Supporting Information for

Role of pendant proton relays and proton-coupled electron transfer on the hydrogen evolution reaction by nickel hangman porphyrins

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General Experimental Details

^{1}H NMR spectra (500 MHz) were recorded on samples in $CDCl_3$ at room temperature unless noted otherwise. Silica gel (60 μm average particle size) was used for column chromatography. 4-Formyl-5-bromo-2,7-di-tert-butyl-9,9-dimethylxanthene,[1] 5-penta-fluorophenyldipyrromethane,[2] were prepared as described in the literature. THF (anhydrous), methanol (anhydrous), CH_2Cl_2 (anhydrous), benzoic acid (≥99.5%), and tetrabutylammonium hexafluoro-phosphate ($TBAPF_6$, ≥99.0%), and all other chemicals were used as received. LD-MS data was measured on porphyrins in the absence of matrix.

The microwave-assisted reactions were performed inside the cavity of a CEM Discover microwave synthesis system equipped with infrared, pressure and temperature sensors for monitoring the synthesis. The reaction vessels were 10 mL crimp-sealed thick-wall glass tubes. The contents of each vessel were stirred with a magnetic stirrer.

UV-vis spectra were recorded at room temperature in quartz cuvettes in CH_2Cl_2 on a Varian Cary 5000 UV-vis-NIR spectrophotometer. UV-vis spectroelectrochemical measurements were made using a quartz thin layer cell (0.5 mm path length) at room temperature in a N_2-filled glovebox with an Ocean Optics USB4000 spectrophotometer and DT-Mini-2GS UV-vis-NIR light source.

Electrochemical measurements were performed on a CH Instruments (Austin, Texas) 760D Electrochemical Workstation using CHI Version 10.03 software. Cyclic voltammetry (CV) experiments were conducted in a nitrogen-filled glovebox at 295 K using a CH Instruments glassy carbon button working electrode (area = 0.071 cm^2), BASi Ag/$AgNO_3$ (0.1 M) reference electrode in 0.1 M $TBAPF_6$ acetonitrile solution at room temperature, and Pt mesh counter electrode in 0.2 M $TBAPF_6$ acetonitrile solutions 2 or 4 mL total volume. Acetonitrile was previously dried by passage through a neutral alumina column under argon. $TBAPF_6$ was dried prior to CV measurements. All CVs were recorded with compensation for solution resistance, and potentials were referenced to the ferrocenium/ferrocene (Fc^+/Fc) couple. Appropriate background scans were subtracted from all CVs. Solutions were stirred between acquisition of individual CVs and the working electrode was polished before each measurement.

Bulk electrolysis was performed using a glassy carbon rod (7 mm × 5 cm) working electrode and a platinum mesh auxiliary electrode in a gas-tight electrochemical cell. The amount of H_2 gas produced in the headspace was analyzed by an Agilent 7890A GC. The potentials for electrolysis were −1.77 V for **1-Ni**, −1.85 V for **2-Ni**, and −1.75 V for **3-Ni** (all potentials are referenced to Fc^+/Fc).

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1. Chang CJ, Yeh CY, Nocera DG (2002) Porphyrin architectures bearing functionalized xanthene spacers. *J Org Chem* 67:1403–1406.
2. Laha JK, Dhanalekshmi S, Taniguchi M, Ambroise A, Lindsey JS (2003) A scalable synthesis of meso-substituted dipyrromethanes. *Org Proc Res Dev* 7:799–812.

X-Ray Crystallographic Details

ZnHPX1Br (2-Zn) X-ray Data. Crystals of **2-Zn** were mounted on a Bruker three circle goniometer platform equipped with an APEX detector. A graphite monochromator was employed for wavelength selection of the Mo Kα radiation (λ = 0.71073 Å). The data were processed and refined using the program SAINT supplied by Siemens Industrial Automation. Structures were solved by direct methods in SHELXS and refined by standard difference Fourier techniques in the SHELXTL program suite (6.10 v., Sheldrick G. M., and Siemens Industrial Automation, 2000). Hydrogen atoms bound to carbon were placed in calculated positions using the standard riding model and refined isotropically. Hydrogen atoms bound to oxygen were located in the difference map and refined semi-freely; they were restrained to a distance of 0.84 Å from the oxygen atom, and the isotropic displacement parameter was constrained to a value of 1.2 times that of the oxygen atom. All non-hydrogen atoms were refined anisotropically.

The complex **2-Zn** crystallized with a water molecule bound to the Zn(II) center, with a geometry that approximates square pyramidal (Figure S1). There are two crystallographically independent molecules per asymmetric unit, which in general are conformationally similar. The zinc atoms sit above the plane of their respective macrocycle, residing 0.192 and 0.206 Å above the mean plane of the four pyrrolic nitrogen atoms. The C_6F_5 substituents are considerably twisted relative to this N4 plane, with dihedral angles of 74.8°, 75.2° and 89.5° for one molecule and 73.2°, 73.4° and 86.9° for the other, as determined by considering the angle between the N4 mean plane and the phenyl ring. The largest of these angles is for the meso substituent that is trans to the xanthene backbone. The major distinction between the two independent molecules is in the dihedral angle of the xanthene substituent, again measured as the angle between the N4 mean plane and the six-membered aryl ring bonded directly to the meso carbon. In one molecule this angle is 52.6°, whereas it is much larger at 67.2° for the second. This latter value is very similar to the dihedral angles of the aqua-bridged dimer $(ZnHPXCO_2H)_2(\mu\text{-}OH_2)$ which we recently reported.[3] In both independent molecules of $Zn(OH_2)$HPX1Br, the bound water molecule is on the same side of the macrocycle as the hanging bromide substituent, though the two are too far apart to consider an intramolecular hydrogen bonding interaction; the distances between the aqua oxygen atoms and the adjacent bromides are 4.458(3) and 4.336(3) Å. However, the crystal structure does suggest an intermolecular hydrogen-bonding interaction between an aqua proton and a symmetry-generated C_6F_5 fluoride (ortho to the meso carbon). The O···F distances of 2.898(4) and 2.996(4) Å, with the associated O–H···F angles of 170(5) and 166(5)°, are indicative of intermolecular hydrogen-bonding stabilization in the crystal structure.

3. Dogutan DK, Bediako DK, Teets TS, Schwalbe M, Nocera DG (2010) Efficient synthesis of hangman porphyrins. *Org Lett* 12:1036–1039.

NiHPXCO$_2$H (1-Ni) X-ray Data. Crystals of **1-Ni** were obtained by slow evaporation from a CH_2Cl_2/hexanes solution of **1-Ni**. The X-ray structure of **1-Ni** is shown in main text Figure 1. The central nickel atom is found in a square planar coordination environment with sum of ∠N–Ni–N equaling 360°, indicating that the Ni is not appreciably displaced from the N4 plane of the pyrrolic nitrogen atoms. The Ni–N distances are not perfectly equivalent as three Ni–N distances are 1.951(3) Å with the remaining Ni–N distance found to be slightly shorter at 1.940(3) Å. The macrocycle distorts only slightly from perfectly square planar with the two pairs of *trans* meso-carbon atoms bending ~10° out of the N4 plane in opposing directions. These solid state metrics are comparable to those of the previous reported cobalt porphyrin (CoHPX3CO$_2$H).[4] This cobalt analog possessing mesityl substituents is similarly planar with the Co atom not appreciably displaced from N4 plane of pyrrolic nitrogen atoms. As mentioned in the text, one notable difference in the crystallographic structures of **1-Ni** and CoHPX3CO$_2$H[4] is the apically coordinated solvent molecule found in the structure of CoHPX3CO$_2$H.[4] This difference can be explained by the d_{z^2} orbital of the d^8 Ni being fully populated and thus not available for interactions with apical ligands. The M–H distances found for NiHPXCO$_2$H and CoHPX3CO$_2$H[4] are also similar as they are found to be 4.46 Å and 4.25 Å respectively. The 0.21 Å difference in M–H distance is due to a larger bending angle in the xanthene backbone for the CoHPX3CO$_2$H[4] (13.9° for Co, 7.1° for Ni), which positions the hanging group closer to the metal center. As this effect is likely due to packing effects in the solid state and not indicative of solution behavior, the Co and Ni complexes can be viewed as structurally analogous with differences in subsequent chemistry being attributed to electronic effects and not underlying structural difference.

Synthetic Details

5-[4-(5-Bromo-2,7-di-*tert*-butyl-9,9-dimethylxanthene)]-10,15,20-tris(pentafluoro-phenyl)porphyrinatonickel (II) (**2-Ni**). A microwave glass tube (10 mL) containing a magnetic stir bar was charged with 8 mL of $CHCl_3$:MeOH (7 mL:1 mL) and sample of HPXBr (**2**) (0.0500 g, 0.0414 mmol). The solution was stirred at room temperature for 10 min to obtain a homogenous mixture. A sample of $NiBr_2$ (0.226 g, 1.035 mmol, 25 mol equiv to **2**) was added. The resulting mixture was stirred at room temperature for 5 min. The reaction vessel was sealed with a septum and subjected to microwave irradiation at 65 °C. The protocol was as follows: (1) heat the reaction vessel from room temperature to 65 °C, (2) hold at 65 °C and irradiate for 20 min (temperature overshoots of 67 - 70 °C were permitted; temperature was re-established at 65 °C by using open flow valve option), (3) allow the reaction mixture to cool to room temperature, (4) check the reaction mixture by silica TLC analysis (Hexanes:CH_2Cl_2 4:1), (5) repeat steps 1 - 4 until all of the free base

4. McGuire Jr R, Dogutan DK, Teets TS, Suntivich J, Shao-Horn Y, Nocera DG (2010) Oxygen reduction reactivity of cobalt(II) hangman porphyrins. *Chem Sci* 1:411–414.

starting material, **2**, was consumed (6 - 8 h). Upon complete reaction, triethylamine (10 mole equiv to metal salt) was added to the solution, which was washed with water and brine, dried over Na_2SO_4, and concentrated to dryness. The resulting crude product was chromatographed [silica, Hexanes:CH_2Cl_2 1:1 → 1:4] to afford dark purple solid (48 mg, 91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ / ppm: 1.25 (s, 9H), 1.53 (s, 9H), 1.88 (s, 6H), 7.08 (d, *J* = 2.0 Hz, 1H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.87 (d, *J* = 2.5 Hz, 1H), 7.94 (d, *J* = 2.5 Hz, 1H), 8.72 (d, *J* = 5.0 Hz, 2H), 8.83 (s, 4H), 8.92 (d, *J* = 5.0 Hz, 2H);. Anal. Calcd. for M = $C_{61}H_{36}BrNiF_{15}N_4O$: Cald. 1264.5382. Found for HR(ESI)-MS: 1265.1297; LD-MS. 1264.15. $\lambda_{max,abs}$ / nm (CH_2Cl_2) = 407, 525, 559.

5-[4-(2,7-Di-*tert*-butyl-5-methoxycarbonyl-9,9-dimethylxanthene)]-10,15,20-tris-(pentafluorophenyl)-porphyrinatonickel(II) (NiHPX-CO_2Me, 4-Ni). A microwave glass tube (10 mL) containing a magnetic stir bar was charged with 5.5 mL of $CHCl_3$:MeOH (4.4 mL:1.1 mL) and sample of HPXCO_2Me (**4**) (0.0300 g, 0.025 mmol). The solution was stirred at room temperature for 10 min to obtain a homogenous mixture. A sample of $NiBr_2$ (0.138 g, 0.632 mmol, 25 mol equiv to **4**) was added. The resulting mixture was stirred at room temperature for 5 min. The reaction vessel was sealed with a septum and subjected to microwave irradiation at 65 °C. The protocol was as follows: (1) heat the reaction vessel from room temperature to 65 °C, (2) hold at 65 °C and irradiate for 20 min (temperature overshoots of 67 - 70 °C were permitted; temperature was re-established at 65 °C by using open flow valve option), (3) allow the reaction mixture to cool to room temperature, (4) check the reaction mixture by silica TLC analysis (Hexanes:CH_2Cl_2 4:1), (5) repeat steps 1 - 4 until all of the free base HPXCO_2Me starting material was consumed (8 - 10 h). Upon complete reaction, triethylamine (10 mol equiv to metal salt) was added to the solution, which was washed with water and brine, dried over Na_2SO_4, and concentrated to dryness. The resulting crude product was chromatographed [silica, hexanes:CH_2Cl_2 silica, hexanes:CH_2Cl_2 1:1 → 1:6] to afford dark purple solid (28 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ / ppm: 0.69 (s, 3H), 1.27 (s, 9H), 1.41 (s, 9H), 1.91 (s, 6H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.64 (d, *J* = 2.5 Hz, 1H), 7.83 (d, *J* = 2.5 Hz, 1H), 8.66 (d, *J* = 5.0 Hz, 2H), 8.77 (s, 4H), 8.84 (d, *J* = 5.0 Hz, 2H);. Anal. Calcd. for M = $C_{63}H_{39}F_{15}N_4NiO_3$: Cald. 1242.2134. Found for HR(ESI)-MS: 1243.2209 (M+H). $\lambda_{max,abs}$ / nm (CH_2Cl_2) = 407, 525, 558.

5-[4-(2,7-Di-*tert*-butyl-5-hydroxycarbonyl-9,9-dimethylxanthene)]-10,15,20-tris-(pentafluorophenyl)-porphyrinatonickel(II) (**1-Ni**). A microwave glass tube (10 mL) containing a magnetic stir bar was charged with 5.5 mL of $CHCl_3$:MeOH (4.4 mL:1.1 mL) and sample of **1** (0.0520 g, 0.044 mmol). The solution was stirred at room temperature for 10 min to obtain a homogenous mixture. A sample of $NiBr_2$ (0.240 g, 1.10 mmol, 25 mol equiv to **1**) was added. The resulting mixture was stirred at room temperature for 5 min. The reaction vessel was sealed with a septum and subjected to microwave irradiation at 65 °C. The protocol was as follows: (1) heat the reaction vessel from room temperature to 65 °C, (2) hold at 65 °C and irradiate for 20 min (temperature overshoots of 67 - 70 °C were

permitted; temperature was re-established at 65 °C by using open flow valve option), (3) allow the reaction mixture to cool to room temperature, (4) check the reaction mixture by silica TLC analysis (hexanes:CH_2Cl_2 4:1), (5) repeat steps 1 - 4 until all of the free base $HPXCO_2H$ starting material was consumed (8 – 10 h). Upon complete reaction, triethylamine (10 mol equiv to metal salt) was added to the solution, which was washed with water and brine, dried over Na_2SO_4, and concentrated to dryness. The resulting crude product was chromatographed [silica, hexanes:CH_2Cl_2 silica, hexanes:CH_2Cl_2 1:1 → 1:9] to afford dark purple solid (51 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ / ppm: 1.26 (s, 9H), 1.49 (s, 9H), 1.93 (s, 6H), 7.32-7.46 (brs, 1H), 7.71 (dd, *J* = 2.5 Hz, 2H), 7.91 (dd, *J* = 8.5 Hz, 2H), 8.69 (d, *J* = 5.0 Hz, 2H), 8.78 (s, 4H), 8.81 (d, *J* = 5.5 Hz, 2H);. Anal. Calcd. for M = $C_{62}H_{37}F_{15}N_4NiO_3$: Cald. 1229.6516. Found for HR(ESI)-MS: 1251.1866 (M+Na); LD-MS. 1229.18. $\lambda_{max,abs}$ / nm (CH_2Cl_2) = 406, 524, 558.

Spectroelectrochemical Studies

UV-vis spectroelectrochemical measurements were made using a quartz thin layer cell (0.5 mm path length) at room temperature in a N_2-filled glovebox with an Ocean Optics USB4000 spectrophotometer and DT-Mini-2GS UV-vis-NIR light source using an optically transparent platinum flag working electrode, platinum wire counter electrode, and Ag wire reference electrode (BASi). Cyclic voltammetry and controlled potential electrolysis in the thin layer cell were carried out using a CH Instruments 730C Electrochemical Workstation. Samples were prepared in 0.1 M $TBAPF_6$ acetonitrile at a 0.6 mL total volume.

Computational Details

Structures were optimized with density functional theory (DFT) using a variety of exchange-correlation functionals: B3P86,[5,6] B3LYP,[6,7] BP86,[5,8] BLYP,[7,8] TPSSh,[9] M06L,[10] and ωB97XD.[11–14] Optimizations were performed with the 6-31+G(d,p)[15] basis set for the

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transferring proton and the 6-31+G(d) basis set[16–18] for all other atoms with default options in Gaussian 09.[19] Optimizations and single point energy calculations in acetonitrile solvent utilized the conductor-like polarizable continuum model (C-PCM)[20,21] with Bondi radii and included nonelectrostatic interactions resulting from dispersion,[22,23] repulsion,[23] and cavity formation.[24] Entropic and zero-point energy effects were calculated from the vibrational frequencies at T = 298.15 K and were included in the calculation of the reaction free energies, which in turn were used to calculate the reduction potentials. When optimized in the gas phase, the free energies of the solvated molecules were calculated with gas phase geometries employing a Born–Haber thermodynamic cycle that combines gas phase free energies with single point solvation free energies of the reduced and oxidized species. The detailed procedure is described in our previous publications.[25] Tables S1, S2, and S5 illustrate that the results are qualitatively similar for these two types of geometries. The results in the main paper utilized the geometries optimized in solution. As stated in the main text, for computation tractability, the *tert*-butyl groups on the xanthene backbone and pentafluorophenyl *meso*-substituents of the porphyrin ring were truncated to methyl groups and chlorine atoms,

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respectively. These truncations were chosen based on the Hammett constants[26,27] (σ) of the substituents, which are similar:

Substituent	σ_m^*	σ_p^*
—Cl	0.37	0.23
—C_6F_5	0.26	0.27
—^{t}Bu	–0.10	–0.20
—CH_3	–0.07	–0.17

*Subscripts "*m*" or "*p*" refer to the position ("*meta*" or "*para*") of the substituent.

Figures of computational results were created with GaussView 5.0.[28]

CV Simulation

All simulated CVs were calculated using DigiElch 7 software.[29] Diffusion coefficients of compounds were determined straightforwardly from the peak currents of reversible waves, and these values were used in the relevant simulations. Symmetry factors/transfer coefficients (α values) were set to 0.5 for all ET steps. Full details of the parameters used in simulation are listed in Tables S3 in the ESI and Table 2 in the manuscript.

For the simulation of trumpet plots, CVs were simulated using the known $E_{1/2}$ values and diffusion coefficient (determined from the peak current as described in the manuscript) as the fixed input parameter in the model. The CV was then simulated for an initial guess value of the standard heterogeneous rate constant (k_{ET}^o) at a particular scan rate, *v* (say, 10 mV/s). The anodic and cathodic peak potentials were noted. The k_{ET}^o value was then maintained and *v* was changed to 30 mV/s, the CV was simulated again and the new peak potentials were noted. This was repeated for *v* = 100, 300, 1000, 3000, … , 10000 mV/s. A plot of peak potentials versus log v was constructed and the simulated data was compared to the experimental result. This procedure is then iterated for different k_{ET}^o values until a good match is obtained between the experimental points and the simulated values over the entire scan rate range.

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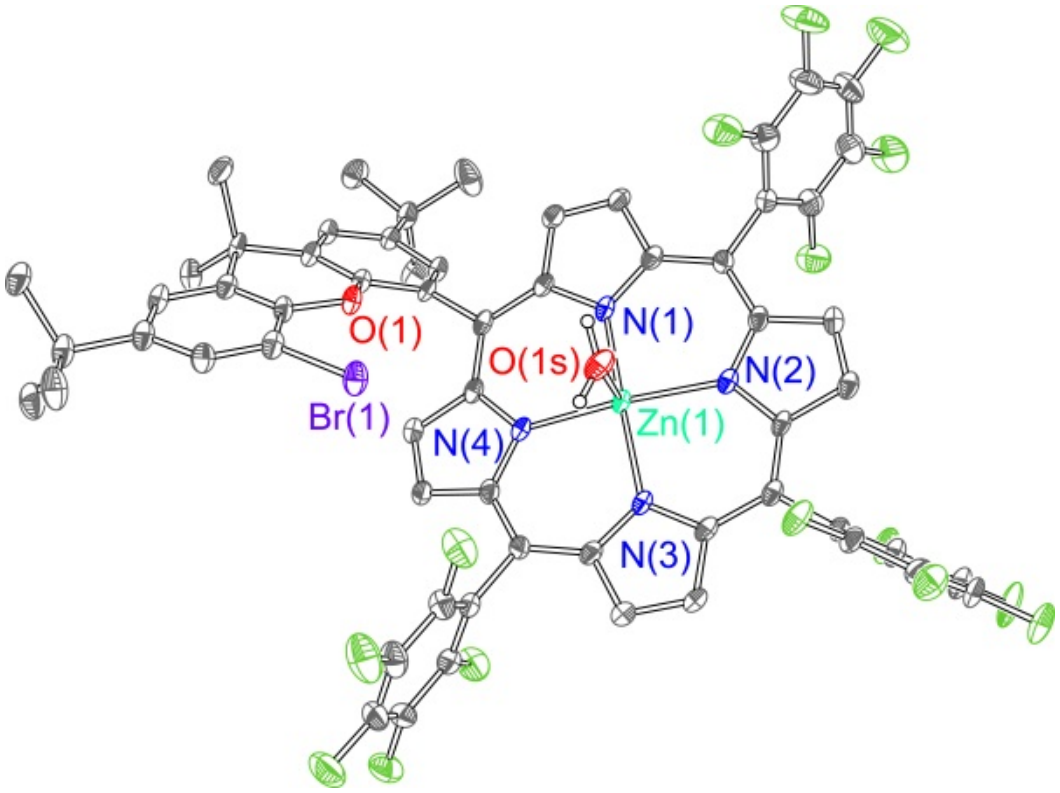

Figure S1. X-ray crytsal structure of **2-Zn** with thermal ellipsoids set at 50% probability.

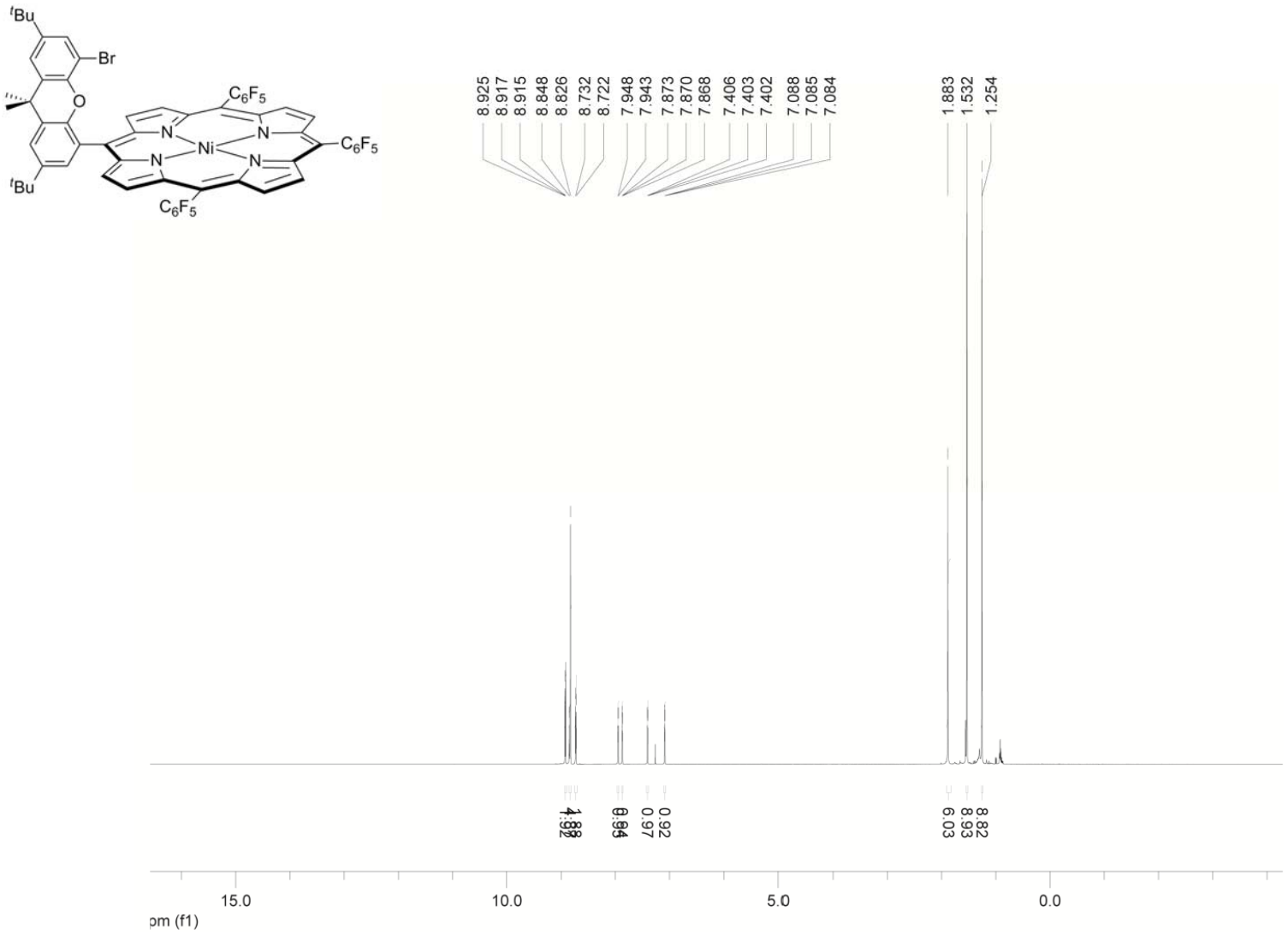

Figure S2a. Full ^{1}H NMR spectrum of NiHPXBr (**2-Ni**).

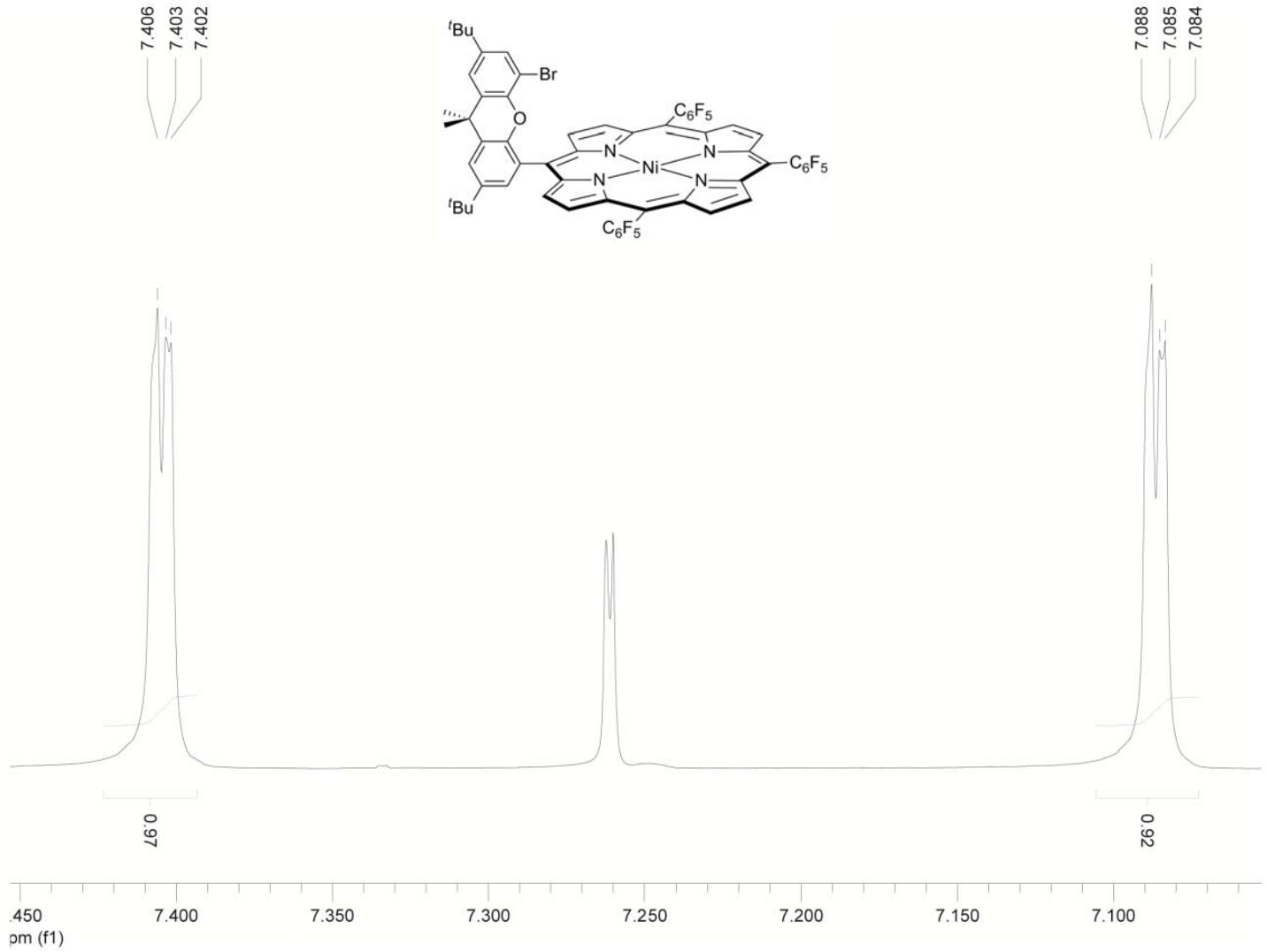

Figure S2b. Aromatic region of the ^{1}H NMR spectrum of NiHPXBr (**2-Ni**) with integrations and chemical shifts.

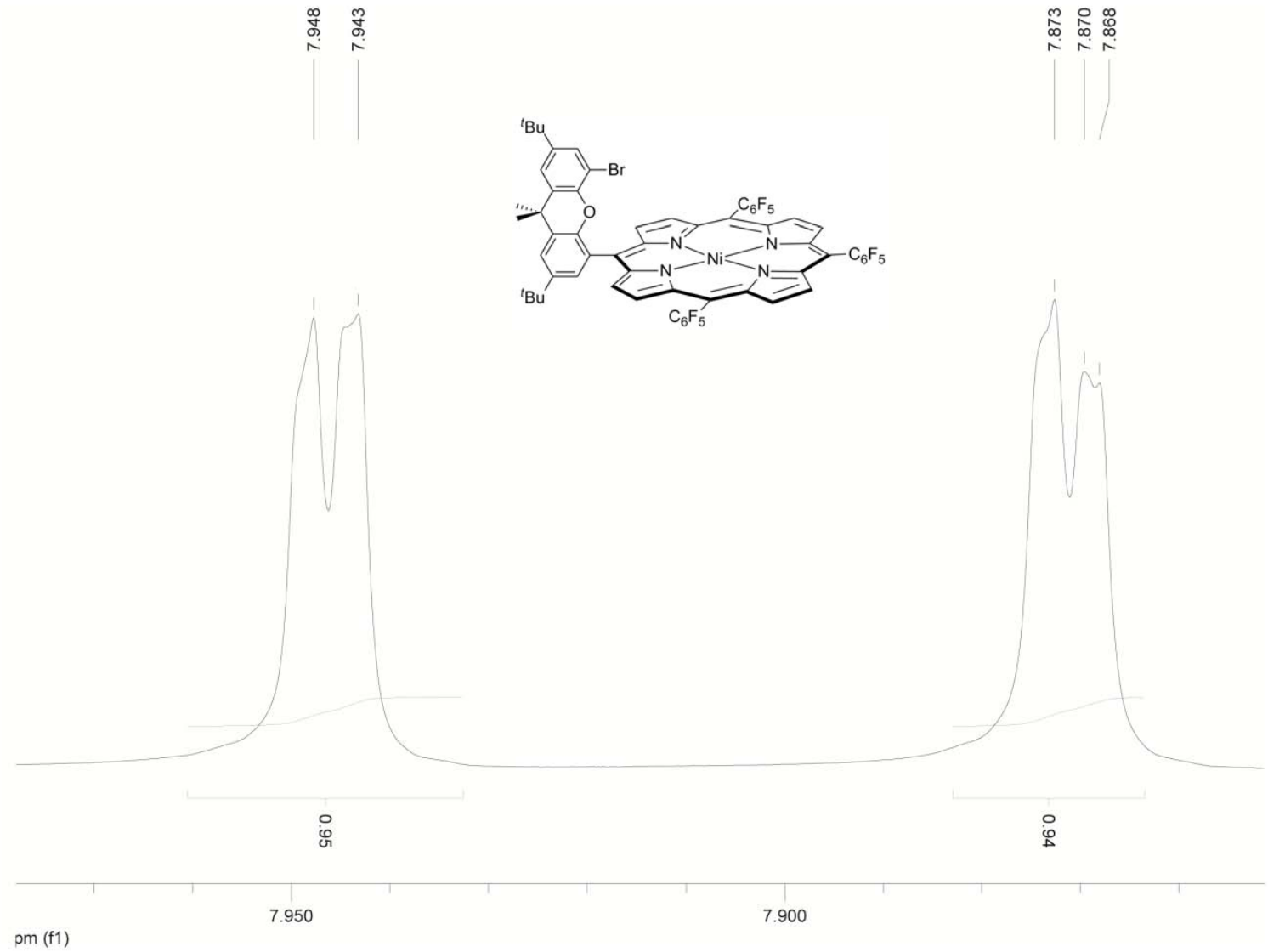

Figure S2c. Aromatic region of the ^{1}H NMR spectrum of NiHPXBr (**2-Ni**) with integrations and chemical shifts.

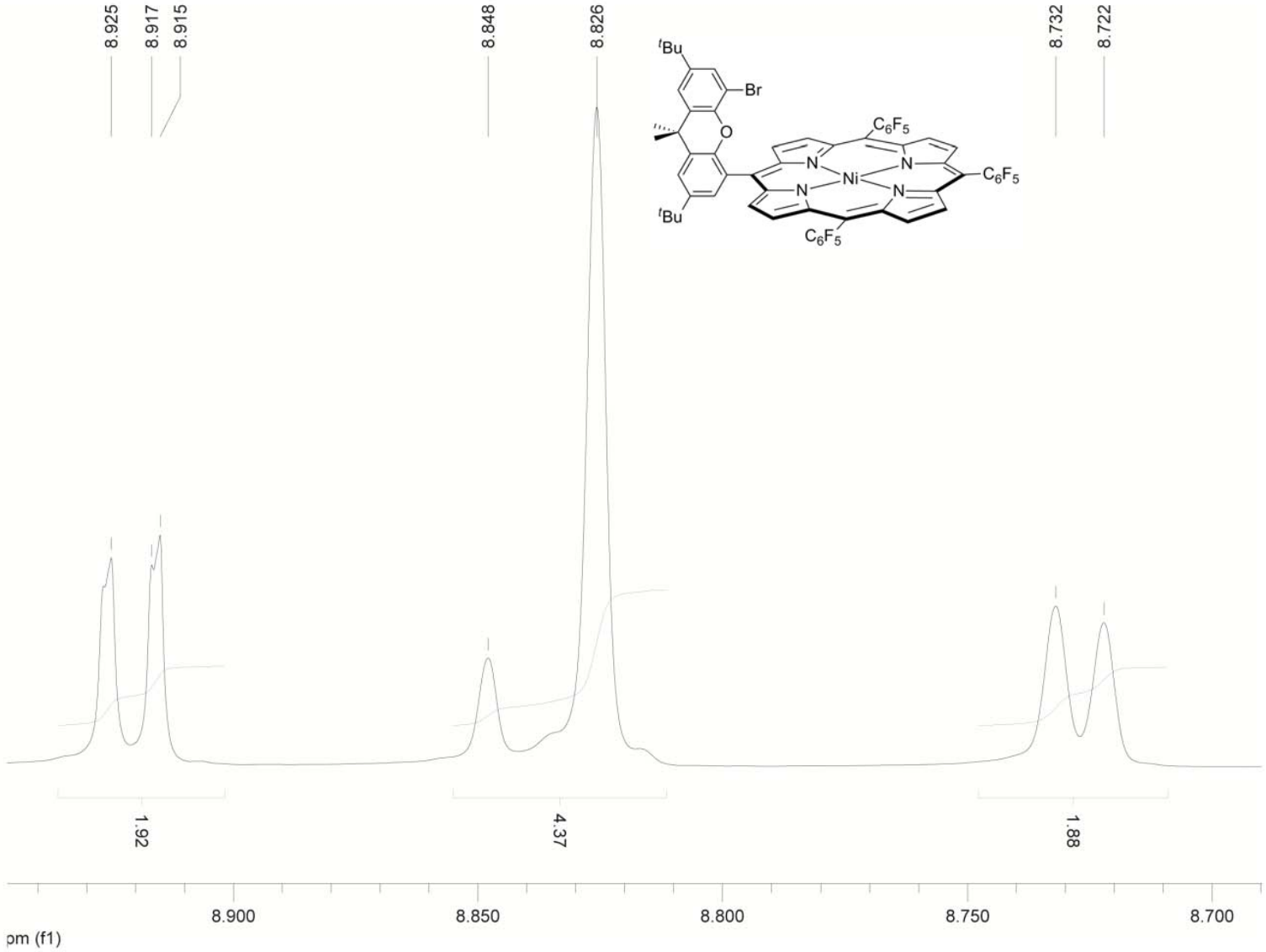

Figure S2d. Aromatic region of the ^{1}H NMR spectrum of NiHPXBr (**2-Ni**) with integrations and chemical shifts.

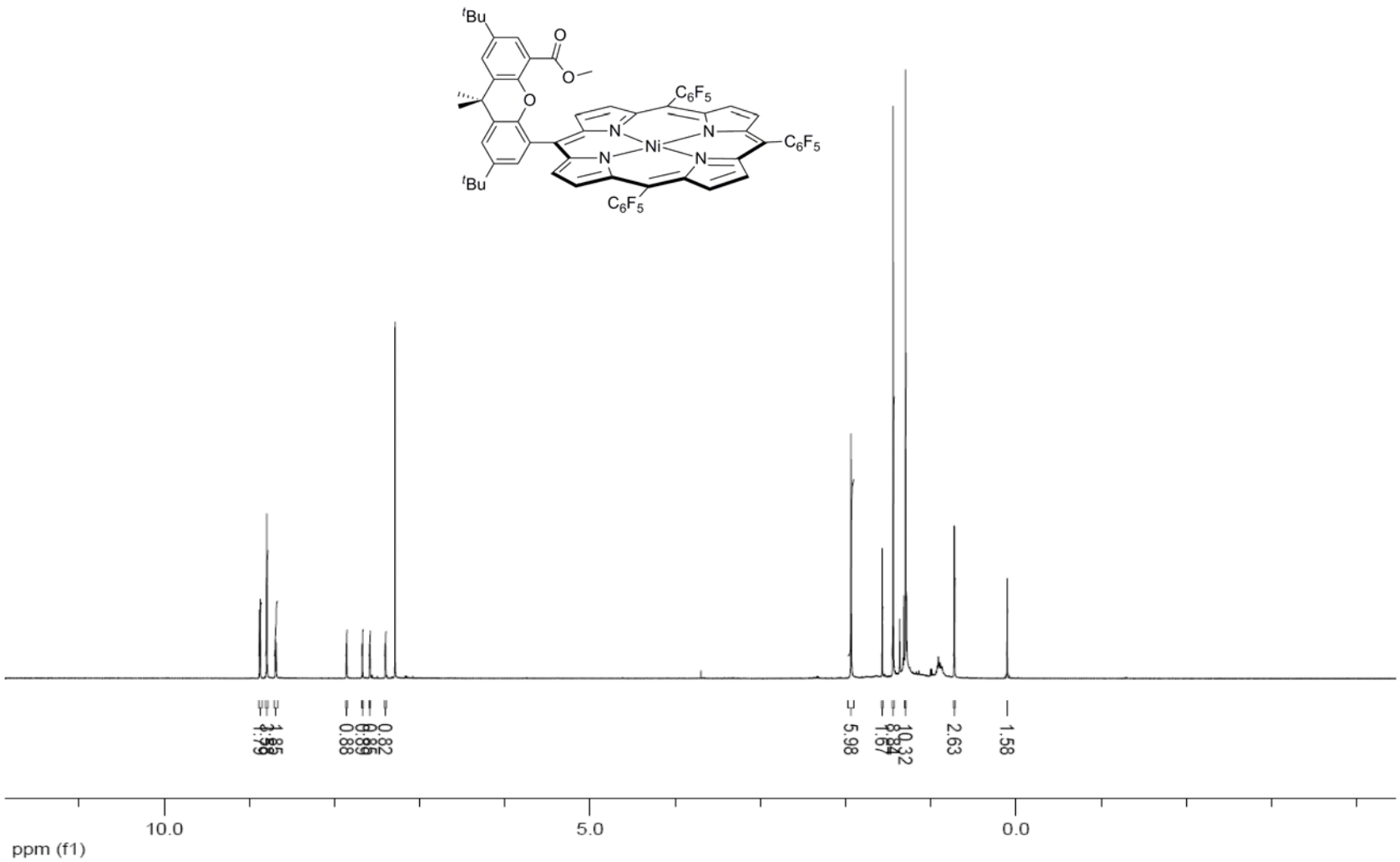

Figure S3a. Full ^{1}H NMR spectrum of NiHPXOMe (**4-Ni**).

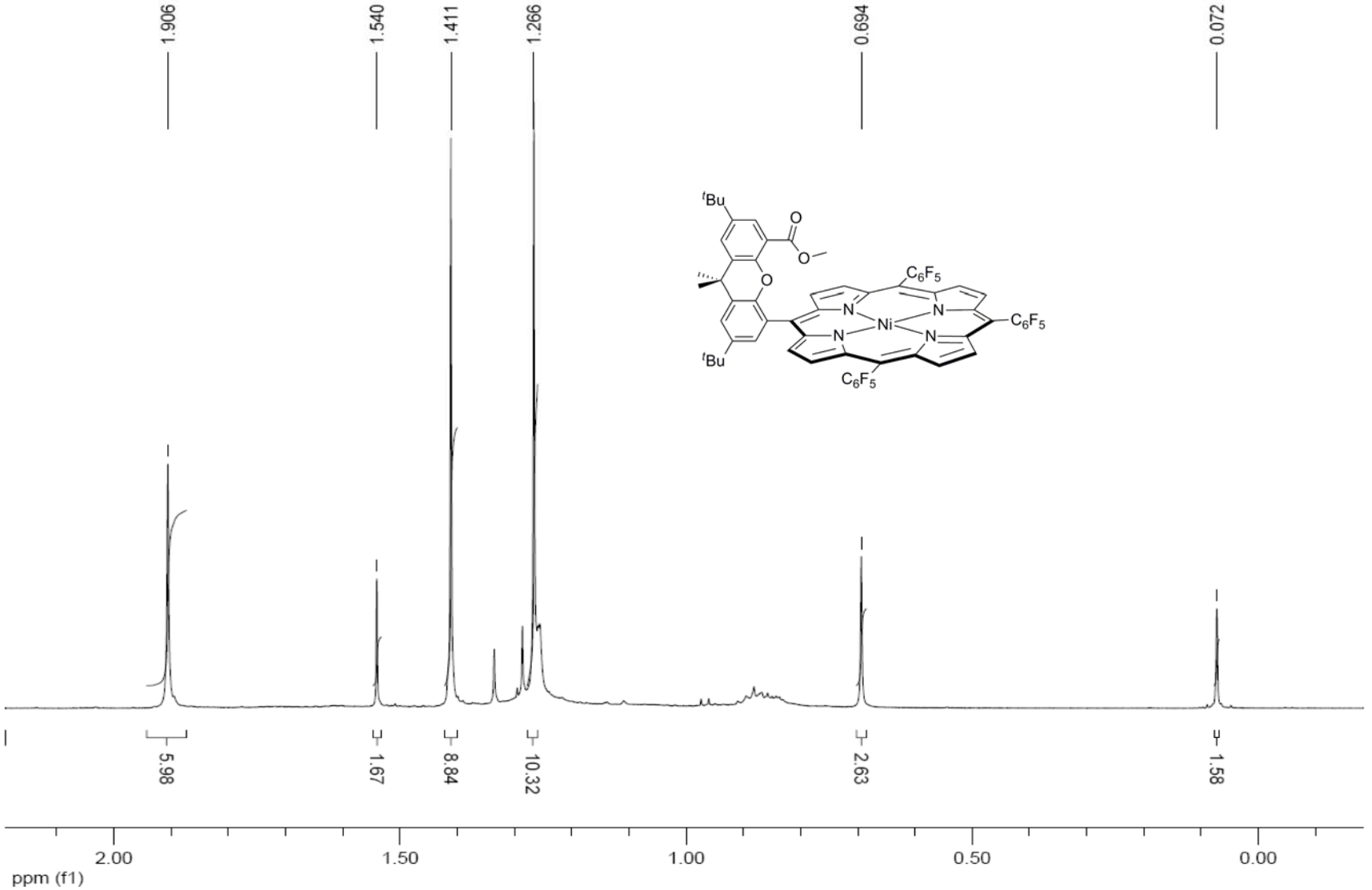

Figure S3b Aliphatic region of the ^{1}H NMR spectrum of NiHPXOMe (**4-Ni**) with integrations and chemical shifts.

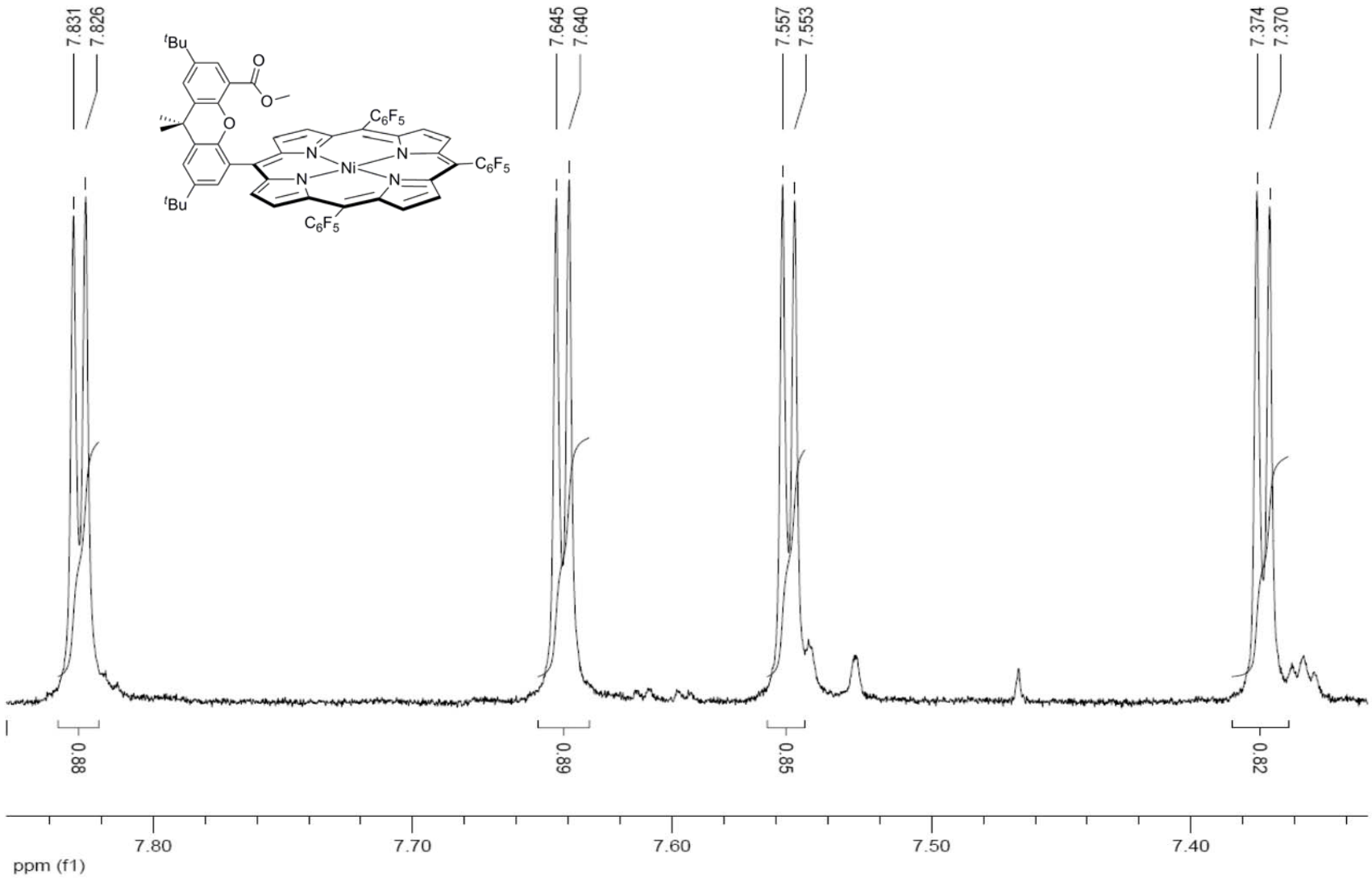

Figure S3c. Aromatic region of the ^{1}H NMR spectrum of NiHPXOMe (**4-Ni**) with integrations and chemical shifts.

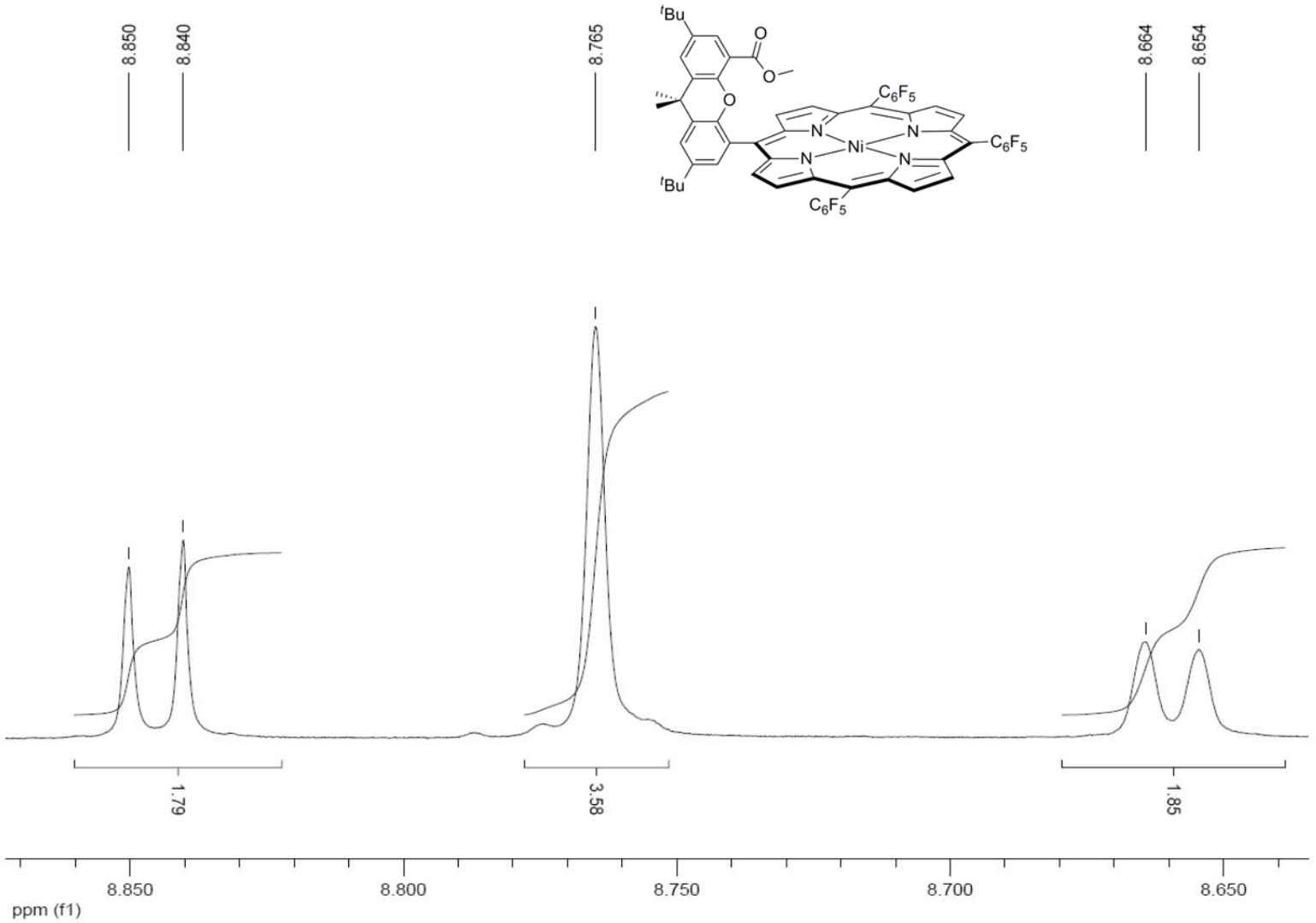

Figure S3d. Aromatic region of the ^{1}H NMR spectrum of NiHPXOMe (**4-Ni**) with integrations and chemical shifts.

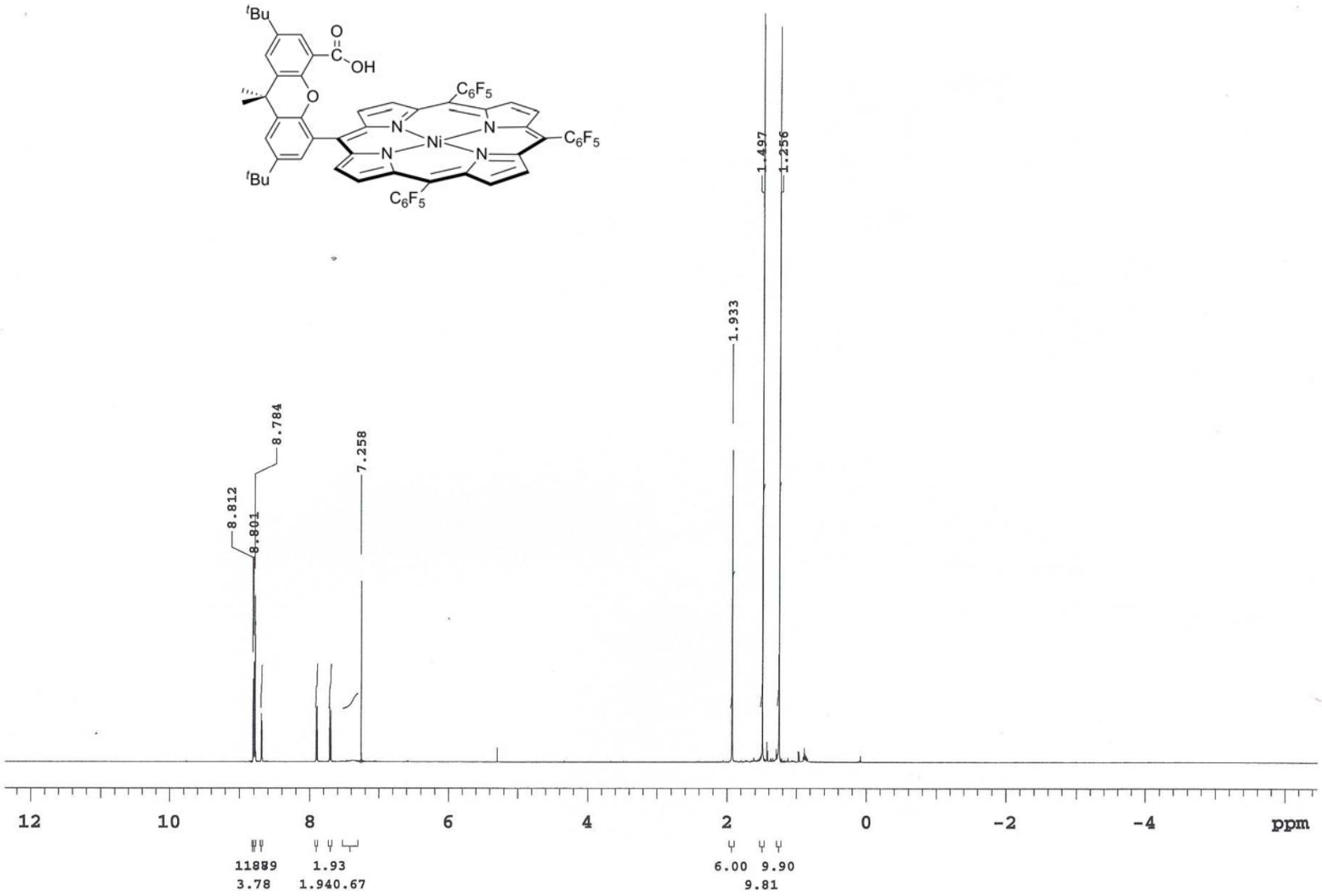

Figure S4a. Full ^{1}H NMR spectrum of NiHPXCO$_2$H (**1-Ni**).

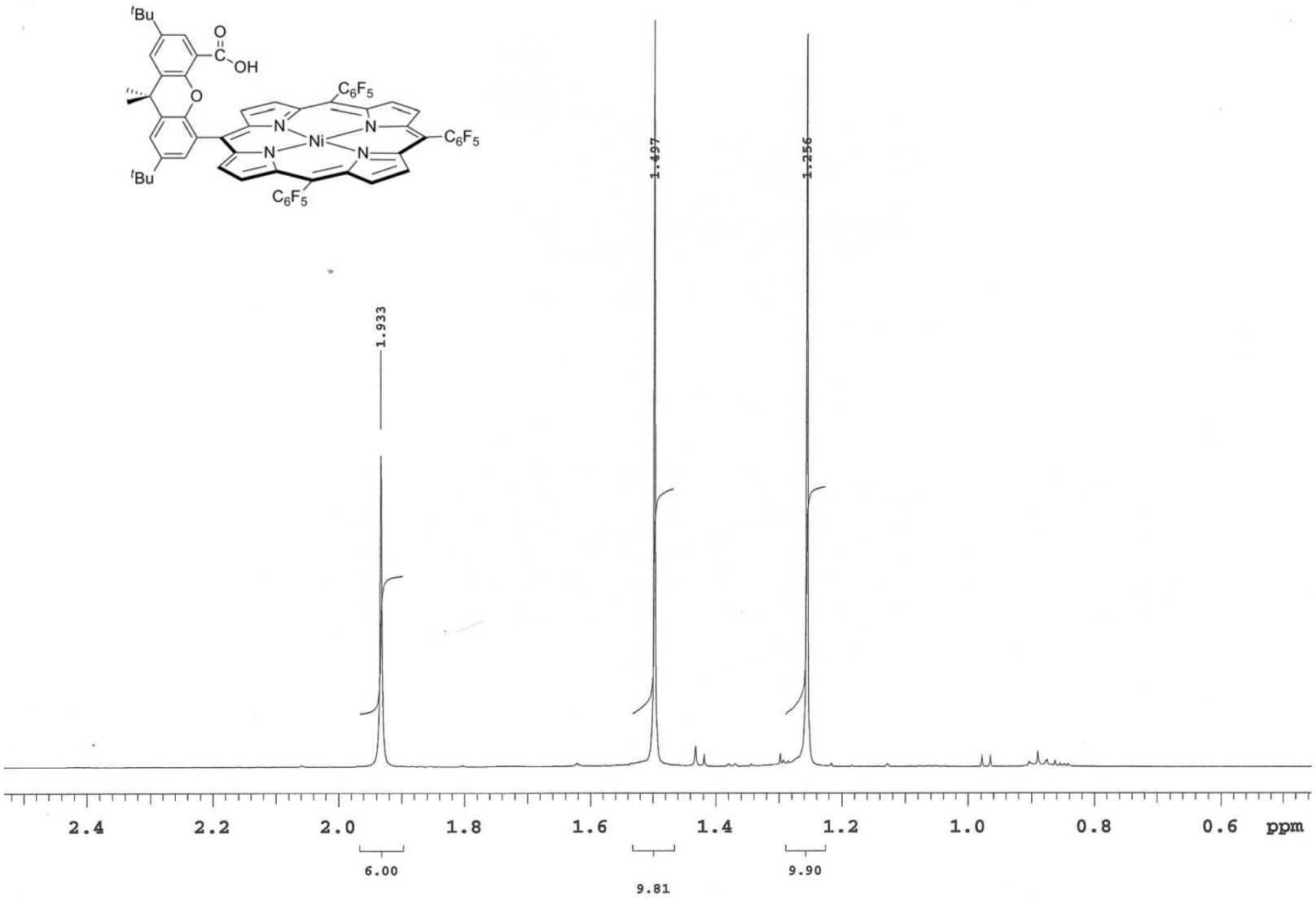

Figure S4b. Aliphatic region of the ^{1}H NMR spectrum of NiHPXCO$_2$H (**1-Ni**) with integrations and chemical shifts.

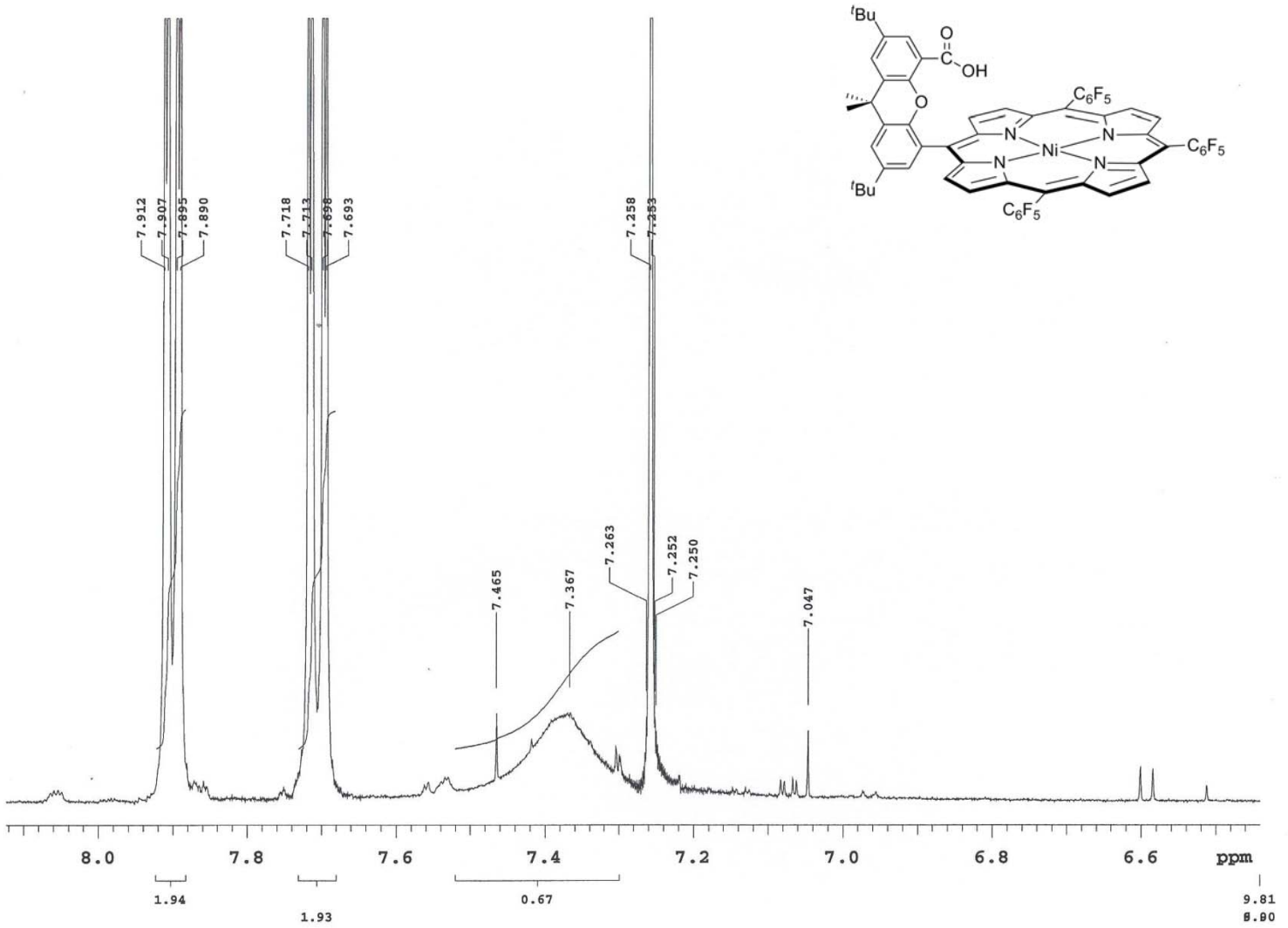

Figure S4c. Aliphatic region of the ^{1}H NMR spectrum of NiHPXCO$_2$H (**1-Ni**)with integrations and chemical shifts.

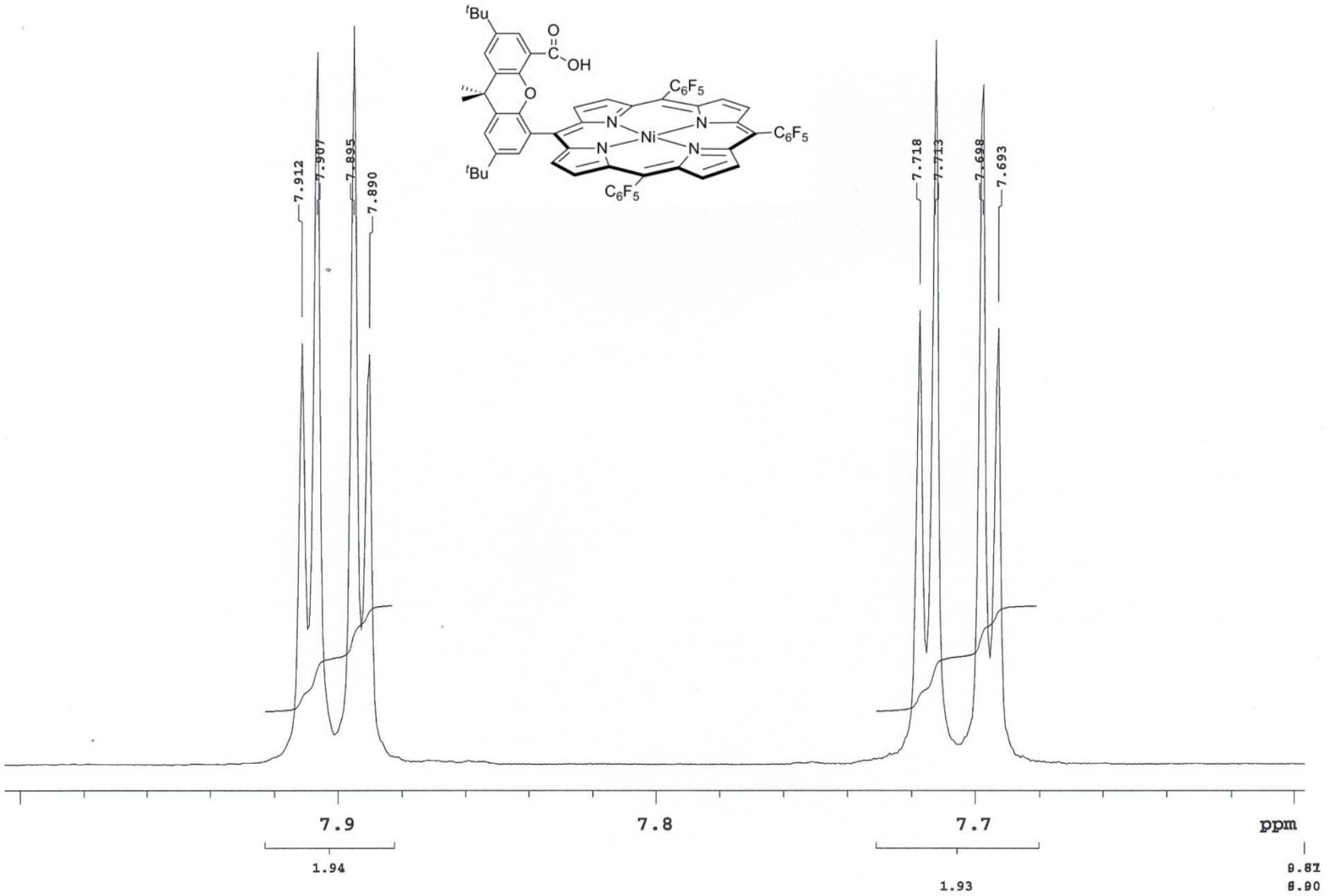

Figure S4d. Aromatic region of the ^{1}H NMR spectrum of NiHPXCO$_2$H (**1-Ni**) with integrations and chemical shifts.

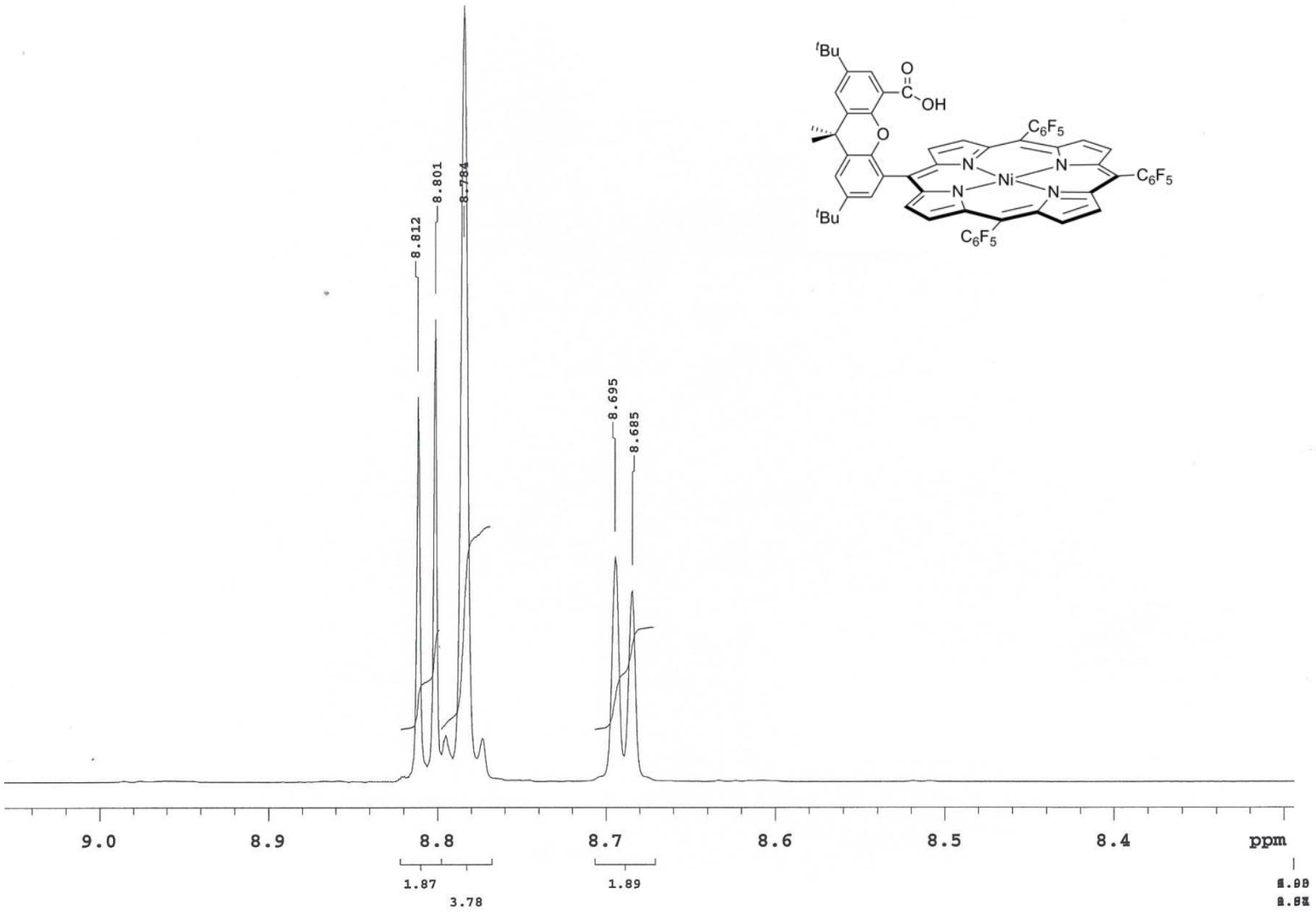

Figure S4e. Aromatic region of the ^{1}H NMR spectrum of $NiHPXCO_2H$ (**1-Ni**) with integrations and chemical shifts.

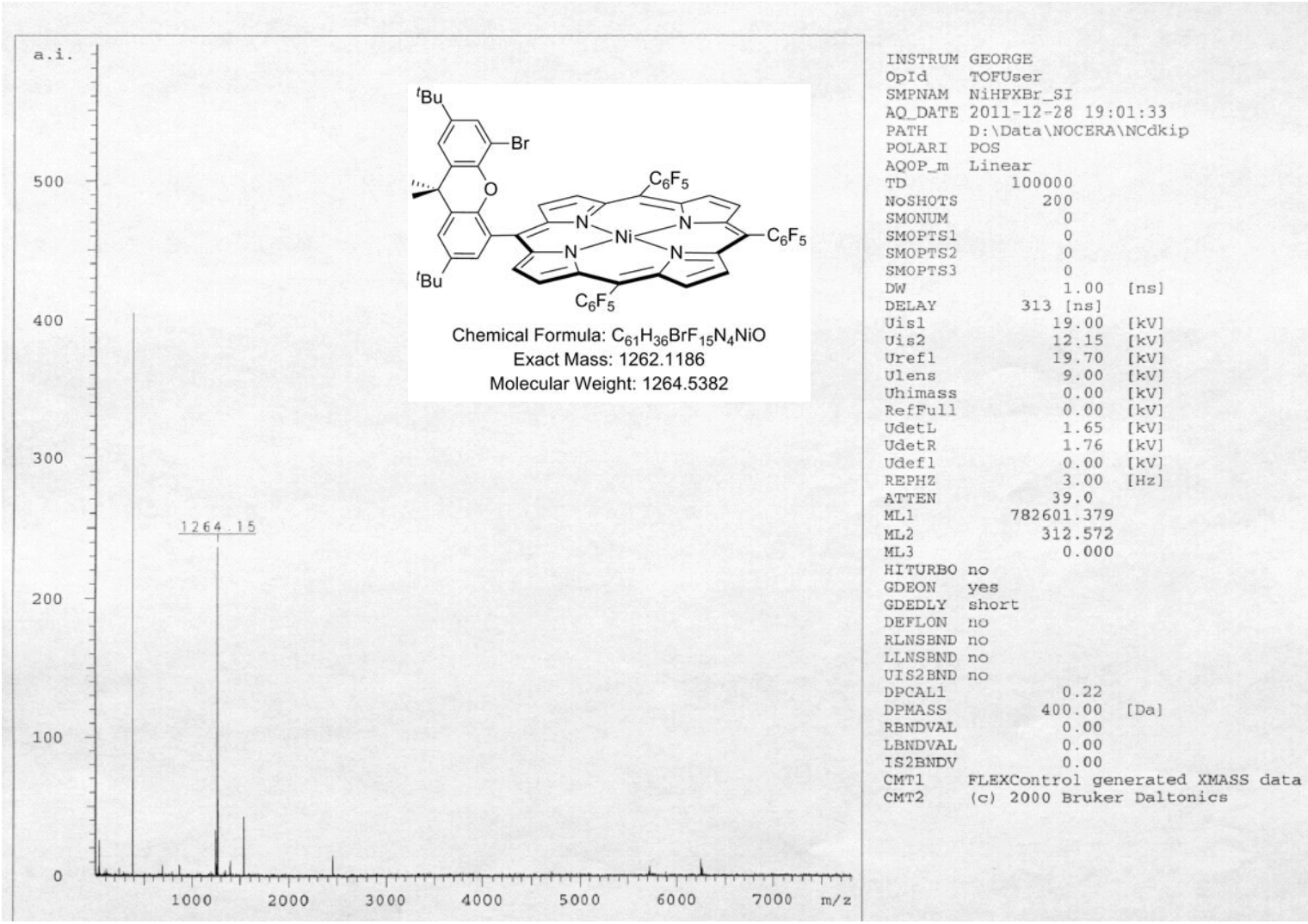

Figure S5a. MALDI spectrum of **2-Ni**.

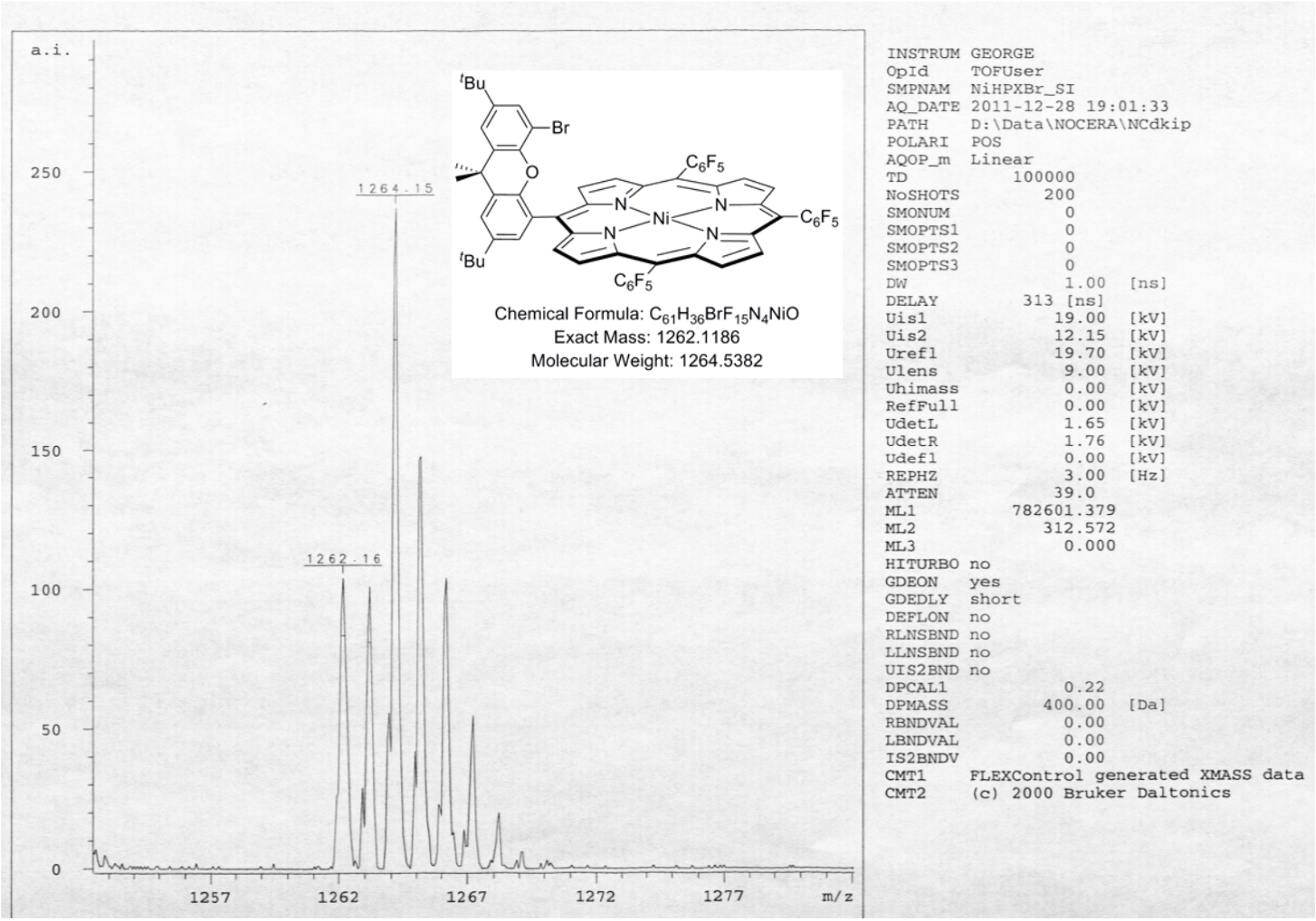

Figure S5b. MALDI spectrum of **2-Ni**.

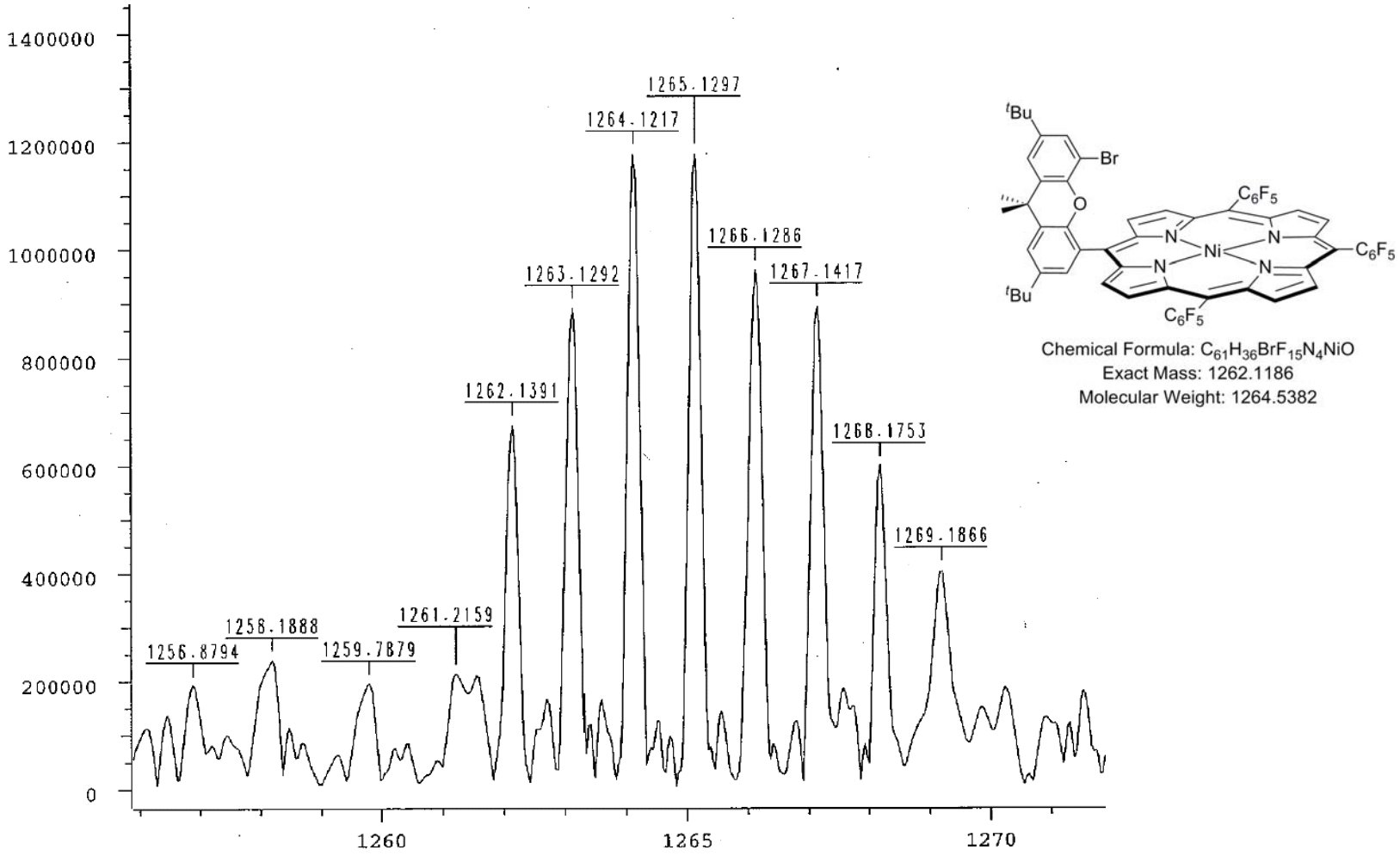

Figure S5c. MALDI spectrum of **2-Ni**.

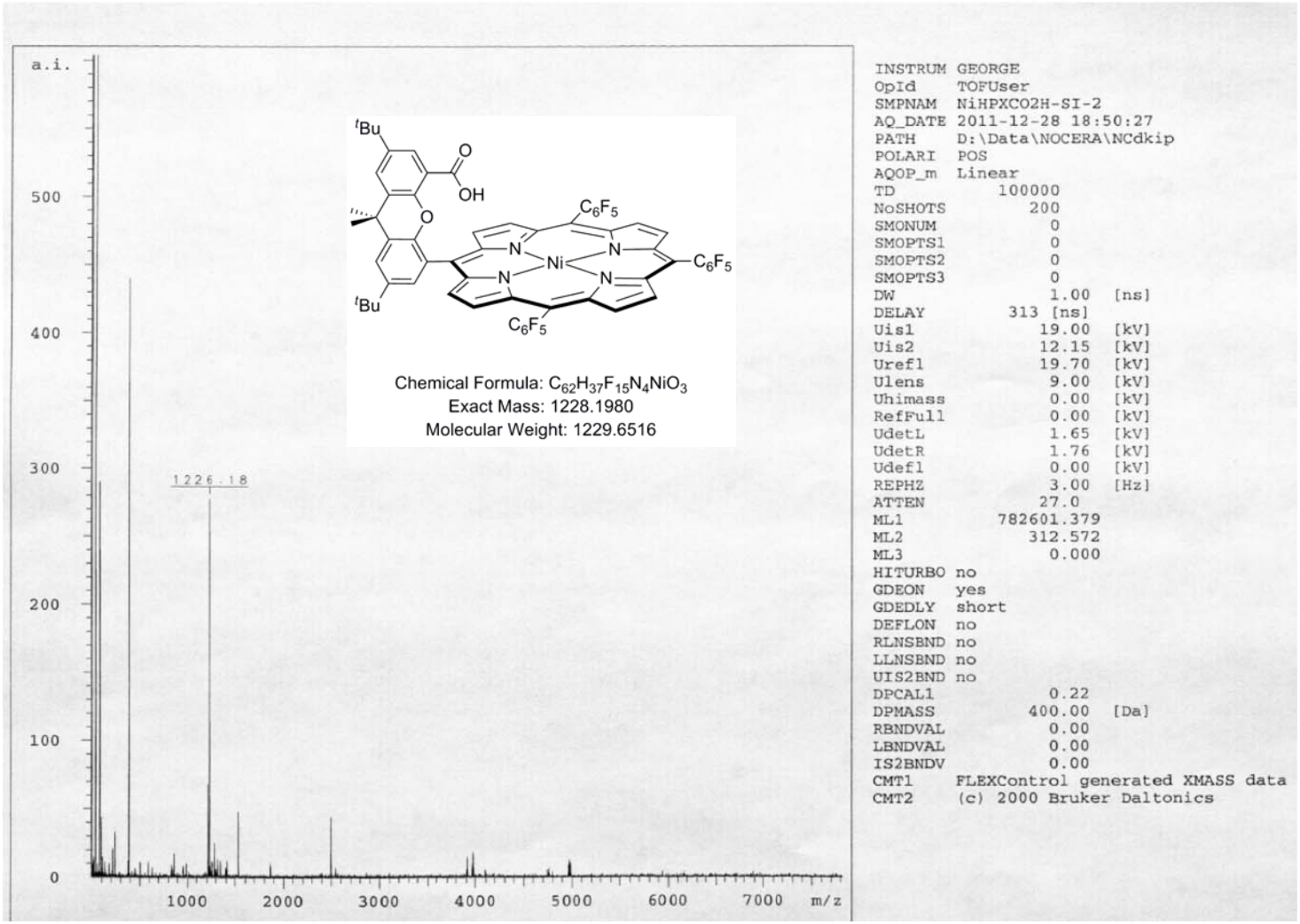

Figure S6a. MALDI spectrum of **1-Ni**.

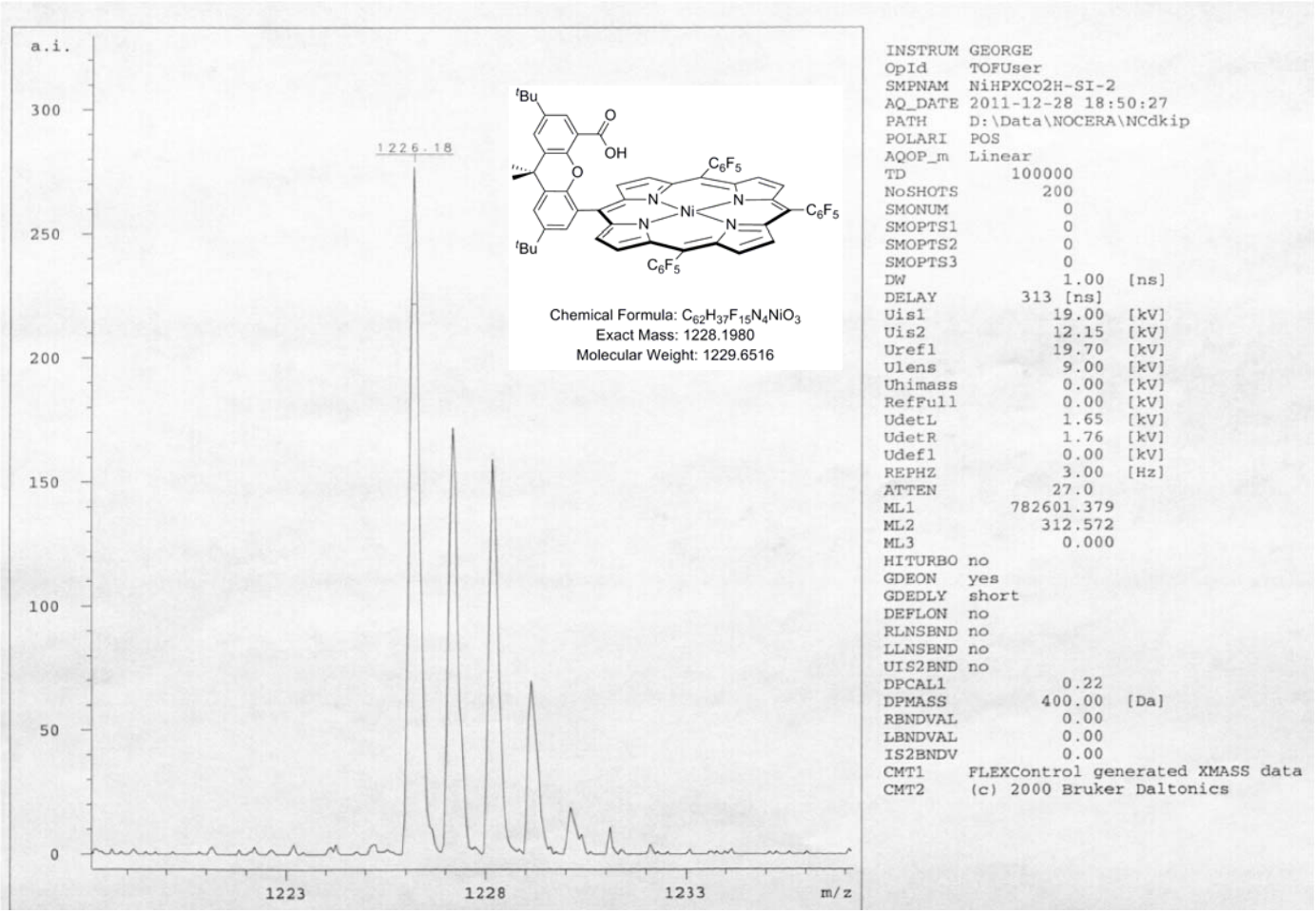

Figure S6b. MALDI spectrum of **1-Ni**.

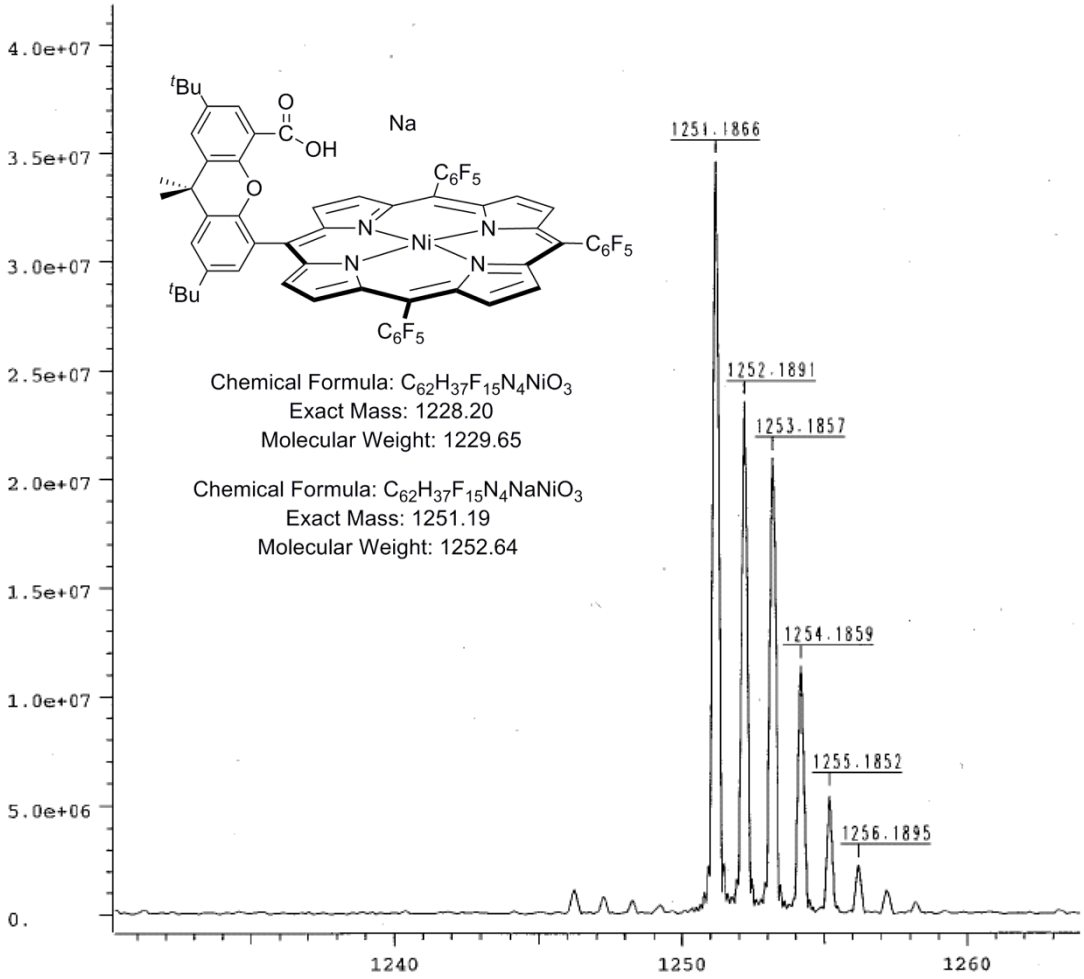

Figure S6c. ESI-MS spectrum of **1-Ni**.

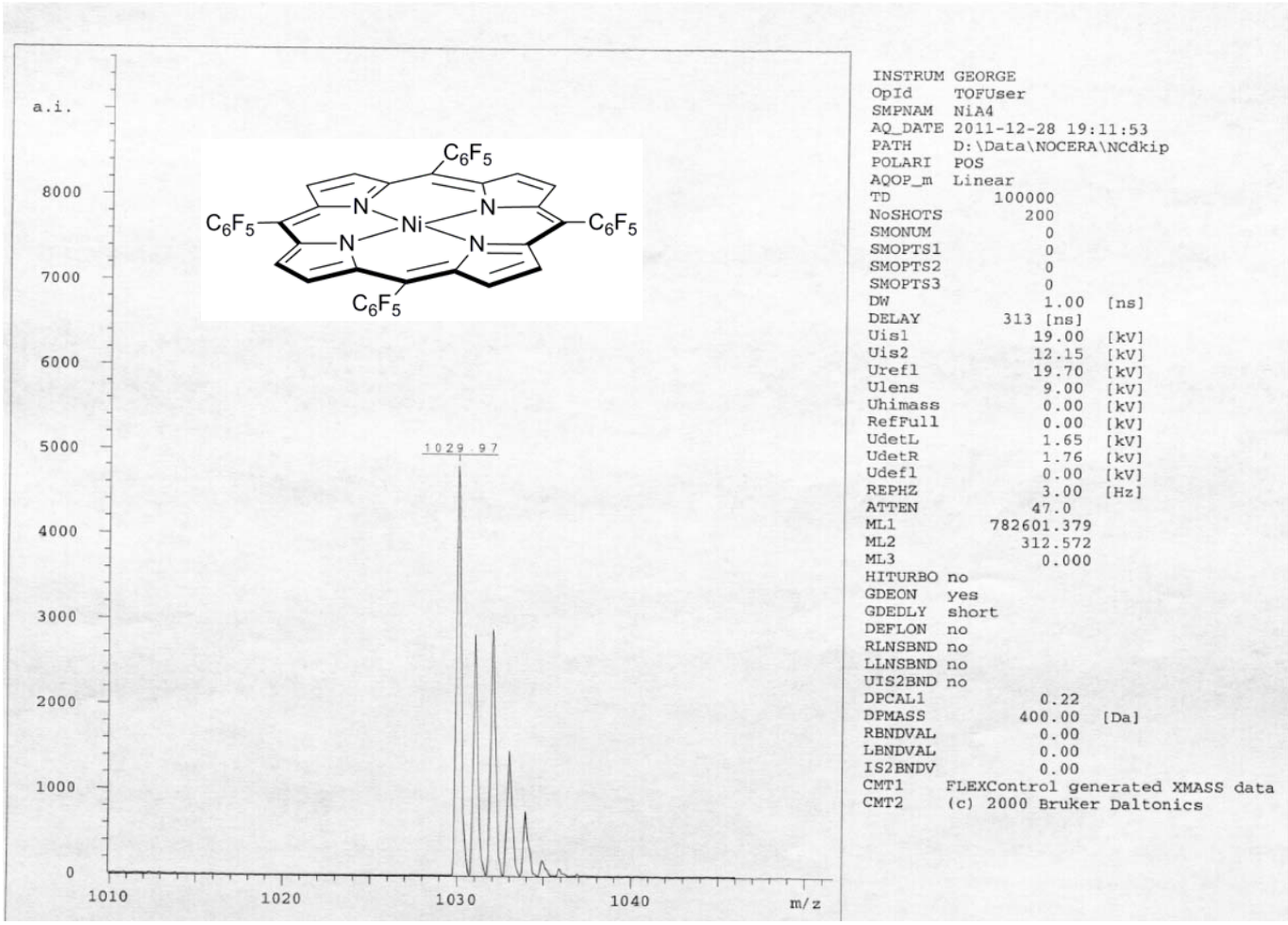

Figure S7. MALDI spectrum of $Ni(C_6F_5)_4$ (**3-Ni**).

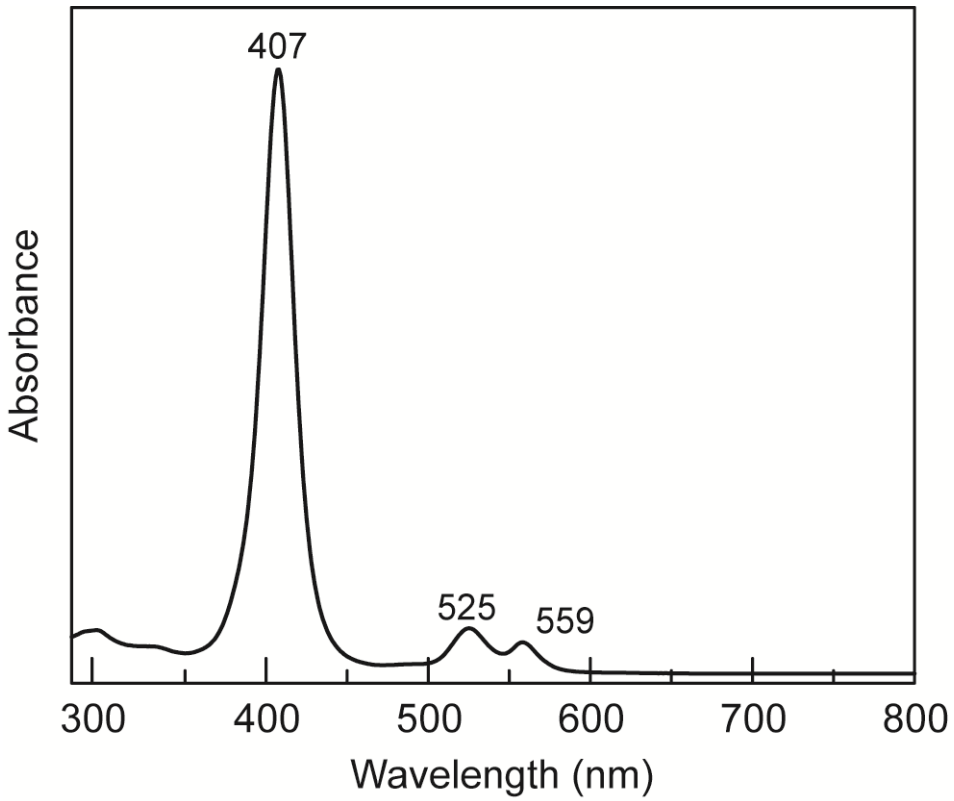

Figure S8. Absorption spectrum of **2-Ni** in CH_2Cl_2 at room temperature.

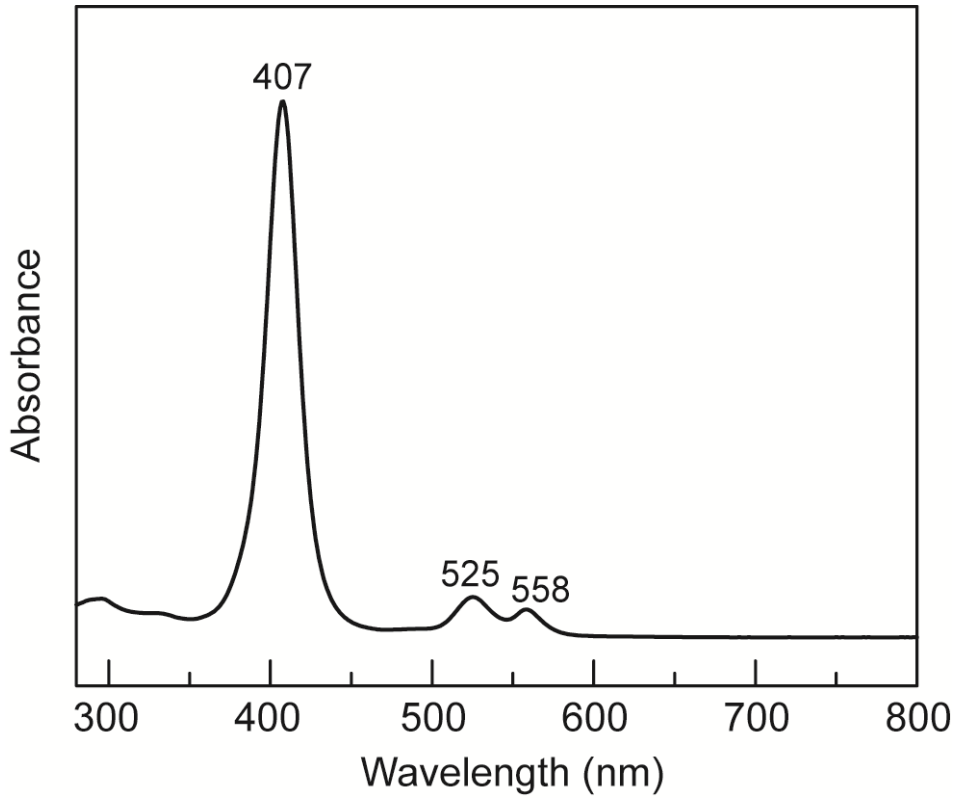

Figure S9. Absorption spectrum of **4-Ni** in CH_2Cl_2 at room temperature.

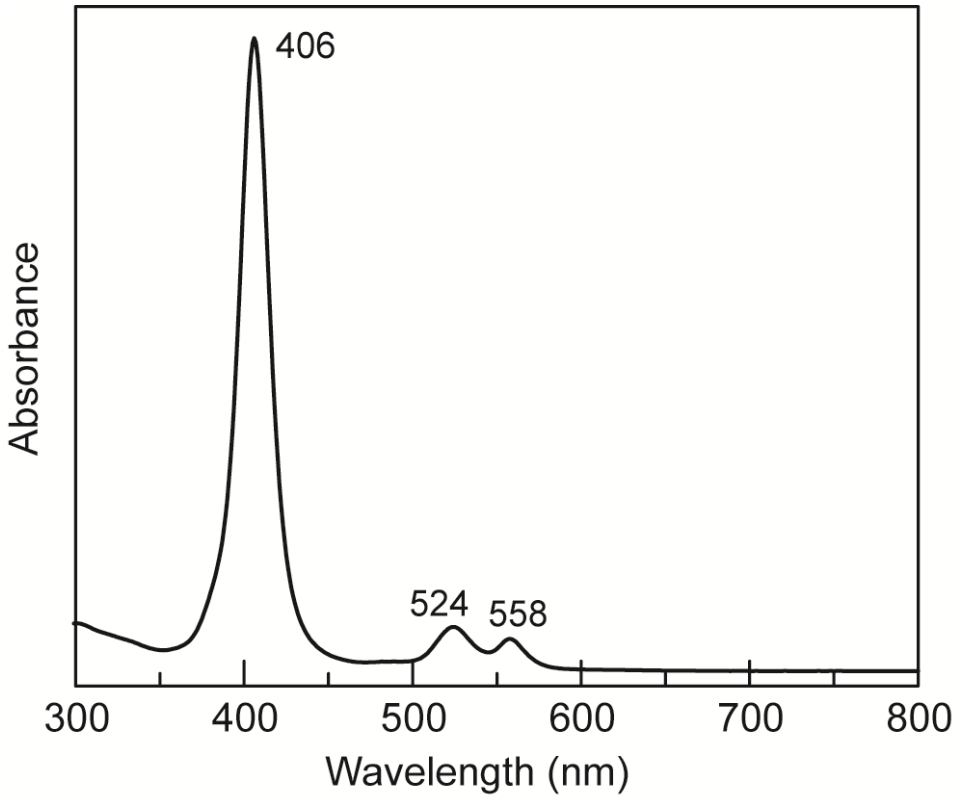

Figure S10. Absorption spectrum of **1-Ni** in CH_2Cl_2 at room temperature.

Cyclic Voltammetry Data

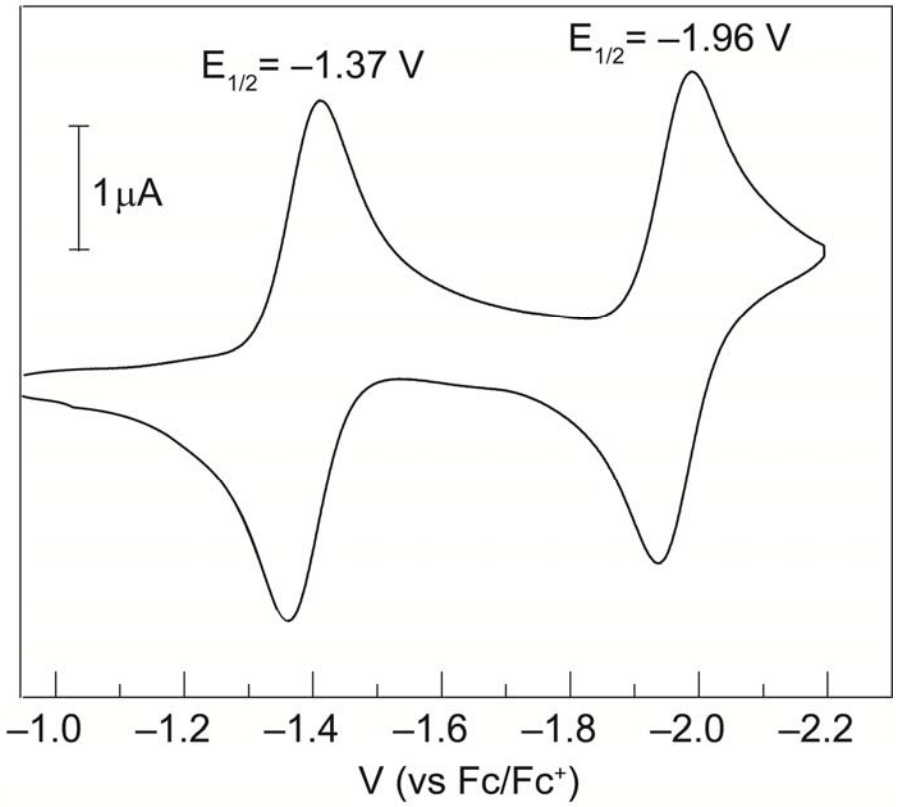

Figure S11. CV of **4-Ni** (2 mM) was recorded in 0.2 M NBu_4PF_6 in acetonitrile in the glove box. A three compartment cell was employed possessing a 0.07 cm^2 glassy carbon button electrode as a working electrode, Pt wire as an auxiliary electrode, and Ag/AgNO as a reference electrode. The CV was collected with scan rate of 30 mV/s with iR compensation.

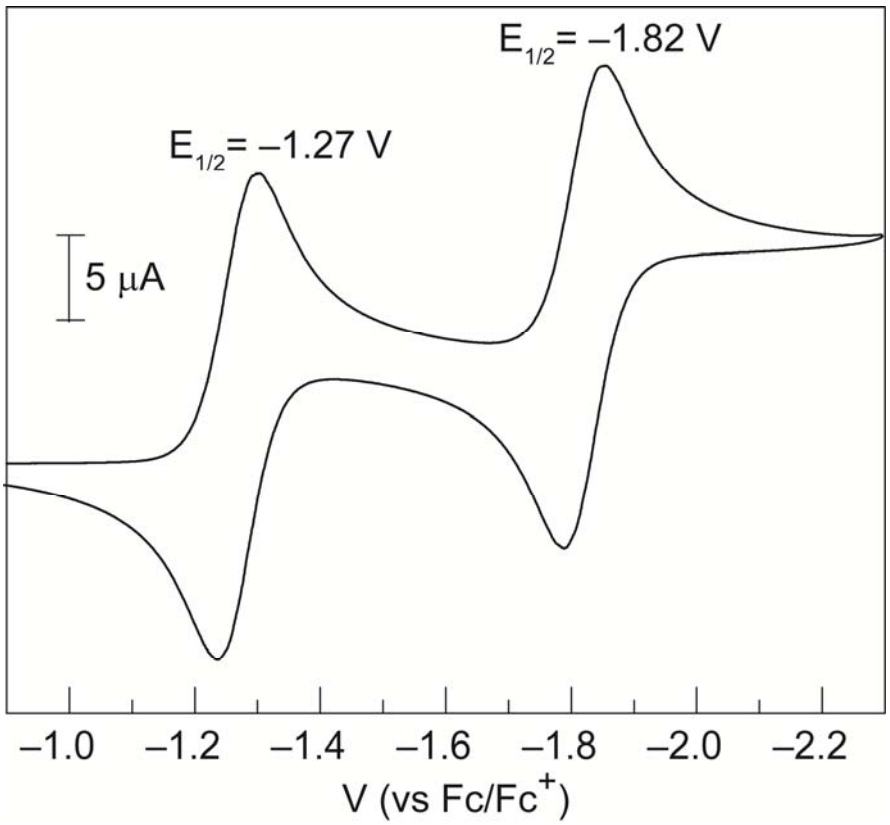

Figure S12. CV of **3-Ni** (0.41 mM) was recorded in 0.1 M NBu_4PF_6 in acetonitrile in the glove box. A three compartment cell was employed possessing a 0.07 cm^2 glassy carbon button electrode as a working electrode, Pt wire as an auxiliary electrode, and $Ag/AgNO_3$ as a reference electrode. The CV was collected with scan rate of 100 mV/s with iR compensation.

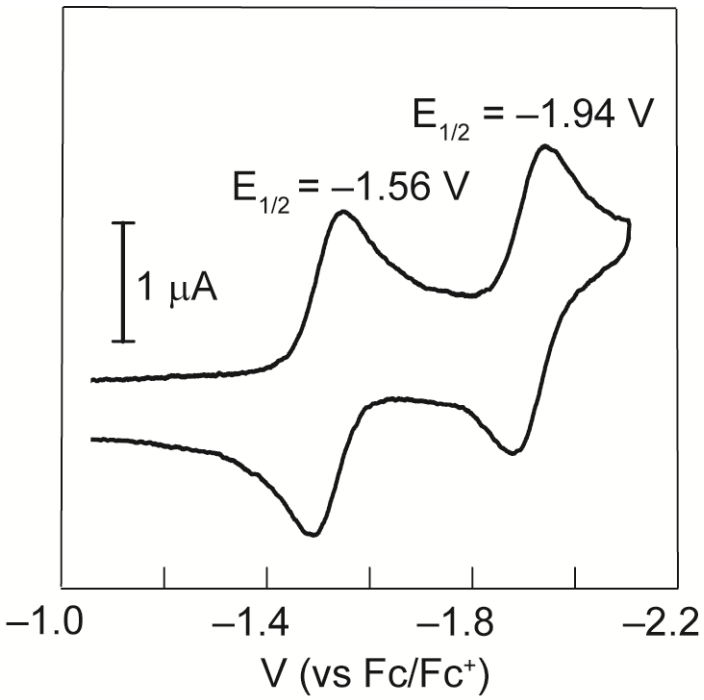

Figure S13. The CV of **2-Zn** shows redox waves at –1.56 V and –1.94 V. This confirms that each electrochemical feature of NiHXBr (–1.38 V, –1.96 V), NiHPXCO_2Me (–1.39 V, –1.97), and NiHPXCO_2H (–1.39 V, –2.01 V) has significant nickel character especially for the first reversible wave. Glassy carbon working electrode (0.07 cm^2), Ag/$AgNO_3$ reference electrode, Pt wire, scan rate 100 mv/s, NBu_4PF_6 electrolyte in acetonitrile.

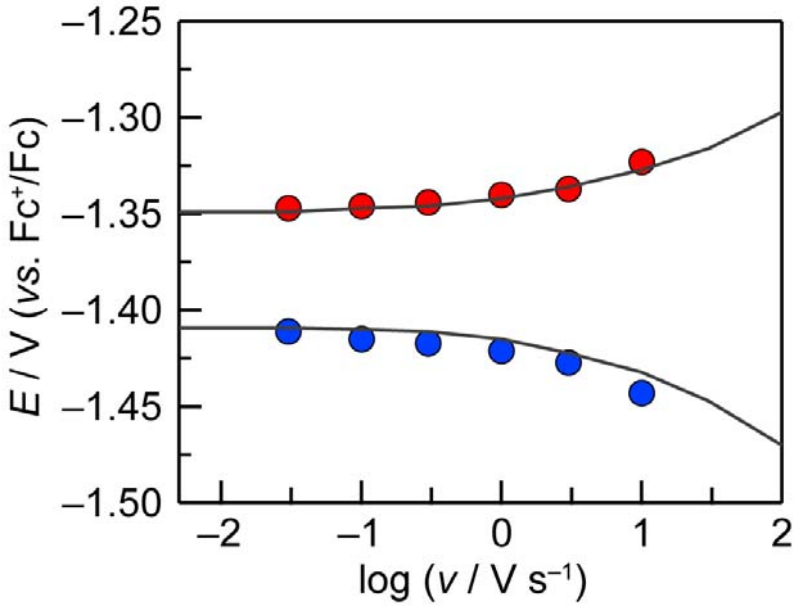

Figure S14. Trumpet plot for the **2-Ni**/[**2-Ni**]⁻ redox couple (E^0 = –1.38 V *vs* Fc^+/Fc). Cathodic (blue circles) and anodic (red circles) peak potentials as a function of the logarithm of the scan rate (v/V s^{-1}). The diffusion coefficient (D) of **2-Ni** was determined to be 8 × 10^{-6} cm^2s^{-1} from the peak current, i, in the reversible limit: $i = 0.446\ FAC^0D^{½}(Fv/RT)^{½}$ (F is the Faraday constant, A is the area of the electrode and C is the bulk **2-Ni** concentration). Solid red lines indicate the variation of peak potential with scan rate simulated for a standard heterogeneous ET rate constant of 0.05 cm s^{-1}.

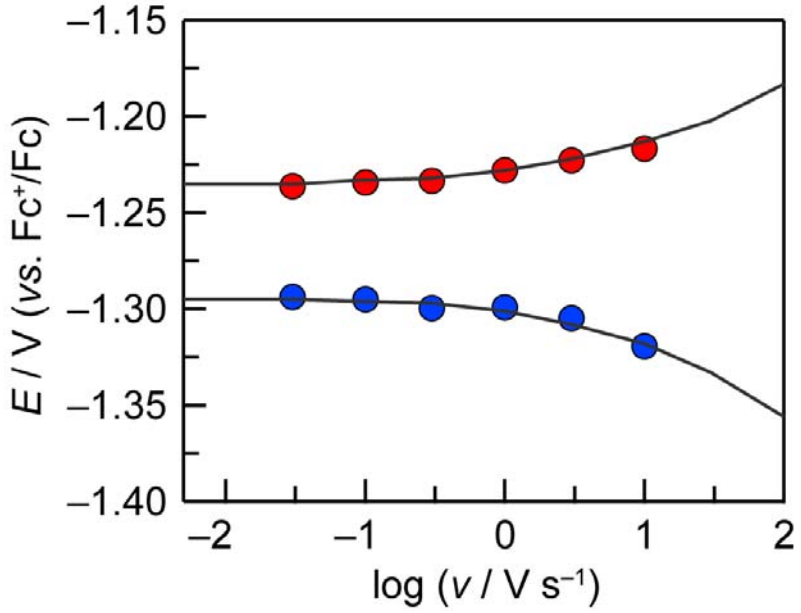

Figure S15. Trumpet plot for the [**2-Ni**]$^{-}$/[**2-Ni**]$^{2-}$ redox couple (E^0 = –1.96 V *vs* Fc^{+}/Fc). Cathodic (blue circles) and anodic (red circles) peak potentials as a function of the logarithm of the scan rate (v/V s^{-1}). Solid red lines indicate the variation of peak potential with scan rate simulated for a standard heterogeneous ET rate constant of 0.05 cm s^{-1}.

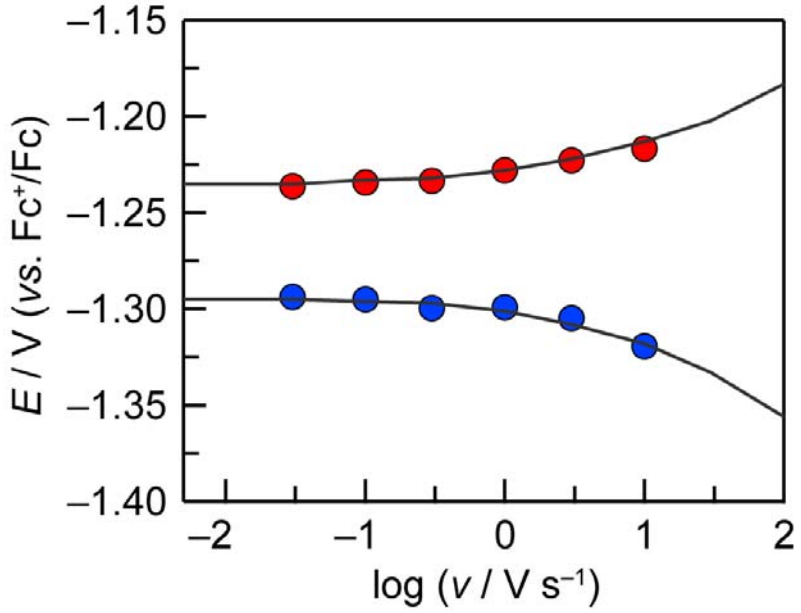

Figure S16. Trumpet plot for the **3-Ni**/[**3-Ni**]$^-$ redox couple (E^0 = –1.26 V *vs* Fc^+/Fc). Cathodic (blue circles) and anodic (red circles) peak potentials as a function of the logarithm of the scan rate (v/V s^{-1}). The diffusion coefficient (D) of **3-Ni** was determined to be 8 × 10^{-6} cm^2 s^{-1} from the peak current, i, in the reversible limit. Solid red lines indicate the variation of peak potential with scan rate simulated for a standard heterogeneous ET rate constant of 0.05 cm s^{-1}.

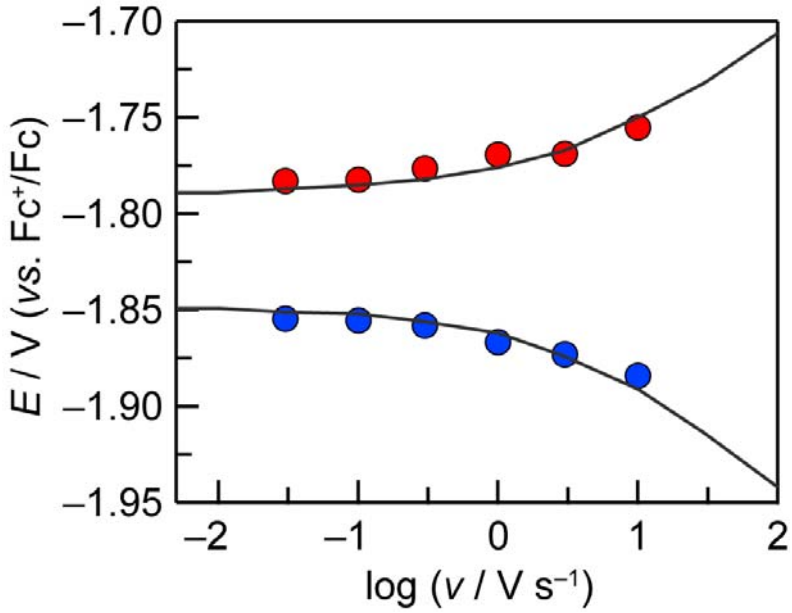

Figure S17. Trumpet plot for the **3-Ni**/[**3-Ni**]$^-$ redox couple (E^0 = –1.82 V *vs* Fc^+/Fc). Cathodic (blue circles) and anodic (red circles) peak potentials as a function of the logarithm of the scan rate (v/V s^{-1}). Solid red lines indicate the variation of peak potential with scan rate simulated for a standard heterogeneous ET rate constant of 0.025 cm s^{-1}.

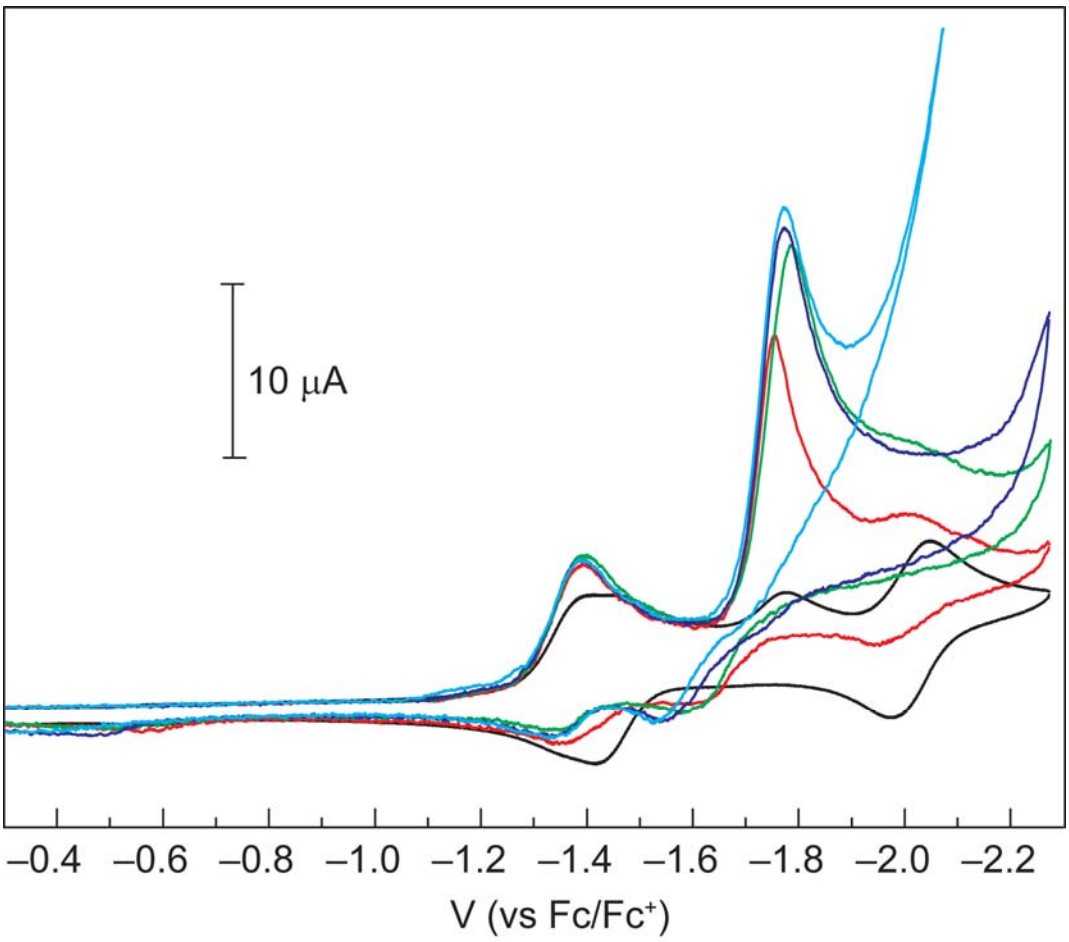

Figure S18. CVs of **NiHPXCO$_2$H** (0.4 mM) in the presence of 0 (–), 2.0 (–), 5.0 (–), 10.0 (–), 20 (–) mM benzoic acid. The scans were recorded in 0.1 M NBu_4PF_6 in acetonitrile in the glove box. A three compartment cell was employed possessing a 0.07 cm^2 glassy carbon button electrode as a working electrode, Pt wire as an auxiliary electrode, and Ag/AgNO as a reference electrode. CV was collected with scan rate of 100 mV/s with iR compensation.

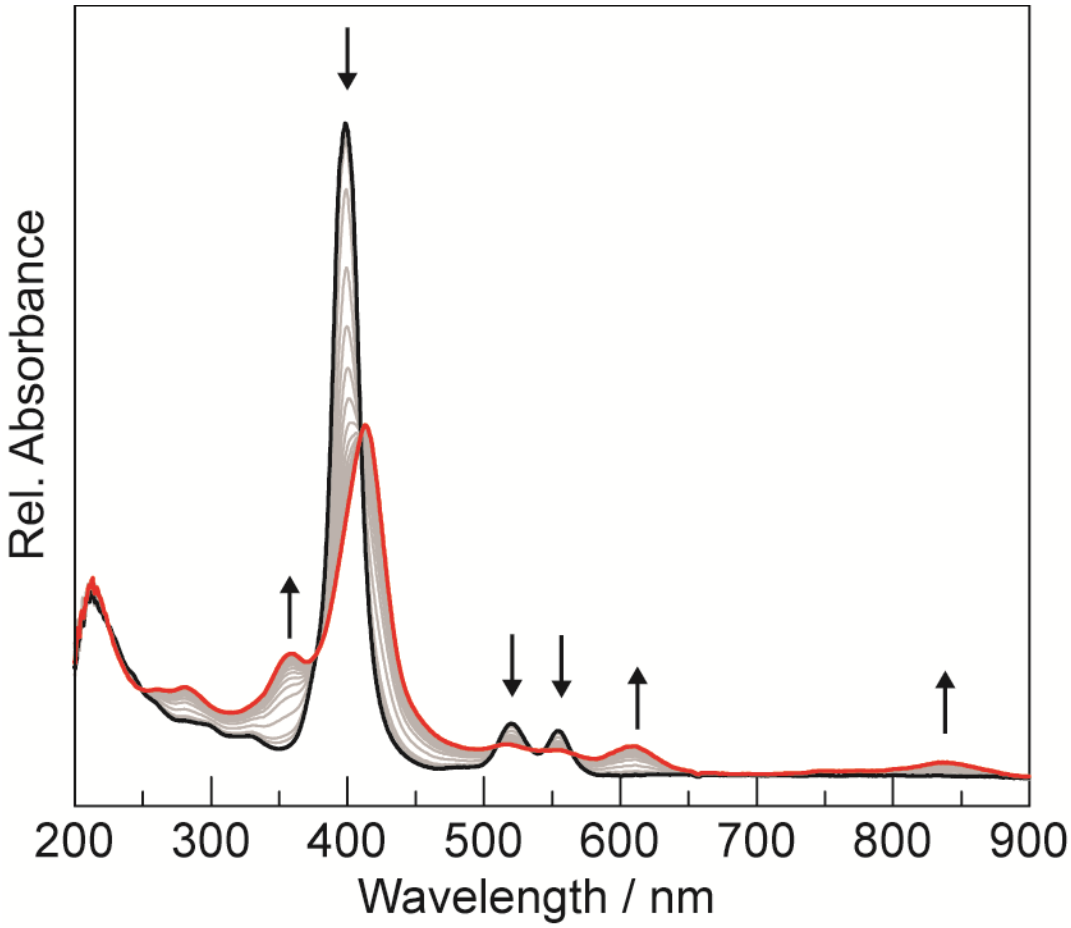

Figure S19a. Thin layer spectroelectrochemistry of 0.3 mM NiTFPP in 0.1 M $TBAPF_6$ in acetonitrile during electrolysis at –1.3 V. Spectra were acquired every 8 sec during electrolysis. Black trace = initial, red trace = final.

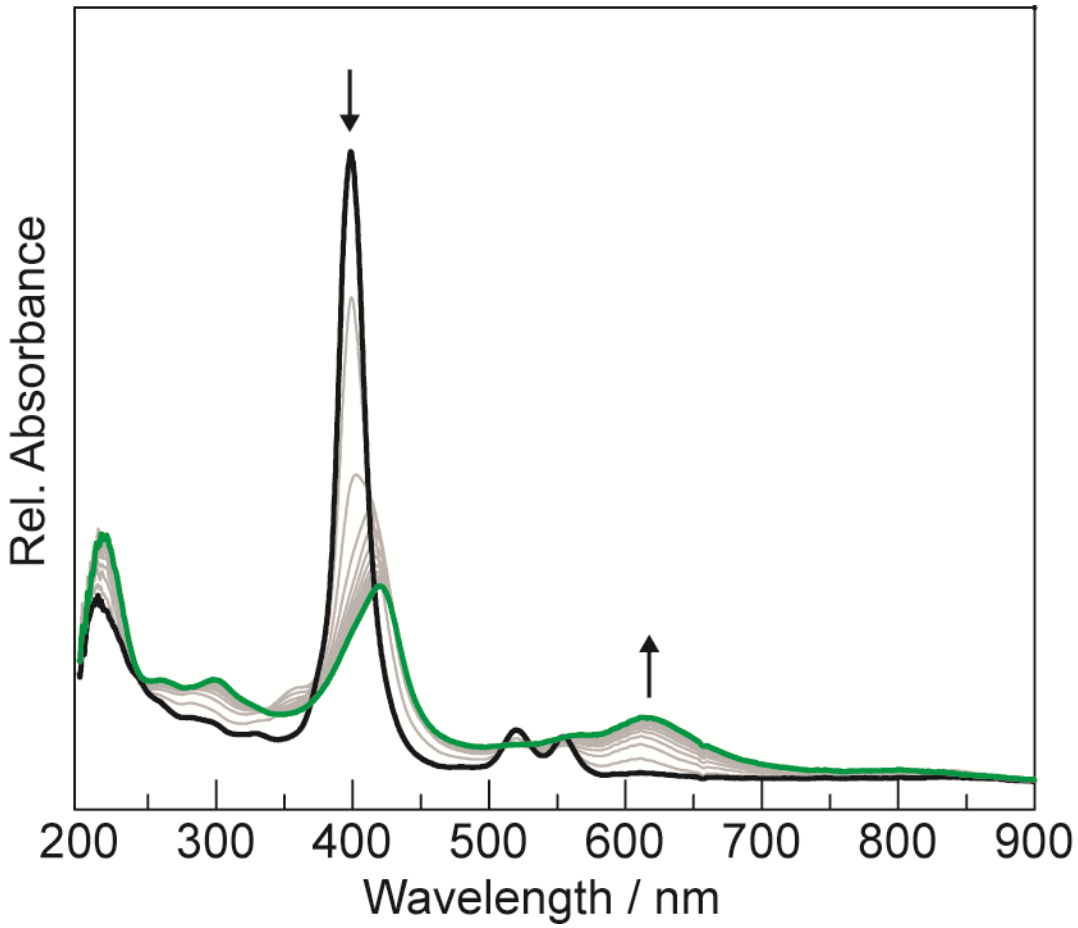

Figure S19b. Thin layer spectroelectrochemistry of 0.3 mM NiTFPP in 0.1 M $TBAPF_6$ in acetonitrile during electrolysis at –1.9 V. Spectra were acquired every 12 sec during electrolysis. Black trace = initial, green trace = final.

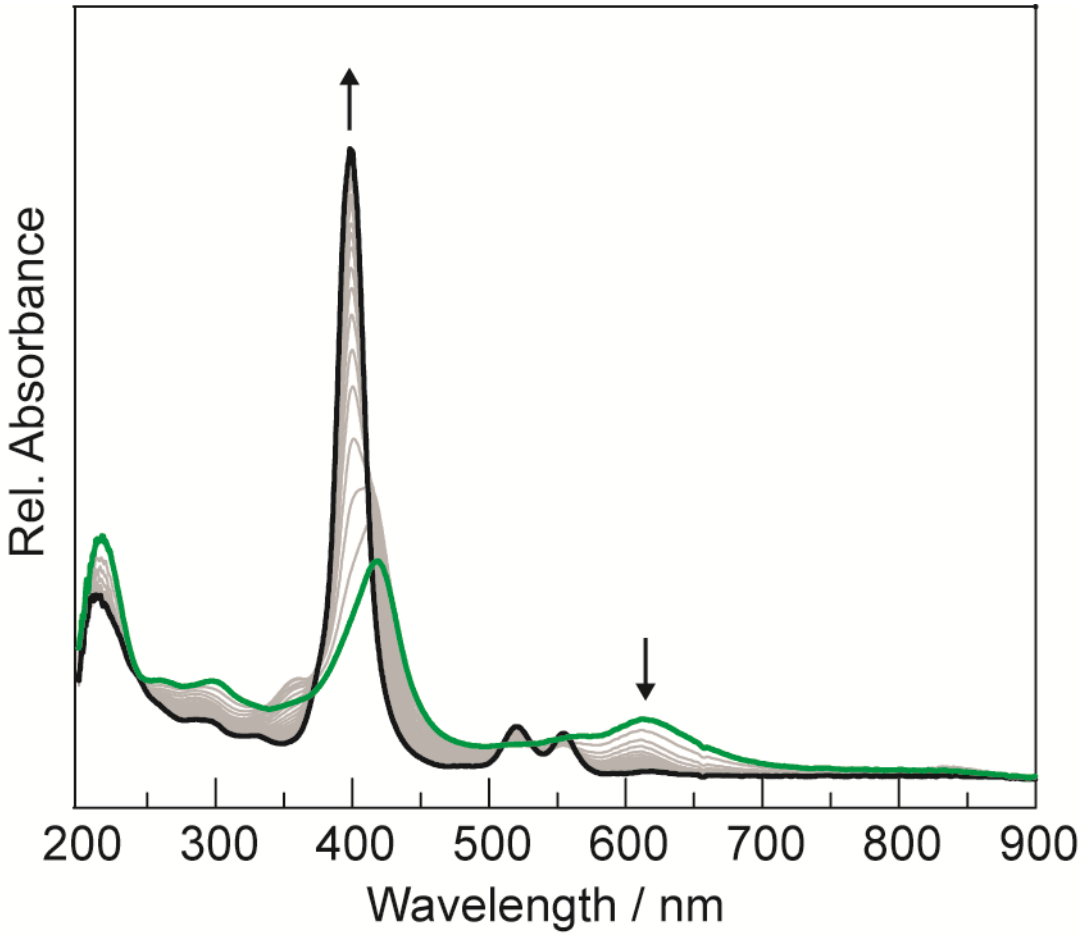

Figure S19c. Thin layer spectroelectrochemistry of 0.3 mM NiTFPP in 0.1 M $TBAPF_6$ in acetonitrile during electrolysis at 0.0 V immediately following electrolysis at –1.9 V. Spectra were acquired every 8 sec. Green trace = initial, black trace = final.

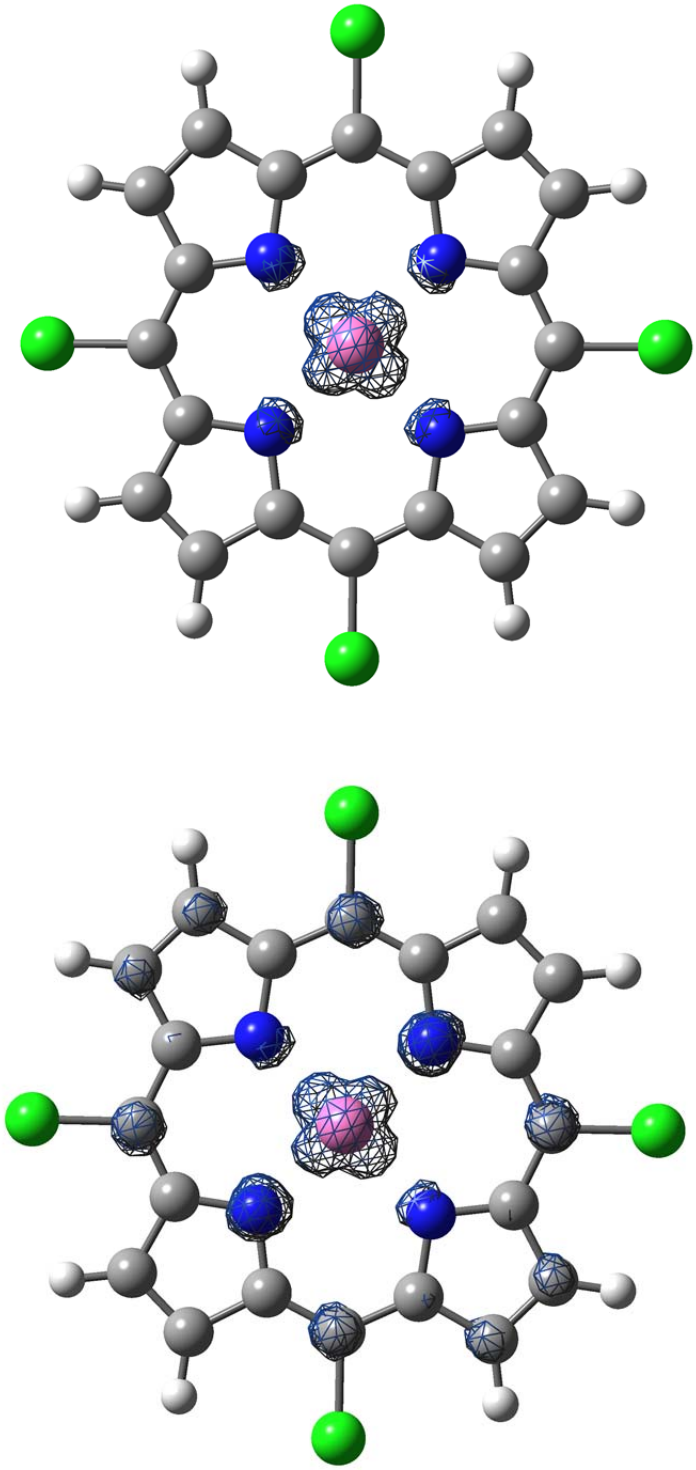

Figure S20. Computed Mulliken atomic spin density (B3P86 with geometry optimized in solution, IsoValue: 0.005) plots of [**3-Ni**]$^{-}$ (top) and [**3-Ni**]$^{2-}$ (bottom). The computed spin density is found to be almost entirely on the metal in the monoanion, top (SD on Ni = 0.936177). In the case of the dianion (bottom), additional spin density from the second electron is localized on the ligands (SD on Ni = 0.963403).

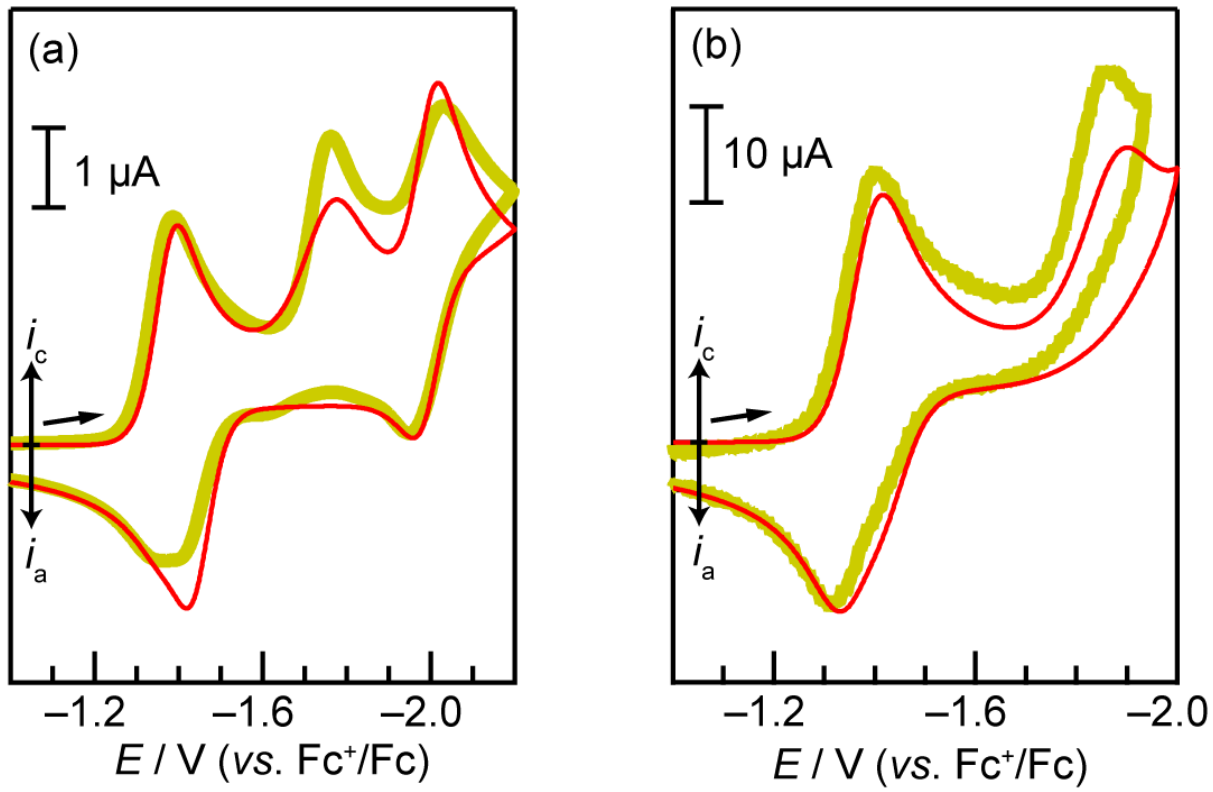

Figure S21. Experimental (thick green curves) and simulated (thin red curves) cyclic voltammograms of a 0.4 mM solution of **1-Ni** at a scan rate of (a) 30 mV/s. and (b) 3 V/s Voltammograms were simulated according to a mechanistic framework consisting of an ETPT pathway (Scheme 2) from [**1-Ni**]$^{-}$ to [**1-Ni$_H$**]$^{2-}$, followed by reduction to [**1-Ni$_H$**]$^{3-}$, which is subsequently protonated by the pendant acid group of another porphyrin molecule to liberate H_2. Parameters used in simulation are tabulated in Table S3.

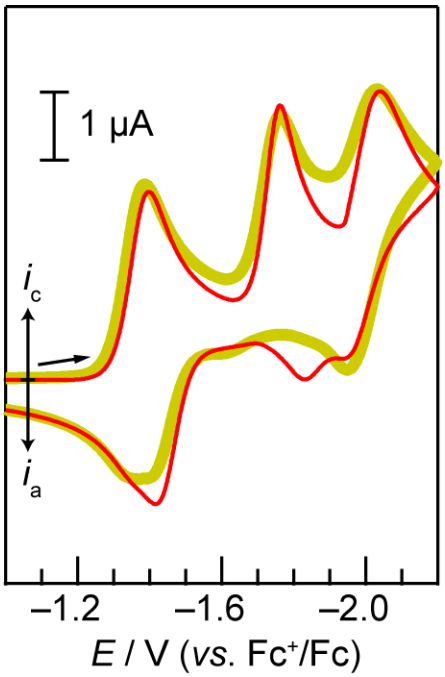

Figure S22. Experimental (thick yellow-green curve) and simulated (thin red curve) CVs of a 0.4 mM solution of **1-Ni** at a scan rate of 30 mV/s. The CV was simulated according to a mechanistic framework consisting of an ETPT pathway (Scheme 2) from **1-Ni**$^-$ to **1-Ni$_H$**$^{2-}$, followed by reduction to **1-Ni$_H$**$^{3-}$, which is subsequently protonated by the pendant acid group of another porphyrin molecule to liberate H_2. Parameters used in simulation are tabulated in Table S4.

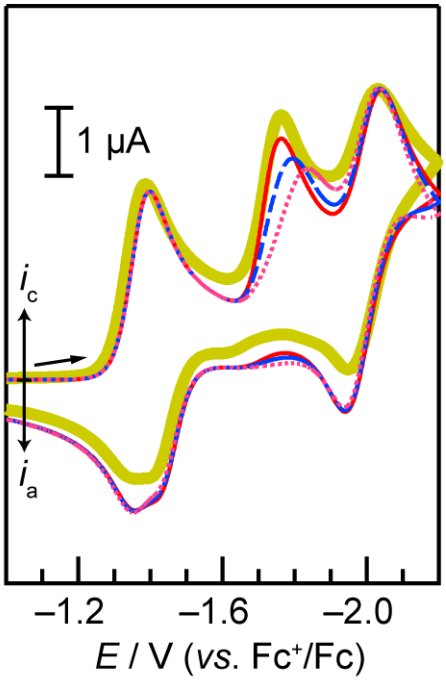

Figure S23. Experimental (thick yellow-green curve) and simulated (thin curves) CVs of a 0.4 mM solution of **1-Ni** at a scan rate of 30 mV/s. The CVs were simulated according to a mechanistic framework consisting of a CPET pathway (Scheme 2) from **1-Ni**$^-$ to **1-Ni$_H$**$^{2-}$ involving a standard CPET rate constant, k_{CPET}, of 6.5 × 10^{-3} cm/s (red, —), 3.25 × 10^{-3} cm/s (blue, – –), and 1.5 × 10^{-3} cm/s (pink, ···) followed by reduction to **1-Ni$_H$**$^{3-}$, which is subsequently protonated by the pendant acid group of another porphyrin molecule to liberate H_2. The other parameters used in simulation are tabulated in Table S5.

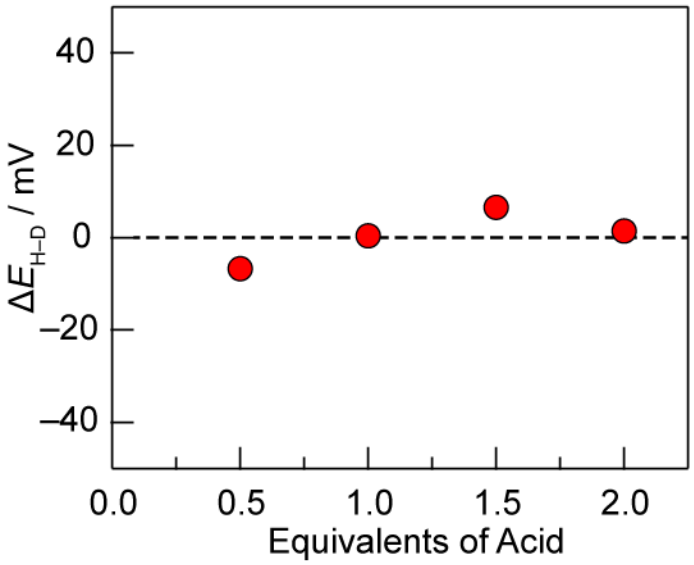

Figure S24. Plot of difference in catalytic peak potential between C_6H_5COOH- and C_6H_5COOD-titrated **1-Ni** (following treatment with K_2CO_3) as a function of the number of acid equivalents introduced.

Table S1. Calculated spin density on Ni of [**3-Ni**]$^-$.

Functional	Spin Density	
	Gas-Phase Geometries [a]	**Solvated Geometries** [b]
B3P86	1.010179	0.936177
B3LYP	1.017783	0.948812
TPSSh	1.060435	0.988065
ωB97xD	0.984440	0.924697
M06L	1.070799	1.017061

[a] Geometry optimizations performed in the *gas* phase. [b] Geometry optimizations performed in solution with C-PCM.

Table S2. Calculated relative free energies and spin density (SD) on Ni of [**3-Ni**]$^{2-}$.

		Gas-Phase Geometries [a]		Solvated Geometries [b]	
Functional	**S**	**Relative Energy (kcal/mol)**	**SD on Ni**	**Relative Energy (kcal/mol)**	**SD on Ni**
B3P86	0	0.00	0.000000	0.00	0.000000
	1	–6.95	1.174651	–6.68	0.963403
B3LYP	0	0.00	0.000000	0.00	0.000000
	1	–8.36	1.181927	–7.21	0.978401
BP86	0	0.00	0.000000	0.00	0.000000
	1	–6.65	1.016560	–6.30	0.931426
BLYP	0	0.00	0.000000	0.00	0.000000
	1	–6.81	1.027134	–7.22	0.959692
TPSSh	0	0.00	0.000000	0.00	0.000000
	1	–8.00	1.145404	–7.44	1.016181
ωB97xD	0	0.00	0.000000	0.00	0.000000
	1	–3.71	1.438658	–3.78	0.990943
M06L	0	0.00	0.000000	0.00	0.000000
	1	–10.42	1.098609	–10.27	1.036479

[a] Geometry optimizations performed in the gas phase. [b] Geometry optimizations performed in solution with C-PCM.

Table S3. CV simulation parameters for ETPT mechanisms using experimentally determined [**2-Ni**]$^-$/[**2-Ni**]$^{2-}$ reduction potential as [**1-Ni**]$^-$/[**1-Ni**]$^{2-}$ potential.

Heterogeneous/Electrochemical Reactions:

Oxidized Species	**Reduced Species**	E^0_{sim} [a]	k^0_{ET} / cm s^{-1}
HOOC--NiP	[HOOC--NiP]$^-$	–1.37	0.025 [b]
[HOOC--NiP]$^-$	[HOOC--NiP]$^{2-}$	–1.96 [c]	0.06 [c]
[OOC--NiP]$^-$	[OOC--NiP]$^{2-}$	–1.45 [d]	0.025 [e]
[OOC--NiP]$^{2-}$	[OOC--NiP]$^{3-}$	–1.99	0.002 [b]
[OOC--NiP(H)]$^{2-}$	[OOC--NiP(H)]$^{3-}$	–1.4 [b]	0.05 [b,e]

Homogeneous/Chemical Reactions:

Reactants	**Products**	K_{eq}	$k_{forward}$
[HOOC--NiP]$^{2-}$	[OOC--NiP(H)]$^{2-}$	>10^6	10^{13}
[OOC--NiP(H)]$^{2-}$ + [OOC--NiP]$^{3-}$	[OOC--NiP(H)]$^{3-}$ + [OOC--NiP]$^{2-}$	9.4 × 10^7 [f]	k_{diff} [g]
[OOC--NiP(H)]$^{3-}$+ acid [h]	H_2 + [OOC--NiP]$^{2-}$ + conjugate base	>10^6	k_{diff} [g]

[a] Reduction potentials are relative to the reduction potential of Fc$^+$. [b] Obtained from simulating experimental CV data. [c] Values estimated from that of non-hangman compound **2-Ni**. [d] Value determined from treatment of **1-Ni** with potassium carbonate, and further refined by simulating shoulder near anodic return peak of **1-Ni**/[**1-Ni**]$^-$ wave. [e] Value set equal to that obtained from trumpet plots of the corresponding protonated species. [f] These equilibrium constants are governed by the difference in reduction potentials of the two sets of species. [g] The forward rate constants of these downhill reactions are assumed to be the diffusion limited rate constant: 10^{10} M^{-1} s^{-1}, [h] All nickel porphyrins with protonated hanging groups are permitted as acid sources in the model.

Table S4. CV simulation parameters for ETPT mechanisms using computed [**1-Ni**]$^-$/[**1-Ni**]$^{2-}$ and [OOC--NiP(H)]$^{2-}$/[OOC--NiP(H)]$^{3-}$ reduction potentials.

Heterogeneous/Electrochemical Reactions:[a]

Oxidized Species	**Reduced Species**	E^0_{sim} [a]	k^0_{ET} / cm s^{-1}
HOOC--NiP	[HOOC--NiP]$^-$	–1.37	0.025 [b]
[HOOC--NiP]$^-$	[HOOC--NiP]$^{2-}$	–1.85[c]	0.06[c]
[OOC--NiP]$^-$	[OOC--NiP]$^{2-}$	–1.45 [d]	0.025 [e]
[OOC--NiP]$^{2-}$	[OOC--NiP]$^{3-}$	–1.99	0.002 [b]
[OOC--NiP(H)]$^{2-}$	[OOC--NiP(H)]$^{3-}$	–1.84 [b]	0.05 [b, e]

Homogeneous/Chemical Reactions:

Reactants	**Products**	K_{eq}	$k_{forward}$
[HOOC--NiP]$^{2-}$	[OOC--NiP(H)]$^{2-}$	>10^6	2000[b]
[OOC--NiP(H)]$^{2-}$ + [OOC--NiP]$^{3-}$	[OOC--NiP(H)]$^{3-}$ + [OOC--NiP]$^{2-}$	9.4 × 10^7 [f]	k_{diff} [g]
[OOC--NiP(H)]$^{3-}$+ acid [h]	H_2 + [OOC--NiP]$^{2-}$ + conjugate base	>10^6	k_{diff} [g]

[a] Reduction potentials are relative to the reduction potential of Fc^+. [b] Obtained from simulating experimental CV data. [c] Value computed using DFT (Table 1). [d] Value estimated from that of non-hangman compound **2-Ni**. [e] Value determined from treatment of **1-Ni** with potassium carbonate, and further refined by simulating shoulder near anodic return peak of **1-Ni**/[**1-Ni**]$^-$ wave. [f] Value set equal to that obtained from trumpet plots of the corresponding protonated species. [f] These equilibrium constants are governed by the difference in reduction potentials of the two sets of species. [g] The forward rate constants of these downhill reactions are assumed to be the diffusion limited rate constant: 10^{10} M^{-1} s^{-1}, [h] All nickel porphyrins with protonated hanging groups are permitted as acid sources in the model.

Table S5. Parameters used in simulating CPET-based pathway

Heterogeneous/Electrochemical Reactions:

Oxidized Species	**Reduced Species**	E^o_{sim} [a]	$k_{ET}{}^o$ / cm s^{-1}
HOOC--NiP	[HOOC--NiP]$^-$	–1.37	0.025 [b]
[HOOC--NiP]$^-$	[HOOC--NiP]$^{2-}$	–1.96[c]	0.06 [c]
[OOC--NiP]$^-$	[OOC--NiP]$^{2-}$	–1.45 [d]	0.025 [e]
[OOC--NiP]$^{2-}$	[OOC--NiP]$^{3-}$	–1.99	0.002 [b]
[HOOC--NiP]$^-$	[OOC--Ni(H)P]$^{2-}$	–1.83 [b]	k_{CPET}*
[OOC--Ni(H)P]$^{2-}$	[OOC--Ni(H)P]$^{3-}$	–1.95 [b]	0.05 [b]

Homogeneous/Chemical Reactions:

Reactants	**Products**	K_{eq}	$k_{forward}$
[OOC--NiP(H)]$^{2-}$ + [OOC--NiP]$^{3-}$	[OOC--NiP(H)]$^{3-}$ + [OOC--NiP]$^{2-}$	4.74 [f]	k_{diff} [g]
[OOC--NiP(H)]$^{3-}$ + acid [h]	H_2 + [OOC-NiP]$^{2-}$conjugate base	> 10^5	k_{diff} [g]

[a] Reduction potentials are relative to the reduction potential of Fc/Fc^+. [b] Obtained from simulating experimental CV data. [c] Values estimated from that of non-hangman compound **2-Ni**. [d] Value determined from treatment of **1-Ni** with potassium carbonate, and further refined by simulating shoulder near anodic return peak of **1-Ni/1-Ni^{-1}** wave. [e] Value set equal to that obtained from trumpet plots of the corresponding protonated species. [f] These equilibrium constants are governed by the difference in reduction potentials of the two sets of species. [g] The forward rate constants of these downhill reactions are assumed to be the diffusion limited rate constant: 10^{10} M^{-1} s^{-1}. [h] All nickel porphyrins with protonated hanging groups are permitted as acid sources in the mechanism.

*See the caption of Figure S23 for the standard CPET rate constant used in simulation.

Table S6. Relative free energies and spin density (SD) on Ni of **[1-Ni]** (B3P86 functional).

		Gas Phase Geometries [a]		Solvated Geometries [b]	
Complex	***S***	**Relative Energy**	**SD on Ni**	**Relative Energy**	**SD on Ni**
[HOOC--NiP]$^{2-}$	0	0.00 kcal/mol	0.000000	0.00 kcal/mol	0.000000
	1	–7.08 kcal/mol	1.201218	–5.51 kcal/mol	1.016012
[OOC--Ni^{II}(H)P]$^{2-}$	0	29.24 kcal/mol	0.000000	28.02 kcal/mol	0.000000
	1	1.99 kcal/mol	1.940001[c]	–0.10 kcal/mol	1.904485[c]
[OOC--(H)P]$^{3-}$	1/2	0.00 kcal/mol	1.975188[c]	0.00 kcal/mol	1.897547[c]
	3/2	–1.21 kcal/mol	1.976108[c]	–1.54 kcal/mol	1.888403[c]

[a] Geometry optimizations performed in the gas phase. [b] Geometry optimizations performed in solution with C-PCM. [c] These spin densities include contributions from the hydride nucleus.

Table S7. Coordinates and energies for complexes optimized in solution with B3P86.

HOOC--NiP (*S*=0)

N	13.683005425905	24.505636854170	–3.539665288299
N	17.122317399133	26.193680363235	–3.895302497585
N	14.730349889813	26.911163581865	–2.837552045958
O	15.579112842484	30.432727872222	–5.191545601269
C	16.519318309743	28.514898022299	–3.365056199637
C	17.412506129831	27.533645306162	–3.783801184413
C	18.809574915195	27.771358483903	–4.014412272358
H	19.280720474234	28.743083604456	–3.997573241700
C	19.389546935918	26.557327036087	–4.201242769729
H	20.429092142566	26.333084441848	–4.388589963367
C	18.330194549112	25.591422375199	–4.163878741918
C	18.465585774195	24.254221428070	–4.503708692553
C	17.392428805059	23.427627628799	–4.807190938974
C	17.489960502103	22.174809661595	–5.495279720060
H	18.412345357405	21.679294972997	–5.759108867730
C	16.217739694700	21.784370233540	–5.771594983285
H	15.891049548645	20.897660929109	–6.293790358699
C	15.353323198859	22.767986227850	–5.191099760818
C	13.974365129797	22.653872053073	–5.093741187531
C	13.197824921257	23.427172413283	–4.243235122988
C	11.850792427588	23.126566522815	–3.859673343346
H	11.248423516502	22.332039961033	–4.273960672975
C	11.528260866136	23.994333908286	–2.864148209076
H	10.603390875563	24.064055131922	–2.311568103414
C	12.657177463509	24.860037462887	–2.695899272404
C	12.672666485895	26.001604351131	–1.906358302574
C	13.613757636087	27.009716404752	–2.038804629012
C	13.470349486835	28.337916333178	–1.517279609866
H	12.676264582721	28.667070426476	–0.863731707217

C	14.480372509497	29.070921343049	–2.053074552405
H	14.698473410265	30.119036048967	–1.908141730579
C	15.278054498491	28.170606086327	–2.837335071443
C	15.349291973529	30.380711345765	–7.571980397358
C	15.981019555617	33.094067053686	–7.665758989379
H	16.221903382592	34.150888238384	–7.711512738452
C	15.909707879340	32.465839825427	–6.422082969077
C	16.065973370962	33.185155897740	–5.089716372170
C	16.783401108463	32.231529151491	–4.145255808732
C	15.614009980811	31.103043403385	–6.397955632391
C	15.020171164436	28.930752130010	–7.620694381219
C	16.448785517974	30.880396145675	–4.205998103772
C	16.949296962802	29.937555236914	–3.305735421411
C	17.696980644544	32.627831904160	–3.167201958822
H	17.985729123121	33.671462314686	–3.096257739505
O	15.042735748312	28.231635190452	–6.484131028262
H	15.284948056469	28.813621395438	–5.730816768146
N	16.079003057494	23.782834088428	–4.610574944963
O	14.735439642478	28.359582600198	–8.662762016415
C	15.411615191192	31.060369956215	–8.792907147595
H	15.200930200541	30.498245639647	–9.696572853999
C	17.852400175128	30.380811699059	–2.336612001497
H	18.250336691171	29.660214382849	–1.628255405962
C	18.249464139786	31.718365469547	–2.260736710955
C	15.741275484386	32.411140618708	–8.863405694533
C	19.247759713049	32.169066965042	–1.230923766867
H	20.265094156002	31.876760170548	–1.513898266671
H	19.233696508431	33.255933576426	–1.120634007073
H	19.041583634382	31.719644047178	–0.255383475324
C	15.841302858033	33.115542151504	–10.187128072791
H	16.685457706349	32.734645923401	–10.771476099873
H	14.938210787284	32.963964828734	–10.785664675001

H	15.984974107336	34.189499671304	–10.048674498460
C	16.787425291773	34.522088575595	–5.226315504032
H	17.798696227671	34.402566218646	–5.625476399513
H	16.230779972357	35.191556658776	–5.886696564136
H	16.852801000598	35.017023297582	–4.254718435866
C	14.651749345763	33.437162737474	–4.518799566505
H	14.725195850862	33.911216195980	–3.535428176858
H	14.090218128964	34.097423776549	–5.186481961604
H	14.100565647827	32.498936012770	–4.410553298259
Cl	13.198362056630	21.368416925949	–5.967781891360
Cl	11.350960757554	26.250414624993	–0.806013818721
Cl	20.070422882027	23.622956264586	–4.722413498083
Ni	15.403905580916	25.348969878509	–3.721801465203

E = –4803.77362761 Hartrees

[HOOC--NiP]$^{-}$ (*S*=1/2)

N	13.672806196421	24.164857012894	–3.107581255637
N	16.866731513189	26.274595453135	–4.395632504625
N	14.477571528676	26.903898742506	–2.967258425804
O	15.636796093458	30.566459069068	–5.358924884724
C	16.262157989034	28.505803763325	–3.538279277589
C	17.102083012694	27.615521499021	–4.215538180948
C	18.356331793909	27.997969209577	–4.818630960548
H	18.767724106722	28.997460438251	–4.820286749507
C	18.886973441236	26.873719637777	–5.368592622273
H	19.818402658386	26.769692124665	–5.905493961778
C	17.956248782883	25.807830031033	–5.090777912073
C	18.122780990646	24.474776576472	–5.463548901146
C	17.259207909084	23.406821937254	–5.210028459341
C	17.479162695624	22.042567023967	–5.615515995297
H	18.336556441565	21.678851846921	–6.162641445465
C	16.405165116526	21.330774573044	–5.180426683486

H	16.220341177286	20.273460453972	–5.301431502004
C	15.537944386710	22.265936735709	–4.511065301970
C	14.318046349453	21.950416257545	–3.911371997703
C	13.443279972136	22.818167669428	–3.256689916008
C	12.192160014551	22.438497024570	–2.652049921823
H	11.781897167231	21.439690457768	–2.628973877917
C	11.655598479307	23.573290635841	–2.128327911907
H	10.721165616832	23.680948429751	–1.597500366705
C	12.581251821124	24.637464231123	–2.420674828676
C	12.415555276430	25.973824427952	–2.052244186634
C	13.286233474623	27.035823413442	–2.295269057456
C	13.085072906319	28.396575307342	–1.864377993867
H	12.229976220789	28.761591182164	–1.314291597768
C	14.176327115901	29.094340685359	–2.276991201579
H	14.386774412075	30.144892737814	–2.132692295937
C	15.032998152720	28.159248465123	–2.966053517682
C	15.519144841643	30.675833672640	–7.733908618837
C	16.321167948432	33.339578072907	–7.639340034687
H	16.637322200360	34.377146759735	–7.614655529264
C	16.158755969445	32.651102864346	–6.438267616951
C	16.298521658340	33.301410457906	–5.067959295177
C	16.817664305815	32.247419440258	–4.098608749834
C	15.776179750145	31.308895669532	–6.509063612786
C	15.110444624618	29.254475724172	–7.885095945716
C	16.409547419755	30.925187536124	–4.263637417820
C	16.736858778158	29.911423616340	–3.361758942184
C	17.621517322934	32.538029016097	–2.993513199149
H	17.962356510373	33.555403945873	–2.834872129210
O	15.077975787020	28.475897562767	–6.801967561451
H	15.336495002612	28.985020881633	–6.001964668724
N	16.068527556167	23.533289651186	–4.537370583638
O	14.811366574092	28.774009654535	–8.968981472374

C	15.670422316442	31.420394654471	–8.911150106242
H	15.460546011010	30.924722621879	–9.852881922108
C	17.531685120959	30.253075435109	–2.265702319780
H	17.793847705624	29.475228581438	–1.554622520968
C	17.995507685221	31.556646128426	–2.071704982382
C	16.085433927512	32.745766345843	–8.886674516143
C	18.886313378238	31.893950637252	–0.908895778569
H	19.924002315582	31.607661452714	–1.114210374305
H	18.875784120761	32.967610648171	–0.705062892236
H	18.579961355090	31.365898101768	–0.001662883062
C	16.281487140346	33.527481916779	–10.154531014027
H	17.337601915047	33.775829788468	–10.303940211925
H	15.944788343474	32.956208214559	–11.022643561566
H	15.728088218650	34.470912494268	–10.128866878072
C	17.196413259125	34.537664022143	–5.109034751680
H	18.205199389239	34.296609422998	–5.455596619073
H	16.771666660313	35.296349430089	–5.770530318773
H	17.268079033276	34.988496180138	–4.116791624816
C	14.890727954503	33.733167599485	–4.597757301417
H	14.950831808008	34.172401715794	–3.597306584029
H	14.480357568135	34.480256079204	–5.283996869493
H	14.202735061126	32.884245907383	–4.560154744749
Cl	13.828587832061	20.267378919338	–3.981805838195
Cl	10.937688354510	26.361808824862	–1.189024102711
Cl	19.598505822861	24.089035345466	–6.331476912776
Ni	15.270493639435	25.220096952089	–3.754378297223

E = –4803.91679558 Hartrees

[HOOC—NiP]$^{2-}$ (*S*=1)

N	13.611804749882	24.292753009961	–3.560145319148
N	17.178980146834	26.137772091091	–4.046119412400
N	14.553018117611	26.999160563732	–3.273074888491

O	15.763487924015	30.484265822982	–5.256299497198
C	16.543321275472	28.464279461102	–3.514397175520
C	17.453592217645	27.483941655849	–3.887622331033
C	18.853695923852	27.742012507223	–4.165558799977
H	19.327683985319	28.713044110296	–4.125912086190
C	19.428491368980	26.552618254949	–4.469684306325
H	20.460447926035	26.362687745191	–4.728746306785
C	18.381792555212	25.553584363832	–4.401368437188
C	18.545061900878	24.206989112908	–4.663248345762
C	17.560060101822	23.187681173224	–4.658504428792
C	17.767005013309	21.819491237584	–4.981340522484
H	18.706656962053	21.366498273615	–5.264289775667
C	16.538401256769	21.196225122728	–4.852564409246
H	16.309418739138	20.152381556510	–5.014735567367
C	15.616986525293	22.201507915664	–4.454789442903
C	14.237443228519	22.016385924109	–4.191969110201
C	13.314325716498	22.959304740815	–3.780076340671
C	11.916535984703	22.700820399848	–3.506881036233
H	11.425536887325	21.742858486590	–3.600723159974
C	11.367730499541	23.877098354503	–3.114180516422
H	10.342771140113	24.062949313256	–2.826393962858
C	12.421729624631	24.867620584232	–3.151957078024
C	12.273817579131	26.204132180262	–2.831263544394
C	13.253094709145	27.224997396422	–2.874329428487
C	13.053193387643	28.593382709518	–2.543159601557
H	12.127395222653	29.037662668892	–2.206300564952
C	14.264619180400	29.224166028607	–2.752933541592
H	14.495780578723	30.270843909054	–2.605426480973
C	15.174668551140	28.226486920671	–3.204431544125
C	15.030145693037	30.663984421566	–7.494200440844
C	15.775986734873	33.340805045467	–7.531580517389
H	16.054196428857	34.389657132158	–7.552770918366

C	15.986279114190	32.612459399419	–6.360493834243
C	16.501625628003	33.266836216454	–5.083180283332
C	17.042976464461	32.199293135209	–4.138899747188
C	15.607369124950	31.267845372633	–6.364405009514
C	14.601734471003	29.242378703873	–7.566475935841
C	16.626180388043	30.876282455123	–4.249419121801
C	17.032366492261	29.863554525724	–3.369383476793
C	17.910148838528	32.506613150350	–3.083333244288
H	18.246016442311	33.529634849969	–2.949306890204
O	14.753313524412	28.460719090916	–6.496619026801
H	15.168972254299	28.949380622074	–5.749927159466
N	16.241339326832	23.425359972337	–4.338560677151
O	14.105866042182	28.764753993845	–8.578299312885
C	14.836907305758	31.443651920927	–8.640623556780
H	14.390156772273	30.967846583004	–9.506530923571
C	17.899240344638	30.226247726640	–2.337042857428
H	18.219775560483	29.458893292732	–1.638237636890
C	18.351306654683	31.539898082890	–2.178679607424
C	15.204356325733	32.782842327166	–8.682219883102
C	19.293457284471	31.901819424932	–1.064016628419
H	20.315689977017	31.578669856427	–1.291022301784
H	19.317547138312	32.982994567357	–0.905853892091
H	19.007270412718	31.419550081838	–0.124828242859
C	14.976632246323	33.617865778133	–9.911287671818
H	15.890043182470	34.139614097116	–10.212480437975
H	14.640882026365	33.001520062441	–10.748671278202
H	14.213661318670	34.383136385202	–9.733152924138
C	17.574907219570	34.316375512072	–5.399574106424
H	18.436975660070	33.866551668691	–5.899447330773
H	17.170051211039	35.100429166431	–6.043389445079
H	17.914805931698	34.807379064238	–4.485436331476
C	15.306123252065	33.963575877086	–4.397049026050

H	15.630716125962	34.453081936848	–3.473821521844
H	14.882527573152	34.721632534387	–5.063495661679
H	14.521782237414	33.242709231676	–4.149935460155
Cl	13.644381442697	20.369042809328	–4.412684951832
Cl	10.666971411171	26.722308556092	–2.319893468485
Cl	20.176631231728	23.670865226682	–5.069307536255
Ni	15.396058204992	25.215126547330	–3.806569758423

E = –4804.04052026 Hartrees

[OOC--NiP]$^{-}$ (S=0)

N	13.913774699339	24.029386055685	–3.061121993640
N	16.626605524332	26.241965481157	–4.647403995129
N	14.302284204316	26.703327960480	–3.334155776359
O	16.058960446492	30.442559066557	–5.568751098232
C	16.041639631547	28.411101456717	–3.653146844557
C	16.864649362272	27.573325356851	–4.396750081169
C	18.008890682390	28.031212770871	–5.130260075258
H	18.401166290236	29.036816281525	–5.091173865518
C	18.430475697153	26.989839492087	–5.893035936889
H	19.253898479167	26.957167384306	–6.590962119017
C	17.593117638778	25.875911069046	–5.554997977206
C	17.814074370229	24.567525216431	–5.955504955312
C	17.237107758241	23.468130210346	–5.335501737601
C	17.697569097782	22.118338921872	–5.464524424037
H	18.465219000505	21.783059710819	–6.145586703018
C	17.017927607783	21.387369552415	–4.542164072522
H	17.104576437497	20.332187992087	–4.330504998692
C	16.098691655886	22.282857116883	–3.907006454058
C	15.092544369024	21.898856619234	–3.033610265637
C	14.013282291961	22.704407295062	–2.704371890968
C	12.798227114348	22.240206672949	–2.105842912889
H	12.631372223896	21.239849794766	–1.735726049722

C	11.923020962820	23.279249193246	–2.147653898323
H	10.900628597978	23.306687948196	–1.801693775047
C	12.633392914252	24.389188095371	–2.710267922395
C	12.161370377284	25.692985042576	–2.765774022286
C	12.975911171535	26.794485504826	–2.979069384255
C	12.611009376805	28.152048507356	–2.697263384344
H	11.621936603382	28.480464663575	–2.414987103555
C	13.747206372017	28.887056876005	–2.817997750279
H	13.879918225998	29.949285672518	–2.673057664946
C	14.782192176315	27.987831487557	–3.242234167550
C	15.508164573623	30.920150285671	–7.810178543546
C	16.320599274694	33.561770381857	–7.489809421860
H	16.637526987371	34.593442061079	–7.365917149803
C	16.404634636593	32.696578857948	–6.392524054290
C	16.942645660031	33.208864324542	–5.065583941706
C	16.909661382490	32.106198799689	–4.020830532098
C	15.988983590953	31.378263917904	–6.572144326029
C	15.012194435324	29.502593968167	–8.023330124974
C	16.489792216487	30.812571933535	–4.325427858430
C	16.473364468611	29.802043306038	–3.348726372181
C	17.313461237423	32.370344215861	–2.706735717263
H	17.648215621058	33.374104395286	–2.457671206401
O	14.136292903911	29.068009849751	–7.228458608302
N	16.243607216002	23.563376363735	–4.389023130543
O	15.488576475571	28.881301818542	–9.012736691508
C	15.468170359166	31.813929993612	–8.878095857125
H	15.118371243543	31.453255937968	–9.841210881860
C	16.873920929775	30.115439407312	–2.051898959177
H	16.855281413386	29.332638064854	–1.298352210522
C	17.302260268259	31.401113874758	–1.706284061953
C	15.858489403768	33.149562598397	–8.737340895536
C	17.722247187470	31.725451560905	–0.300295946948

H	18.129420929799	32.737532406961	–0.239904584108
H	16.876490448095	31.663658445947	0.392969023083
H	18.484363282580	31.028725685963	0.062421714282
C	15.783030580198	34.111577220648	–9.889847315792
H	16.305877669556	33.724150574843	–10.770008727697
H	14.745967528948	34.298628735202	–10.188246300205
H	16.234823641301	35.071289725983	–9.625402096821
C	18.395191640188	33.686979156176	–5.250715131566
H	19.028087584472	32.873201619566	–5.615899958978
H	18.437398404735	34.508709209379	–5.971934509674
H	18.804445232684	34.043061358124	–4.300976520397
C	16.082685548323	34.394449477489	–4.588776777768
H	16.452141368631	34.777583946892	–3.633539807300
H	16.118413987139	35.209779976258	–5.316799063989
H	15.040042112236	34.092285942304	–4.458540293876
Cl	15.099663115070	20.260611479077	–2.449375678331
Cl	10.489850736511	25.974650430847	–2.377850077301
Cl	19.008823445090	24.275924919080	–7.185911654883
Ni	15.271116897369	25.134439302471	–3.859297446212

E = –4803.34607814 Hartrees

[OOC--NiP]$^{2-}$ (S=1/2)

N	13.636127040145	24.231929704341	–3.591828600532
N	17.198034123707	26.098997395791	–4.029430626743
N	14.542354125986	26.939335602871	–3.416382495599
O	15.875083628980	30.432622901194	–5.399174166244
C	16.507072121475	28.423889119634	–3.578774686487
C	17.451370017709	27.443678210646	–3.906535564415
C	18.847894330662	27.719210112207	–4.144331309047
H	19.302435817290	28.699196685378	–4.117455060705
C	19.448428766220	26.526410177339	–4.396806450174
H	20.489557066115	26.339606441840	–4.616465009171

C	18.411647275009	25.527340372928	–4.327463337771
C	18.592790586586	24.160021589413	–4.534051411800
C	17.620847973971	23.158582545393	–4.500527188397
C	17.854979593710	21.761358967020	–4.760845578564
H	18.805160012088	21.316422891225	–5.017930965284
C	16.656278020128	21.134856107973	–4.621130418704
H	16.441477742469	20.083238050750	–4.742600993142
C	15.699277473278	22.153412929308	–4.274661444630
C	14.341659491951	21.937785979182	–4.038347857318
C	13.372780723195	22.889422382573	–3.718527773297
C	11.977119477298	22.615084435023	–3.496021254664
H	11.513362466415	21.640290160800	–3.534359667529
C	11.383935113029	23.811274157435	–3.237537826330
H	10.341729138165	23.999868517825	–3.024901166108
C	12.423974945549	24.805797437325	–3.294350865893
C	12.249627761718	26.172729227235	–3.072110787534
C	13.224433345851	27.169422478673	–3.102102814079
C	13.001328005020	28.562625249120	–2.805767451229
H	12.056367378638	29.004875278493	–2.525744134146
C	14.202592448427	29.181035353682	–2.949933553331
H	14.429655483302	30.228425187316	–2.807060959023
C	15.151984783359	28.167170903973	–3.339094126804
C	14.979437289037	30.774575247513	–7.548564243907
C	15.604955791413	33.483179678802	–7.428462634913
H	15.846524497229	34.541642607004	–7.384770318536
C	15.930986613858	32.671254196989	–6.337034202762
C	16.611220369933	33.264169038593	–5.110680960738
C	17.054317627201	32.156244739471	–4.165412580618
C	15.594319158252	31.316923459953	–6.411419534975
C	14.592866502627	29.312627829706	–7.658831705469
C	16.636401101374	30.836783630561	–4.335117829406
C	16.986669876941	29.827096420337	–3.420812759181

C	17.851706403893	32.447555500880	–3.051169556033
H	18.182580039534	33.469845767945	–2.891143401549
O	13.865354774961	28.832210020337	–6.749656815131
N	16.298276980980	23.388685916030	–4.209762801949
O	14.999658460202	28.700488122894	–8.684914976200
C	14.703172460630	31.619903966642	–8.622719402228
H	14.241568079331	31.195388181405	–9.509580197797
C	17.790754444284	30.167244688732	–2.335085563881
H	18.062865668519	29.388958279694	–1.627846941084
C	18.238095005796	31.476049059123	–2.130537267647
C	14.995041562867	32.984259905663	–8.580602104881
C	19.101125412525	31.819480462641	–0.948450117833
H	20.053320382167	31.279817855799	–0.978910718252
H	19.319834709669	32.889875602246	–0.922198750010
H	18.611104101476	31.551818371772	–0.006714715960
C	14.674480850305	33.886215202171	–9.740644462493
H	15.559169431315	34.441923666330	–10.067667725655
H	14.302205141941	33.310974599909	–10.592119020630
H	13.910634077937	34.624984780617	–9.475654783671
C	17.820290580332	34.110694939133	–5.545552284353
H	18.534652776076	33.507964041100	–6.112791047167
H	17.496161203216	34.945708389512	–6.171237050523
H	18.334666236092	34.532155296511	–4.678588138510
C	15.610010216119	34.168232768185	–4.364420223437
H	16.089050026974	34.624632227304	–3.492904675544
H	15.254302400048	34.969364118448	–5.019707153512
H	14.745444648381	33.592584096679	–4.021929997990
Cl	13.788325981340	20.274654109560	–4.145051394565
Cl	10.615358989808	26.694071690479	–2.697662864171
Cl	20.231718672899	23.637748202215	–4.889210257586
Ni	15.418296175074	25.166150767206	–3.813708274558

E = –4803.48527041 Hartrees

[OOC--NiP]$^{3-}$ (S=1)

N	13.643630197284	24.188515796701	–3.610093166510
N	17.202456889956	26.059146096745	–4.036239411187
N	14.522116584744	26.927562411966	–3.497297265211
O	15.963230261377	30.439160962403	–5.514728012600
C	16.512669017483	28.402916216839	–3.657258553735
C	17.448813782046	27.420025674667	–3.940345838255
C	18.853764318736	27.686272479825	–4.168710306566
H	19.308206753786	28.667385012587	–4.157145496859
C	19.459712072520	26.493191623839	–4.388749327240
H	20.505359741528	26.306964452797	–4.589360343187
C	18.426954665186	25.480092080724	–4.305902310823
C	18.627835612723	24.119465535182	–4.457293787559
C	17.668611000822	23.078943040375	–4.377571624732
C	17.923211483460	21.688851663727	–4.529311791352
H	18.883090814972	21.235920633756	–4.734652876442
C	16.707635469631	21.047350619757	–4.367406382489
H	16.511210851014	19.985718873755	–4.418918441785
C	15.747253407005	22.062543437997	–4.120771147120
C	14.360008652079	21.872348999620	–3.917907171771
C	13.389953328831	22.829556477836	–3.696182082281
C	11.978960112333	22.566427553571	–3.522730527715
H	11.517208668999	21.589831369003	–3.548914671496
C	11.374805936353	23.765334163304	–3.328434910622
H	10.323360066344	23.955473334622	–3.165410261359
C	12.413550084597	24.772393251229	–3.372634127719
C	12.222647868876	26.130096701459	–3.189573151172
C	13.196454179318	27.157542387746	–3.205360229161
C	12.967452652700	28.534654447464	–2.928982660761
H	12.018432540266	28.981944537715	–2.668299328449
C	14.189519746210	29.164376893023	–3.062054249619

H	14.407231254309	30.216007958163	–2.930629592006
C	15.131914852972	28.162624590844	–3.424481448621
C	14.962710221499	30.869736687060	–7.604256947412
C	15.546464788084	33.578701096830	–7.378755763504
H	15.770848141379	34.637973804965	–7.284845414388
C	15.947480360191	32.718129328629	–6.352168520040
C	16.698201160167	33.270456931468	–5.150876913291
C	17.081974053611	32.145546585642	–4.203295148003
C	15.626994824492	31.364077882630	–6.471401488859
C	14.586662308696	29.409519767886	–7.763781511583
C	16.673795667788	30.827862843106	–4.407532777276
C	16.992953064075	29.804872657983	–3.493728463606
C	17.842602453922	32.426886428955	–3.061290185044
H	18.159067780428	33.450972534966	–2.882548765747
O	13.871947671381	28.895813948372	–6.863102474434
N	16.335946784477	23.311618284186	–4.125219053226
O	14.984088400384	28.834032194424	–8.814670272395
C	14.610235215238	31.763263051439	–8.615060703893
H	14.102880805836	31.378355701322	–9.495355595556
C	17.762408617189	30.139718047126	–2.380113620887
H	18.006014992664	29.354077313057	–1.670353590550
C	18.205928929114	31.445169508102	–2.144064760528
C	14.872240362308	33.131789493499	–8.514583056634
C	19.036175384852	31.774510794451	–0.934621359176
H	19.996939558739	31.249430130457	–0.953111462949
H	19.239313990966	32.847260584151	–0.881311014052
H	18.528653310663	31.481937957161	–0.009633051376
C	14.428481226297	34.094879929784	–9.580940481920
H	15.180922457521	34.868754796615	–9.757398385564
H	14.235945742344	33.579098955353	–10.525560634403
H	13.501957001307	34.605302724439	–9.292957612997
C	17.962592121735	34.008708680781	–5.629392922466

H	18.634875169364	33.327129163240	–6.158038932131
H	17.696555124101	34.825215175954	–6.306152408316
H	18.505068427687	34.437724864193	–4.782411508310
C	15.792910973679	34.264450668863	–4.396771826699
H	16.318319088118	34.664800513059	–3.524634443061
H	15.514590274740	35.099958190467	–5.046248110560
H	14.877624028590	33.771380197794	–4.057579598536
Cl	13.816065851987	20.193248357359	–3.957229731089
Cl	10.568871225713	26.661571918179	–2.869249231351
Cl	20.278135335313	23.594464402325	–4.806189538710
Ni	15.425585234893	25.123007624486	–3.821721223073

E = –4803.60537825 Hartrees

[OOC--Ni^{II}(H)P]$^{2-}$ (*S*=1)

N	13.579279135770	24.206342504748	–3.267618381649
N	16.974967171992	26.181791617212	–4.312871709794
N	14.401447163649	26.966429250718	–3.309988437382
O	15.617633339630	30.615455677493	–5.357066913972
C	16.321399237484	28.471900057201	–3.667095265225
C	17.233249901038	27.513769522101	–4.134069608608
C	18.586872871504	27.818565174062	–4.536120558204
H	19.045397703777	28.795915109198	–4.492594475479
C	19.138698984002	26.655525626031	–4.974726261399
H	20.137080839342	26.494619050369	–5.353767346766
C	18.124337007441	25.642290644760	–4.821946147983
C	18.290561510755	24.282834641511	–5.103272148876
C	17.400634733213	23.239576230800	–4.826947832596
C	17.669554737586	21.836805634840	–5.019026164017
H	18.586019446673	21.417396279510	–5.406873173772
C	16.561521422241	21.169285422749	–4.597658881341
H	16.400293123796	20.101582438828	–4.580523013774
C	15.620050551660	22.170675255322	–4.162759175900

C	14.335167241965	21.918138375039	–3.673375151559
C	13.385856764611	22.851863986744	–3.243597946664
C	12.076441839482	22.535029153669	–2.732599312054
H	11.675157525379	21.541654414890	–2.596740338766
C	11.471239858395	23.721774979900	–2.456515538936
H	10.482751866668	23.882473538000	–2.052420772873
C	12.418677108863	24.753914147554	–2.793787765278
C	12.209640467501	26.128653313553	–2.638506700676
C	13.127952493510	27.161193403910	–2.848669191827
C	12.899391095577	28.556357191868	–2.561083435428
H	11.977654301541	28.980952347784	–2.191648470858
C	14.067149187322	29.198934714499	–2.830570494607
H	14.284542730647	30.252178732889	–2.721186152469
C	14.995683548544	28.198542302073	–3.300729496796
C	15.192015577415	30.881154654430	–7.675869028132
C	16.138888307070	33.501456648928	–7.560029126573
H	16.495694193854	34.525743651375	–7.525309101953
C	16.089562914980	32.751337751507	–6.380372430120
C	16.432594871917	33.340022142100	–5.017856882417
C	16.942619138029	32.217248292293	–4.124172061542
C	15.631662786741	31.434003043007	–6.464307432243
C	14.625788892746	29.478621592834	–7.795806809618
C	16.468172303480	30.918079810626	–4.322512235596
C	16.828340701720	29.861616158322	–3.473754425058
C	17.811133603619	32.437573675065	–3.051040722437
H	18.192055559012	33.436693002235	–2.869058948263
O	13.730943992417	29.138744555697	–6.975960924193
H	14.621755784953	25.363544535796	–5.591115278064
N	16.150339972141	23.424128201630	–4.304716968259
O	15.067801818164	28.774881224486	–8.745788194148
C	15.269412249434	31.667116893607	–8.825582119394
H	14.961748599970	31.224084782925	–9.768423050508

C	17.695116845058	30.132610069554	–2.412777020545
H	17.976951968377	29.317182491240	–1.752600166872
C	18.202035477206	31.413907667972	–2.186247209866
C	15.736976142588	32.982635602103	–8.791723678782
C	19.147950392585	31.683441451223	–1.048971715797
H	20.148487884420	31.293475061314	–1.267998456084
H	19.245573249367	32.756505242606	–0.865132452986
H	18.815033563688	31.201565985755	–0.125010651081
C	15.820433127425	33.809411175766	–10.044797386367
H	16.409853438555	33.304359522016	–10.816668461017
H	14.828695771269	33.997312733309	–10.470340373519
H	16.287412497315	34.777204870750	–9.843133386418
C	17.442662684768	34.484029665012	–5.131458049573
H	18.380642326703	34.156521346758	–5.589013597341
H	17.031526893000	35.296870246000	–5.734667251370
H	17.663242158739	34.906859779083	–4.148723187469
C	15.135740253517	33.904600239956	–4.394733741762
H	15.349687829414	34.331260092310	–3.409477319484
H	14.726510717937	34.692478642428	–5.034901667122
H	14.376540427276	33.125929716536	–4.277774984995
Cl	13.854702298224	20.235051708545	–3.597124125569
Cl	10.626527194750	26.606400498731	–2.058130269348
Cl	19.819634737716	23.822990631495	–5.825268939408
Ni	15.174209190878	25.223849322841	–4.078789033179

E = –4804.02591363 Hartrees

[OOC--Ni^{II}(H)P]$^{3-}$ (*S*=3/2)

N	13.659732456579	24.113998794731	–3.121892675475
N	16.928468266144	26.249309004428	–4.409707045130
N	14.470722970605	26.892910412544	–3.036523285862
O	15.652154242603	30.575190430381	–5.419188815907
C	16.266402830799	28.496646058355	–3.595253537172

C	17.151754760867	27.597249634159	–4.244769780156
C	18.408942138595	27.962594442416	–4.805947968164
H	18.829713135678	28.958705061395	–4.809927958003
C	18.962194071473	26.810514351682	–5.329133612068
H	19.914270426552	26.698146882529	–5.827908633369
C	18.032488980160	25.764545746583	–5.062462811050
C	18.198324991838	24.396311582286	–5.394444008189
C	17.351356034337	23.336173622746	–5.105536163284
C	17.600170692473	21.948583073442	–5.436626319786
H	18.481643039082	21.572774244634	–5.935872556128
C	16.524591083781	21.242040694494	–5.004994502134
H	16.361519485729	20.176577161227	–5.081396360308
C	15.611667070029	22.190759938051	–4.406927670332
C	14.380336696989	21.883895274057	–3.854051062613
C	13.456380159822	22.756379182160	–3.228931656755
C	12.228467654511	22.382866698441	–2.619344947681
H	11.830920263513	21.380048847915	–2.556205326745
C	11.670318724824	23.544780446517	–2.118221840188
H	10.738324225059	23.651577442900	–1.581855334696
C	12.569876708318	24.598200550452	–2.445036976580
C	12.405649645549	25.969251709375	–2.118738200015
C	13.276764131833	27.020364832449	–2.369838528322
C	13.081994340429	28.391601554764	–1.944952281513
H	12.228578973808	28.760881948942	–1.394259632218
C	14.174671564833	29.084757641455	–2.355285677468
H	14.386242948453	30.135027719534	–2.206975123116
C	15.041059593848	28.150686043669	–3.041871464291
C	15.557094945128	30.735886583336	–7.784757387731
C	16.341523436552	33.410966703627	–7.641947771826
H	16.643300710814	34.452287502162	–7.597984074689
C	16.164708103006	32.695142740137	–6.453177830690
C	16.286030780205	33.319940242978	–5.070347770586

C	16.814827963022	32.249631776299	–4.124606389594
C	15.784298164521	31.354147927396	–6.548471367039
C	15.095596454200	29.297530314464	–7.908217088440
C	16.406572339012	30.925240289664	–4.322334327586
C	16.734542512960	29.905298097548	–3.422901040642
C	17.617217183060	32.529295559530	–3.017111315253
H	17.950614555915	33.547541413357	–2.844755467989
O	14.049139923265	28.970471658099	–7.286575192697
N	16.138570970612	23.464306851498	–4.471519271356
O	15.776970652867	28.548977252421	–8.661804698086
C	15.749912143025	31.488601485509	–8.943865103702
H	15.585328179682	31.008847446415	–9.904990733374
C	17.532206428896	30.237771905727	–2.323418216946
H	17.796405692696	29.450708259877	–1.622582063798
C	17.996299178546	31.536057556420	–2.108488549744
C	16.142762341218	32.828707157865	–8.895405083697
C	18.885575562864	31.857514500554	–0.939181108661
H	19.931798263139	31.949032325563	–1.252317746539
H	18.606792643876	32.805793089282	–0.470153430725
H	18.837679004814	31.072237726621	–0.179987030335
C	16.349346473976	33.618650924007	–10.158200363367
H	17.170290494928	33.206734564699	–10.755042939757
H	15.455948368392	33.603753964275	–10.790748004098
H	16.588503050264	34.661718788544	–9.934705663235
C	17.163349592665	34.571674120679	–5.074488590740
H	18.179854705842	34.354576079080	–5.415496051381
H	16.734879858891	35.337926243733	–5.725210270667
H	17.218710047366	35.002908922707	–4.072127976732
C	14.869039961511	33.718445374619	–4.598438626728
H	14.913000367957	34.139787061286	–3.589026796341
H	14.446539934413	34.469749460556	–5.273147502952
H	14.198584628505	32.854837973264	–4.581319150742

Cl	13.899488181188	20.190011393892	–3.892593144334
Cl	10.914802963338	26.364704991696	–1.264919961782
Cl	19.695762525622	24.002084286716	–6.236166218568
Ni	15.160070050502	25.228763940153	–4.036212074779
H	14.458742121630	25.468066325027	–5.483882927354

E = –4804.15274614 Hartrees

2–Ni (*S*=0)

N	13.771423076963	24.434297056662	–3.366151711734
N	16.944961982709	26.466635886050	–4.075894850986
N	14.801643965591	26.779678855423	–2.452449718181
O	16.007245514286	30.174516568078	–5.170628948494
C	16.334668131689	28.606010110166	–3.026680724232
C	17.186685969960	27.777640884684	–3.753448835477
C	18.518823625421	28.155205379954	–4.128559865535
H	18.947448715655	29.133634223176	–3.965852017483
C	19.110131572448	27.049845724084	–4.652785876685
H	20.115132617323	26.941357998338	–5.031822274254
C	18.111098866055	26.022575389092	–4.658162110639
C	18.223705014549	24.805291853222	–5.311785366678
C	17.140920124786	23.981545129260	–5.587485598137
C	17.137641820099	22.921629451224	–6.550025298561
H	18.000649424495	22.583741061821	–7.103920869536
C	15.855308613805	22.479153450209	–6.636515880794
H	15.460210755580	21.691728253674	–7.260814003437
C	15.100468099887	23.225046865900	–5.674425510427
C	13.801264479013	22.934123573660	–5.283908073076
C	13.219965668845	23.429299853172	–4.126365980373
C	12.058256509365	22.881887448941	–3.490580442904
H	11.448421164141	22.086576707364	–3.892778976647
C	11.926679248898	23.526699055752	–2.301512223429
H	11.174529750977	23.383444776579	–1.540401882944

C	12.966275326447	24.511564965748	–2.254270794135
C	13.057982209917	25.523240133113	–1.309228629837
C	13.845248380284	26.652975005464	–1.474256988460
C	13.680961960545	27.880593367594	–0.751793956511
H	12.987216223035	28.029855450906	0.061984088697
C	14.510948703683	28.783524739059	–1.335761065314
H	14.656544341437	29.823534606220	–1.083147107491
C	15.240229627215	28.080318237017	–2.352927797464
C	15.612320869967	30.010904538658	–7.468664297529
C	16.175287774941	32.674692969148	–7.843409583646
H	16.384838508334	33.728458029885	–8.001679181236
C	16.266193644231	32.153919682981	–6.546962091626
C	16.630436378720	33.040299092614	–5.361905492823
C	16.816994835551	32.195715723629	–4.107822566427
C	15.971437368905	30.803107296626	–6.375703623317
C	16.499996789003	30.842284295726	–4.082160792191
C	16.658391791649	30.052678922722	–2.932720173212
C	17.299221171902	32.757196314225	–2.918833169867
H	17.559070560434	33.811996861937	–2.904022285664
N	15.888568081880	24.164367940561	–5.049869980508
C	15.525018649670	30.544468775551	–8.742263535744
H	15.232185373154	29.914635630507	–9.575300277028
C	17.136054903094	30.655312871649	–1.773596510924
H	17.274137145865	30.049977685515	–0.882803840110
C	17.466589169278	32.016123286468	–1.749538762246
C	15.817120547930	31.898733887969	–8.945693464837
C	17.995485611475	32.651315777010	–0.494224546789
H	18.846039181433	32.089672854223	–0.095771429022
H	18.320440016037	33.677354627252	–0.682062769784
H	17.231201550271	32.678108599446	0.290017855979
C	15.735280330356	32.495194554347	–10.322919746479
H	16.519813270521	32.093793880718	–10.973095907510

H	14.776601501892	32.267340164046	–10.798301778651
H	15.852300597738	33.580650774632	–10.285456700884
C	17.931121456687	33.804433986788	–5.663236532949
H	18.758618904234	33.110162316523	–5.831562714183
H	17.816861979230	34.429443729661	–6.551998857490
H	18.193746795684	34.456900668050	–4.826613000249
C	15.493919532376	34.053242500327	–5.122634222102
H	15.744567857428	34.704534129495	–4.280130874737
H	15.348152974741	34.676004058632	–6.010150114409
H	14.554134331822	33.541454644022	–4.897726755173
Cl	12.916798945256	21.749892670681	–6.199037451520
Cl	12.000613189235	25.456231919810	0.069946240697
Cl	19.771474111964	24.370822541947	–5.975231102071
Ni	15.348862563018	25.464045909272	–3.741462957320
Br	15.216875198984	28.184959495133	–7.158130075259

E = –7186.75490703 Hartrees

[2-Ni]$^{-}$ (S=1/2)

N	13.604575343685	24.322999065698	–3.520659115354
N	17.143546847299	26.203662867003	–4.055846599628
N	14.559851857015	26.990485773405	–3.140903788825
O	15.759078114752	30.418516501431	–5.157706350381
C	16.507430178089	28.485591010731	–3.376913047853
C	17.424382290246	27.528438134583	–3.824807954746
C	18.807138998937	27.813369666929	–4.124918616036
H	19.279708454109	28.780573918648	–4.029825667172
C	19.369473913441	26.645697964038	–4.534271666834
H	20.389852729247	26.471186396320	–4.842737535059
C	18.324717742776	25.653692565193	–4.490736675289
C	18.467719234270	24.315519755829	–4.856456056703
C	17.483138203819	23.325859278673	–4.862513506045
C	17.680047189984	21.958059744704	–5.268100798624

H	18.610620085371	21.529052829263	–5.609633949037
C	16.480520255416	21.334407922951	–5.123156816153
H	16.243372659402	20.300592129505	–5.327871368266
C	15.560234876500	22.325065909178	–4.627114710145
C	14.220291351578	22.096978271911	–4.312410859534
C	13.304250951723	23.008593736417	–3.786095140278
C	11.942083261115	22.709045610155	–3.426360742236
H	11.458915252765	21.748610915461	–3.530678668710
C	11.411915170444	23.858148880459	–2.928287178441
H	10.412486252488	24.016229370616	–2.550519322666
C	12.451263560974	24.852510256533	–2.994790880523
C	12.322288695417	26.183398145322	–2.593584983492
C	13.289128433351	27.186417566705	–2.655096845924
C	13.099511629003	28.555651593802	–2.247110681409
H	12.195473312838	28.966479835967	–1.822239467654
C	14.272949188247	29.194608690976	–2.496144512332
H	14.514439911034	30.233357948471	–2.317046067638
C	15.173573710806	28.214615599614	–3.051755996121
C	15.123783252095	30.529663447740	–7.412583666212
C	15.852548130872	33.175778483234	–7.564254013966
H	16.132970225302	34.221633989273	–7.634584221222
C	16.013161189119	32.513259183013	–6.345730155980
C	16.485794141425	33.221860385932	–5.080139928429
C	17.009604158985	32.190833885104	–4.085202729446
C	15.640055062089	31.168021834469	–6.287011422272
C	16.589743391980	30.864314285763	–4.159440202975
C	16.983428679411	29.891443158957	–3.231722811760
C	17.852744591449	32.532934014186	–3.021629354518
H	18.189611669057	33.559803881812	–2.919824394552
N	16.183108540145	23.540430399856	–4.473981566526
C	14.954463439140	31.210155840826	–8.609826937357
H	14.550513853350	30.689914601405	–9.471471772958

C	17.826521486612	30.280802320301	–2.193374723558
H	18.136841931071	29.537061866962	–1.465047488637
C	18.272158532935	31.600818062642	–2.070723871304
C	15.323176171984	32.553969776893	–8.699605845198
C	19.193379265722	31.999917999870	–0.951451016420
H	20.229083263282	31.717492699771	–1.171481058112
H	19.174047646277	33.081190308262	–0.794167056744
H	18.918447944012	31.508889054047	–0.013725342017
C	15.139073521317	33.317322960584	–9.981223116732
H	16.063004900516	33.822983482396	–10.277607538817
H	14.834059843250	32.655015495352	–10.794582605861
H	14.369960610081	34.089608264598	–9.873862225385
C	17.554451831392	34.272727614820	–5.404881165698
H	18.434407913225	33.816096942843	–5.865807224895
H	17.157046131092	35.027937968062	–6.086758647784
H	17.866392339314	34.797401532630	–4.499244848209
C	15.266951687224	33.927895227715	–4.446575318344
H	15.565547873702	34.440963510953	–3.527174325705
H	14.856348690331	34.666498833878	–5.142108356953
H	14.480606240721	33.208440192827	–4.202073567760
Cl	13.620218160987	20.472813573942	–4.601860263270
Cl	10.761944504865	26.646412832817	–1.934968291667
Cl	20.071279978224	23.817088490639	–5.367590717775
Ni	15.369822257823	25.268974019650	–3.810739639276
Br	14.652481293476	28.705228719486	–7.277354996599

E = –7186.89491146 Hartrees

[2-Ni]$^{2-}$ (*S*=1)

N	13.601229669786	24.310051002634	–3.503965713317
N	17.127984693635	26.207686101495	–4.060751571285
N	14.542207297282	26.999447321193	–3.102716540113
O	15.766985858699	30.425173877527	–5.160719413543

C	16.505760225837	28.493196378531	–3.363662010616
C	17.406262505051	27.544366744266	–3.821229984371
C	18.789409663415	27.828977231752	–4.142585166274
H	19.262573144522	28.796588650575	–4.046565116069
C	19.349553987442	26.668998875036	–4.566960349930
H	20.367467972282	26.502192816248	–4.889475472744
C	18.309618066381	25.661473645910	–4.519867924929
C	18.461363213014	24.338624201333	–4.895798686182
C	17.481119522078	23.314822357089	–4.904810652078
C	17.678654194124	21.968368577559	–5.315663962954
H	18.605454766456	21.541955801044	–5.672417507637
C	16.463296665673	21.327116959598	–5.156285587675
H	16.233264344108	20.291576483237	–5.363854798859
C	15.558909694725	22.298136797024	–4.652199845104
C	14.202626990571	22.082859852260	–4.311201635431
C	13.303056633607	22.984656231169	–3.777229924002
C	11.937594667687	22.686739871218	–3.405216287331
H	11.453675428327	21.726262602096	–3.511831711162
C	11.409209122988	23.828298411748	–2.897418408472
H	10.410915110183	23.979261985392	–2.512117536642
C	12.445007645027	24.836993339552	–2.961178292265
C	12.308708037593	26.151031514179	–2.549597042152
C	13.272848995169	27.186457345406	–2.603061957760
C	13.083217287296	28.533589229585	–2.186597138516
H	12.182354517590	28.941860397001	–1.750792750370
C	14.272639305270	29.188832992351	–2.441699514492
H	14.508287179890	30.228279172702	–2.254365540105
C	15.156726550057	28.230012195167	–3.008795886159
C	15.151292009609	30.526894490016	–7.420749543446
C	15.878487475801	33.172900251526	–7.576488368019
H	16.157796863776	34.218954545795	–7.648583549048
C	16.028888036707	32.515506757240	–6.353865276563

C	16.489539476130	33.228411267022	–5.086322322667
C	17.007860681759	32.200771208362	–4.084572763109
C	15.657422027285	31.169586704197	–6.292594905942
C	16.589604793622	30.873584118503	–4.155016422830
C	16.978568280724	29.900054794344	–3.224096843411
C	17.846078307281	32.549053694925	–3.018153247178
H	18.181735847578	33.576683518879	–2.919101523731
N	16.182265294368	23.520733661170	–4.498445110489
C	14.992399304401	31.202201342774	–8.622332556547
H	14.596948159382	30.678079603039	–9.485636564520
C	17.814116905207	30.299657745922	–2.182789317337
H	18.120708311295	29.559541291851	–1.448818810313
C	18.260738837403	31.620284496356	–2.062722527788
C	15.360753967230	32.545957746107	–8.714353887220
C	19.178007784238	32.021993170612	–0.940835077632
H	20.214706541351	31.738792462988	–1.155658266030
H	19.158728166890	33.103703371028	–0.785601223822
H	18.899614415942	31.533160141225	–0.002822543107
C	15.188383349857	33.303622656336	–10.000992683717
H	16.116368122142	33.804275689002	–10.293635453735
H	14.887129027471	32.637980813535	–10.813070838100
H	14.421367395600	34.079278954245	–9.903435425204
C	17.558003848028	34.281130354151	–5.406254052278
H	18.441892464494	33.825192657201	–5.860370564592
H	17.163810481505	35.034404054744	–6.092235558613
H	17.863650646259	34.807814126104	–4.499646489372
C	15.264934478736	33.933848260830	–4.463118280611
H	15.556569755364	34.447983558318	–3.541982923524
H	14.857799506335	34.671434688864	–5.161877293033
H	14.477955872609	33.213531372760	–4.223060529379
Cl	13.606244944457	20.447171734753	–4.601045297108
Cl	10.745673618698	26.609132888492	–1.867010022952

Cl	20.069618187095	23.846330827969	–5.432717444240
Ni	15.360362241069	25.264630299251	–3.805155078156
Br	14.678755616535	28.702858717685	–7.281885486093

E = –7187.01736302 Hartrees

3-Ni (*S*=0)

N	13.623488599666	24.287799479633	–3.482462404529
N	16.894209871406	26.195183106652	–4.142526891200
N	14.408035294382	26.880965262513	–3.283988964954
C	16.040583328164	28.475793761568	–4.130152540241
C	17.055721615438	27.549884428210	–4.317484278441
C	18.427258860955	27.875787557575	–4.572458713773
H	18.806346639557	28.870168684093	–4.753632580467
C	19.122996076607	26.711748962579	–4.495834593155
H	20.184449965207	26.557793491506	–4.619633237572
C	18.161450464526	25.675522842123	–4.264875309620
C	18.432883073496	24.316730738694	–4.317718698681
C	17.452988974171	23.344939118449	–4.453285378828
C	17.690669330708	21.997530906073	–4.878003572294
H	18.664289887068	21.557685029030	–5.034571381815
C	16.470992286877	21.437070702930	–5.087647642369
H	16.244221036045	20.438498341501	–5.429869792567
C	15.499007487973	22.424157565857	–4.722393397210
C	14.134981642427	22.196052672145	–4.618603958245
C	13.266638049457	23.043725684345	–3.947582709832
C	11.950103296216	22.688213024287	–3.508383795495
H	11.441573578156	21.768272147665	–3.755047384499
C	11.521135146601	23.701200065472	–2.711442254720
H	10.580648018799	23.787640672484	–2.188525427628
C	12.547561899545	24.700500611682	–2.732330745323
C	12.420289824503	25.977678437659	–2.207193033514
C	13.250732020481	27.032138397182	–2.557056814472

C	12.941679445872	28.417521855660	–2.361859863736
H	12.087033322495	28.791062171699	–1.817949630313
C	13.894792831823	29.123972712683	–3.024110798063
H	13.990276489760	30.195263456181	–3.117991127994
C	14.817232886867	28.165540541773	–3.556113644493
N	16.105898423609	23.600745352295	–4.348366037982
Cl	16.382325832076	30.143224996246	–4.479591602585
Cl	11.052935759429	26.312894139125	–1.190406996720
Cl	20.095012147025	23.815624103083	–4.370798470465
Cl	13.509543210578	20.688263174080	–5.213256807876
Ni	15.259196382036	25.240979805268	–3.811553518327

E = –4339.75197267 Hartrees

[3-Ni]$^{-}$ (*S*=1/2)

N	13.540760798154	24.233667552157	–3.457969347142
N	16.974440141053	26.245532495160	–4.168787000820
N	14.367831002769	26.965333012258	–3.246222001872
C	16.251414554448	28.490971896323	–3.536881375371
C	17.216388281892	27.584264285814	–3.976979382445
C	18.577820129734	27.914840770483	–4.313963979755
H	19.022277365435	28.896858480132	–4.246820825420
C	19.165275615734	26.761223479962	–4.727075081449
H	20.181224547486	26.618589932317	–5.064179418219
C	18.160510622292	25.733578944217	–4.634839032018
C	18.349724446355	24.391505189144	–4.964816467027
C	17.427102039923	23.351015262653	–4.854588246852
C	17.690758732057	21.968918749677	–5.163575989414
H	18.624985039342	21.574196398316	–5.534913600361
C	16.549856237137	21.284996191069	–4.883558090041
H	16.371719449936	20.224937735152	–4.989143527251
C	15.594894051729	22.256507877858	–4.414108622267
C	14.284092293710	21.977677134516	–4.026491265034

C	13.315429777360	22.885864176205	–3.597557996807
C	11.955956773382	22.552984606493	–3.255893472180
H	11.524855630294	21.563165588453	–3.283113794923
C	11.346645027787	23.717943455381	–2.912387522635
H	10.323614305774	23.863474677683	–2.598714098855
C	12.341523907022	24.752307946995	–3.034825698352
C	12.133762556183	26.104919034762	–2.764458505273
C	13.063318793650	27.141323393937	–2.853506961702
C	12.795144690805	28.526144634716	–2.560727117906
H	11.845916768277	28.931298339688	–2.241887863845
C	13.956621061848	29.198995793684	–2.775603033589
H	14.138968057099	30.257086813957	–2.658631669262
C	14.924460658365	28.220475361668	–3.201260655227
N	16.142049222730	23.516421188489	–4.398292080779
Cl	13.795159765882	20.294098695441	–4.096299276196
Cl	10.519736778963	26.552677915611	–2.244323041840
Cl	16.759297001753	30.165702545868	–3.406368674837
Cl	19.933758831293	23.963614971543	–5.586504488943
Ni	15.256828042350	25.240034472218	–3.816484794093

E = –4339.89694312 Hartrees

[3-Ni]$^{2-}$ (*S*=1)

N	13.539704993398	24.235943636836	–3.465825435221
N	16.973846841111	26.245502799571	–4.166813442379
N	14.355915728355	26.989951501926	–3.238681500675
C	16.262804149523	28.501021276408	–3.548203390164
C	17.212361926869	27.596111293336	–3.982574576421
C	18.580548929078	27.919891931669	–4.328148349842
H	19.025448858466	28.902808959585	–4.268712806813
C	19.168718499612	26.767996853306	–4.732638981301
H	20.185506711362	26.627727704756	–5.069958740020
C	18.168019672863	25.727261816568	–4.635106043520

C	18.366575667727	24.398722918229	–4.956520491947
C	17.446829353624	23.327092925607	–4.853707524113
C	17.710321704040	21.963947074586	–5.154233125816
H	18.647111550404	21.562437832638	–5.513722150539
C	16.545788273401	21.270016882010	–4.880827260306
H	16.370732598763	20.209149513122	–4.990633938616
C	15.603010859067	22.230723831834	–4.425502797769
C	14.265626984972	21.972911497008	–4.038319692587
C	13.312934197165	22.878941484406	–3.613299910601
C	11.945590803193	22.554016093378	–3.266049902374
H	11.510141740392	21.565550972966	–3.296792624981
C	11.341334625588	23.714498057509	–2.913390973822
H	10.318910311017	23.857322890856	–2.594515491478
C	12.335414592814	24.759583860176	–3.030956776399
C	12.124104719043	26.095384338351	–2.750210289729
C	13.049468472556	27.163785497335	–2.836020140104
C	12.783239886459	28.528652346821	–2.545298871907
H	11.836361080522	28.937078210217	–2.221459988225
C	13.961997584321	29.214901117993	–2.773645006995
H	14.139416275090	30.274599170072	–2.657156422848
C	14.913961821207	28.249214733744	–3.197847748313
N	16.154286193806	23.493430326347	–4.405614109463
Cl	13.772228340968	20.280735550824	–4.120426753127
Cl	10.506708505190	26.544285549888	–2.207658334316
Cl	16.770241226305	30.186680648979	–3.421957942642
Cl	19.962625739857	23.964144429715	–5.571011369449
Ni	15.256287581871	25.241123471428	–3.818310095176

E = –4340.02204598 Hartrees