629062409	17.30358359467671	7.79324815421569
C	9.90045836879328	16.65158916433108	8.68135007507992
C	9.41174760326473	15.69612443064146	9.60868451201608
C	8.01662764553297	15.47084086985163	9.60001609225150
C	7.16049260203312	16.12193076498341	8.70555156704536
N	10.27400285060200	14.99161879927115	10.4631440909811
C	11.61298434942037	15.52633856436622	10.6792910795053
H	-0.84085368220412	20.97382107875447	4.22849242697648
H	7.37893718568831	18.41802241451026	6.27298383258814
H	10.96209937460070	16.89285156251300	8.64518896989161
H	-2.88815952370150	21.53236933164621	3.39327513187208
H	-5.20965760320669	20.97373830138640	2.92710847918776
H	-4.55940935526896	17.01378111364586	4.55626800589557
H	9.47233704512722	18.03297788918038	7.09605048206695
H	-2.22342956122718	17.60314448748938	5.02543760645529
H	-0.81197840621802	16.41339554728480	7.59605101084150
H	0.07919533517909	14.87585539813206	7.64740922562405
H	-0.64893040237083	15.45327891911399	6.12685113155361
H	6.09156599675816	15.91523890232434	8.71739700358114
H	3.56901298977675	14.35644969770360	7.32945014441309
H	1.97175805725129	14.28186287444205	8.10668881588475
H	3.32678964490600	15.12999140448354	8.89462239749717
H	7.57283524353994	14.76334411836568	10.2998817019165
H	-7.95087046641274	17.17166732739246	3.40293692742305
H	-6.63422298946114	16.78709053230615	4.52649611515006
H	-6.37032337643811	16.62406401741541	2.76802115252107

H	12.16809252866228	15.59118367539238	9.73291172708558
H	12.16104355128710	14.84347337553158	11.33953847791482
H	11.60870526145955	16.53352413292279	11.14323097498547
C	9.68769648250022	14.29657580103673	11.60219049437070
H	10.48487070795466	13.77134811728244	12.14188686200422
H	9.17576124425761	14.97936959296374	12.31041494604819
H	8.95777437418555	13.54504665898173	11.26936953007293
C	-7.23096176562948	19.47719006245466	2.59605850207204
H	-8.27022422028174	19.12726767358192	2.57933602284584
H	-7.23712363209403	20.52294535042101	2.93417866001738
H	-6.83754010899802	19.45489869088927	1.55949975234206

Ni($N(CH_3)_2$, CN): starting complex (q=0)

C	-2.93045580338081	18.41436300056080	4.75202562385135
C	-2.28843183100705	19.48193671150096	4.10028871311580
C	-3.03667661120062	20.25846644973065	3.19350370557184
C	-4.37401428808713	19.98934537291316	2.94245084613002
C	-5.04074475787283	18.91663552972225	3.59658155280121
C	-4.27197367426021	18.13950250609113	4.50448981782262
N	-0.94002507617719	19.84524036814532	4.28281330690485
C	0.05660673793294	19.31096375252344	5.02767083874579
S	1.62292636105603	20.15668410596434	4.92889440176232
Ni	2.62202241490676	18.79719284790548	6.28644860221082
N	0.99774816780003	17.87301549637982	6.42713116503402
N	-0.13573488731701	18.23114132050861	5.77417465284303
N	-6.36675677601038	18.64689918044282	3.36163083228929
C	-7.01283993749819	17.51719286045135	4.01585850348833
N	3.22797362113825	17.49455354853817	7.46883990547524
C	2.32588331320350	16.59607625115153	7.83571041411875
C	1.02424474017844	16.81229773303753	7.22703159718204
C	-0.15393286590964	15.93065749859628	7.47822174176116
N	4.50244509065446	17.42256878006184	7.95313958274392
C	5.24416168979419	18.39977039726181	7.47208784393050
S	4.63069059540527	19.62604641128756	6.34496143102043
N	6.56340516466715	18.53501235646606	7.81627584929721
C	7.38291547660719	17.78527492413662	8.65940860416683
C	6.95328939535157	16.65106895694344	9.37865041363378
C	7.84849152474286	15.97162644550728	10.1963488699792
C	9.18464439810853	16.40198195091486	10.3169407692875
C	9.61418345035606	17.53716580762569	9.59534189977416
C	8.72400431005474	18.21551625351824	8.78029282234480
C	10.09324861513889	15.69958603160976	11.1584315858695
C	2.63742587131167	15.48151705069454	8.77758660968544
N	10.83840085619329	15.12476947892499	11.8503078455232
C	-7.11668469029660	19.44062309406835	2.39755473967828
H	7.02445016607229	19.32901905610779	7.37434863699025
H	-0.65812624591301	20.66745124927683	3.75016466998674
H	-4.90713351076434	20.61728766896798	2.23085565778400
H	9.05929378569047	19.09210256154284	8.22299724021845

H	10.64560867442013	17.87866424429538	9.68017654396790
H	7.51163789676674	15.09541614477540	10.7504965244915
H	-2.55351900122805	21.08924352052409	2.67347793597551
H	5.92366677111868	16.31577573045837	9.28810916126020
H	3.38464771444080	14.80253758667327	8.33795051343792
H	1.73897409633682	14.90451596490275	9.01959267861874
H	3.07225343412588	15.87520984080072	9.70797381747354
H	-2.37316181781848	17.80005126274507	5.45509121837068
H	-0.44749720349462	15.96408731341149	8.53918277936429
H	0.08636042809834	14.88328000389127	7.24088036391628
H	-1.00465139607378	16.24743991575678	6.86762032651434
H	-4.72963155512903	17.30264273074735	5.02964601032638
H	-7.12831255091305	20.50778232222458	2.67446516784122
H	-8.15078670367698	19.08299564995493	2.37282897538508
H	-6.69657608663843	19.35700850370817	1.38029261910954
H	-8.06328010346187	17.48467122457222	3.70996767396035
H	-6.54160068224527	16.55803334993272	3.74002391080803
H	-6.97689770529741	17.61087768154523	5.11385948615545

Ni($N(CH_3)_2$, CN): 1-electron reduced complex (q=-1)

C	-2.90662767807343	18.43989675788805	4.73644582455113
C	-2.30215604865136	19.55003489490429	4.11972260077244
C	-3.10016907335432	20.34552423315372	3.27280716673872
C	-4.44260467367443	20.05769887128633	3.05502933019057
C	-5.07261946898636	18.95423742455352	3.68799303421033
C	-4.25500449909354	18.14956808277447	4.51794534766729
N	-0.95634929063347	19.91858329881716	4.27690427976105
C	0.05733697471189	19.36448291322040	5.02060751850737
S	1.63167034846037	20.19707055301939	4.91228007462763
Ni	2.65052682910298	18.82707032788699	6.26337744356439
N	1.03104047289607	17.92718608367732	6.40985111017194
N	-0.11670550815352	18.29298967753183	5.76439571770813
N	-6.42729789423719	18.69104113751543	3.51422684203876
C	-6.95871014820985	17.40887514273540	3.95782737964315
N	3.23802588965763	17.51945907267772	7.44629449134205
C	2.30132484352509	16.60840719590443	7.82353591157093
C	1.03538781421744	16.84541755755765	7.23003988804262
C	-0.20611697360474	16.03593299531476	7.43892631660258
N	4.51163810180306	17.43401195896528	7.92415281092358
C	5.27854276274046	18.38823470125065	7.45128598236142
S	4.67745530523852	19.62112792635857	6.31823878197643
N	6.61695274714624	18.50489096646989	7.80022279573733
C	7.41515429823169	17.76120892525254	8.64602031938355
C	6.95966642680490	16.63949746976451	9.38284404743772
C	7.83305665668540	15.95160902019648	10.2128399384940
C	9.18287547298134	16.34868392637564	10.3407316300383
C	9.63942487327854	17.46962160709138	9.60293470677127
C	8.77254818132276	18.15734408018961	8.77556399497379
C	10.06660169216456	15.63780187253187	11.1930496395984

C	2.64453811763627	15.50174595211156	8.77020035161189
N	10.79644269778030	15.05132103676922	11.8959994976661
C	-7.14573541481909	19.36293353272540	2.43878494796624
H	7.08471511528684	19.28708485916087	7.34640438386285
H	-0.67783437206177	20.74527858741742	3.75402462398829
H	-5.00594393945960	20.70440567120771	2.38427666818925
H	9.13245871858370	19.01911799660601	8.20968736433716
H	10.67835335133933	17.78842371713777	9.68974007852595
H	7.47229390037549	15.08998162813103	10.7758024312382
H	-2.65335760370770	21.20650885407639	2.76865408689786
H	5.92171548099669	16.32996211198803	9.28651285964265
H	3.45962901653780	14.87668020800085	8.37153890528220
H	1.77842198434066	14.85808553021420	8.96067340884786
H	2.99833334946504	15.89949320129084	9.73504422473636
H	-2.30972036517786	17.80106749259038	5.38400272818006
H	-1.01608712389062	16.65259100973635	7.86051848860126
H	-0.02409011848744	15.19554495032076	8.11837584116775
H	-0.58299608661345	15.63469016642848	6.48464742823834
H	-4.67246802198783	17.27390760943900	5.01289642914096
H	-7.09207997406937	20.45539577548159	2.55162353909450
H	-8.20177434843484	19.07403237624476	2.48782581845075
H	-6.75779797791757	19.10250042221266	1.43486576866637
H	-8.04273192961131	17.40276011513538	3.79666725706432
H	-6.51879239163152	16.55031109725664	3.41401242606061
H	-6.77820149876876	17.25945342345140	5.032222517135074

Ni($N(CH_3)_2$, CN): 2-electron reduced complex (q=-2, S = 0)

C	-2.91332759692985	18.45284364693478	4.73237580447791
C	-2.37696120617924	19.67371335704889	4.27724410758765
C	-3.22105739031470	20.50300942591031	3.50615487993798
C	-4.53130106769090	20.14166275641855	3.20901822594199
C	-5.08845024782120	18.92455259288476	3.67852578271008
C	-4.23007465271525	18.09003984408550	4.43004723240611
N	-1.07618600090170	20.11271621848110	4.53060712806042
C	-0.01838107550330	19.51167694730019	5.21143325364301
S	1.53437140231277	20.37808108749029	5.13347316875577
Ni	2.66886014405235	18.84354962985496	6.22090768130519
N	1.05811922789780	17.88213607878095	6.31326992939696
N	-0.14907982040667	18.38443705980591	5.86494944781692
N	-6.42674404078527	18.58658596111610	3.43432225300227
C	-6.83357968437269	17.20342495213862	3.64847219129069
N	3.20678282171977	17.64946949701403	7.56793124667841
C	2.26595589965525	16.68527660830059	7.89917562220787
C	1.02452393128158	16.91524550898034	7.30601702294721
C	-0.26511577304197	16.23589353272229	7.66146725134135
N	4.51235268340706	17.43438139734177	7.90569886739810
C	5.34037494065542	18.23590884864529	7.27312075064568
S	4.79671379466854	19.31918921184654	5.97748870206809

N	6.70068539844168	18.30789768452466	7.59473977913356
C	7.46869332676600	17.64779808929425	8.51886841492233
C	6.96146978274463	16.66800895652940	9.41984816780217
C	7.80587723143644	16.04514055741048	10.3230716549717
C	9.18849367588933	16.35790557856035	10.3791209606661
C	9.69718842925918	17.33435937706912	9.47556955359790
C	8.85954990463870	17.95755259233633	8.57452866585995
C	10.03916119316545	15.71698072186540	11.3068884460771
C	2.64108998588091	15.52607466402772	8.77350024098491
N	10.74720607286622	15.18641438935292	12.0792387089228
C	-7.13186798396320	19.29213308887754	2.37081946148822
H	7.20535308404004	18.96564795642204	7.00334184563628
H	-0.83899052176870	21.01779722388757	4.13441136190659
H	-5.12661949445232	20.82382285955162	2.60353685597869
H	9.26407752028806	18.70459925283174	7.88745531027600
H	10.75732626360759	17.58966720799866	9.49882881336476
H	7.40074545776455	15.29784358407517	11.0074085266399
H	-2.83311961427234	21.45118329112623	3.12361879703454
H	5.90156466879467	16.42449437915982	9.38124795453016
H	3.38772160718873	14.87244233827739	8.28897934359380
H	1.76414788340708	14.91069060694658	9.01240953369623
H	3.09532697912058	15.85834916540811	9.72208933251204
H	-2.28243802120817	17.79031497740955	5.32243128471294
H	-0.98679061030959	16.94103389585522	8.10844821986180
H	-0.09939766942040	15.42475844134073	8.38209023971230
H	-0.76213650808281	15.81156679890220	6.77327759907661
H	-4.58845734862612	17.13091733196300	4.80247070920082
H	-7.16112442947794	20.37309888784585	2.56815655735923
H	-8.16716921642765	18.93220522320253	2.33755811937490
H	-6.67550105957567	19.13862051993900	1.37219143932422
H	-7.90876538476378	17.11876797297429	3.45072098051774
H	-6.29890333389688	16.48788044170989	2.99156852190046
H	-6.66003455804202	16.90102378022308	4.69096104974330

Ni($N(CH_3)_2$, CN): 2-electron reduced complex (q=-2, S = 1)

C	-2.89934380649940	18.47788372729715	4.72352173290391
C	-2.31685957977535	19.52462585835256	3.98270648777435
C	-3.15718170025300	20.24408888206723	3.10611140903750
C	-4.51035288519976	19.94812575499322	2.98005515368018
C	-5.11421285821629	18.91325281285043	3.739717900684774
C	-4.25946491128488	18.18084416504964	4.59615349669114
N	-0.96828881223511	19.89746853378072	4.04116913120533
C	0.09684473529446	19.41733962475329	4.78606952594667
S	1.63601292386388	20.27619477827703	4.52821232799989
Ni	2.78765869105075	19.03921547406341	6.07395420348761
N	1.09377464263114	18.09492952940402	6.29035274799717
N	-0.06197429954718	18.40022369085701	5.61032618841860
N	-6.48479794522854	18.65087901322425	3.66169098677960
C	-6.98305588041723	17.39861824432251	4.21601986818246

N	3.32513613276341	17.64950768078493	7.34196338292478
C	2.36153669501413	16.77903432446520	7.73146686316880
C	1.09974196492592	17.01326353741099	7.10212545085184
C	-0.12594538095669	16.16327387750986	7.27849248457790
N	4.55416803741983	17.57900741226309	7.93403279822399
C	5.37588317125819	18.51691542360469	7.49922318502542
S	4.94924487694589	19.76456611330464	6.30775466968412
N	6.67731254091038	18.59585508705738	7.99119106966616
C	7.42796116443623	17.75771861278121	8.78786342478549
C	6.96520010321868	16.51702618859499	9.30731561404817
C	7.79593275813196	15.73069836855121	10.0883650178734
C	9.12187592683068	16.13607691708244	10.3974311132455
C	9.58511127853136	17.37844534093130	9.87612168012867
C	8.75934772020377	18.16136330493768	9.09583236853754
C	9.95823699777747	15.33084026440318	11.2004277019230
C	2.64502156783592	15.70620772147794	8.74247821916673
N	10.65553623237880	14.66044200662365	11.8679410999231
C	-7.23473319073656	19.19311764019355	2.53544483110722
H	7.16913535052070	19.41689492148773	7.64048628047341
H	-0.70676674242895	20.67400992616498	3.43790228385665
H	-5.10203929374337	20.53703919018586	2.28072152810870
H	9.12934353265228	19.11190691409973	8.70422841648053
H	10.59966489987137	17.71179528294648	10.0979529922232
H	7.42411452278478	14.78144724462749	10.4774202129041
H	-2.73366854620930	21.05231427604855	2.50364316632378
H	5.94629471399060	16.20700905254506	9.08493373020434
H	3.47787596385389	15.06042338400970	8.41768930207822
H	1.76984539890005	15.07044524443538	8.92180408958381
H	2.95502918208277	16.13903257648127	9.70882925673280
H	-2.26979222127844	17.89663583430691	5.39434248660724
H	-0.97022391129906	16.75321002439170	7.67249248242791
H	0.05260040643665	15.32465039498417	7.96191167292215
H	-0.46656362338608	15.75178260440175	6.31380832777745
H	-4.65484283369154	17.35607410897871	5.18781251272389
H	-7.15697813786039	20.28899143632091	2.50239082192321
H	-8.29377222392127	18.93939552898723	2.66311886779476
H	-6.89516550848260	18.79531441913314	1.55844637277848
H	-8.07495092226236	17.37979021710771	4.11851670984790
H	-6.57046551505275	16.50568436876488	3.70547070424271
H	-6.74184240254990	17.31988913832022	5.28564264633345

Ni($N(CH_3)_2$, CN): 2-electron reduced complex (q=-2, M_s = 0)

C	-2.90523917649992	18.44158887185305	4.71157377394245
C	-2.36044342445559	19.65035988397521	4.23402679417142
C	-3.20433377843447	20.47831438478298	3.46101228613599
C	-4.52178030755820	20.12761522003439	3.18360288931681
C	-5.08691864406123	18.92329851732048	3.67579274938988
C	-4.22922835595052	18.08955898777064	4.42891051216164
N	-1.05192055084688	20.07786595184401	4.46515136212921

C	0.00143027473602	19.48385444832504	5.15888075022644
S	1.55762656523413	20.34268144851877	5.07090537922620
Ni	2.68183776175478	18.82326056645087	6.19360783618660
N	1.06861730058629	17.86768340319504	6.28959686049423
N	-0.13544078137401	18.36693691257467	5.82910983093529
N	-6.43145494181179	18.59644518709683	3.45108195673537
C	-6.85086416235739	17.22114204864899	3.68907173309889
N	3.20934824324554	17.65134894036170	7.56151631131085
C	2.26581918569206	16.69137454217926	7.89914787830392
C	1.02816731699050	16.91406891481398	7.29499913731717
C	-0.26467274490933	16.24227753094893	7.65264441590132
N	4.51294220174068	17.43982465693440	7.91046338312652
C	5.34524494463508	18.23250233661829	7.27204207501089
S	4.81084031293837	19.29824629120856	5.95871965842201
N	6.70363374445034	18.30755823336566	7.60133306818912
C	7.46654518579055	17.65276531862980	8.53349845558031
C	6.95472777312866	16.67811291178532	9.43730051557629
C	7.79451488706926	16.05960853643062	10.3479393983472
C	9.17698243584853	16.37256941459376	10.4086146925608
C	9.69058351239337	17.34428378225135	9.50270685566569
C	8.85712251988658	17.96269846346248	8.59433923157776
C	10.02303487945215	15.73592382081894	11.3434513989415
C	2.63670693874911	15.54073818906214	8.78639727266633
N	10.72734215302185	15.20697906753953	12.1204377727644
C	-7.14220111108762	19.29564271252432	2.38739909919098
H	7.21175936367537	18.96075955065986	7.00785570518386
H	-0.81236041915820	20.97897685020919	4.06139216935063
H	-5.11639338678550	20.80835335884056	2.57577120313095
H	9.26530226474775	18.70585943269091	7.90514211947774
H	10.75062451297007	17.59956346326780	9.52946044339430
H	7.38591794040087	15.31591329250660	11.0340959478839
H	-2.81093199686078	21.41728772512457	3.06157745333524
H	5.89487944713642	16.43470372726563	9.39472030591035
H	3.40144611086850	14.89576644103886	8.31906815127678
H	1.76266095479798	14.91558607679346	9.01006435242065
H	3.06832652243135	15.88109174978476	9.74294098088136
H	-2.27505694229405	17.78018629934704	5.30365875495628
H	-0.98584157008898	16.95345518718251	8.09098783556290
H	-0.10325420852309	15.43753764519871	8.38148341091796
H	-0.76045296570913	15.81136866866782	6.76686884758775
H	-4.59409157977433	17.13966278663071	4.81840063520238
H	-7.15261685796008	20.37979232565647	2.56800895876698
H	-8.18319477742894	18.95101214175071	2.37534636851915
H	-6.70359562700554	19.11970243313015	1.38444404810099
H	-7.92911217832485	17.14532973942529	3.50458081245801
H	-6.33149702364393	16.49069383982616	3.03625305226794
H	-6.66892674146784	16.93104876908221	4.73369510881025