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Elucidating electron-transfer events in polypyridine nickel complexes for reductive coupling reactions

In the format provided by the authors and unedited

Contents

Supplementary Methods

General Considerations

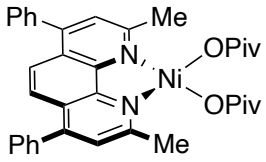
Solvents. Reactions were carried out under N_2 in a glovebox or on a Schlenk line, in solvents (THF, Et_2O, toluene) that had been dried and degassed using an Innovative Technologies solvent purification system, then stored under N_2 over 4 Å molecular sieves for at least 16 h prior to use. Pentane was degassed by bubbling with N_2 and stored under N_2 over 4 Å molecular sieves for at least 16 h prior to use. C_6D_6, C_7D_8, THF-d_8, (Eurisotop) were freeze/pump/thaw degassed (4x) and likewise stored under N_2 over 4 Å molecular sieves for at least 16 h prior to use.

Reagents. Neocuproine and bathocuproine were purchased from Fluorochem. Zinc dichloride ($ZnCl_2$), and sodium phenoxide, lithium tert-butoxide, and manganese dichloride were purchased from Sigma-Aldrich. Potassium benzoate was purchased from Thermo Fisher. $ZnBr_2$ and potassium pivalate (KOPiv) were purchased from Alfa Aesar. [$Ni(COD)_2$] was purchased from Strem Chemicals. Trimethoxylbenzene (TMB) was purchased from TCI Chemicals. Salts $ZnBr_2$, $ZnCl_2$, and KOPiv were dried at 150 °C under high vacuum overnight. Complexes (bipy)$NiCl_2$,[1] (bipy)$NiBr_2$,[1] (phen)$NiCl_2$,[1] (neocuproine)$NiCl_2$,[2] (bathocuproine)$NiCl_2$,[2] (neocuprooine)$_2$Ni,[2] (bathocuproine)$_2$Ni,[2] and (bipy)Ni(OPiv)$_2$[3] were synthesized according to literature procedures.

Analytical methods. Flash chromatography was performed with Sigma Aldrich technical grade silica gel 60 (230-400 mesh). Thin layer chromatography was carried out using Merck TLC Silica gel 60 F254. NMR spectra were recorded on Bruker Avance Ultrashield 300, 400, or 500 MHz spectrometers, with chemical shifts reported in parts per million (ppm) and coupling constants, *J*, reported in hertz. Quantitative NMR experiments were performed with d1 set to 10s (^{1}H). Gas chromatographic analyses were performed on an Agilent 6890N gas chromatograph with an FID detector. Continuous wave (CW) X-band EPR spectra were obtained using a Bruker EMX Micro X-band spectrometer using a Bruker ER 1164 HS resonator. Spectra were simulated using SpinFit within Xenon. The samples were cooled to 77 K in a Suprasil finger dewar (Wilmad-LabGlass) filled with liquid nitrogen. The spectral data were collected with the following spectrometer settings: microwave power = 0.56mW; centre field = 3250 G, sweep width = 2500 G, sweep time = 35.07 s, modulation frequency = 100 KHz, modulation amplitude = 10 G, power attenuation= 25 dB, time constant = 20.48 ms. Simulations, g values, and frequencies are provided alongside the characterization data of the complexes. IR spectra were obtained with a Bruker FT-IR Alpha spectrometer. MALDI-TOF mass spectra were collected on a Bruker Autoflex MALDI-TOF mass spectrometer. Samples were prepared by the dried-droplet protocol, from solutions containing the charge-transfer matrix pyrene or DCTB in THF.

Synthesis and Characterization of Complexes

Synthesis of (L4)Ni(OPiv)$_2$



In the glovebox, (**L4**)NiCl$_2$ (224 mg, 0.46 mmol) was added to a 12 mL vial with potassium pivalate (206 mg, 1.66 mmol). A stir bar was added, and the vial was charged with 6 mL of toluene turning the pink powder to a pink suspension and let stir overnight. After 16 hours the green solution was filtered through a celite plug with salt being filtered off and a green solution collected. The solvent was then removed to afford a green solid and washed with pentane (1 mL x 3) to give (**L4**)Ni(OPiv)$_2$ (199 mg, 70 % yield) as a green powder.

Stability: Stable in air

^{1}H NMR (^{1}H NMR (400 MHz, C_6D_6) δ 49.57, 20.78, -9.05. **^{13}C NMR**, no signals are observed due to paramagnetism of (L4)Ni(OPiv)$_2$. [spectrum]

X-Band EPR = EPR Silent

UV-VIS (nm) = 685 nm [spectrum]

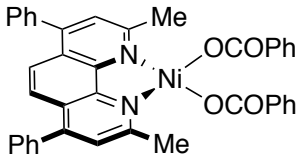
Key IR Stretches = 1619 cm^{-1} (weak), 1527 cm^{-1} (strong) [spectrum]

EA Calcd. C, 69.58; H, 6.16; N, 4.51; Found: C, 69.34; H, 6.14; N, 4.38

Cyclic Voltammetry = $E_{p/2}$ values for (L4)Ni(OPiv)$_2$ are Ni(II)/Ni(0) = -1.43 V. The reduction appears chemically reversible (E_p oxidation = -1.27 V vs SCE) and electrochemically irreversible. [spectrum]

Single Crystal XRD [structure]

Synthesis of (L4)Ni(OCOPh)$_2$



In the glovebox, (**L4**)NiCl$_2$ (122 mg, 0.25 mmol) and potassium benzoate (83 mg, 0.52 mmol, 2.08 equiv.) were added to a 10 mL vial. A stirbar was added and charged with 3 mL of THF and left to stir overnight in which a colour change from pink to orange to green is observed. The solvent was then removed and the solid was dissolved in DCM and filtered through a celite plug where a white solid was filtered off. The green filtrate was concentrated to dryness and filtered. The solid was washed with pentane (3 mL x 3) to afford (**L4**)Ni(OCOPh)$_2$ as a green powder (128 mg, 78 % yield).

Stability: Stable in air

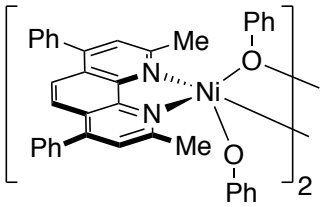
^{1}H NMR (500 MHz, THF-d_8) δ 52.21, 21.77, -9.11. **^{13}C NMR**, no signals are observed due to paramagnetism of (L4)Ni(OCOPh)$_2$. [spectrum]

X-Band EPR = EPR Silent

UV-VIS (nm) = 700 nm [spectrum]

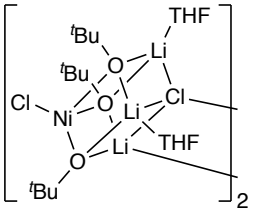
Key IR Stretches = 1593 cm^{-1} (weak), 1528 cm^{-1} (strong) [spectrum]
Single crystal XRD [structure]

Synthesis of [(L4)Ni(OPh)$_2$]$_2$



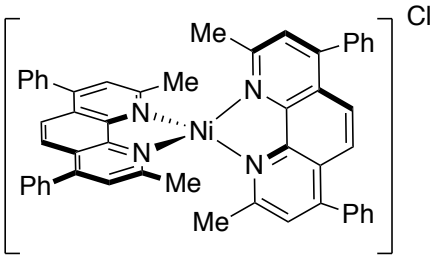
In the glovebox, (**L4**)$NiCl_2$ (158 mg, 0.32 mmol) and sodium phenoxide (116 mg, 1.00 mmol, 3.1 equiv.) were added to a 10 mL vial. A stirbar was added and charged with 5 mL of toluene and left to stir overnight. The solvent was then removed and redissolved in DCM (sparingly soluble) and filtered through a celite plug. The solvent was removed, filtered and washed with pentane (3 mL x 3) to afford (**L4**)$Ni(OPh)_2$ as a brown powder (88 mg, 45 % yield).
^{1}H NMR (400 MHz, CD_2Cl_2) δ 54.35, 49.37, 19.92, 18.28, 0.30, 0.09. **^{13}C NMR**, no signals are observed due to paramagnetism of [(L4)Ni(OPh)$_2$]$_2$. [spectrum]
X-Band EPR = EPR Silent
Key IR Stretches = 1256 cm^{-1} (strong) [spectrum]
Single crystal XRD [structure]

Synthesis of NiLi$_3$Cl$_2$(O^{t}Bu)$_3$•2THF



In the glovebox, (**L4**)$NiCl_2$ (113 mg, 0.23 mmol) and lithium tert-butoxide (41 mg, 0.51 mmol) were added to a 10 mL vial. A stirbar was added and charged with 3 mL of THF and left to stir overnight. The solvent was then removed and dissolved in minimal THF, and then filtered through a celite plug. The solvent was removed, filtered and washed with pentane (3 mL x 3) to afford NiLi$_3$Cl$_2$(O^{t}Bu)$_3$•2THF as a blue powder (88 mg, quantitative).
Stability: Unstable in air
^{1}H NMR (400 MHz, THF-d_8) δ 33.31, 32.48, 13.01. **^{13}C NMR**, no signals are observed due to paramagnetism of NiLi$_3$Cl$_2$(O^{t}Bu)$_3$•2THF. [spectrum]
X-Band EPR = EPR Silent
Single crystal XRD [structure]

Synthesis of [(L4)$_2$Ni]Cl



Following a modification of literature procedures,[4] in the glovebox, (**L4**)$NiCl_2$ (44 mg, 0.09 mmol), $Ni(COD)_2$ (25 mg, 0.09 mmol, 1 equiv) and L4 (96 mg, 0.27 mmol, 3 equiv) were added to a 10 mL vial. A stirbar was added and charged with 5 mL of THF and left to stir overnight. The solvent was removed, filtered and washed with pentane (1 mL x 3, cold -36 ºC) to afford [(**L4**)$_2$Ni]Cl as a purple powder (132 mg, 91 % yield).

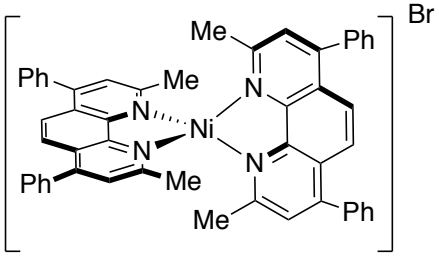
Stability: Unstable in air

^{1}H NMR (400 MHz, THF-d_8) δ 75.78, 53.72, 25.67, 18.75, 14.13. **^{13}C NMR**, no signals are observed due to paramagnetism of [(L4)$_2$Ni]Cl. [spectrum]

X-Band EPR = g(x) = 2.109, g(y) = 2.106, g(z) = 2.445 [spectrum]

UV-VIS (nm) = 560 nm, 735 nm [spectrum]

Synthesis of [(L4)$_2$Ni]Br



Following a modification of literature procedures,[4] in the glovebox, (**L4**)$NiBr_2$ (60 mg, 0.10 mmol), $Ni(COD)_2$ (29 mg, 0.10 mmol, 1 equiv) and L4 (112 mg, 0.31 mmol, 3 equiv) were added to a 10 mL vial. A stirbar was added and charged with 5 mL of THF and left to stir overnight. The solvent was removed, filtered and washed with pentane (1 mL x 3, cold -36 ºC) to afford [(L4)$_2$Ni]Br as a blue powder (167 mg, 94 % yield).

Stability: Unstable in air

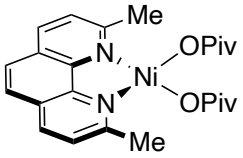
^{1}H NMR (400 MHz, THF-d_8) δ 24.45, 12.22. **^{13}C NMR**, no signals are observed due to paramagnetism of [(L4)$_2$Ni]Br. [spectrum]

X-Band EPR = g(x) = 2.115, g(y) = 2.114, g(z) = 2.456 [spectrum]

UV-VIS (nm) = 560 nm, 690 nm [spectrum]

Single crystal XRD [structure]

Synthesis of (L3)Ni(OPiv)$_2$

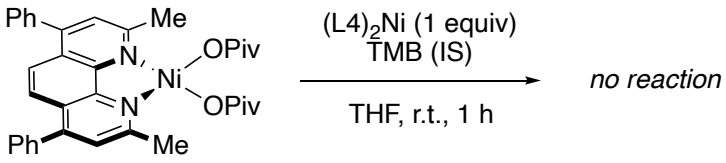


In the glovebox, (L3)$NiCl_2$ (97 mg, 0.29 mmol) was added to a 12 mL vial with potassium pivalate (143 mg, 1.15 mmol, 4 equiv). A stir bar was added, and the vial was charged with 7 mL of toluene turning the pink powder to a pink suspension and let stir overnight. After 16 hours the green suspension was filtered through a celite plug and washed with DCM (8 mL) with the salt being filtered off and a green solution collected. The solvent was then removed to afford a green solid and washed with pentane (1 mL x 3) to give (**L3**)Ni(OPiv)$_2$ (123 mg, 90 % yield) as a green powder.

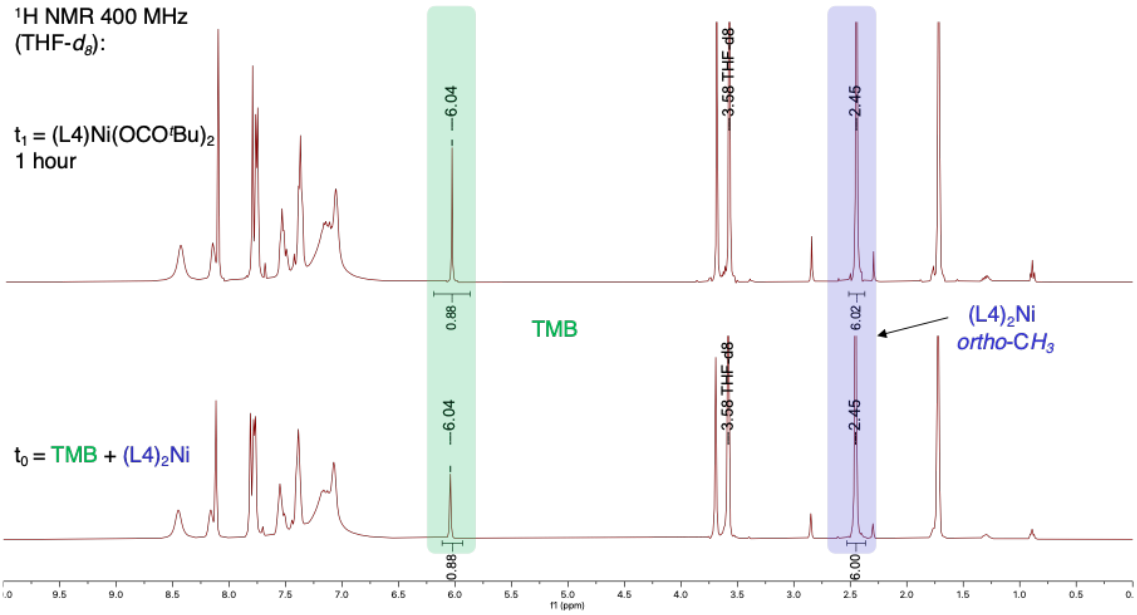
^{1}H NMR (^{1}H NMR (400 MHz, C_6D_6) δ 48.92, 18.43, 15.50, -9.49. **^{13}C NMR**, no signals are observed due to paramagnetism of (L3)Ni(OPiv)$_2$. [spectrum]
X-Band EPR = EPR Silent
Single Crystal XRD [structure]

Stochiometric Reactions.

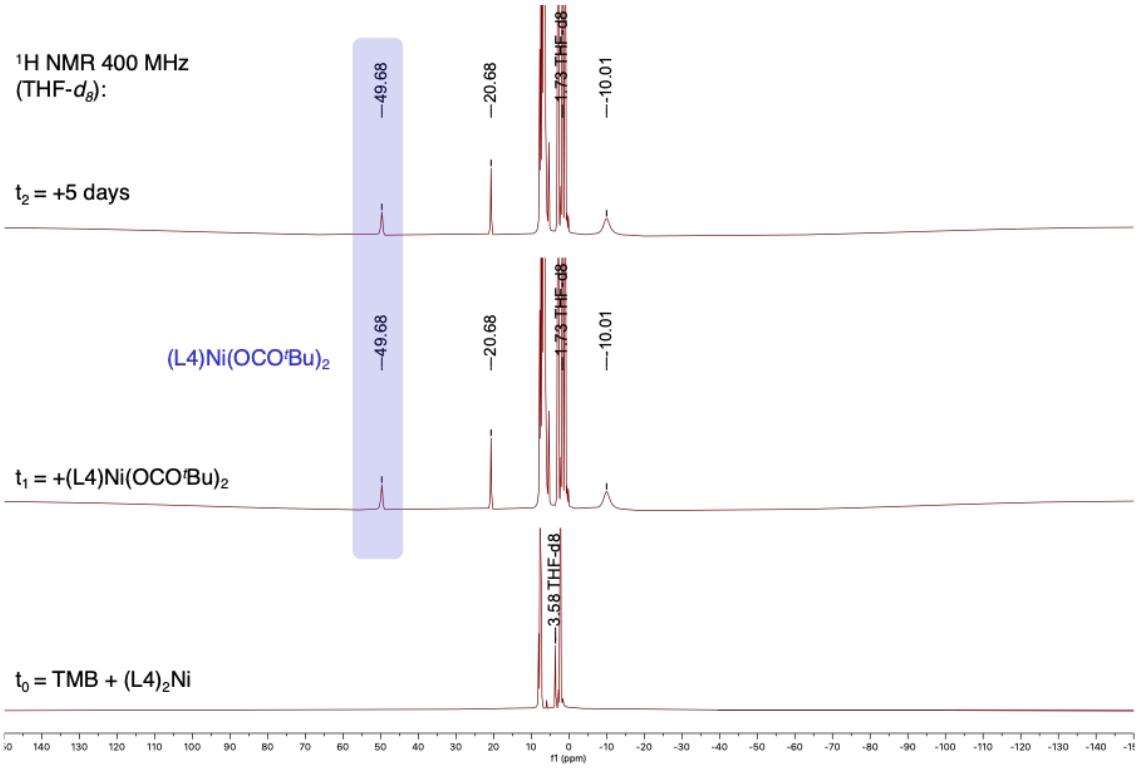
No reaction between (L4)Ni(OPiv)$_2$ and (L4)$_2$Ni



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (L4)$_2$Ni (12 mg, 0.02 mmol) and TMB (1 mg, internal standard) were added to a 4 mL vial with 1 mL of THF-d_8. The solution was transferred to a J-Young NMR tube and the initial integration of (**L4**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing (**L4**)Ni(OPiv)$_2$ (10 mg, 0.02 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. No conversion of (**L4**)$_2$Ni was observed and paramagnetic signals of (**L4**)Ni(OPiv)$_2$ remained with no additional signals of paramagnetic species observed. Conclusion: This is consistent with no reaction between (**L4**)$_2$Ni and (**L4**)Ni(OPiv)$_2$.

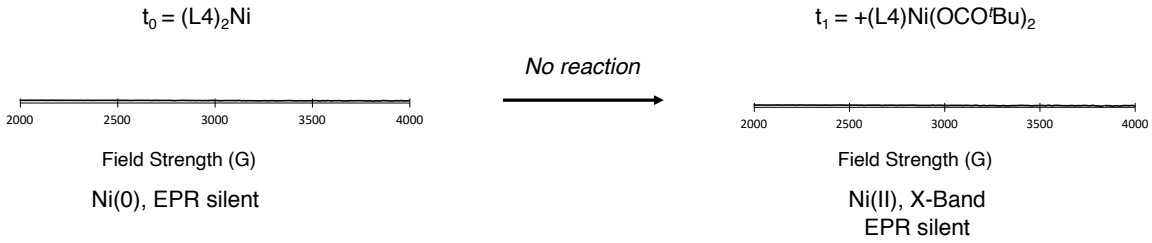


Supplementary Figure 1. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni indicating no conversion of (**L4**)$_2$Ni upon adding (**L4**)Ni(OPiv)$_2$. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).



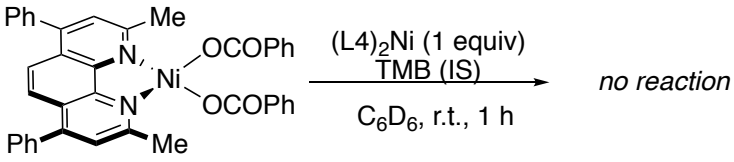
Supplementary Figure 2. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)Ni(OPiv)$_2$ and (**L4**)$_2$Ni indicating no conversion of (**L4**)Ni(OPiv)$_2$. (**L4**)Ni(OPiv)$_2$ (blue).

Monitored by EPR. In the glovebox, a solution of (**L4**)$_2$Ni was prepared and the EPR spectrum of (L4)$_2$Ni was recorded which was EPR silent. Separately, (**L4**)Ni(OPiv)$_2$ (10 mg, 0.02 mmol) and (L4)$_2$Ni (12 mg, 0.02 mmol) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF. After 1 hour, a 100 uL aliquot was removed and diluted to 800 uL in THF and then analyzed by EPR, in which no EPR signals corresponding to Ni(I) species were observed. As described in the synthesis of (**L4**)Ni(OPiv)$_2$, this Ni(II) complex is X-band EPR silent.

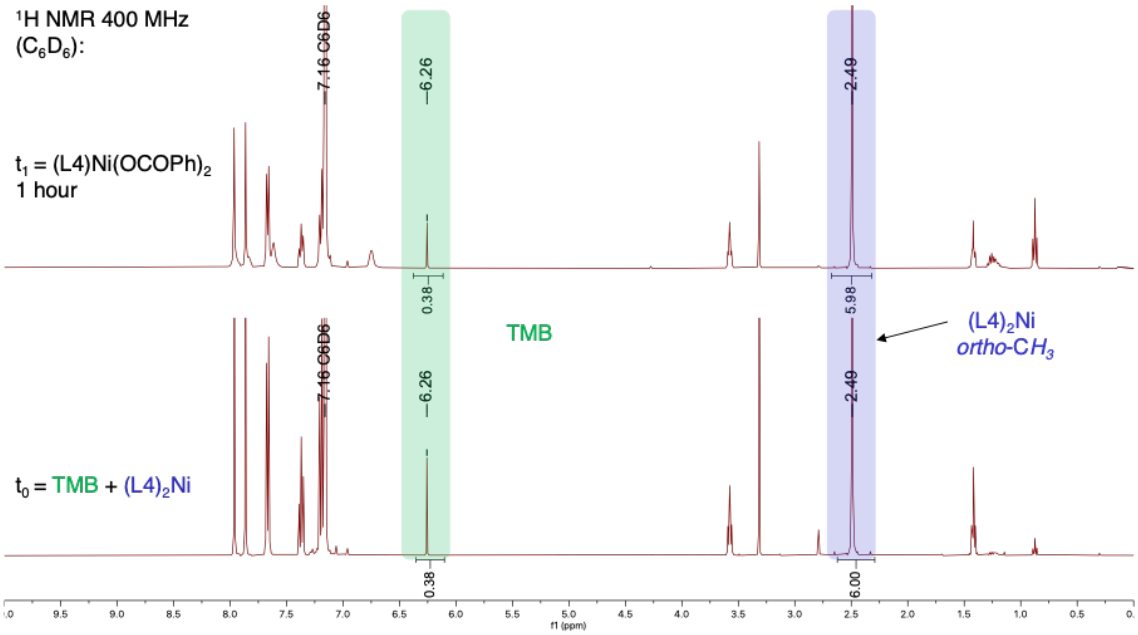


Supplementary Figure 3. Continuous wave (CW) X-Band EPR spectra of (**L4**)$_2$Ni and upon mixing (**L4**)Ni(OPiv)$_2$ and (**L4**)$_2$Ni indicating no formation of Ni(I) species. (**L4**)$_2$Ni and (**L4**)Ni(OPiv)$_2$ are both X-Band EPR silent, while Ni(I) species would be EPR active.

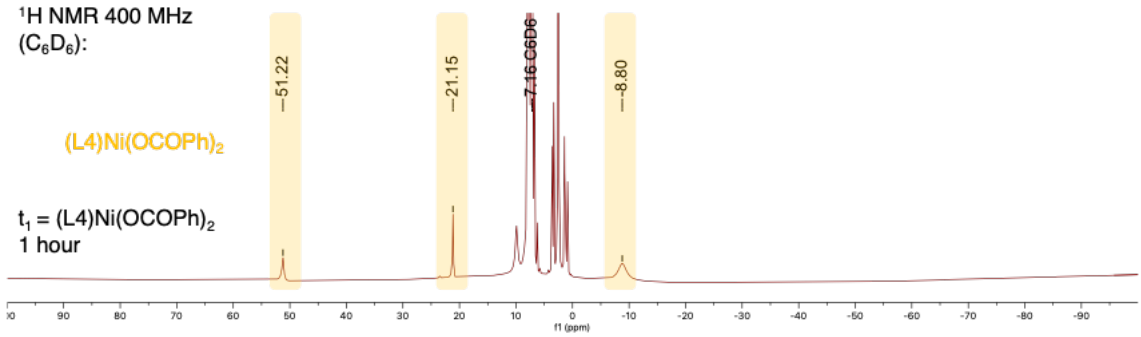
No reaction between (L4)Ni(OCOPh)$_2$ and (L4)$_2$Ni



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (**L4**)$_2$Ni (10 mg, 0.01 mmol) and TMB (1 mg, internal standard) were added to a 4 mL vial with 1 mL of C_6D_6. The solution was transferred to a J-Young NMR tube and the initial integration of (**L4**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing (**L4**)Ni(OCOPh)$_2$ (9 mg, 0.01 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. No conversion of (**L4**)$_2$Ni was observed and paramagnetic signals of (**L4**)Ni(OCOPh)$_2$ remained with no additional signals of paramagnetic species observed. Conclusion: This is consistent with no reaction between (**L4**)$_2$Ni and (**L4**)Ni(OCOPh)$_2$.

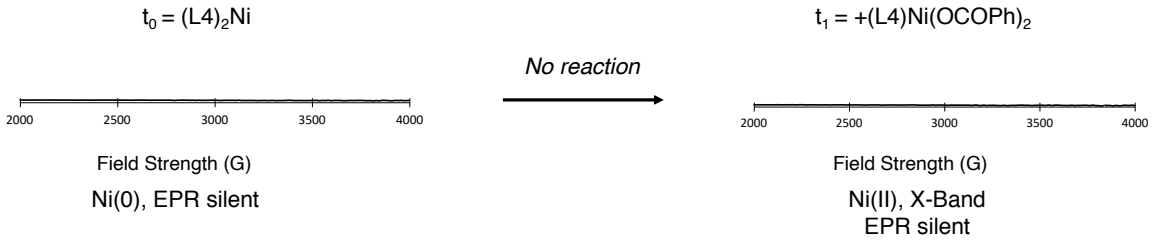


Supplementary Figure 4. Quantitative ^{1}H NMR spectra of TMB and (L4)$_2$Ni indicating no conversion of (L4)$_2$Ni upon adding (L4)Ni(OCOPh)$_2$. Internal standard trimethoxybenzene, TMB (green) and (L4)$_2$Ni (blue).



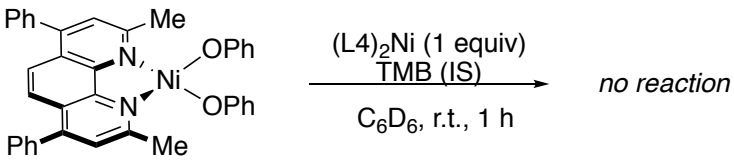
Supplementary Figure 5. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)Ni(OCOPh)$_2$ and (L4)$_2$Ni indicating no conversion of (**L4**)Ni(OCOPh)$_2$. (**L4**)Ni(OCOPh)$_2$ (orange).

Monitored by EPR. In the glovebox, (**L4**)Ni(OCOPh) $_2$ (8 mg, 0.02 mmol) and (**L4**)$_2$Ni (9 mg, 0.01 mmol) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF. After 1 hour, a 100 uL aliquot was removed and diluted to 800 uL in THF and then analyzed by EPR.

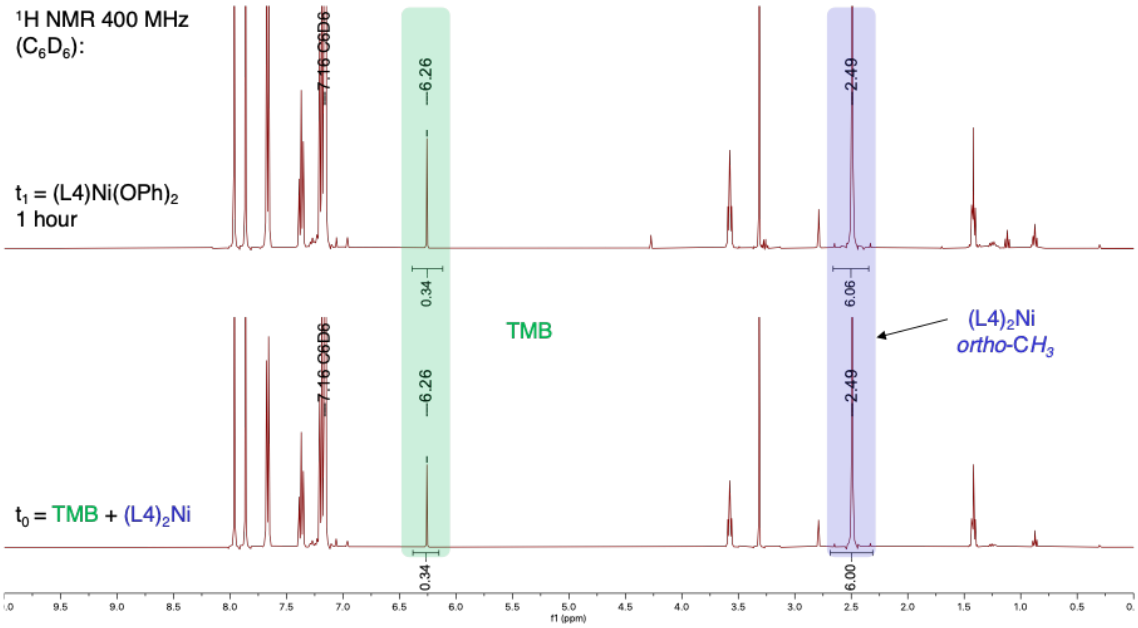


Supplementary Figure 6. Continuous wave (CW) X-Band EPR spectra of (**L4**)$_2$Ni and upon mixing (**L4**)Ni(OCOPh)$_2$ and (**L4**)$_2$Ni indicating no formation of Ni(I) species. (**L4**)$_2$Ni and (**L4**)Ni(OCOPh)$_2$ are both X-Band EPR silent, while Ni(I) species would be EPR active.

No reaction between [(L4)Ni(OPh)$_2$]$_2$ and (L4)$_2$Ni

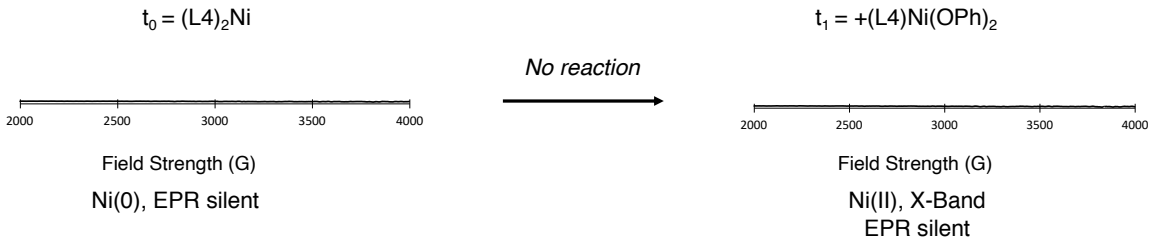


Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (**L4**)$_2$Ni (10 mg, 0.01 mmol) and TMB (1 mg, internal standard) were added to a 4 mL vial with 1 mL of C_6D_6. The solution was transferred to a J-Young NMR tube and the initial integration of (**L4**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing [(**L4**)Ni(OPh)$_2$]$_2$ (8 mg, 0.01 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. No conversion of (**L4**)$_2$Ni was observed with no additional signals of paramagnetic species observed, signals for [(**L4**)Ni(OPh)$_2$]$_2$ were observed in low intensity due to the poor solubility in C_6D_6. Conclusion: This is consistent with no reaction between (**L4**)$_2$Ni and [(**L4**)Ni(OPh)$_2$]$_2$.



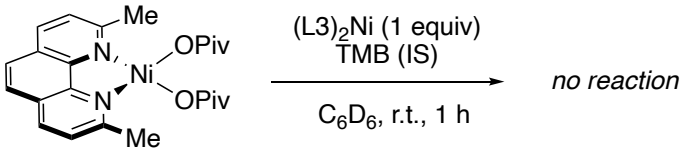
Supplementary Figure 7. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni indicating no conversion of (**L4**)$_2$Ni upon adding [(**L4**)Ni(OPh)$_2$]$_2$. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

Monitored by EPR. In the glovebox, [(**L4**)Ni(OPh)$_2$]$_2$ (10 mg, 0.02 mmol) and (**L4**)$_2$Ni (12 mg, 0.02 mmol) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF. After 1 hour, a 100 uL aliquot was removed and diluted to 800 uL in THF and then analyzed by EPR.



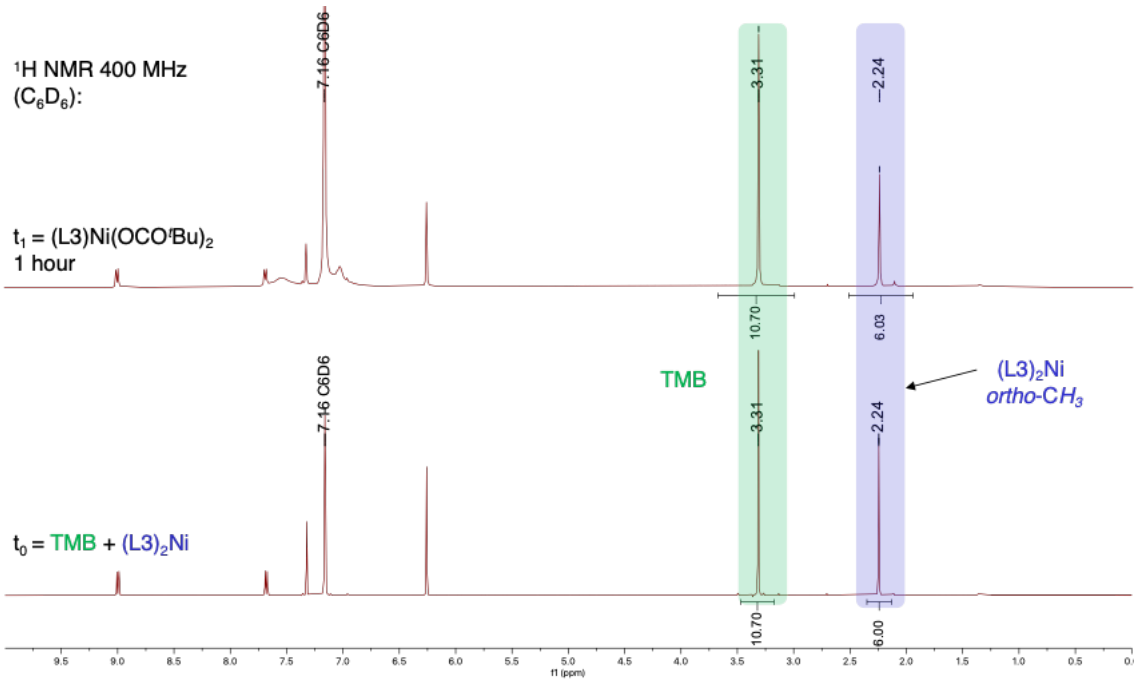
Supplementary Figure 8. Continuous wave (CW) X-Band EPR spectra of (**L4**)$_2$Ni and upon mixing [(**L4**)Ni(OPh)$_2$]$_2$and (L4)$_2$Ni indicating no formation of Ni(I) species. (**L4**)$_2$Ni and [(**L4**)Ni(OPh)$_2$]$_2$are both X-Band EPR silent, while Ni(I) species would be EPR active.

No reaction between (L3)Ni(OPiv)$_2$ and (L3)$_2$Ni

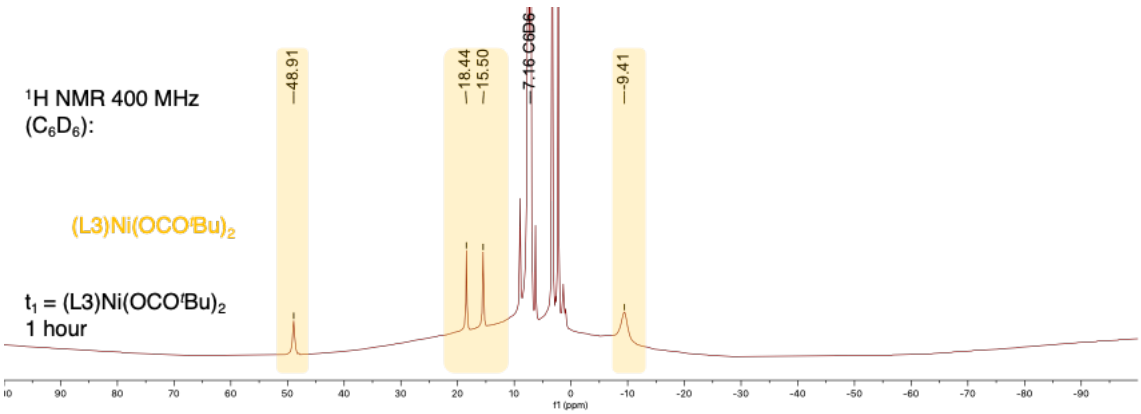


Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (L3)$_2$Ni (4.4 mg, 0.01 mmol) and TMB (1 mg, internal standard) were added to a 4 mL vial with 0.7 mL of C_6D_6 and filtered through a celite plug to remove traces of undissolved material and the filtrate

was diluted further with 0.4 mL of C_6D_6 to prevent (**L3**)$_2$Ni from precipitating out of solution. The solution was transferred to a J-Young NMR tube and the initial integration of (**L3**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing (**L3**)Ni(OPiv)$_2$ (4.3 mg, 0.01 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. No conversion of (**L3**)$_2$Ni was observed and paramagnetic signals of (**L3**)Ni(OPiv)$_2$ remained with no additional signals of paramagnetic species observed. Conclusion: This is consistent with no reaction between (**L3**)$_2$Ni and (**L3**)Ni(OPiv)$_2$.



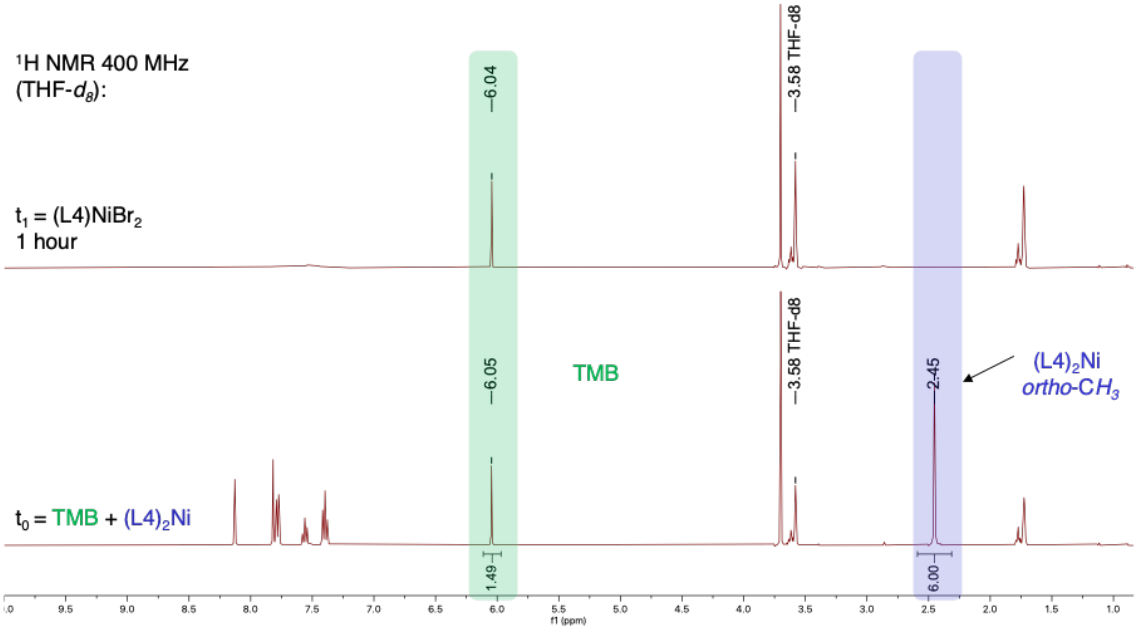
Supplementary Figure 9. Quantitative ^{1}H NMR spectra of TMB and (**L3**)$_2$Ni indicating no conversion of (**L3**)$_2$Ni upon adding (**L3**)Ni(OPiv)$_2$. Internal standard trimethoxybenzene, TMB (green) and (**L3**)$_2$Ni (blue).



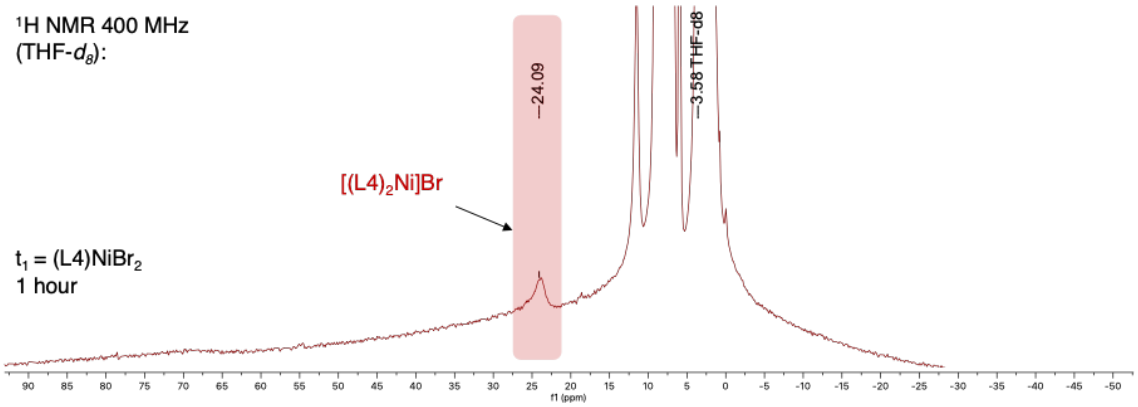
Supplementary Figure 10. Paramagnetic ^{1}H NMR spectra upon mixing (**L3**)Ni(OPiv)$_2$ and (**L3**)$_2$Ni indicating no conversion of (**L3**)Ni(OPiv)$_2$. (**L3**)Ni(OPiv)$_2$ (orange).

Reaction between (L4)$NiBr_2$ and (L4)$_2$Ni

Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (**L4**)$_2$Ni (10 mg, 0.01 mmol) and TMB (1 mg, internal standard) were added to a 4 mL vial with 1 mL of THF-d_8. The solution was transferred to a J-Young NMR tube and the initial integration of (**L4**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing (**L4**)$NiBr_2$ (7 mg, 0.01 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. Full conversion of (**L4**)$_2$Ni was observed with additional signals of paramagnetic species observed. Conclusion: This is consistent with reaction between (**L4**)$_2$Ni and (**L4**)$NiBr_2$ to form Ni(I) complex [(**L4**)$_2$Ni]Br.

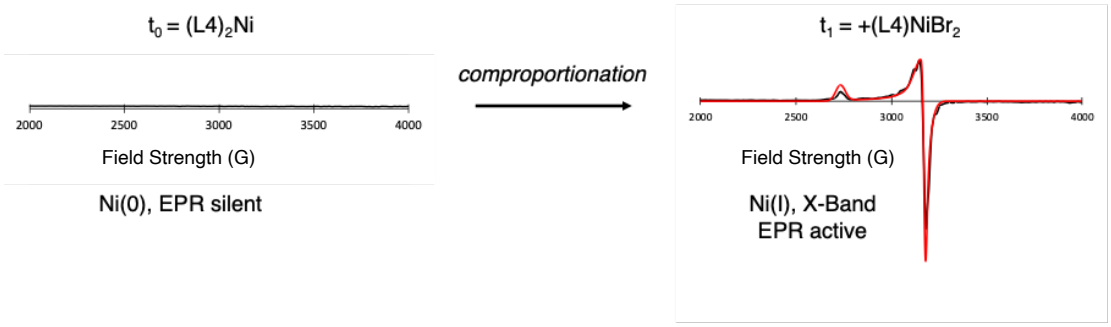


Supplementary Figure 11. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni indicating full conversion of (**L4**)$_2$Ni upon adding (**L4**)$NiBr_2$. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).



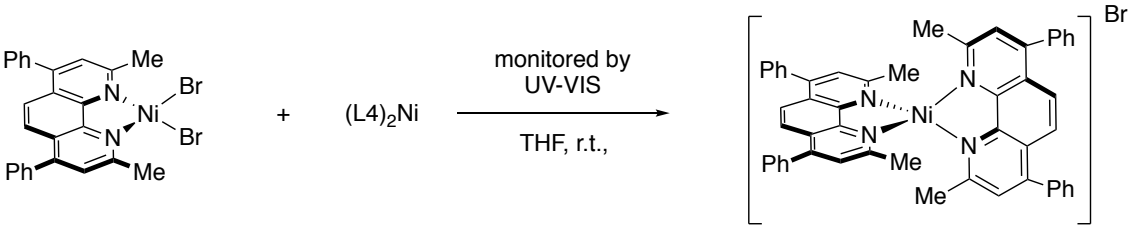
Supplementary Figure 12. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)$NiBr_2$ and (**L4**)$_2$Ni indicating full conversion of (**L4**)$_2$Ni and formation of [(**L4**)$_2$Ni]Br. [(**L4**)$_2$Ni]Br (red).

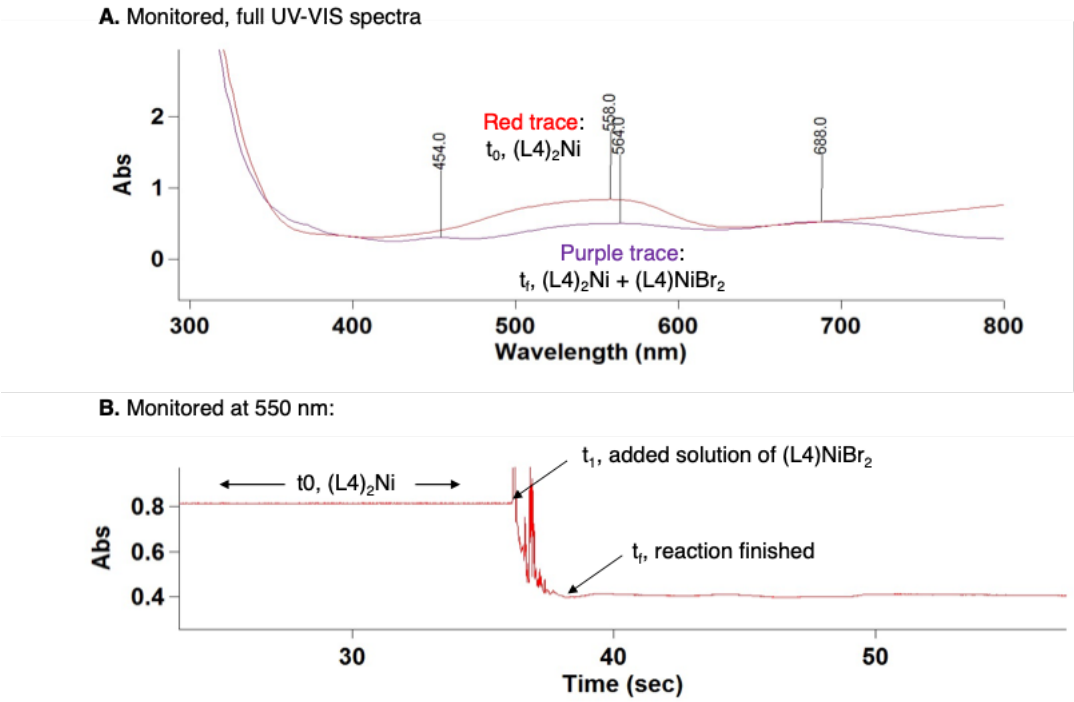
Monitored by EPR. In the glovebox, (**L4**)$NiBr_2$ (8 mg, 0.01 mmol) and (**L4**)$_2$Ni (11 mg, 0.01 mmol) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF. After 1 hour, a 100 uL aliquot was removed and diluted to 800 uL in THF and then analyzed by EPR.



Supplementary Figure 13. Continuous wave (CW) X-Band EPR spectra of (**L4**)$_2$Ni and upon mixing (**L4**)$NiBr_2$ and (**L4**)$_2$Ni indicating formation of Ni(I) species. (**L4**)$_2$Ni and (**L4**)$NiBr_2$ are both X-Band EPR silent, while Ni(I) species [(**L4**)$_2$Ni]Br would be EPR active.

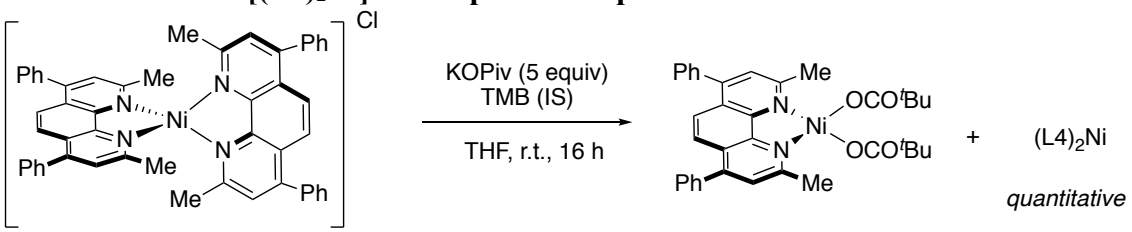
Monitored rate of reaction by UV-VIS. In the glovebox, a solution of (**L4**)$_2$Ni (0.04 mM, 2.5 mL) in THF was transferred to a sealed cuvette. The UV-VIS spectra was monitored at 550 nm an a solution of (**L4**)$NiBr_2$ (0.4 mM, 0.25 mL) was injected via microsyringe in which the reaction was complete within 4 seconds. Noise from injecting the solution of (**L4**)$NiBr_2$ precluded accurate rate measurements. Conclusion: This is consistent with reaction between (**L4**)$_2$Ni and (**L4**)$NiBr_2$ to form Ni(I) complex [(**L4**)$_2$Ni]Br occurs rapidly.



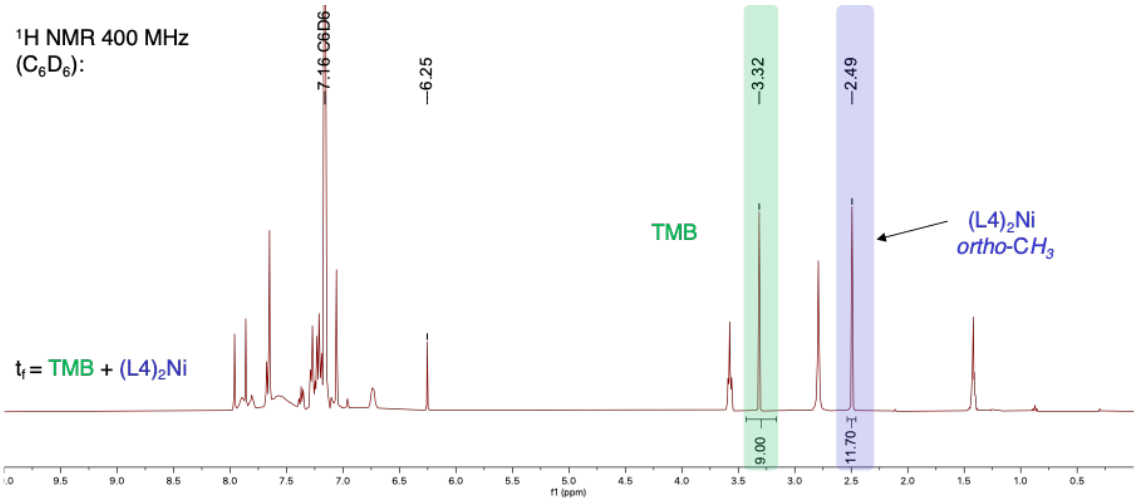


Supplementary Figure 14. Monitoring the reaction of (**L4**)$_2$Ni and (**L4**)NiBr$_2$ by UV-VIS spectroscopy. **A**. Initial UV-VIS spectrum of (**L4**)$_2$Ni (red trace) and the resulting spectrum after addition of (**L4**)NiBr$_2$. **B**. Monitoring the reaction at 550 nm.

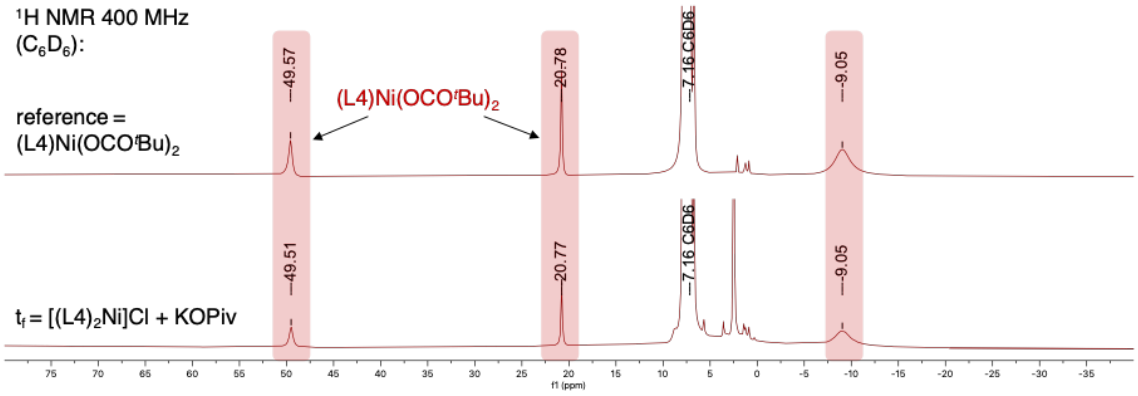
Reaction between [(L4)$_2$Ni]Cl and potassium pivalate in THF



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, ([(**L4**)$_2$Ni]Cl (22 mg, 0.03 mmol) and potassium pivalate (18 mg, 0.15 mmol, 5 equiv) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF. After 16 hour, the solvent was removed and redissolved in 3 mL of C_6D_6. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in quantitative yield and the only species observed in the paramagnetic NMR was (**L4**)Ni(OPiv)$_2$. Attempts to follow these reactions by EPR and paramagnetic NMR were performed to identify the formation of transient (**L4**)Ni^I-OPiv, however we were unable to identify any new signals that would correspond to this species suggested it undergo rapid disproportionation once formed. Conclusion: This is consistent with reaction between Ni(I) complex [(**L4**)$_2$Ni]Cl and potassium pivalate to form (**L4**)$_2$Ni and (**L4**)Ni(OPiv)$_2$.

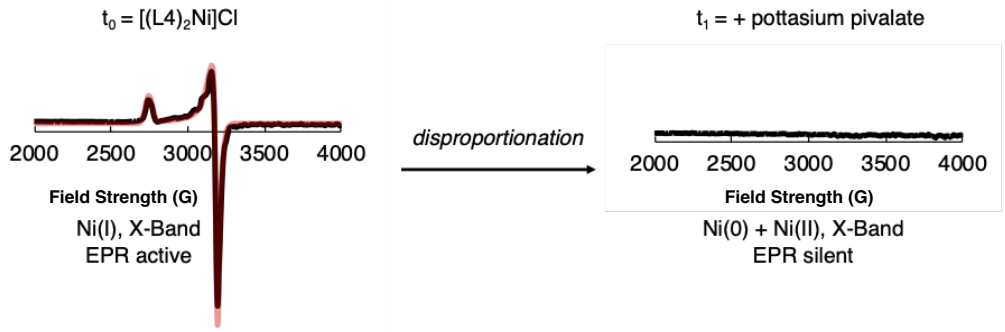


Supplementary Figure 15. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting [(**L4**)$_2$Ni]Cl with potassium pivalate. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).



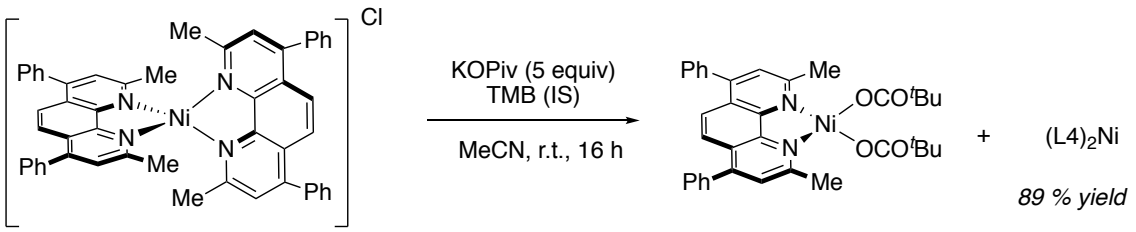
Supplementary Figure 16. Paramagnetic ^{1}H NMR spectra upon mixing [(**L4**)$_2$Ni]Cl with potassium pivalate formation of (**L4**)Ni(OPiv)$_2$. (**L4**)Ni(OPiv)$_2$ (red).

Monitored by EPR. In the glovebox, [(**L4**)$_2$Ni]Cl (10 mg, 0.01 mmol) and potassium pivalate (8 mg, 0.06 mmol, 6 equiv) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF. After 16 hour, a 100 uL aliquot was removed and diluted to 800 uL in THF and then analyzed by EPR.

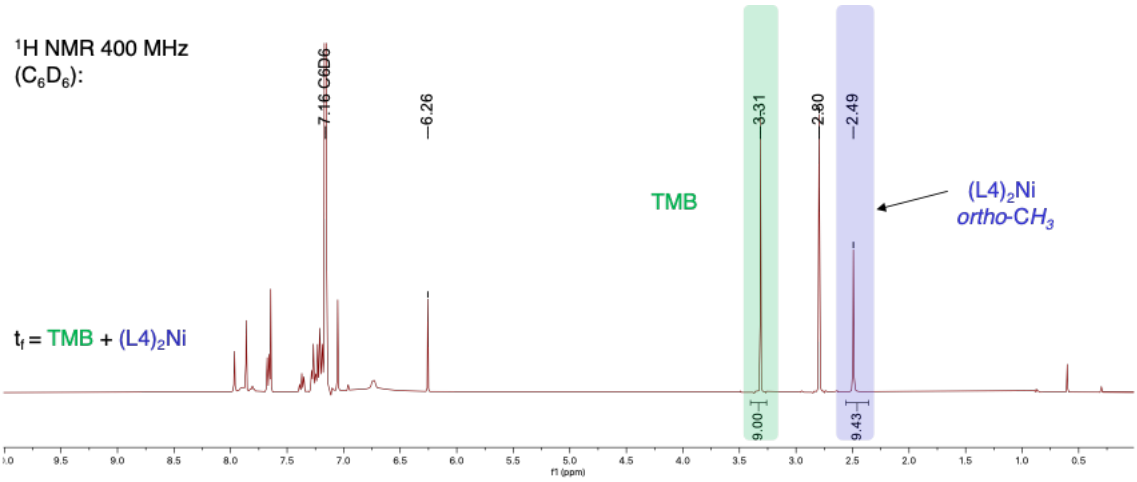


Supplementary Figure 17. Continuous wave (CW) X-Band EPR spectra of [(**L4**)$_2$Ni]Cl and upon mixing [(**L4**)$_2$Ni]Cl with potassium pivalate indicating loss of Ni(I) species [(**L4**)$_2$Ni]Cl. (**L4**)$_2$Ni and (**L4**)Ni(OPiv)$_2$ are both X-Band EPR silent, while Ni(I) species [(**L4**)$_2$Ni]Cl would be EPR active.

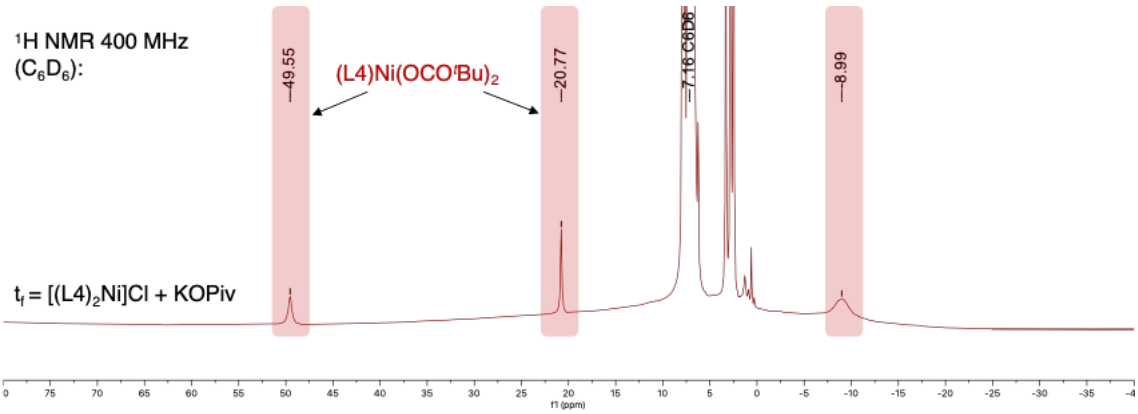
Reaction between [(L4)$_2$Ni]Cl and potassium pivalate in MeCN



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, ([(**L4**)$_2$Ni]Cl (18 mg, 0.02 mmol) and potassium pivalate (14 mg, 0.11 mmol, 5 equiv) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 3 mL of MeCN. After 16 hour, the solvent was removed and redissolved in 3 mL of C_6D_6. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 89 % yield and the only species observed in the paramagnetic NMR was (**L4**)Ni(OPiv)$_2$. Conclusion: This is consistent with reaction between Ni(I) complex [(**L4**)$_2$Ni]Cl and potassium pivalate to form (**L4**)$_2$Ni and (**L4**)Ni(OPiv)$_2$.

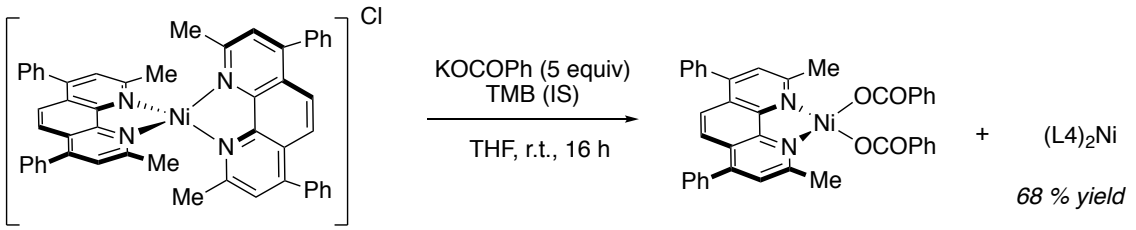


Supplementary Figure 18. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting [(**L4**)$_2$Ni]Cl with potassium pivalate. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

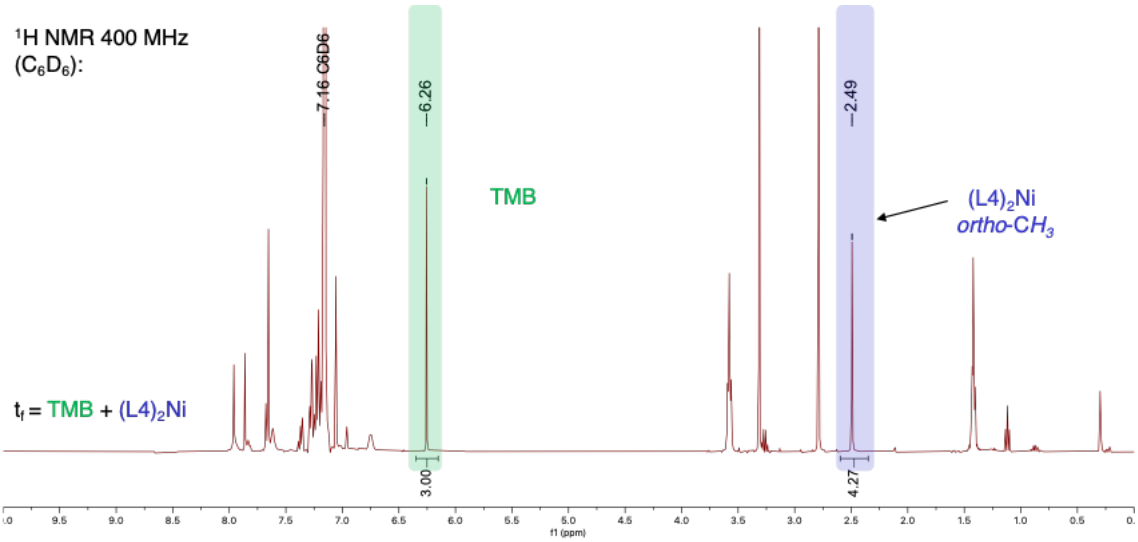


Supplementary Figure 19. Paramagnetic ^{1}H NMR spectra upon mixing [(**L4**)$_2$Ni]Cl with potassium pivalate formation of (**L4**)Ni(OPiv)$_2$. (**L4**)Ni(OPiv)$_2$ (red).

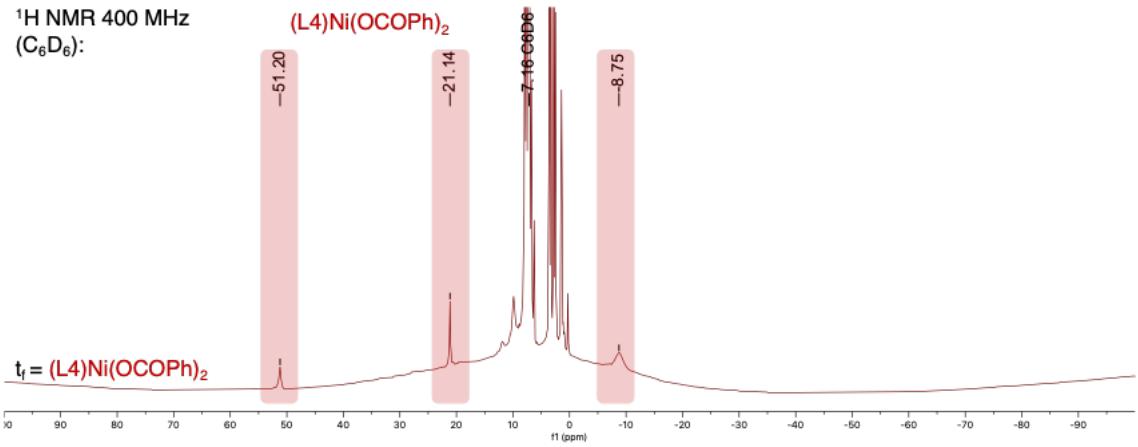
Reaction between [(L4)$_2$Ni]Cl and potassium benzoate



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, ([(**L4**)$_2$Ni]Cl (10 mg, 0.01 mmol), potassium benzoate (10 mg, 0.06 mmol, 6 equiv), and **L4** (5 mg, 0.01 mmol) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF. After 16 hour, the solvent was removed, redissolved in 3 mL of C_6D_6 and filtered through a celite plug. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 68 % yield and the only species observed in the paramagnetic NMR was (**L4**)Ni(OCOPh)$_2$. Conclusion: This is consistent with reaction between Ni(I) complex [(**L4**)$_2$Ni]Cl and potassium benzoate to form (**L4**)$_2$Ni and (**L4**)Ni(OCOPh)$_2$.

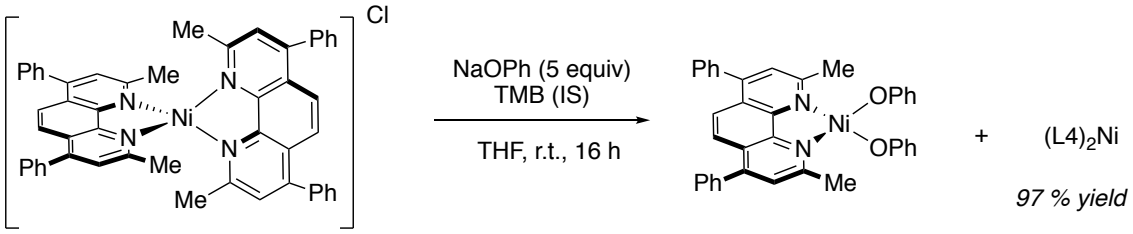


Supplementary Figure 20. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting [(**L4**)$_2$Ni]Cl with potassium benzoate. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

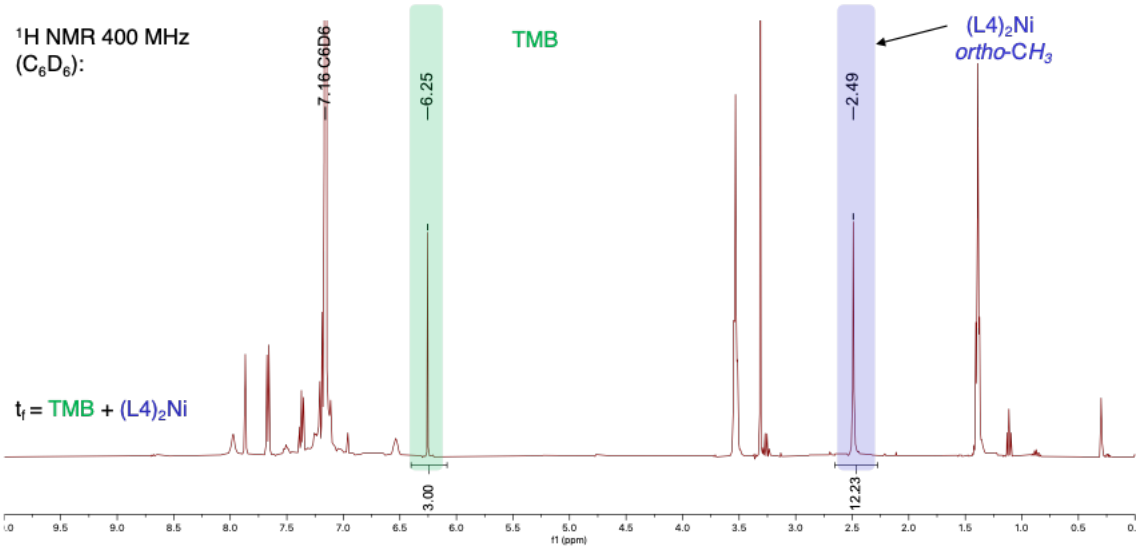


Supplementary Figure 21. Paramagnetic ^{1}H NMR spectra upon mixing [(**L4**)$_2$Ni]Cl with potassium benzoate and formation of (**L4**)Ni(OCOPh)$_2$. (**L4**)Ni(OCOPh)$_2$ (red).

Reaction between [(L4)$_2$Ni]Cl and sodium phenoxide

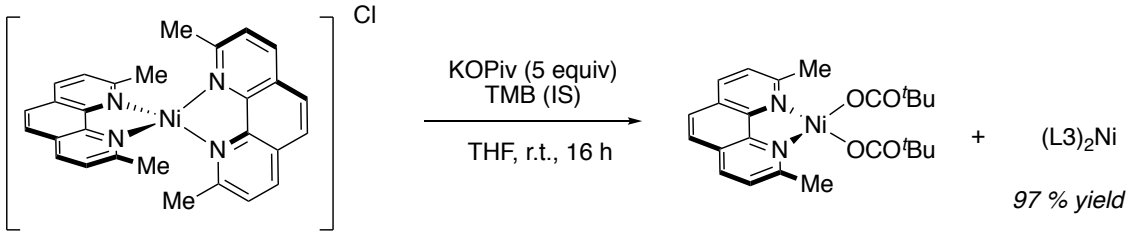


Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, ([(**L4**)$_2$Ni]Cl (21 mg, 0.03 mmol), sodium phenoxide (15 mg, 0.13 mmol, 5 equiv), and **L4** (9 mg, 0.03 mmol) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF. After 16 hour, the solvent was removed, redissolved in 3 mL of C_6D_6 and filtered through a celite plug. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 97 % yield and the only species observed in the paramagnetic NMR was (**L4**)Ni(OPh)$_2$. Due to the insolubility of [(**L4**)Ni(OPh)$_2$]$_2$ in C_6D_6, only faint traces of paramagnetic species are observed. Conclusion: This is consistent with reaction between Ni(I) complex [(**L4**)$_2$Ni]Cl and sodium phenoxide to form (**L4**)$_2$Ni and [(**L4**)Ni(OPh)$_2$]$_2$.

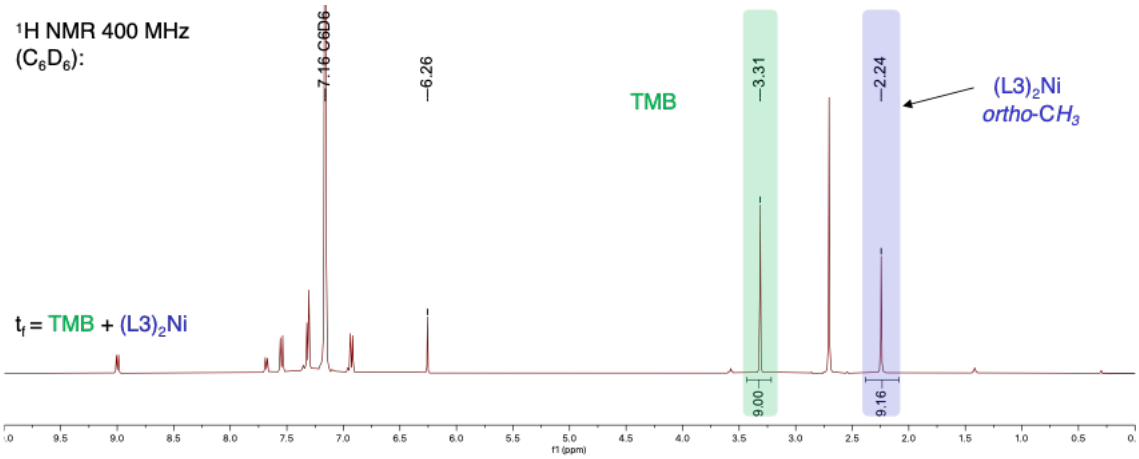


Supplementary Figure 22. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting [(**L4**)$_2$Ni]Cl with sodium phenoxide. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

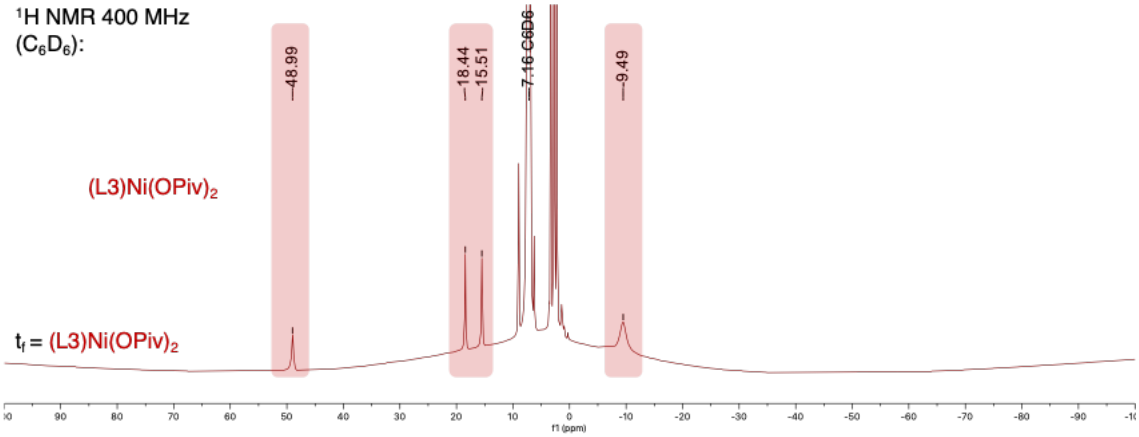
Reaction between [(L3)$_2$Ni]Cl and potassium pivalate



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, ([(**L3**)$_2$Ni]Cl (10 mg, 0.02 mmol), potassium pivalate (12 mg, 0.10 mmol, 5 equiv), and **L3** (4 mg, 0.02 mmol) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF. After 16 hour, the solvent was removed, redissolved in 3 mL of C_6D_6 and filtered through a celite plug. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L3**)$_2$Ni was measured by ^{1}H NMR to determine (**L3**)$_2$Ni had formed in 96 % yield and the only species observed in the paramagnetic NMR was (**L3**)Ni(OPiv)$_2$. Conclusion: This is consistent with reaction between Ni(I) complex [(**L3**)$_2$Ni]Cl and potassium pivalate to form (**L3**)$_2$Ni and (**L3**)Ni(OPiv)$_2$.



Supplementary Figure 23. Quantitative ^{1}H NMR spectra of TMB and (**L3**)$_2$Ni after reacting [(**L3**)$_2$Ni]Cl with pottasium pivalate. Internal standard trimethoxybenzene, TMB (green) and (**L3**)$_2$Ni (blue).

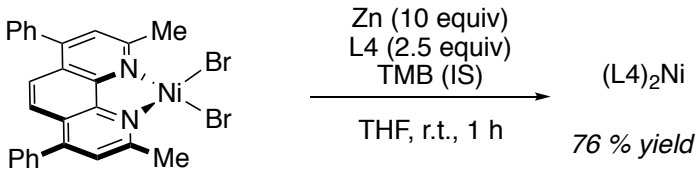


Supplementary Figure 24. Paramagnetic ^{1}H NMR spectra upon mixing [(**L3**)$_2$Ni]Cl with potassium pivalate and formation of (**L3**)Ni(OPiv)$_2$. (**L3**)Ni(OPiv)$_2$ (red).

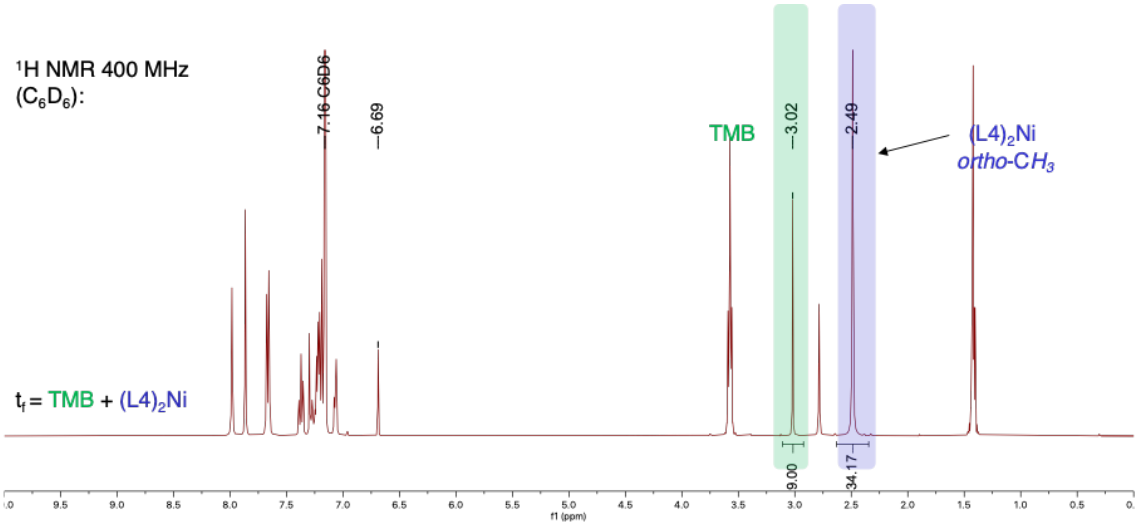
Solubility of Ni(II) complexes

In the glovebox (bipyridine)NiCl$_2$ (25 mg) was added to a 10 mL vial. A stir bar was added, and the vial was charged with 3 mL of THF and stirred at 900 rpm. After 1 hour, a 1.5 mL aliquot was removed and filtered through a celite plug to afford a saturated solution of (bipyridine)NiCl$_2$ in which 1 mL was transferred to a tared vial. The solvent was removed to afford the resultant solid. This representative procedure was repeated for (phenanthroline)NiCl$_2$, (**L3**)NiCl$_2$ and (**L4**)NiCl$_2$.

Reaction between (L4)$NiBr_2$ and zinc

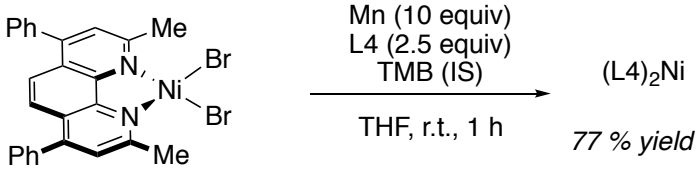


Quantified by ^{1}H NMR. In the glovebox, (**L4**)$NiBr_2$ (22 mg, 0.04 mmol), **L4** (35 mg, 0.10 mmol, 2.5 equiv) and zinc (25 mg, 0.38 mmol, 10 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug and the solvent was removed and redissolved in 3 mL of C_6D_6. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 76 % yield. Conclusion: This is consistent with full reduction of Ni(II) to Ni(0) with Zn.



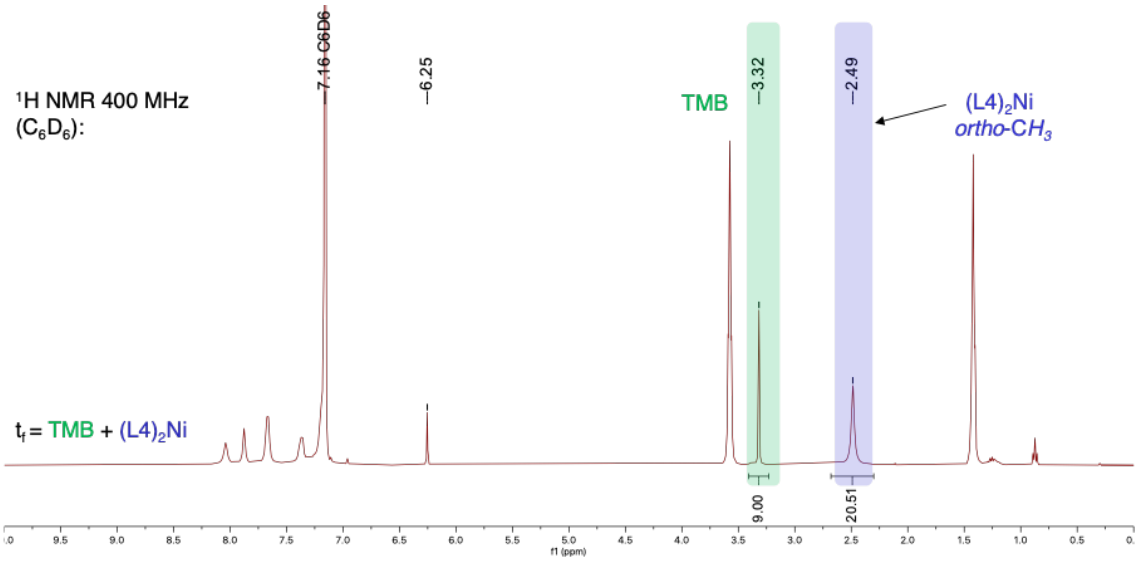
Supplementary Figure 25. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting (**L4**)$NiBr_2$ with zinc (10 equiv). Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

Reaction between (L4)$NiBr_2$ and manganese



Quantified by ^{1}H NMR. In the glovebox, (**L4**)$NiBr_2$ (16 mg, 0.03 mmol), **L4** (25 mg, 0.07 mmol, 2.5 equiv) and manganese (15 mg, 0.27 mmol, 10 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug and the solvent was removed and redissolved in 3 mL of C_6D_6. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio

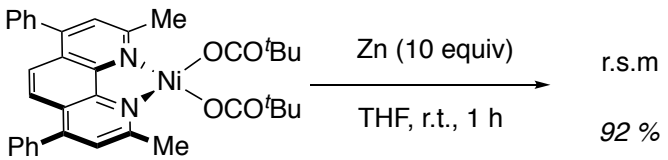
of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 77 % yield. Conclusion: This is consistent with full reduction of Ni(II) to Ni(0) with Mn.

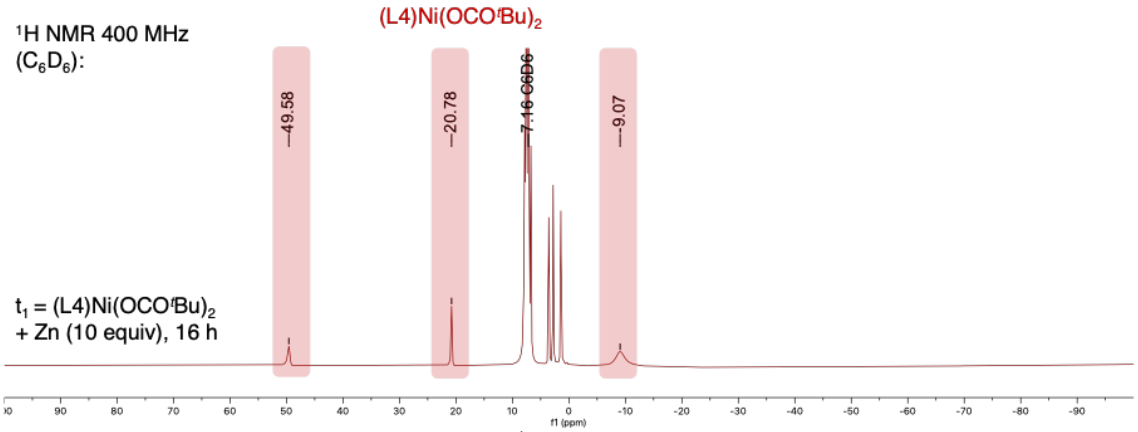


Supplementary Figure 26. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting (**L4**)NiBr$_2$ with manganese (10 equiv). Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

No reaction between (L4)Ni(OPiv)$_2$ and Zn

Quantified by isolation. In the glovebox, (**L4**)Ni(OPiv)$_2$ (19 mg, 0.03 mmol), and zinc (20 mg, 0.31 mmol, 10 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug to afford a green filtrate in which the solvent was removed. The solid was then filtered to afford (**L4**)Ni(OPiv)$_2$ as a green solid (18 mg, 92 % recovered yield). These reactions were performed without added **L4** to assist in isolation. They were repeated with additional L4 as a control to verify this did not change the reaction outcome in which only starting material is observed, even at 16 h in which only starting material is observed (Supplementary Figure 27). Conclusion: This is consistent with no reduction of Ni(II)-(OPiv)$_2$ to Ni(0) with Zn.

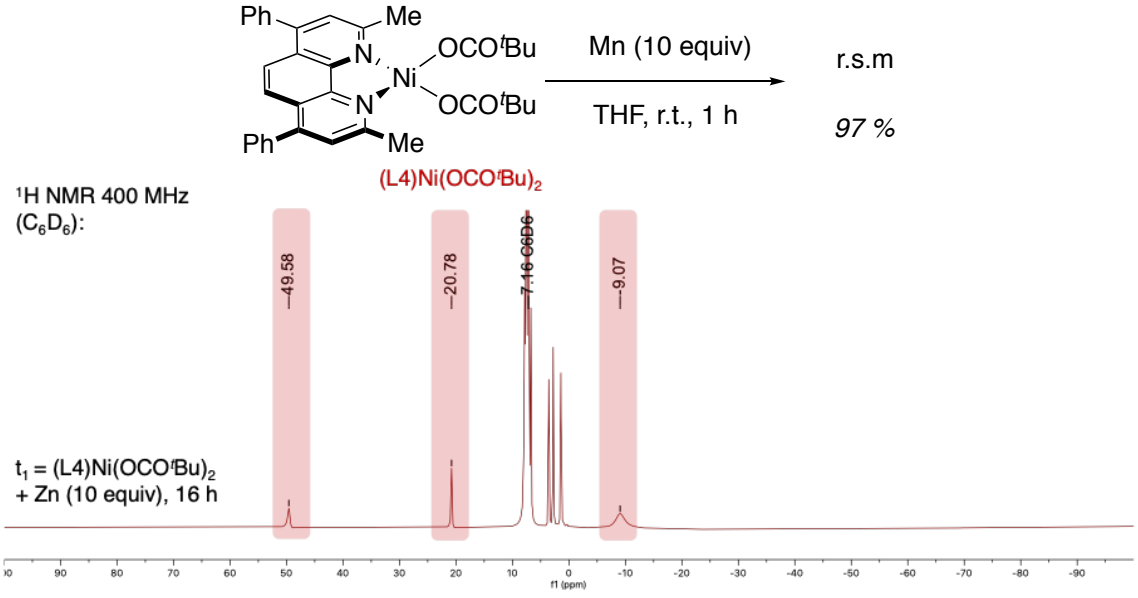




Supplementary Figure 27. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)Ni(OPiv)2 with zinc (10 equiv) and isolating unreacted (**L4**)Ni(OPiv)$_2$ with no formation of (**L4**)$_2$Ni. (**L4**)Ni(OPiv)$_2$ (red).

No reaction between (L4)Ni(OPiv)$_2$ and Mn

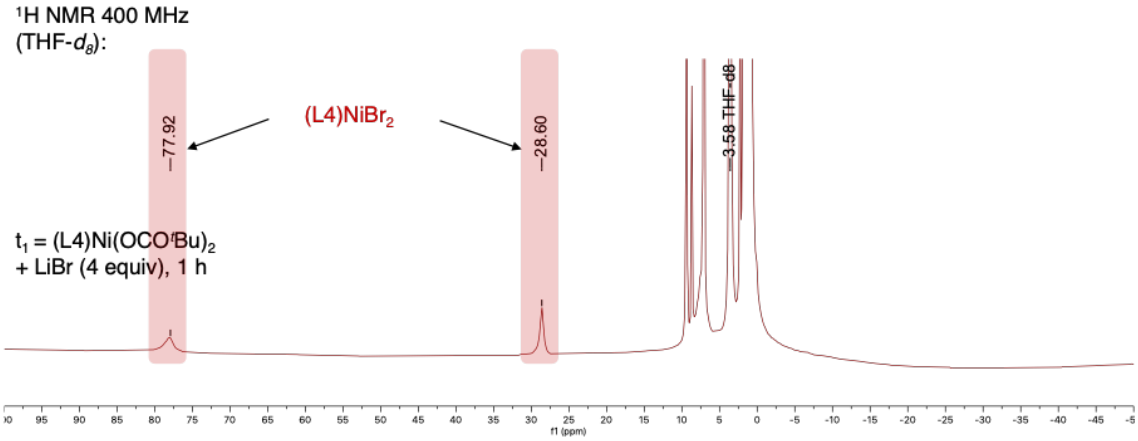
Quantified by isolation. In the glovebox, (**L4**)Ni(OPiv)$_2$ (19 mg, 0.03 mmol), and manganese (17 mg, 0.30 mmol, 10 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug to afford a green filtrate in which the solvent was removed. The solid was then filtered to afford (**L4**)Ni(OPiv)$_2$ as a green solid (18 mg, 97 % recovered yield). These reactions were performed without added **L4** to assist in isolation. They were repeated with additional L4 as a control to verify this did not change the reaction outcome in which only starting material is observed, even at 16 h in which only starting material is observed (Supplementary Figure 28). Conclusion: This is consistent with no reduction of Ni(II)-(OPiv)$_2$ to Ni(0) with Zn.



Supplementary Figure 28. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)Ni(OPiv)$_2$ with manganese (10 equiv) and isolating unreacted (**L4**)Ni(OPiv)$_2$ with no formation of (L4)$_2$Ni. (**L4**)Ni(OPiv)$_2$ (red).

Reaction between (L4)Ni(OPiv)$_2$ and LiBr

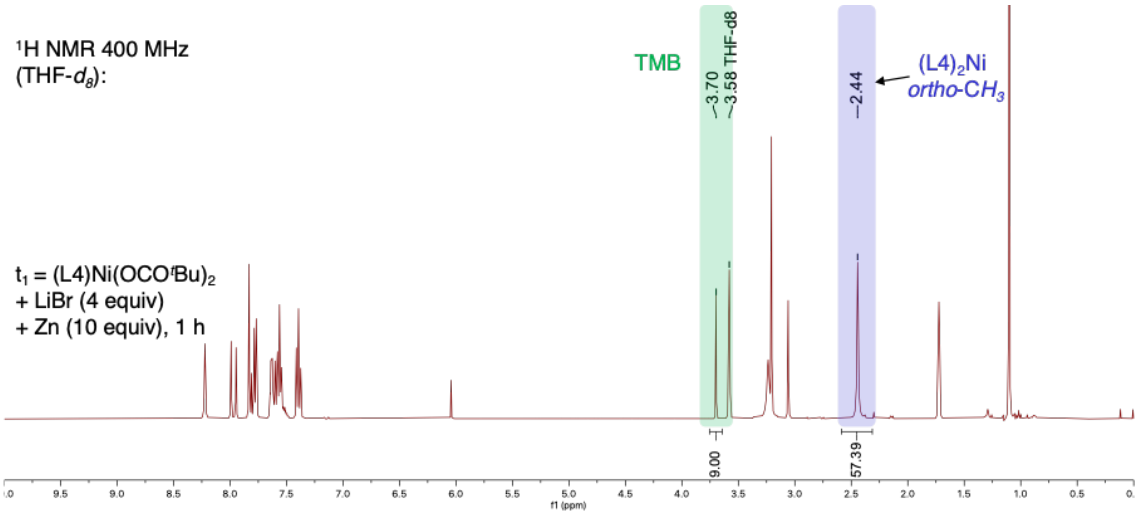
Quantified by isolation. In the glovebox, (**L4**)Ni(OPiv)$_2$ (31 mg, 0.05 mmol), and LiBr (17 mg, 0.20 mmol, 4 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 2 mL of THF and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug to afford a pink filtrate from which the solvent was removed. The solid was then re-dissolved in toluene and filtered the solvent was again removed to afford (**L4**)Ni(Br)$_2$ as a pink solid (27 mg, 93 % yield).
Conclusion: This is consistent with full conversion of Ni(II)-(OPiv)$_2$ to Ni(II)-(Br)$_2$ with LiBr.



Supplementary Figure 29. Paramagnetic ^{1}H NMR spectra upon mixing (**L4**)Ni(OPiv)$_2$ with LiBr (4 equiv) indicating full conversion of (**L4**)Ni(OPiv)$_2$ to (**L4**)NiBr$_2$. (**L4**)NiBr$_2$ (red).

Reaction between (L4)Ni(OPiv)$_2$, Zinc and LiBr

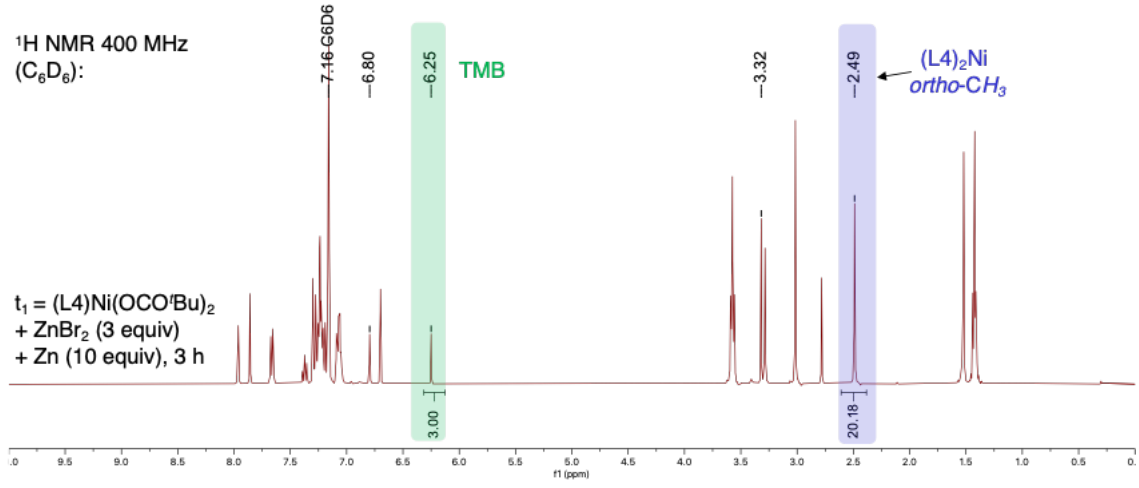
Quantified by ^{1}H NMR. In the glovebox, (**L4**)Ni(OPiv)$_2$ (12 mg, 0.02 mmol), L4 (18 mg, 0.05 mmol, 2.5 equiv), LiBr (9 mg, 0.1 mmol, 4 equiv) and zinc (13 mg, 0.20 mmol, 10 equiv) were added to a 4 mL vial. A stir bar was added, and the vial was charged with 1 mL of THF-d_8 and stirred at 900 rpm. After 1 hour, the suspension was filtered through a celite plug. To this solution, a stock solution of TMB in THF-d_8 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in 80 % yield. Conclusion: This is consistent with full reduction of Ni(II) to Ni(0) with Zn. Excess ligand was used to prevent ligand sequestering by coordinatively unsaturated Zn salts.



Supplementary Figure 30. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting (**L4**)Ni(OPiv)$_2$ with LiBr (4 equiv) and zinc (10 equiv). Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

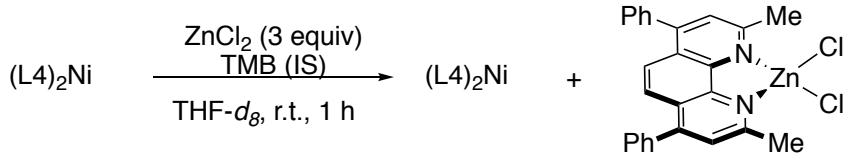
Reaction between (L4)Ni(OPiv)$_2$, Zinc and ZnBr$_2$

Quantified by ^{1}H NMR. In the glovebox, (**L4**)Ni(OPiv)$_2$ (13 mg, 0.02 mmol), **L4** (42 mg, 0.12 mmol, 5.9 equiv), ZnBr$_2$ (15 mg, 0.07 mmol, 3 equiv) and zinc (14 mg, 0.21 mmol, 10 equiv) were added to a 10 mL vial. A stir bar was added, and the vial was charged with 3 mL of THF and stirred at 900 rpm. After 3 hours, the solvent was removed and redissolved in 1.5 mL of C_6D_6 which was then filtered through a celite plug. To this solution, a stock solution of TMB in C_6D_6 was added and the integral ratio of TMB to (**L4**)$_2$Ni was measured by ^{1}H NMR to determine (**L4**)$_2$Ni had formed in a quantitative yield. Conclusion: This is consistent with ZnBr$_2$ undergoing anion exchange with Ni(II)-OPiv species which enables the full reduction of Ni(II) to Ni(0) with Zn. Excess ligand was used to prevent ligand sequestering by coordinatively unsaturated Zn salts.



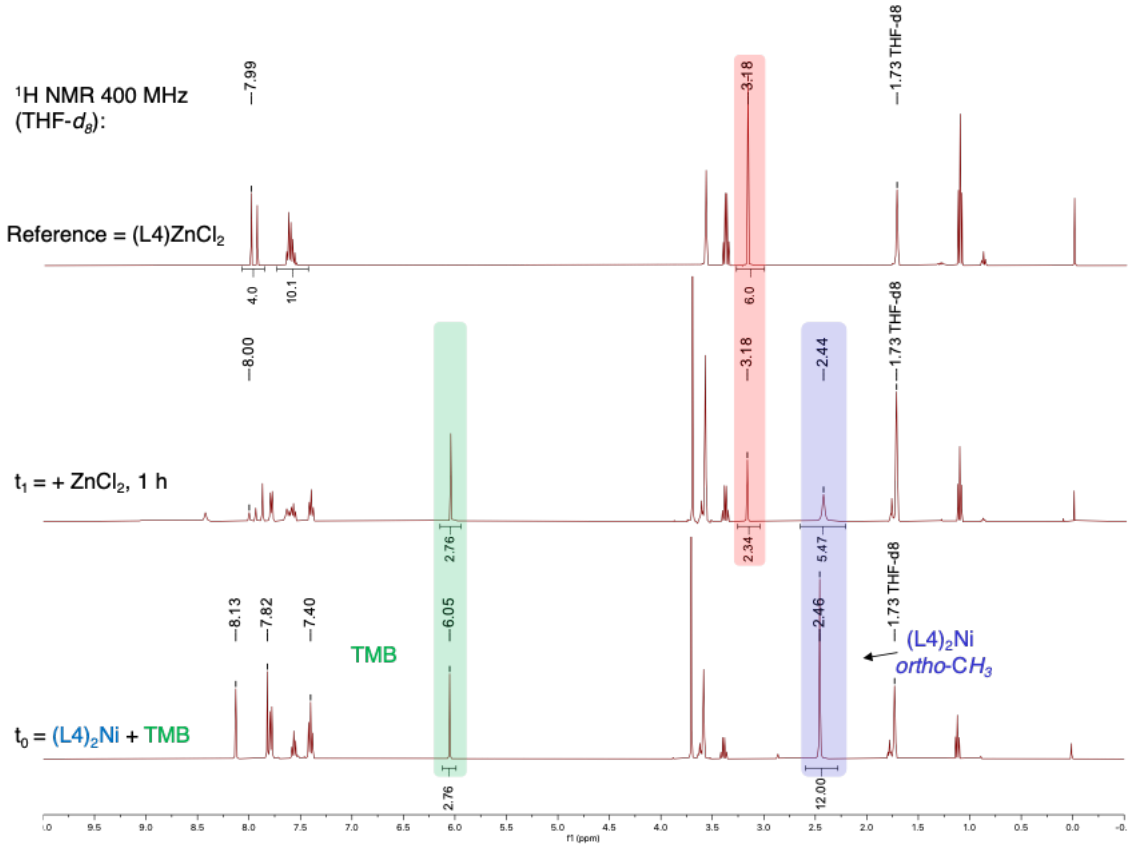
Supplementary Figure 31. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni after reacting (**L4**)Ni(OPiv)$_2$ with ZnBr$_2$ (3 equiv) and zinc (10 equiv). Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

Reaction between $(L4)_2Ni$ and Zinc Chloride



Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, $(\mathbf{L4})_2Ni$ (11.2 mg, 0.01 mmol) and TMB (2 mg, internal standard) were added to a 4 mL vial with 1.5 mL of THF-d_8. The solution was transferred to a J-Young NMR tube and the initial integration of $(\mathbf{L4})_2Ni$ and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing $ZnCl_2$ (5.6 mg, 0.04 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. After 1h, $(\mathbf{L4})_2Ni$ remained (46 %) along with formation of $(\mathbf{L4})ZnCl_2$ (39 %) with no paramagnetic species generated (Supplementary Figure 32. t1. Conclusion: This is consistent with ligand sequestering of $ZnCl_2$ from $(\mathbf{L4})_2Ni$.

Independent synthesis of $(L4)ZnCl_2$. In the glovebox, $ZnCl_2$ (66 mg, 0.48 mmol), L4 (177 mg, 0.49 mmol, 1.02 eq) were added to a 10 mL vial with a stirbar. The vial was charged with THF (3 mL) to afford a yellow suspension that was stirred overnight to afford a white suspension. After 16 h the suspension was filtered and washed with THF (1 mL) and pentane (3 ml x 2) and dried under vacuum to afford $(\mathbf{L4})ZnCl_2$ (88 mg, 37 % yield) as a white solid. **^{1}H NMR** (400 MHz, THF-d_8) δ 7.99 (s, 2H), 7.93 (s, 2H), 7.74 – 7.45 (m, 11H), 3.17 (s, 6H).

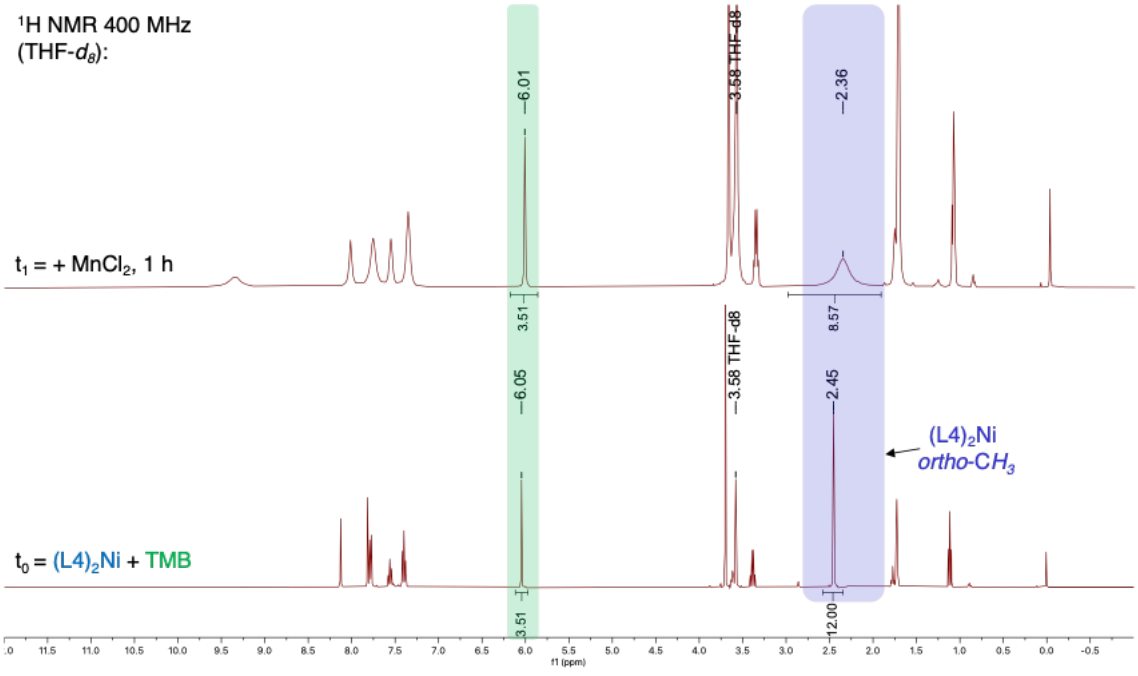


Supplementary Figure 32. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni indicating ligand sequestering by $ZnCl_2$ from (**L4**)$_2$Ni. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue), (**L4**)$ZnCl_2$.

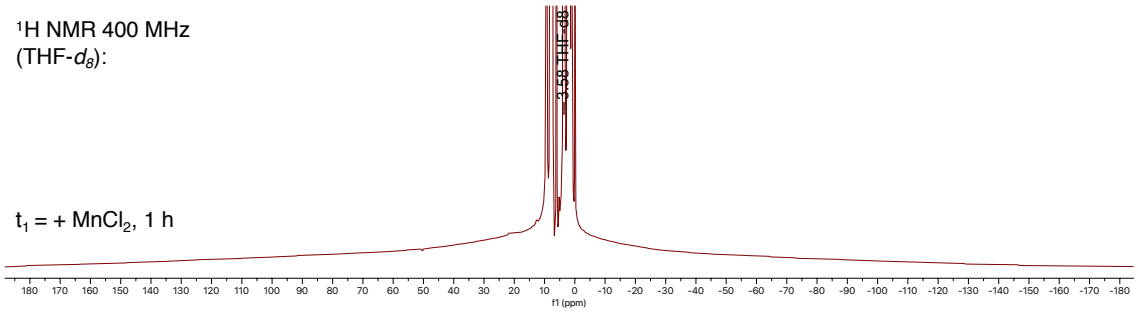
Reaction between (L4)$_2$Ni and Manganese Chloride

$$(L4)_2Ni \xrightarrow[\text{THF-}d_8\text{, r.t., 1 h}]{MnCl_2\ (3\ \text{equiv})\ \text{TMB (IS)}} (L4)_2Ni + \text{other species}$$

Monitored by quantitative ^{1}H NMR and paramagnetic ^{1}H NMR. In the glovebox, (**L4**)$_2$Ni (10.0 mg, 0.01 mmol) and TMB (2 mg, internal standard) were added to a 4 mL vial with 1.5 mL of THF-d_8. The solution was transferred to a J-Young NMR tube and the initial integration of (**L4**)$_2$Ni and TMB was recorded. The J-Young NMR tube was brought back into the glovebox and added to a vial containing $MnCl_2$ (4.3 mg, 0.03 mmol) and stirred for 1 h before transferring back into the J-Young NMR tube and analyzed by ^{1}H NMR. After 1h, (**L4**)$_2$Ni remained (71 %) with no paramagnetic species observable. Conclusion: This is consistent with ligand sequestering of $MnCl_2$ from (**L4**)$_2$Ni, in which the Mn complexes formed are either insoluble or have very broad paramagnetic ^{1}H NMR spectra. A very broad paramagnetic spectra would be consistent with low spin d^5 complex (L4)$MnCl_2$. The existence of these paramagnetic species is also consistent with extensive line broadening observed in the diamagnetic ^{1}H NMR spectra.



Supplementary Figure 33. Quantitative ^{1}H NMR spectra of TMB and (**L4**)$_2$Ni indicating ligand sequestering by $MnCl_2$ from (**L4**)$_2$Ni. Internal standard trimethoxybenzene, TMB (green) and (**L4**)$_2$Ni (blue).

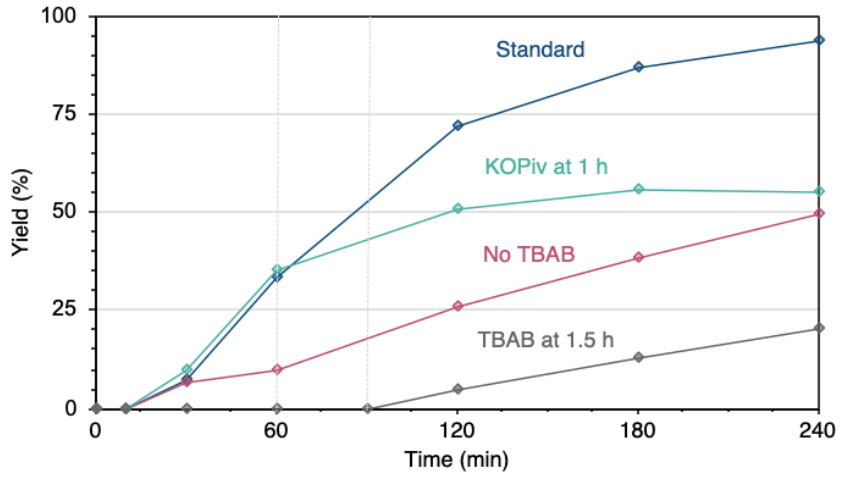


Supplementary Figure 34. Paramagnetic ^{1}H NMR spectra indicating no oxidation of (**L4**)$_2$Ni to [(**L4**)$_2$Ni]Cl.

Catalytic reactions

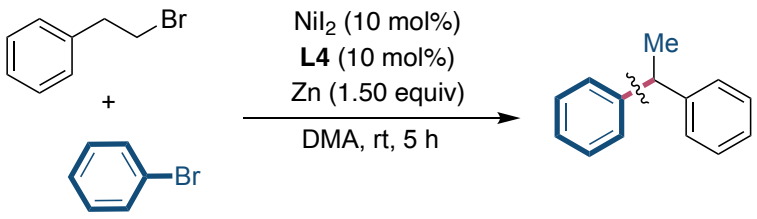
Migratory reductive coupling of aryl and alkyl bromides using L4

Representative Procedure: In the glovebox NiI_2 (8 mg, 0.025 mmol, 10 mol%) and L4 (9 mg, 0.025 mmol, 10 mol%) or (**L4**)Ni(OPiv)$_2$ (16 mg, 0.025 mmol, 10 mol%) were added to a 10 mL vial. In addition, zinc dust (25 mg, 0.38 mmol, 1.5 equiv.), *n*-Bu_4NBr (81 mg, 0.25 mmol, 1.0 equiv.) and KOPiv (35 mg, 0.25 mmol, 1 equiv) when applicable, were added with DMA (1 mL). In a separate 4 mL vial a stock solution of decane (72 mg, 0.5 mmol) and (2-bromoethyl)benzene (93 mg, 0.5 mmol) was dissolved in 2 mL DMA from which 1 mL (0.25 mmol, 1 equiv.) was added to the reaction vial, additionally 50 µl aliquot of the stock solution was removed for GC-FID analysis to establish an initial ratio of starting material to internal standard. Finally, aryl bromide (47 mg, 0.3 mmol, 1.2 equiv.) was added to the reaction vial. The reaction was stirred at 900 rpm at room temperature for 5 h in the glovebox. At given time intervals reaction monitoring was carried out by quenching 50 µl aliquots with HCl, after dilution with EtOAc and filtration, samples were analyzed by GC-FID to determine conversion of starting material and yield of cross coupled product.

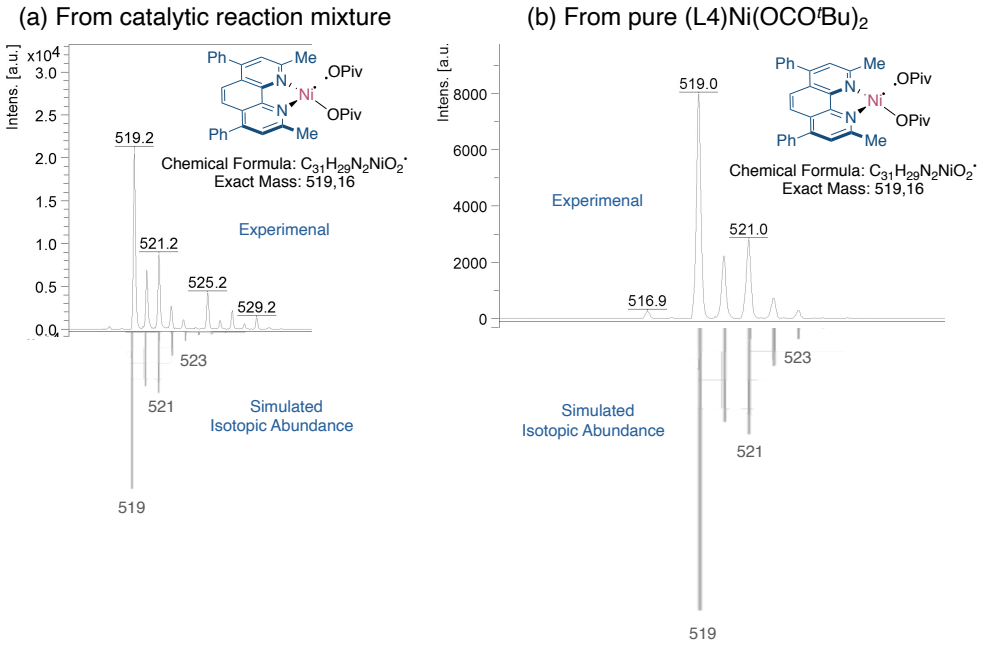


Supplementary Figure 35. Monitoring the reductive cross-coupling of alkyl bromides and aryl bromides by GC-FID.

Poisoning Experiments: Following the representative procedure as above using 0.5 mmol (2-bromoethyl)benzene without TBAB and decane added, the reactions were performed with additives (KOPiv (14 mg, 20 mol %), NaOPh (12 mg, 20 mol %), NaOCOPh (14 mg, 20 mol %)) from the onset and analyzed by ^{1}H NMR after 5 hours. In each case a significant reduction in yield is observed when compared to the reaction monitored without TBAB (Supplementary Figure 35, pink trace).

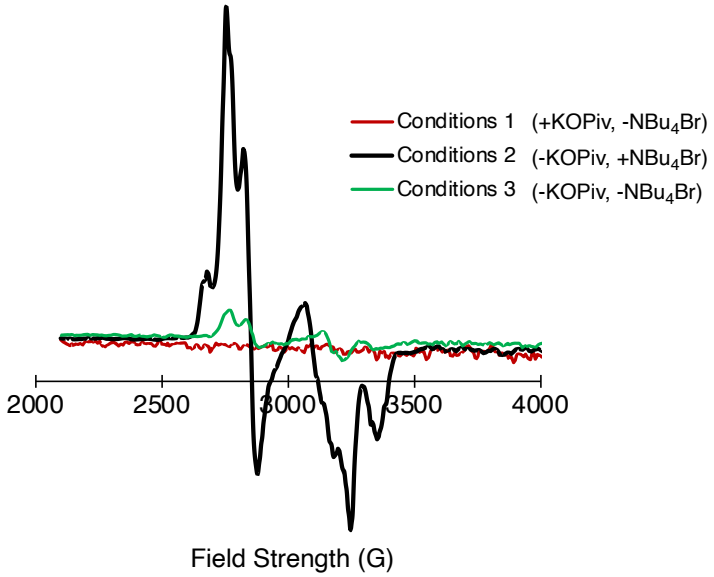


Entry	Deviation from standard conditions	Yield (%)
1	0.4 equiv KOPiv	16
2	0.4 equiv NaOPh	20
3	0.4 equiv NaOCOPh	8



Supplementary Figure 36. MALDI-MS spectra of (**L4**)Ni(OPiv)$_2$. (a) Mass fragment of (**L4**)Ni(OPiv)$_2$ from the standard reaction with added potassium pivalate after 2 hours. (b) Mass fragment of isolated (**L4**)Ni(OPiv)$_2$.

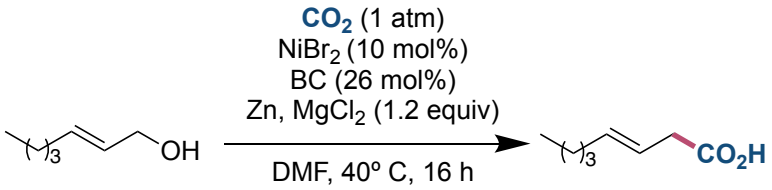
EPR analysis: 3 sets of experiments were performed and analyzed by EPR following the representative procedure as above using 0.5 mmol (2-bromoethyl)benzene to gain additional information about Ni speciation. In each experiment, the reaction was stirred at 900 rpm at room temperature for 2 h in the glovebox. A 0.5 mL aliquot was taken and diluted with 0.5 mL THF and analyzed by EPR (–196°C). *Experiment 1*: Added KOPiv (35 mg, 1 equiv), without NBu$_4$Br *Experiment 2*: Without KOPiv, with NBu$_4$Br (81 mg, 1 equiv). *Experiment 3*: Without KOPiv and without NBu$_4$Br. **Analysis:** In experiments 2 and 3 that do not contain KOPiv, an EPR signal is observed that is consistent with a resting state Ni(I) species. While the exact operative mechanism is still ambiguous and we are unsure of the exact nature of this species, we identify it is not [(L4)$_2$Ni]Br as the spectra do not match and could not identify an analogous EPR spectra reported in the literature. In the reaction conditions with KOPiv added, no EPR signal is observed which we suspect is due to anion exchange with this resting state complex followed by disproportionation as MALDI-MS of the reaction previously identified the formation of (**L4**)Ni(OPiv)$_2$.



Supplementary Figure 37. Continuous wave (CW) X-Band EPR spectra of the various reaction conditions with KOPiv or NBu_4Br added.

Catalytic carboxylation of allylic alcohols with CO_2 using L4

Representative Procedure: In the glovebox to an oven-dried schlenk tube containing a stirring bar was added $NiBr_2DME$ (6 mg, 0.020 mmol, 10 mol%) and L4 (19 mg, 0.052 mmol, 26 mol%) or (**L4**)$Ni(OPiv)_2$ (12 mg, 0.020 mmol, 10 mol%) and L4 (12 mg, 0.032 mmol, 16 mol%). Additionally, Zn dust (14 mg, 0.240 mmol, 1.2 equiv.), $MgCl_2$ (19 mg, 0.200 mmol, 1 equiv.) and KOPiv (34 mg, 0.240 mmol, 1.2 equiv.) were added when applicable. The tube was taken out of the glovebox and connected to a Schlenk line where it was evacuated and back-filled under CO_2 flow 3 times. (E)-oct-2-en-1-ol (26 mg, 0.200 mmol, 1 equiv.), and DMF (2 mL) were added under CO_2 flow. Once added, the schlenk tube was closed under a flow of CO_2 (approx. 1 bar overpressure) and stirred at 40 ºC for 16 h. The mixture was quenched with 2M HCl and diluted with EtOAc. An aliquot of the solution was analyzed by ^{1}H-NMR spectroscopy using TMB as internal standard to determine the yield of the expected product.



Entry	Deviation from standard conditions	Yield (%)[a]
1	None	64
2	No $MgCl_2$	15
3	0.4 equiv KOPiv, No $MgCl_2$	9
4	$Ni(OPiv)_2$ i.o. $NiBr_2$, No $MgCl_2$	0
5	$Ni(OPiv)_2$ i.o. $NiBr_2$	45
6	$Ni(COD)_2$ i.o. $NiBr_2$, No $MgCl_2$	0
7	$Ni(COD)_2$ i.o. $NiBr_2$	61

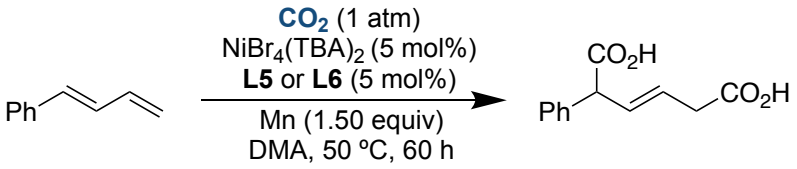
Supplementary Figure 38. Various conditions of the reductive carboxylation of allylic alcohols with CO_2. [a] ^1H NMR yields using 1,3,5-trimethoxybenzene as internal standard. i.o., instead of.

Catalytic carboxylation of dienes with CO_2 using L5 and L6

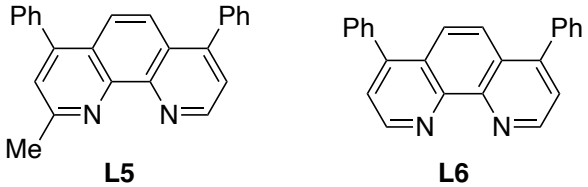
Preface: Extending these results to reductive coupling reactions that form Ni-carboxylate complexes on-cycle with different *N*-based ligands than we used in this case study we investigated the reductive carboxylation of dienes with CO_2.[5] In this report the authors performed control experiments (Supplementry Table 1 entries 1, 2, 3) that highlighted the importance of halide sources for productive catalysis using 2-methyl-4,7-diphenyl-1,10-phenanthroline (L5) which we show below for convenience (Supplementary Figure 39). Halide containing precatalyst $NiBr_4(TBA)_2$ was optimal (Supplementary Figure 39, entry 1) but importantly, no product was obtained without inorganic halide sources (i.e using $Ni(COD)_2$ without TBAB; Supplementary Figure 39 entry 2) and catalytic activity could be recovered by adding TBAB as a halide source (60 % yield, Supplementary Figure 39 entry 3). They further show non-ortho substituted phenathroline ligands could afford the dicarboxylated product (56 % yield, Supplementary Figure 39 entry 4). Investigating if these reactivity trends extended to non-ortho substituted ligands, entry 4 was repeated which afforded the dicarboxylated product formed in 52 % yield and using $Ni(COD)_2$ as the precatalyst afforded no product (Supplementary Figure 39 entry 5) consistent with inorganic halide sources being a requirement for productive catalysis in reductive carboxylation reactions that form on-cycle Ni-carboxylate complexes with **L4** (bathocuproine), **L5** (2-methyl-4,7-diphenyl-1,10-phenanthroline) and **L6** (bathrophenanthroline).

Representative Procedure: An oven-dried Schlenk tube equipped with a magnetic stirring bar was charged with Mn dust (16.5 mg, 0.3 mmol, 1.5 equiv), ligand (either 2-methyl-4,7-diphenyl-1,10-phenanthroline (L5) (3.5 mg, 0.01 mmol, 0.05 equiv) or bathrophenanthroline (L6) (3.3 mg, 0.01 mmol, 0.05 equiv) and Ni source (0.01 mmol, 0.05 equiv). The schlenk tube was filled with carbon dioxide by applying three cycles of evacuation and filling with CO_2. Subsequently, 1-phenyl-1,3-butadiene (1a, 0.20 mmol, 1 equiv) was added by syringe followed by DMA (0.40 mL) with a constant flow of CO_2. The Schlenk flask was tightly sealed and stirred at 50 ºC for 60 hours after which it was quenched by careful addition of 2 M aq. HCl sol and internal standard

added. The crude was extracted with EtOAc, and a sample of such solution was concentrated and analyzed by ^{1}H NMR.



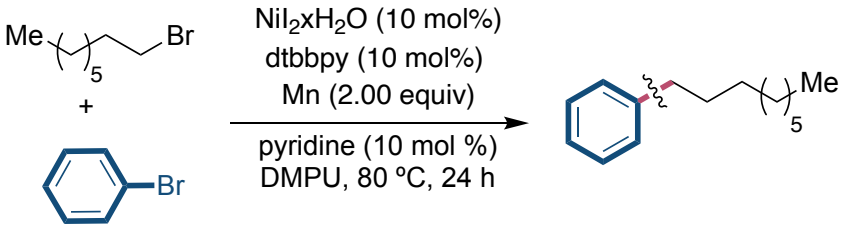
Entry	Deviation from standard conditions	Yield (%)
1	using **L5**,	79[a]
2	using **L5** and $Ni(COD)_2$ i.o. $NiBr_4(TBA)_2$	0[a]
3	$Ni(COD)_2$ and 10 % TBAB	60[a]
4	using **L6**	56[a]
5	using **L6** and $Ni(COD)_2$ i.o. $NiBr_4(TBA)_2$	0[b]



Supplementary Figure 39. Various conditions of the reductive carboxylation of dienes with CO_2. [a] yields from control experiments previously published (Supplementary Table 1, entries 1, 2, 3).[5] [b] ^{1}H NMR yields using 1,3,5-trimethoxybenzene as internal standard. i.o = instead of

Reductive Coupling of Aryl and Alkyl Bromides Using dtbbpy

Representative Procedure: In the glovebox, an oven-dried Schlenk tube equipped with a magnetic stirring bar was charged with Mn dust (54.9 mg, 1.0 mmol, 2.0 equiv), dtbbpy (13.4 mg, 0.05 mmol, 0.1 equiv) and NiI_2xH_2O (20.2 mg, 0.05 mmol, 0.1 equiv), 1-bromooctane (96.6 mg, 0.5 mmol, 1 mmol), phenyl bromide (78.6 mg, 0.5 mmol, 1 equiv), pyridine (4 ul, 0.05 mmol, 0.1 equiv). DMPU was then added and the reaction was heated at 80 ºC for 16 hours after which it was quenched by careful addition of 2 M aq. HCl sol and internal standard TMB added. The crude was extracted with EtOAc, and a sample of such solution was concentrated and analyzed by ^{1}H NMR.

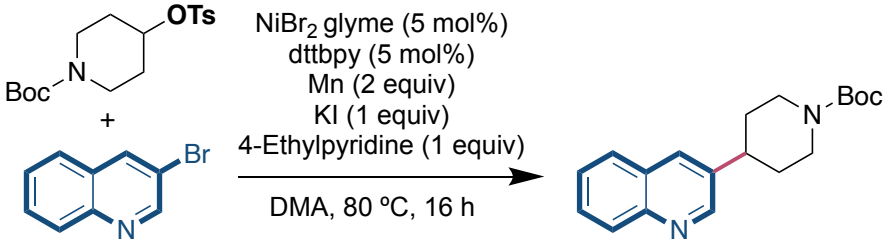


Entry	Deviation from standard conditions	Yield (%)[a]
1	none	60
2	0.2 equiv NaOPh	5
3	0.2 equiv NaOCOPh	5

Supplementary Figure 40. Various conditions of the reductive coupling of aryl and alkyl bromides. [a] ^{1}H NMR yields using 1,3,5-trimethoxybenzene as internal standard.

Reductive Coupling of Aryl Bromides and Alkyl Tosylates Using dtbbpy

Representative Procedure: In the glovebox, an oven-dried Schlenk tube equipped with a magnetic stirring bar was charged with alkyl tosylate (0.1 mmol), $NiBr_2$·glyme (0.005 mmol, 1.5 mg) or $Ni(COD)_2$ (0.005 mmol, 1.4 mg), 4,4′-ditert-butyl-2,2′-bipyridine (0.005 mmol, 1.3 mg), Mn powder (0.2 mmol, 11.0 mg) and when appropriate KI (0.1 mmol, 16.6 mg), and/or potassium pivalate (0.02 mmol, 2.8 mg). Dimethylacetamide (0.5 mL) and 4-ethylpyridine (0.1 mmol, 10.8 mg) were added via syringe, followed by the phenyl bromide (0.1 mmol, 15.7 mg). The reaction was stirred under Ar at 80 °C for 18 h, after which the solution was cooled and diluted with MeCN and filtered through a pad of Celite. This solution was concentrated and a stock solution of TMB in $CDCl_3$ was added as internal standard, and analyzed by ^{1}H NMR.

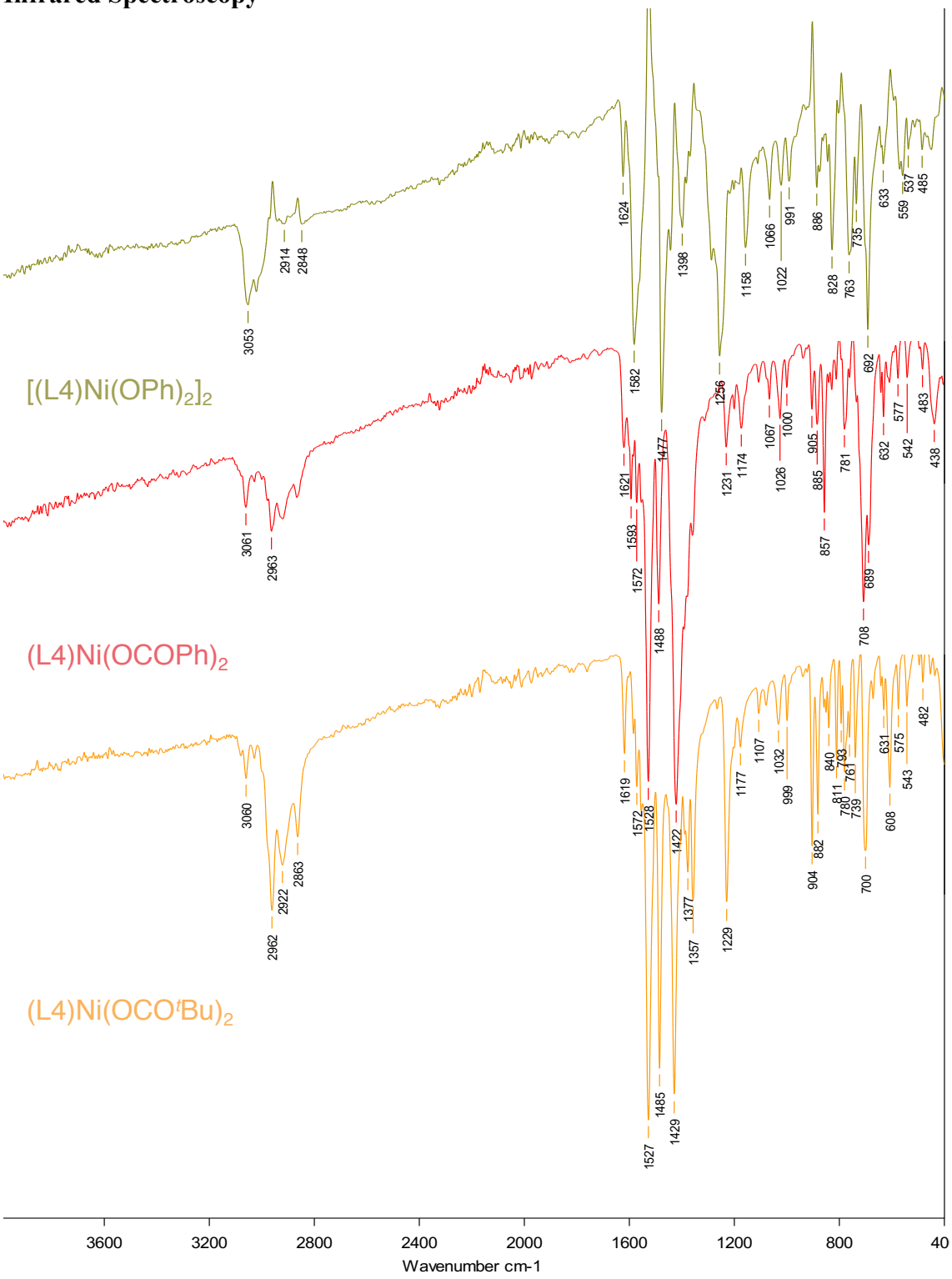


Entry	Deviation from standard conditions	Yield (%)[a]
1	None	75
2	No KI	19
3	0.2 equiv KOPiv, No KI	14
4	0.2 equiv KOPiv	35
5	$Ni(COD)_2$ i.o. $NiBr_2$(glyme), no KI	5
6	$Ni(COD)_2$ i.o. $NiBr_2$(glyme)	56

Supplementary Figure 41. Various conditions of the reductive coupling of aryl bromides and alkyl tosylates. [a] ^{1}H NMR yields using 1,3,5-trimethoxybenzene as internal standard.

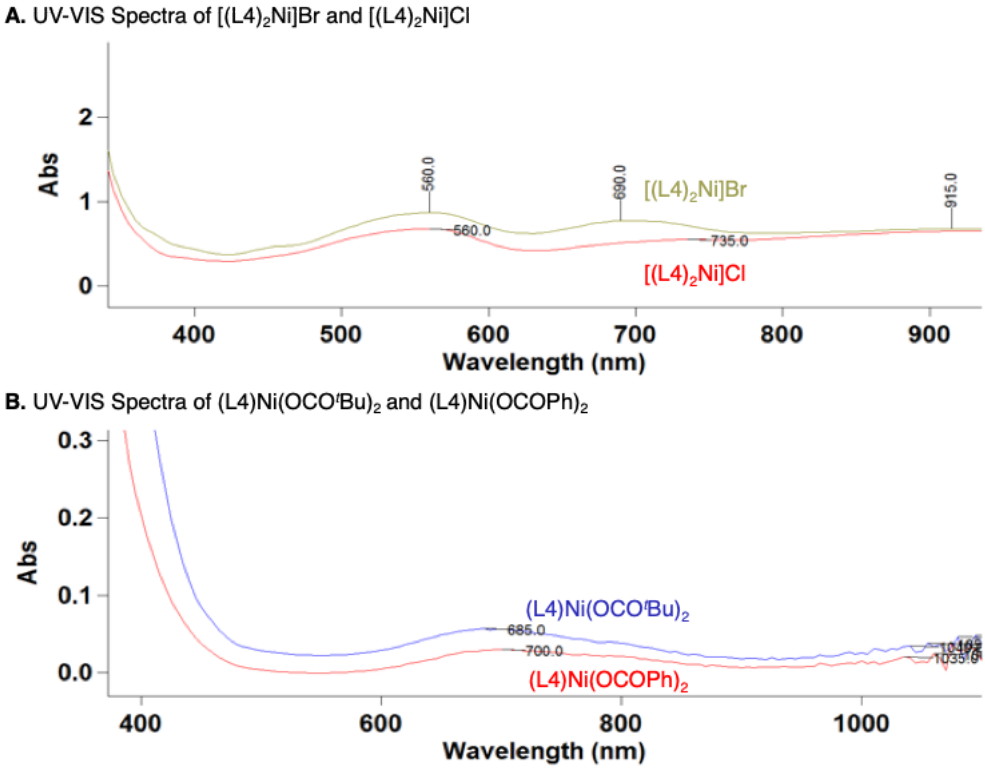
IR, UV-VIS, and Cyclic Voltammetry

Infrared Spectroscopy



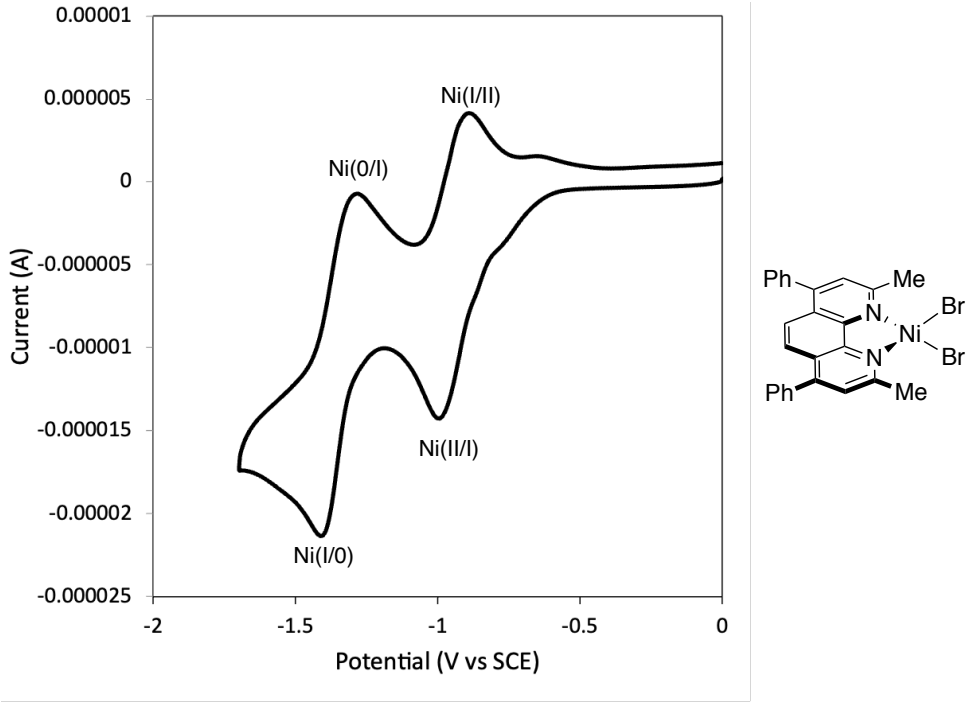
Supplementary Figure 42. Stack IR spectra of [(**L4**)Ni(OPh)$_2$]$_2$, (**L4**)Ni(OCOPh)$_2$, and (**L4**)Ni(OPiv)$_2$.

UV-VIS Spectroscopy

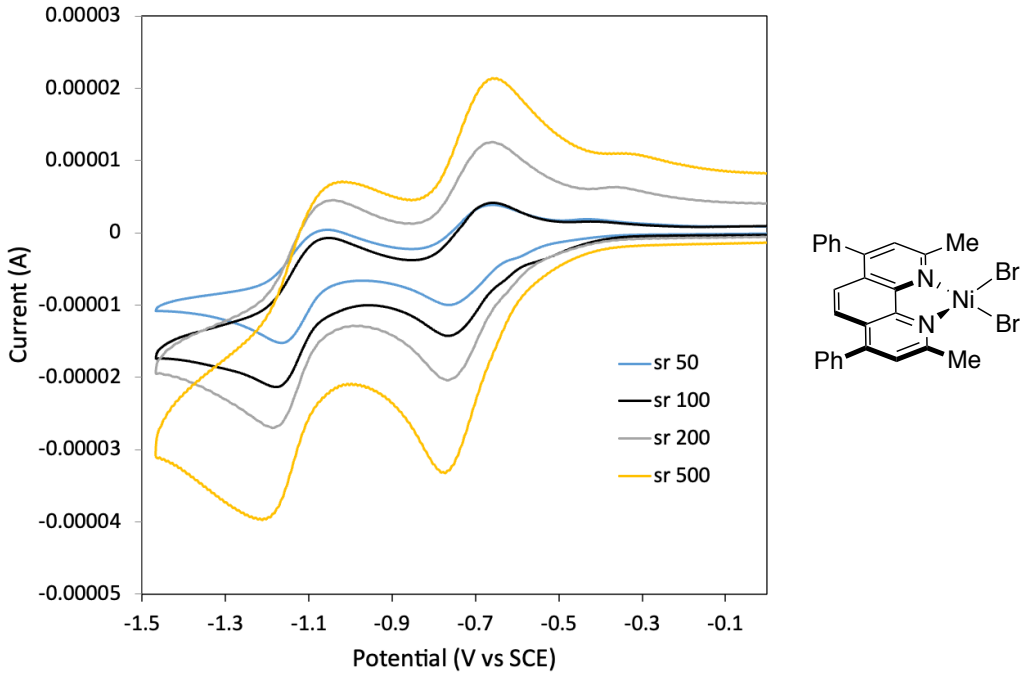


Supplementary Figure 43. UV-VIS spectra of [(**L4**)$_2$Ni]Br, [(**L4**)$_2$Ni]Cl, (**L4**)Ni(OPiv)$_2$ and (**L4**)Ni(OCOPh)$_2$.

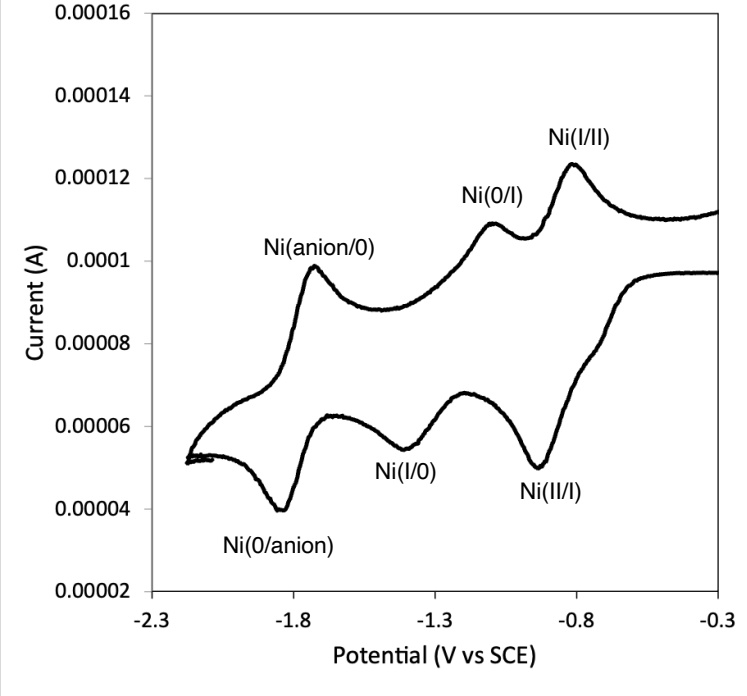
Cyclic Voltammetry



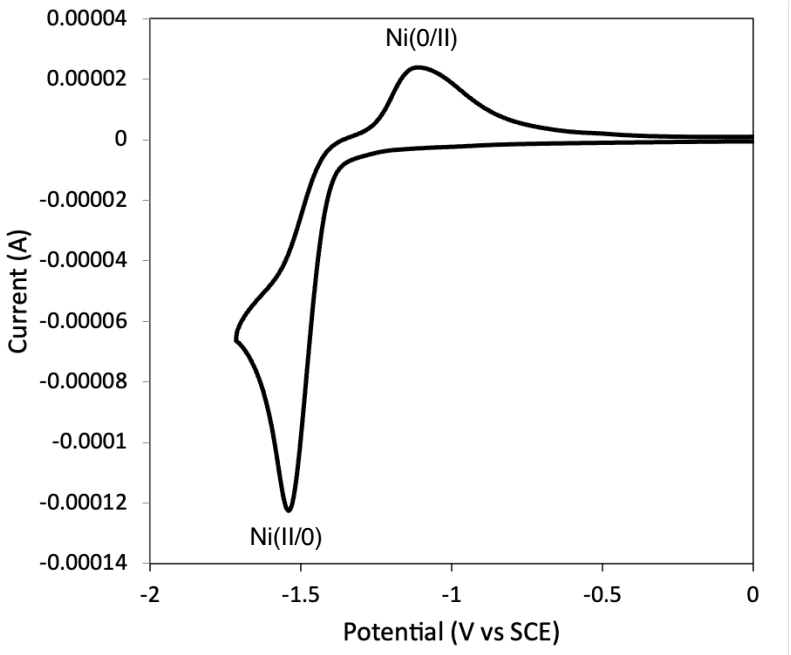
Supplementary Figure 44. Cyclic voltammogram of (**L4**)$NiBr_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][PF_6] supporting electrolyte MeCN solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first; the second cycle is shown here. $E_{1/2}$ values for (L4)$NiBr_2$ are Ni(II)/Ni(I) = -0.71 V, Ni(I)/Ni(0) = -1.10 V. Literature reports CV of 2,9-substituted phen ligated Ni complexes are reported with $E_{p/2}$ values of Ni(II)/Ni(I) = -0.69 V, Ni(I)/Ni(0) = -1.37 V vs SHE in THF.[6]



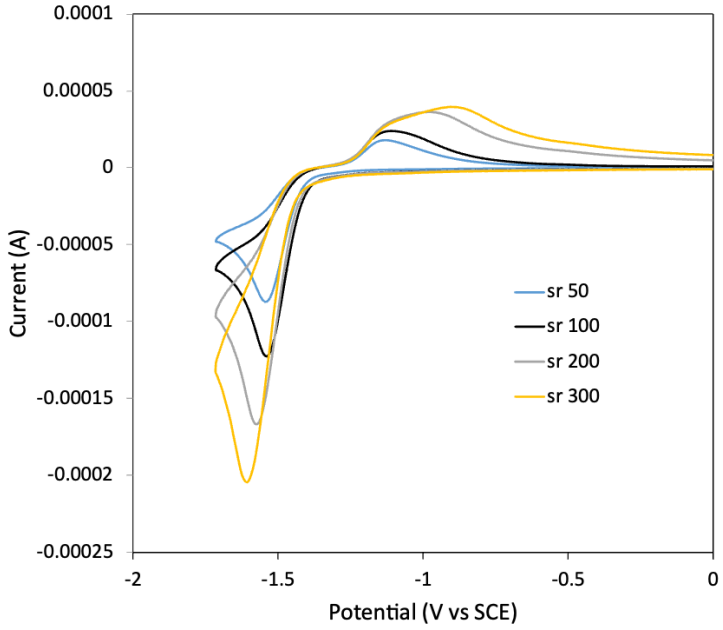
Supplementary Figure 45. Cyclic voltammogram of (**L4**)$NiBr_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][PF_6] supporting electrolyte MeCN solution with a varied scan rates and 0.01 M of sample referenced to Fc (+0.380 V vs SCE).

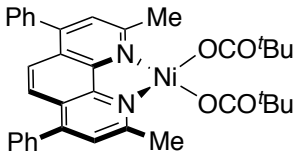


Supplementary Figure 46. Cyclic voltammogram of (**L4**)$NiCl_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][PF_6] supporting electrolyte MeCN solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first; the second cycle is shown here. $E_{1/2}$ values for (**L4**)$NiCl_2$ are Ni(II)/Ni(I) = -0.86 V, Ni(I)/Ni(0) = -1.24 V. While the first reduction $E_{1/2}$ ($Ni^{II/I}$) appears reversible, the second reduction $E_{1/2}$ ($Ni^{I/0}$) appears quasireversible. Reduction of the ligand or to an anionic complex is observed in further reduction.

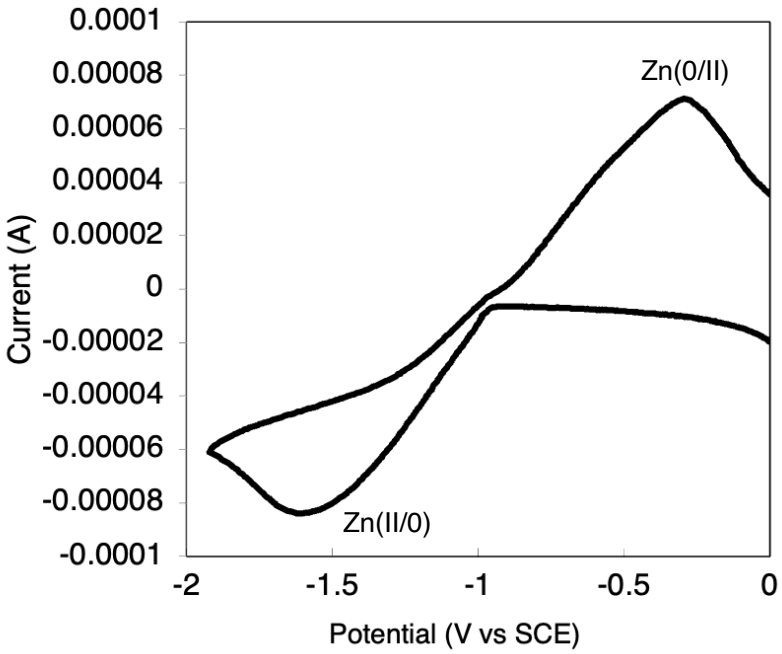


Supplementary Figure 47. Cyclic voltammogram of (**L4**)$Ni(OPiv)_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][PF_6] supporting electrolyte MeCN solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first; the second cycle is shown here. $E_{p/2}$ value for (**L4**)$Ni(OPiv)_2$ are Ni(II)/Ni(0) = -1.43 V. The reduction appears chemically reversible (E_p oxidation = -1.27 V vs SCE) and electrochemically irreversible.



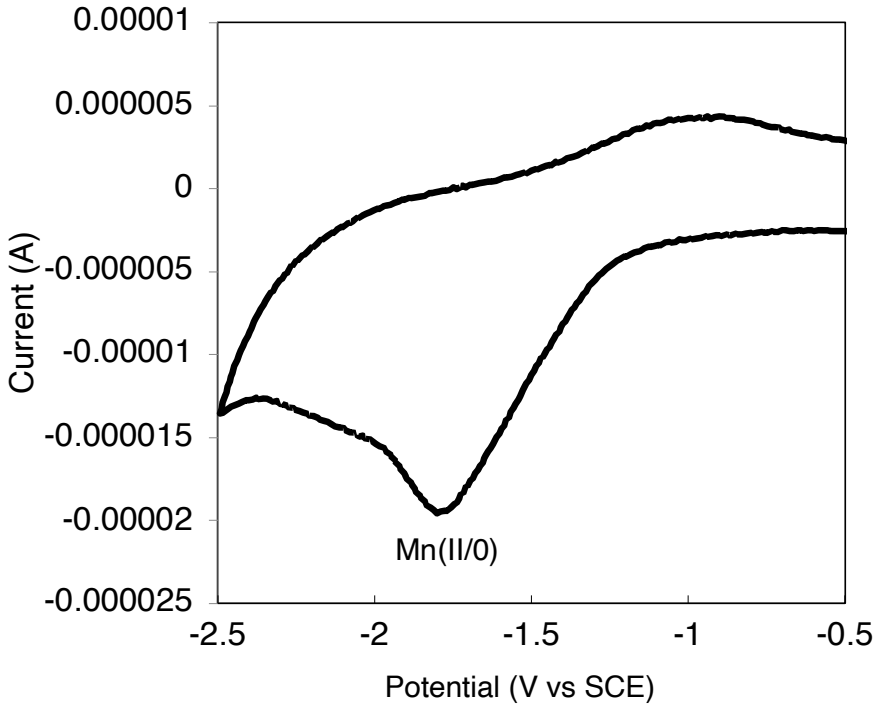


Supplementary Figure 48. Cyclic voltammogram of (**L4**)Ni(OPiv)$_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [^{n}Bu$_4$N][PF$_6$] supporting electrolyte MeCN solution with various scan rates and 0.01 M of sample referenced to Fc (+0.380 V vs SCE).



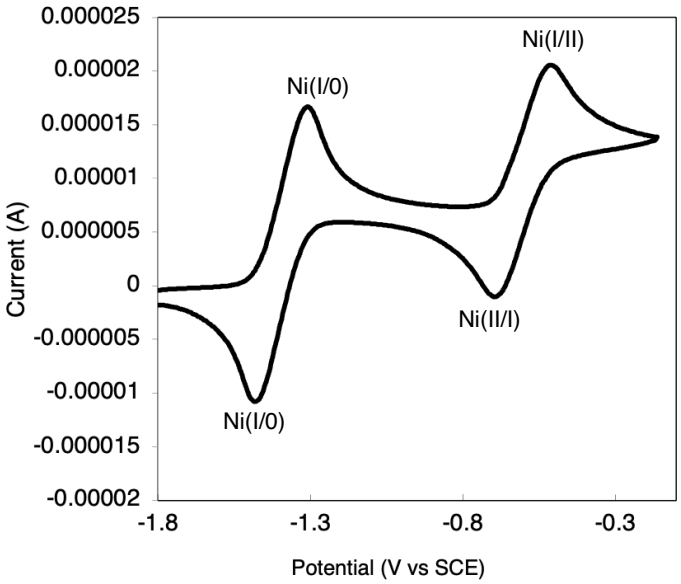
$ZnCl_2(MeCN)_n$

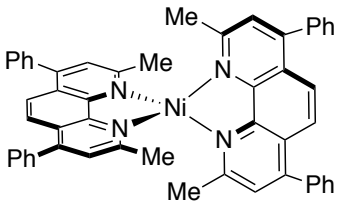
Supplementary Figure 49. Cyclic voltammogram of $ZnCl_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [^{n}Bu$_4$N][PF$_6$] supporting electrolyte MeCN solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first. $E_{p/2}$ values for $ZnCl_2$ are Zn(II)/Zn(0) = -1.26 V vs SCE. The reduction appears chemically reversible (E_p oxidation = -0.26 V vs SCE), and electrochemically irreversible. Literature reports CV of $ZnBr_2$ are reported with $E_{p/2}$ values of Zn(II)/Zn(0) = -1.26 V vs SHE, in DMA.[6]



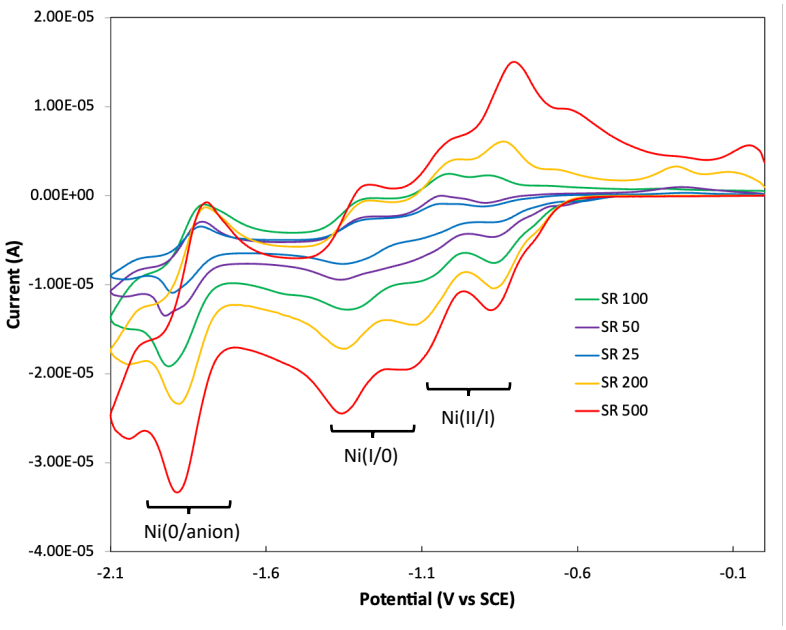
$MnCl_2(MeCN)_n$

Supplementary Figure 50. Cyclic voltammogram of $MnCl_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [^{n}Bu$_4$N][PF_6] supporting electrolyte MeCN solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first. $E_{p/2}$ values for $MnCl_2$ are Mn(II)/Mn(0) = -1.38 V. Unlike the case of $ZnCl_2$, $MnCl_2$ reduction appears chemically irreversible and electrochemically irreversible.

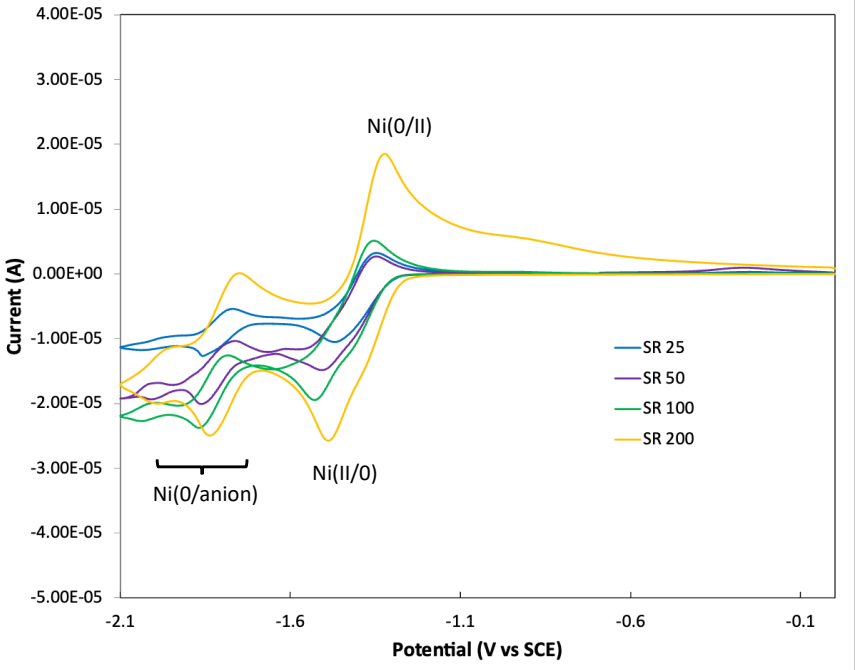




Supplementary Figure 51. Cyclic voltammogram of (**L4**)$_2$Ni. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [^{n}Bu$_4$N][PF_6] supporting electrolyte THF solution with a 100 mV/s scan rate and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the cathodic direction first; the second cycle is shown here. $E_{1/2}$ values for (L4)$_2$Ni are Ni(II)/Ni(I) = -0.59 V, Ni(I)/Ni(0) = -1.39 V. **Note:** This complex studied is poorly soluble in MeCN so CVs were performed in THF.

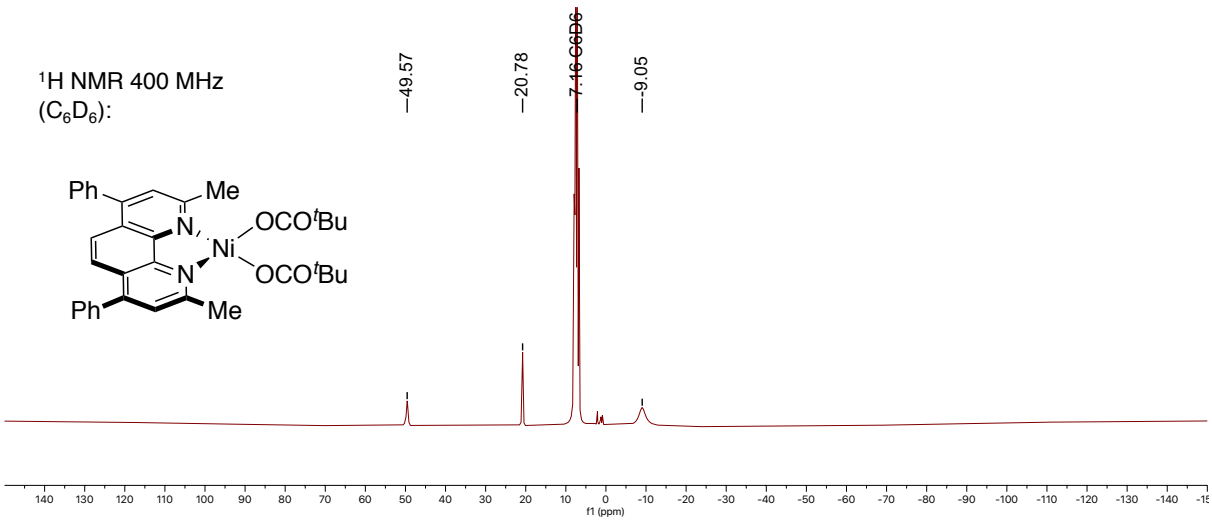


Supplementary Figure 52. Cyclic voltammogram of (**L2**)$NiBr_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][BF_4] supporting electrolyte MeCN solution with varied scan rates and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first; the first cycle is shown here. While the redox steps are less clear for (**L2**)$NiBr_2$ due to the multiple species generated insitu (i.e solvates or higher order species/nickelates), estimates are given as; $E_{1/2}$ values for Ni(II)/Ni(I) = -0.83 V, Ni(I)/Ni(0) = -1.30 V. Literature reports CV of $(bipy)_2Ni$ or $(bipy)_3Ni(ClO_4)_2$ MeCN (0.2 M, TEAP)[7] as two close redox steps from Ni(II/0) at -1.27 V and Ni(0/anion) at -1.97 V vs SCE or $(bipy)NiCl_2$ (MeCN, 0.1 M)[8] as two close redox steps from Ni(II/0) at -1.33 V and Ni(0/anion) at -2.09 V vs SCE.

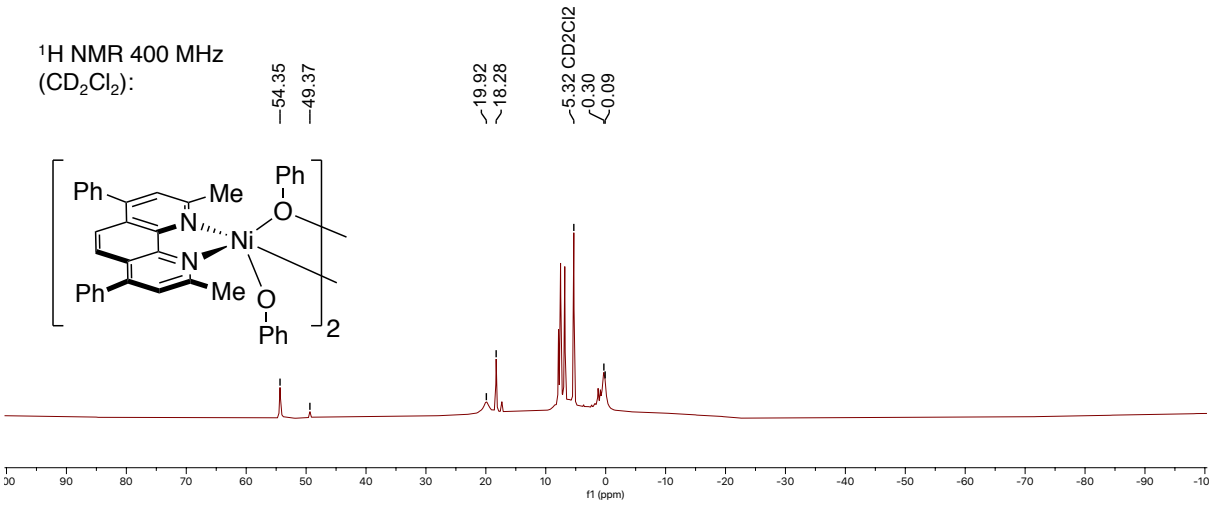


Supplementary Figure 53. Cyclic voltammogram of (**L2**)$Ni(OPiv)_2$. Voltammograms were taken using a glassy carbon working electrode in a 0.1 M [$^nBu_4N$][BF_4] supporting electrolyte MeCN solution with varied scan rates and 0.01 M of sample referenced to Fc (+0.380 V vs SCE). Scans were started at the open-circuit potential and scanned in the anode direction first; the first cycle is shown here. $E_{1/2}$ values for (**L2**)$Ni(OPiv)_2$ are Ni(II)/Ni(0) = -1.48 V vs SCE.

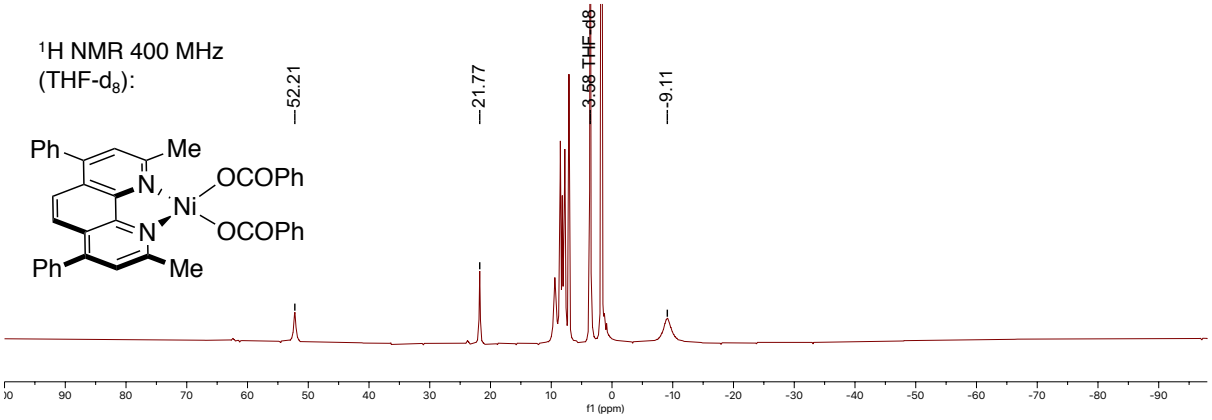
NMR and EPR Spectra of Synthesized Complexes



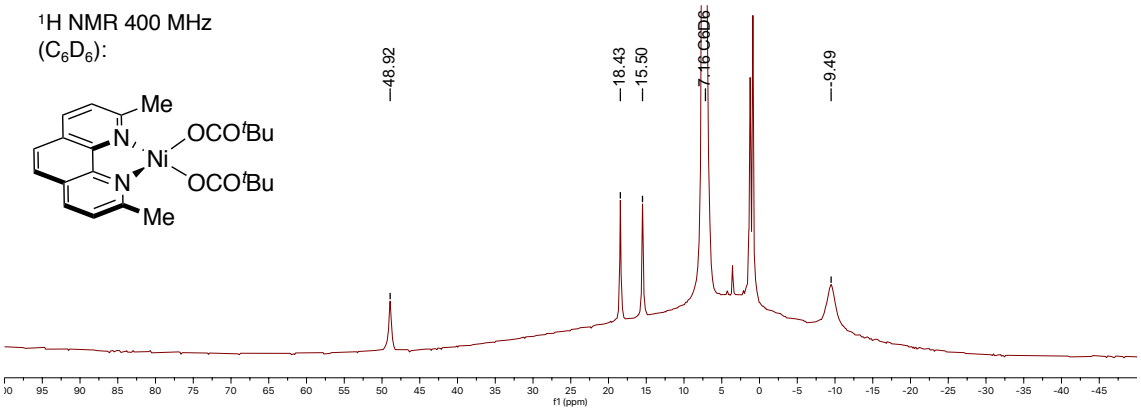
Supplementary Figure 54. NMR spectra (C_6D_6, 400 MHz) of (L4)Ni(OPiv)$_2$.



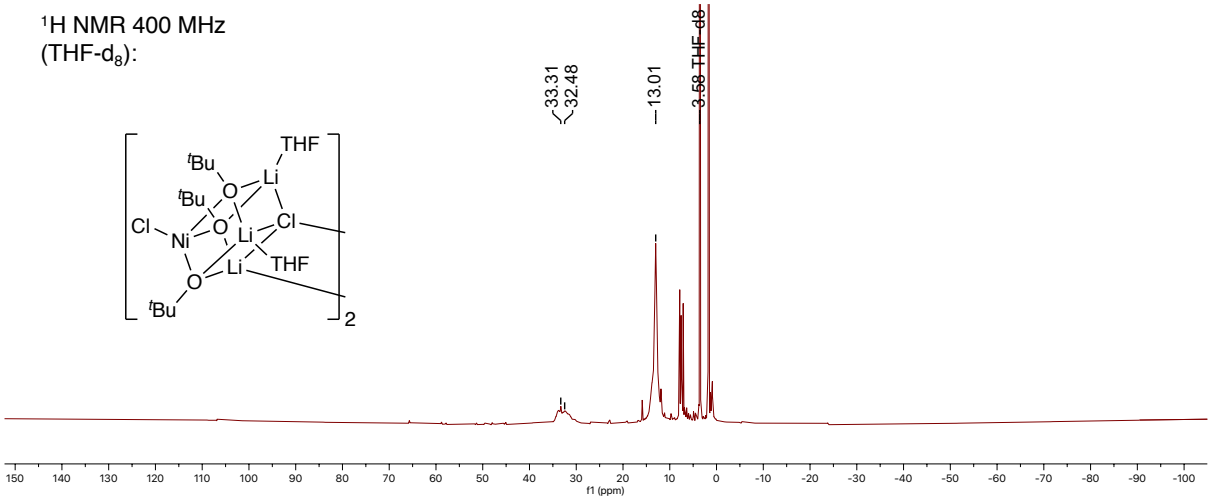
Supplementary Figure 55. NMR spectra (CD_2Cl_2, 400 MHz) of [(**L4**)Ni(OPh)$_2$]$_2$.



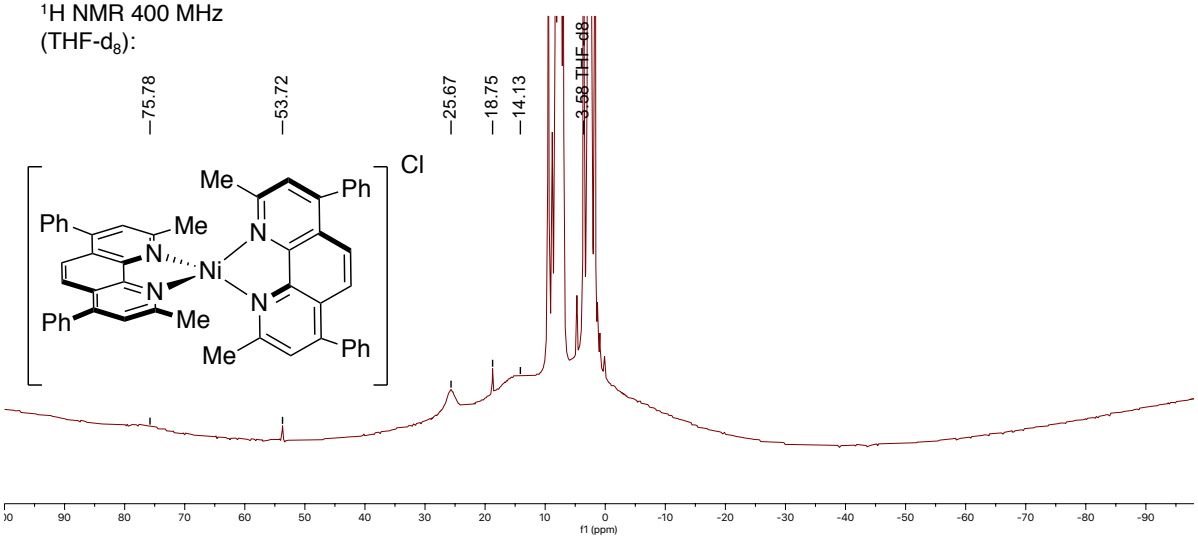
Supplementary Figure 56. NMR spectra (THF-d_8, 400 MHz) of (**L4**)Ni(OCOPh)$_2$.



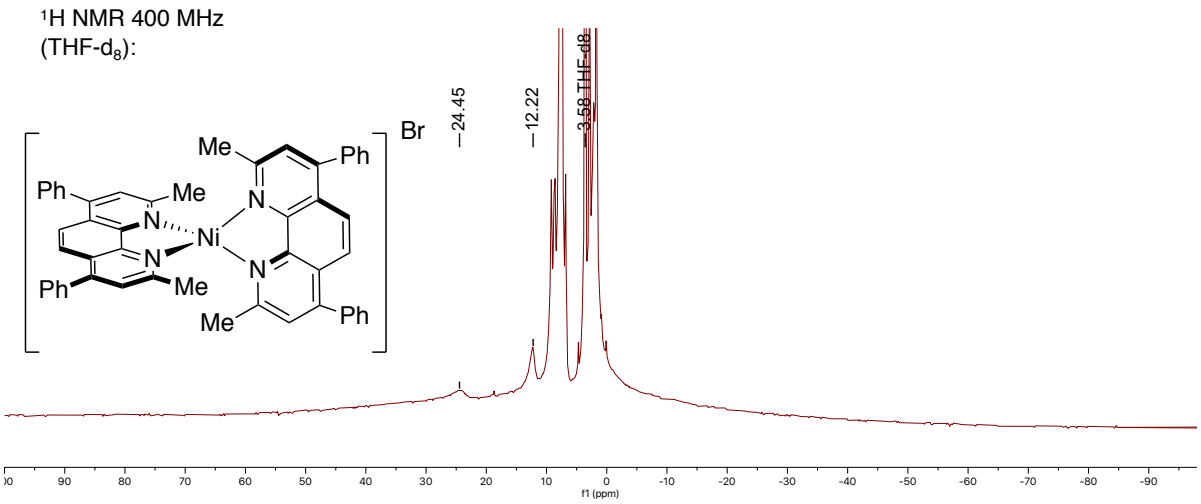
Supplementary Figure 57. NMR spectra (C_6D_6, 400 MHz) of (**L3**)Ni(OPiv)$_2$



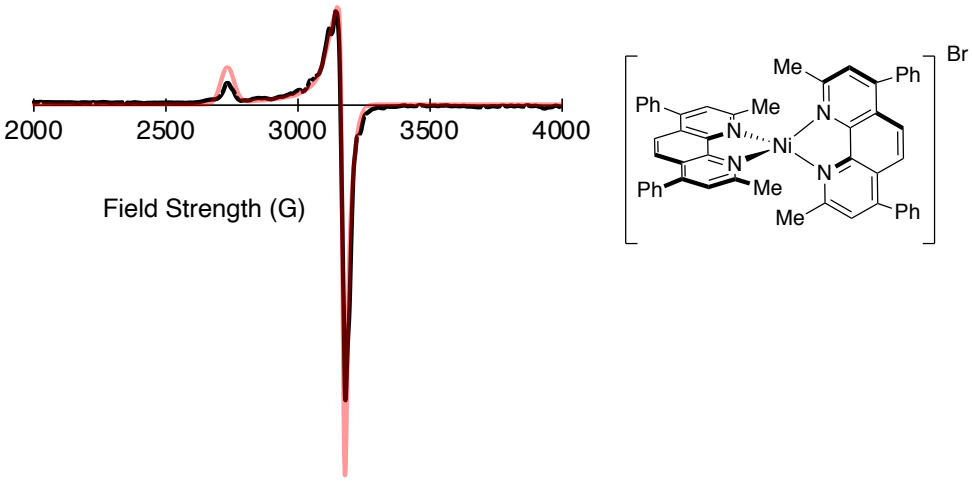
Supplementary Figure 58. NMR spectra (THF-d_8, 400 MHz) of $NiLi_3Cl_2(O^tBu)_3$•2THF.



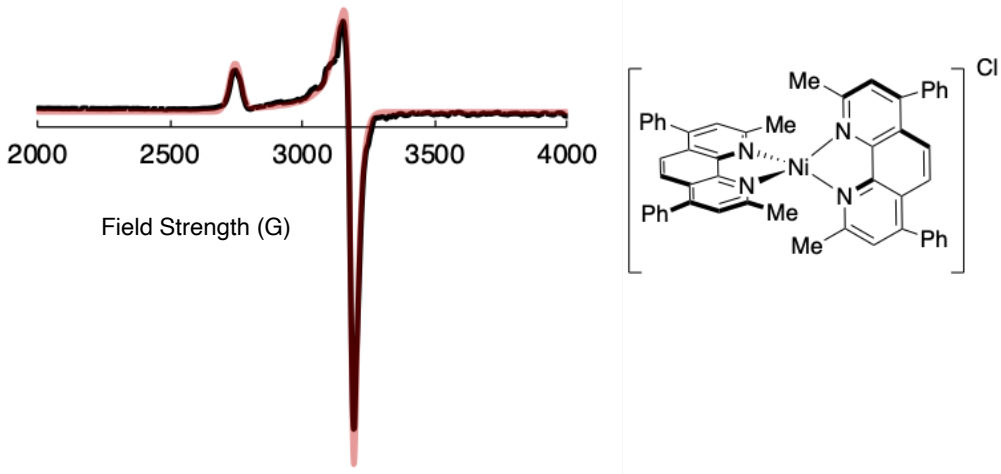
Supplementary Figure 59. NMR spectra (THF-d_8, 400 MHz) of [(**L4**)$_2$Ni]Cl.



Supplementary Figure 60. NMR spectra (THF-d_8, 400 MHz) of [(**L4**)$_2$Ni]Br.



Supplementary Figure 61. Continuous wave (CW) X-Band EPR spectra of [(**L4**)$_2$Ni]Br with g values fit to g(x) = 2.115, g(y) = 2.114, g(z) = 2.456.



Supplementary Figure 62. Continuous wave (CW) X-Band EPR spectra of [(**L4**)$_2$Ni]Cl with g values fit to g(x) = 2.109, g(y) = 2.106, g(z) = 2.445.

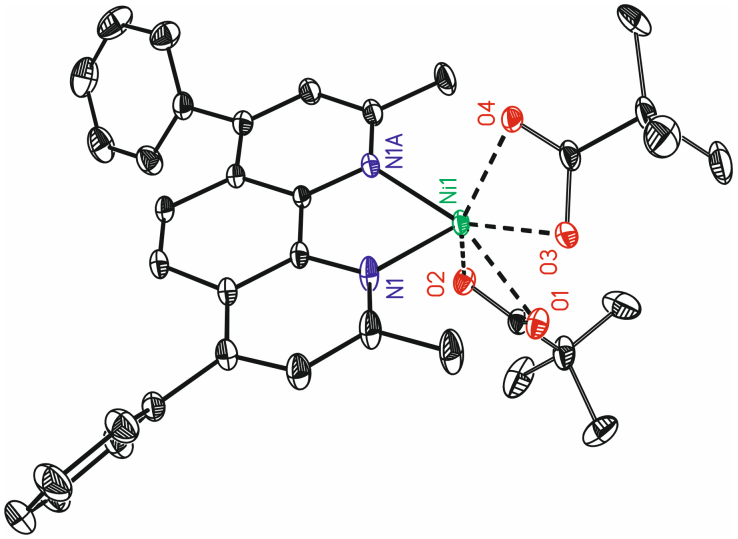
Crystallographic Data

Data collection: The measured crystals were prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation.

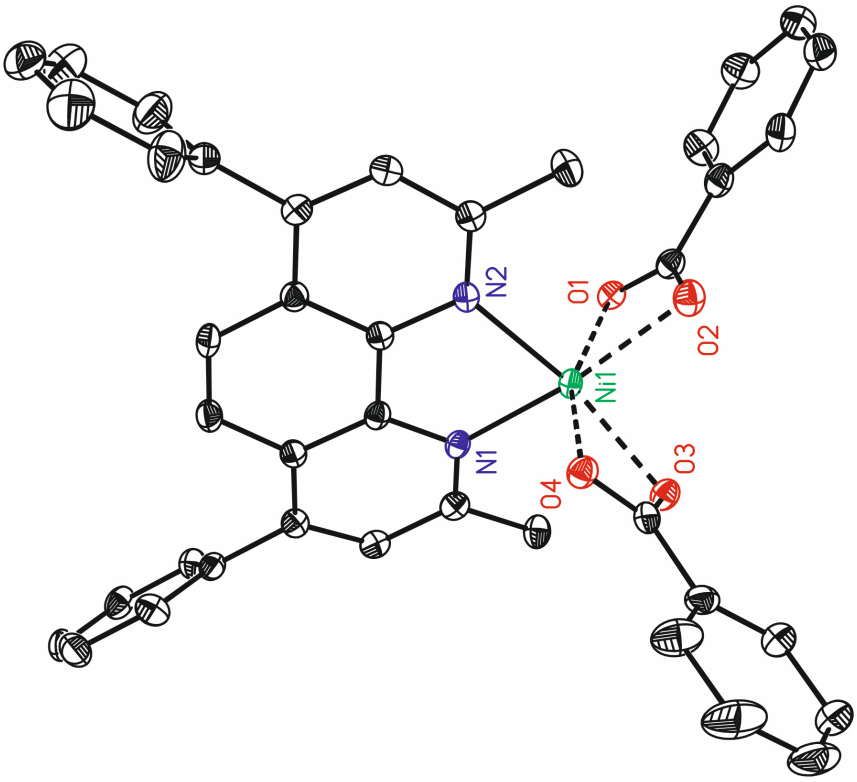
Crystal structure determination for (**L3**)Ni(OPiv)$_2$, (**L4**)Ni(OPiv)$_2$, [NiLi$_3$Cl$_2$(O^{t}Bu)$_3$•2THF]$_2$ and (**L4**)Ni(OCOPh)$_2$ was carried out using a Rigaku diffractometer equipped with a Pilatus 200K area detector, a Rigaku MicroMax-007HF microfocus rotating anode with MoK_α radiation, Confocal Max Flux optics and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = -173 °C). Full-sphere data collection was used with ω and φ scans. *Programs used:* Data collection data reduction with CrysAlisPro[9] and absorption correction with Scale3 Abspack scaling algorithm.[10]

Crystal structure determination for [(**L4**)$_2$Ni]Br, [(**L4**)Ni(OPh)$_3$(THF)]$_2$ and (**L4**)NiBr$_2$ was carried out using an Apex DUO Kappa 4-axis goniometer equipped with an APPEX 2 4K CCD area detector, a Microfocus Source E025 IuS using CuK_α radiation, Quazar MX multilayer Optics as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = -173 °C). Full-sphere data collection was used with ω and φ scans. *Programs used:* Data collection APEX II,[11] data reduction Bruker Saint[12] V/.60A and absorption correction TWINABS.[13-14]

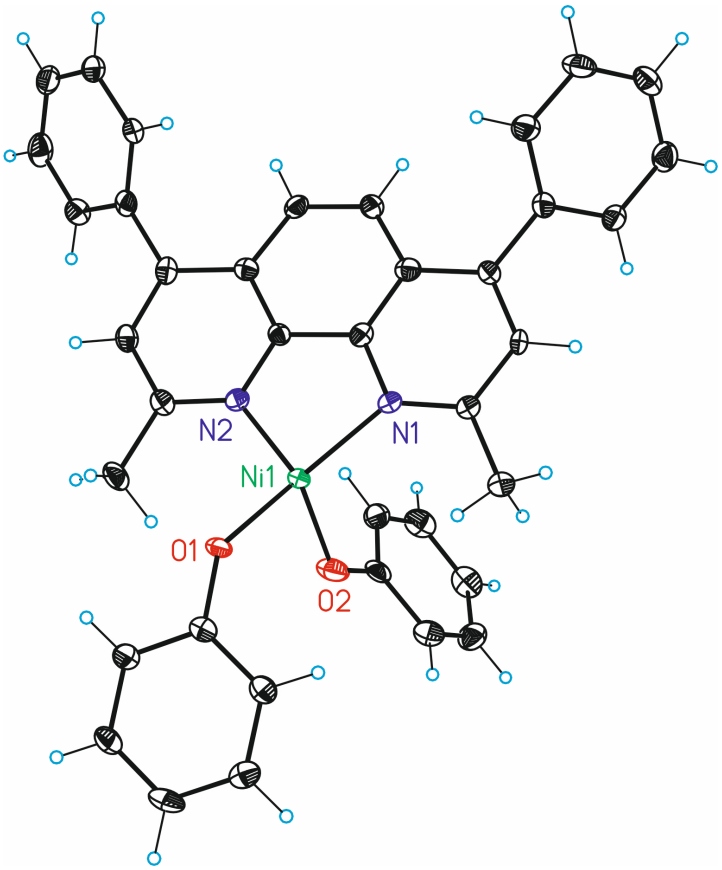
Structure Solution and Refinement: Crystal structure solution was achieved using the computer program SHELXT.[15] Visualization was performed with the program SHELXle.[16] Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F^2 using all measured intensities was carried out using the program SHELXL 2015.[17] All non-hydrogen atoms were refined including anisotropic displacement parameters.



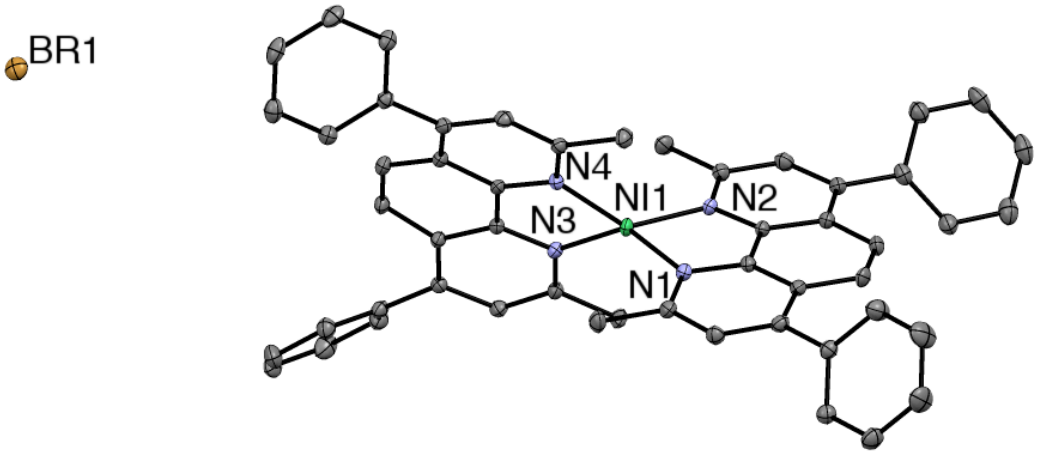
Supplementary Figure 63. ORTEP drawing (50 %) showing (**L4**)Ni(OPiv)$_2$. Hydrogen atoms and disordered parts have been omitted in the sake of clarity. CCDC deposition number **CCDC-2175355.**



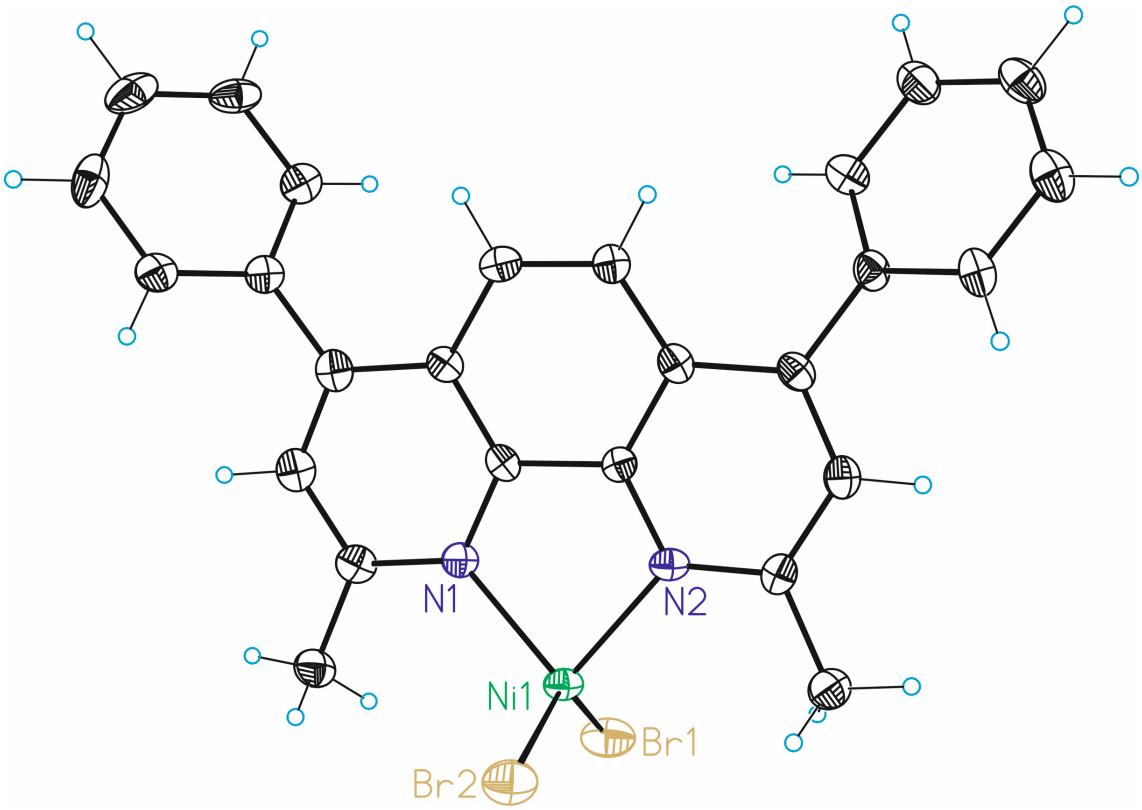
Supplementary Figure 64. ORTEP drawing (50 %) showing (**L4**)Ni(OCOPh)$_2$. Hydrogen atoms and disordered THF solvent molecule have been omitted in the sake of clarity. CCDC deposition number **CCDC-2175356.**



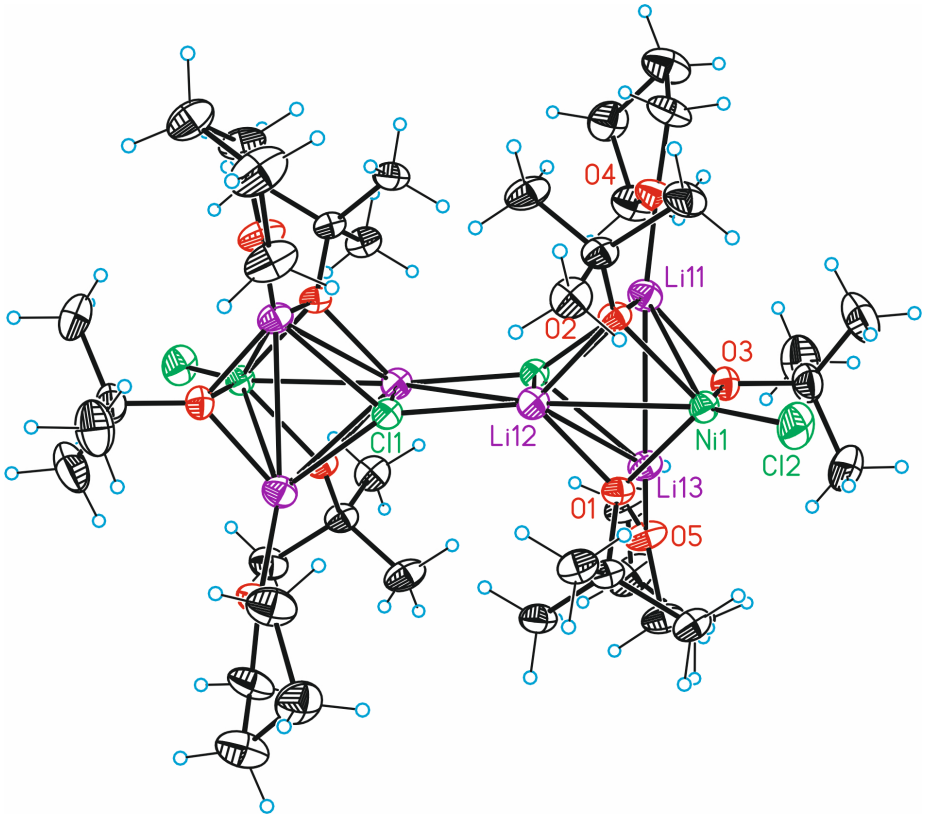
Supplementary Figure 65. ORTEP drawing (50 %) showing asymmetric unit of [(**L4**)Ni(OPh)$_2$(THF)]$_2$. Disordered THF solvent molecules have been omitted in the sake of clarity. CCDC deposition number **CCDC-2175354.**



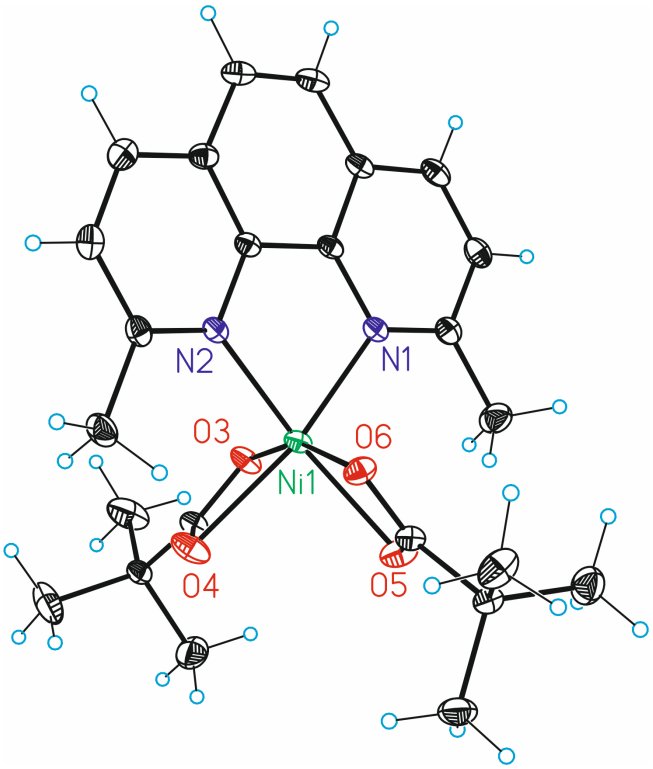
Supplementary Figure 66. ORTEP drawing (50 %) showing [(**L4**)$_2$Ni]Br. Hydrogen atoms and CH_3CN solvent molecules have been omitted in the sake of clarity. CCDC deposition number **CCDC-2175353.**



Supplementary Figure 67. ORTEP drawing (50 %) showing (L4)$NiBr_2$. CCDC deposition number **CCDC-2175357.**



Supplementary Figure 68. ORTEP drawing (50 %) showing $[NiLi_3Cl_2(O^tBu)_3•2THF]_2$. Disordered parts have been omitted in the sake of clarity. CCDC deposition number **CCDC-2175358.**



Supplementary Figure 69. ORTEP drawing (50 %) showing (**L3**)Ni(OPiv)$_2$. CCDC deposition number **CCDC-2175352.**

Supplementary Table 1. Crystallographic Data

	(**L4**)Ni(OPiv)$_2$	(**L4**)Ni(OCOPh)$_2$ •0.5THF	[(**L4**)Ni(OPh)$_2$• THF]$_2$
Formula	$C_{36}H_{38}N_2NiO_4$	$C_{44}H_{38}N_2NiO_{4.5}$	$C_{84}H_{76}N_4Ni_2O_6$
Formula weight	621.39	697.42	1354.87
T (K)	100(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Triclinic
Space group	*Pnma*	*C*2/*c*	*P*-1
***a* (Å)**	8.6390(3)	44.5471(15)	9.4680(15)
***b* (Å)**	17.4573(10)	11.9193(5)	12.252(2)
***c* (Å)**	20.8047(5)	12.5427(4)	14.803(3)
α (deg)	90	90	100.401(5)
β (deg)	90	96.780(3)	97.331(5)
γ (deg)	90	90	96.907(5)
V (Å^3)	3137.6(2)	6613.2(4)	1657.0(5)
Z	4	8	1
Density (calc.) (Mg/m^3)	1.315	1.401	1.358
μ (mm^{-1})	0.660	0.636	0.629
F(000)	1312	2912	712
Crystal size (mm^3)	0.040 x 0.040 x 0.020	0.090 x 0.060 x 0.010	0.050 x 0.030 x 0.010
Theta range for data collection (deg)	2.553 to 37.284	2.446 to 28.951	1.708 to 27.896
Index ranges	-13<=h<=14, -22<=k<=15, -35<=l<=19	-47<=h<=59, -12<=k<=16, -15<=l<=14	-11<=h<=12, -16<=k<=16, -19<=l<=19
Reflections collected	22056	28776	16033
Independent reflections	7206 [R(int) = 0.0375]	7433[R(int) = 0.0357]	7626[R(int) = 0.0715]
Completeness to theta	86.3% 37.284°	85.0% 28.951 °	96.2 % 27.896 °
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	1.00 and 0.85	1.00 and 0.46	0.74 and 0.65
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7206/ 0/ 257	7433/ 194/ 494	7626/ 220/ 481
Goodness-of-fit on F^2	1.017	1.026	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.0901	R1 = 0.0450, wR2 = 0.1049	R1 = 0.0666, wR2 = 0.1330
R indices (all data)	R1 = 0.0698, wR2 = 0.0993	R1 = 0.0762, wR2 = 0.1162	R1 = 0.1242, wR2 = 0.1557
Largest diff. peak and hole	0.475 and -0.468 e.Å^{-3}	1.038 and -0.659 e.Å^{-3}	0.703 and -0.692 e.Å^{-3}

Supplementary Table 2. Crystallographic Data

	[(**L4**)$_2$Ni]Br• 3MeCN	(**L4**)NiBr$_2$	[NiLi$_3$Cl$_2$(O^{t}Bu)$_3$ •2THF]$_2$
Formula	$C_{58}H_{49}BrN_7Ni$	$C_{26}H_{20}Br_2N_2Ni$	$C_{40}H_{86}Cl_4Li_6Ni_2O_{10}$
Formula weight	982.66	578.97	1027.94
T (K)	100(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	*C*2/*c*	*P*2$_1$/*c*	*P*-1
***a* (Å)**	32.275(3)	12.861(5)	9.9981(3)
***b* (Å)**	11.1373(11)	22.587(8)	11.4148(4)
***c* (Å)**	27.385(3)	7.834(3)	13.5283(3)
α (deg)	90	90	103.805(2)
β (deg)	101.187(2)	98.804(11)	103.504(2)
γ (deg)	90	90	102.091(2)
V (Å^3)	9656.8(16)	2249.0(14)	1399.21(7)
Z	8	4	1
Density (calc.) (Mg/m^3)	1.352	1.710	1.220
μ (mm^{-1})	1.276	4.432	0.908
F(000)	4072	1152	548
Crystal size (mm^3)	0.500 x 0.030 x 0.020	0.200 x 0.100 x 0.010	0.080 x 0.060 x 0.050
Theta range for data collection (deg)	1.516 to 31.357	1.602 to 29.346	2.299 to 31.958
Index ranges	-42<=h<=43, -16<=k<=16, -39<=l<=40	-17<=h<=14, -28<=k<=31, -10<=l<=9	-14<=h<=14, -16<=k<=16, -20<=l<=19
Reflections collected	38133	23083	22057
Independent reflections	15247 [R(int) = 0.0431]	5709 [R(int) = 0.0814]	9056 [R(int) = 0.0452]
Completeness to theta	96.1% 31.357°	92.4 % 29.346 °	93.7 % 31.958 °
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.74 and 0.66	0.74 and 0.52	1.00 and 0.44
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	15247/ 0/ 611	5709/ 0/ 282	9056/ 480/ 381
Goodness-of-fit on F^2	1.020	1.031	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.0918	R1 = 0.0555, wR2 = 0.1488	R1 = 0.0529, wR2 = 0.1353
R indices (all data)	R1 = 0.0735, wR2 = 0.1008	R1 = 0.0944, wR2 = 0.1723	R1 = 0.0692, wR2 = 0.1440
Largest diff. peak and hole	0.552 and -0.442 e.Å^{-3}	1.285 and -1.305 e.Å^{-3}	1.640 and -1.049 e.Å^{-3}

Supplementary Table 3. Crystallographic Data

	(**L3**)Ni(OPiv)$_2$
Formula	$C_{24}H_{30}N_2NiO_4$
Formula weight	469.21
T (K)	100(2)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	*P*-1
***a* (Å)**	9.4391(3)
***b* (Å)**	9.6315(2)
***c* (Å)**	14.0382(3)
α (deg)	88.863(2)
β (deg)	82.422(2)
γ (deg)	62.883(2)
V (Å^3)	1124.87(5)
Z	2
Density (calc.) (Mg/m^3)	1.385
μ (mm^{-1})	0.895
F(000)	496
Crystal size (mm^3)	0.080 x 0.050 x 0.040
Theta range for data collection (deg)	2.378 to 33.032
Index ranges	-14<=h<=14, -14<=k<=13, -21<=l<=21
Reflections collected	22403
Independent reflections	7703 [R(int) = 0.0173]
Completeness to theta	90.4 % 33.032°
Absorption correction	Multi-scan
Max. and min. transmission	1.00 and 0.87
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7703/ 0/ 288
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0253, wR2 = 0.0699
R indices (all data)	R1 = 0.0284, wR2 = 0.0713
Largest diff. peak and hole	0.528 and -0.360 e.Å^{-3}

Computational details

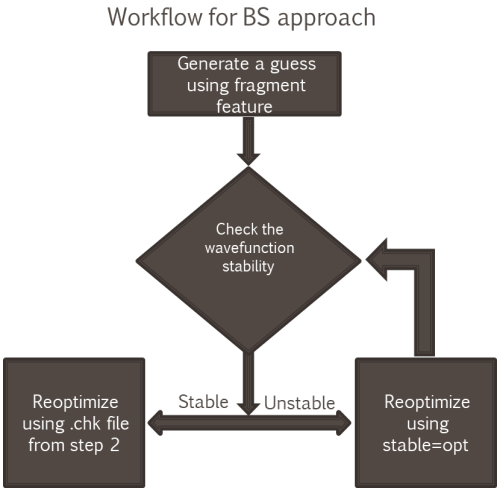
All geometry optimizations of intermediates and transition states were achieved using spin-unrestricted (U)B3LYP[18-19] -D3[20-23]/def2-SVP[24-25] method, in THF solvent using the CPCM solvent model[26-30] with "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian16.[31] Vibrational frequencies were computed at the same level to get thermal corrections (at 298 K; enthalpy and free energy) and to characterize the obtained stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). Different spins were considered for the nickel species. Also, extensive conformational search was performed for all intermediates and transition states, and only the lowest-energy species were shown and discussed. Intrinsic reaction coordinate (IRC) calculations were performed for all transition states to ensure they are connected to the corresponding intermediates. To compare energetics, we also carried out single-point energy calculations for the lowest energy structures using (U)B3LYP-D3/def2-TZVPP-CPCM(THF); (U)PBE0-D3/def2-TZVPP-CPCM(THF) and domain based local pair natural orbital coupled cluster method with single-, double-, and perturbative triple excitations and def2-SVP basis set along with def2-SVP/C[32] as auxiliary basis set [noted as DLPNO-CCSD(T)/def2-SVP-CPCM(THF)//(U)B3LYP-D3/def2-SVP-CPCM(THF)] with ORCA (version 4.1.1).[33] All structural figures were generated with CYLview.[34] Distances in structural figures are shown in Å and energies are in kcal/mol.

Broken-Symmetry approach for optimization Ni(0) species

Our initial DFT calculations on (**L4**)$_2$Ni^0 indicated a triplet ground state in stark contrast to the experimental observation wherein Ni^0 species is diamagnetic in nature. To resolve this dilemma and to ascertain that the optimized geometries are indeed the lowest energy structures, the wavefunction stability associated with each structure were further examined. This resulted in an interesting observation that the DFT optimized Ni^0 singlet species has an unstable wavefunction, thus increasing its energy significantly. However, the wavefunction associated with Ni^0 triplet species is stable, thus triplet species ends up having lower energy and in turn may lead to a false interpretation of triplet state being the Ni^0 ground state. Therefore, all the optimized structures throughout this project were examined for its wavefunction stability using *stable=opt* keyword to ascertain the true energetics. To understand, the underlying reason for this inability of DFT to capture the true ground state of Ni-complexes, an extensive literature search on N-ligated Ni complexes were also carried out which in turn revealed that Ni complexes containing bipyridine ligands are best described as Ni^{I}(bpy$^{\cdot}$)(bpy^0) wherein the central Ni^{I} ion (d^9) is antiferromagnetically coupled to the charge-delocalized π-radical anion (bpy$^{\cdot -1}$).[35] Therefore, defining 0 as charge and 1 as the multiplicity is not exactly true for these type of N-ligated Ni complexes. To capture the antiferromagnetic coupling between the Ni center and the associated ligands, Broken Symmetry DFT calculations must be used. So, we also optimized the Ni^0 species using BS-DFT calculations, and it was observed that the BS-DFT solution converges to the stable=opt solution as shown in **Supplementary Figure 70**. The energy obtained for using stable=opt keyword is lowest and thus highlighted in yellow.

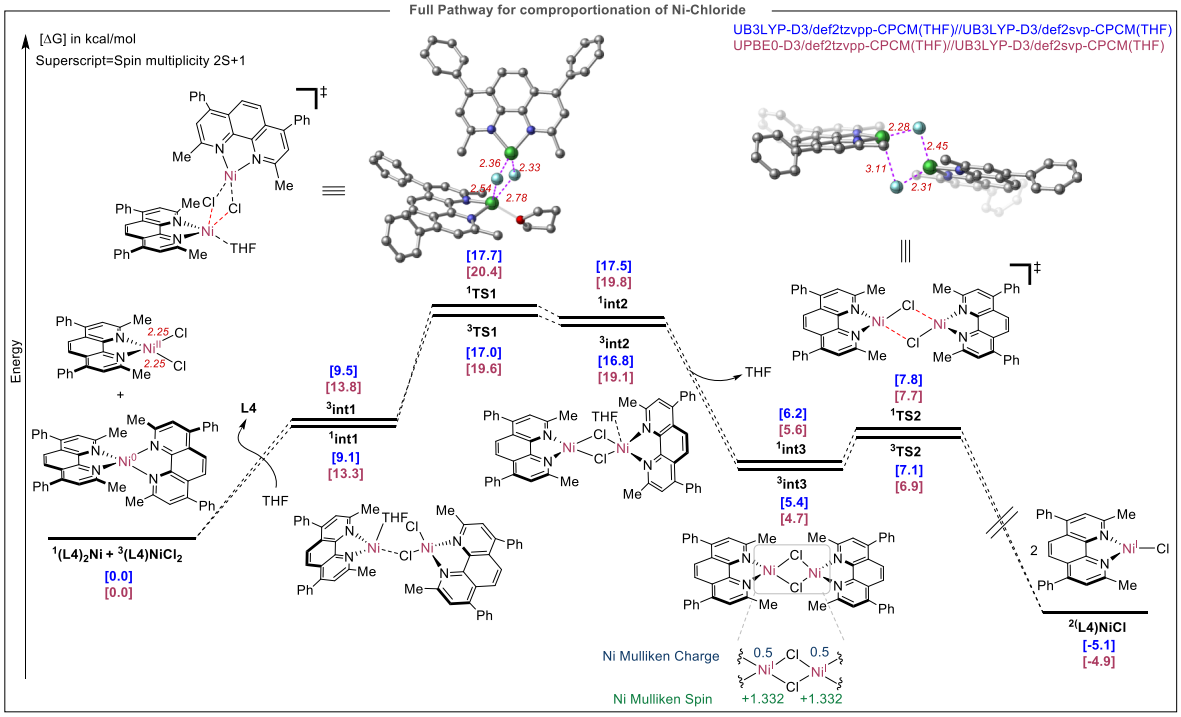
Method Used	Spin state	Wavefunction stable ?	E
UKS	1	No	-3731.496636
UKS	3	Yes	-3731.508782
UKS with stable=opt	1	Yes	-3731.516634
BS(1,-1) (converges to stable=opt solution)	1	Yes	-3731.516615
BS(1,1) (Converges to UKS solution)	3	Yes	-3731.508782

Here, BS(m,n) refers to m unpaired electron in the Ni center and n unpaired electron in the ligand. Positive sign indicates α spin, negative sign indicates β spin.



Supplementary Figure 70. Workflow for Broken-Symmetry DFT approach and the electronic energy obtained for various methods.

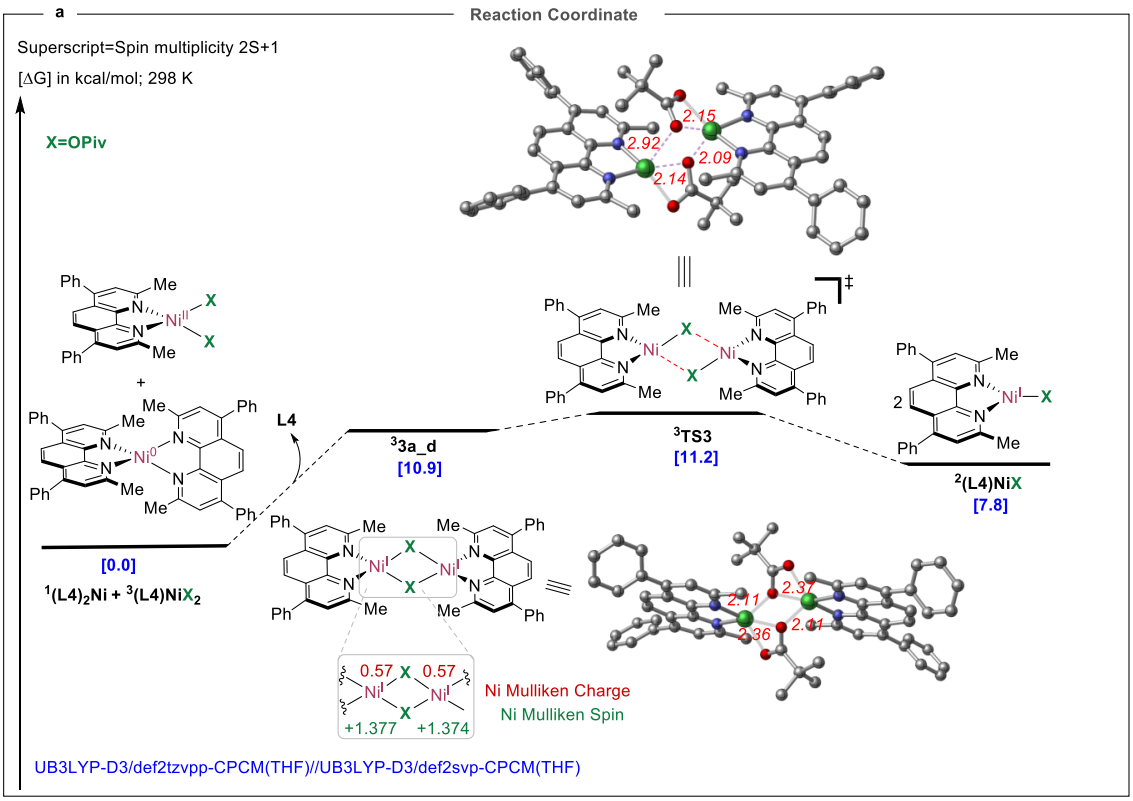
Complete free energy profile for comproportionation of Ni-Chloride



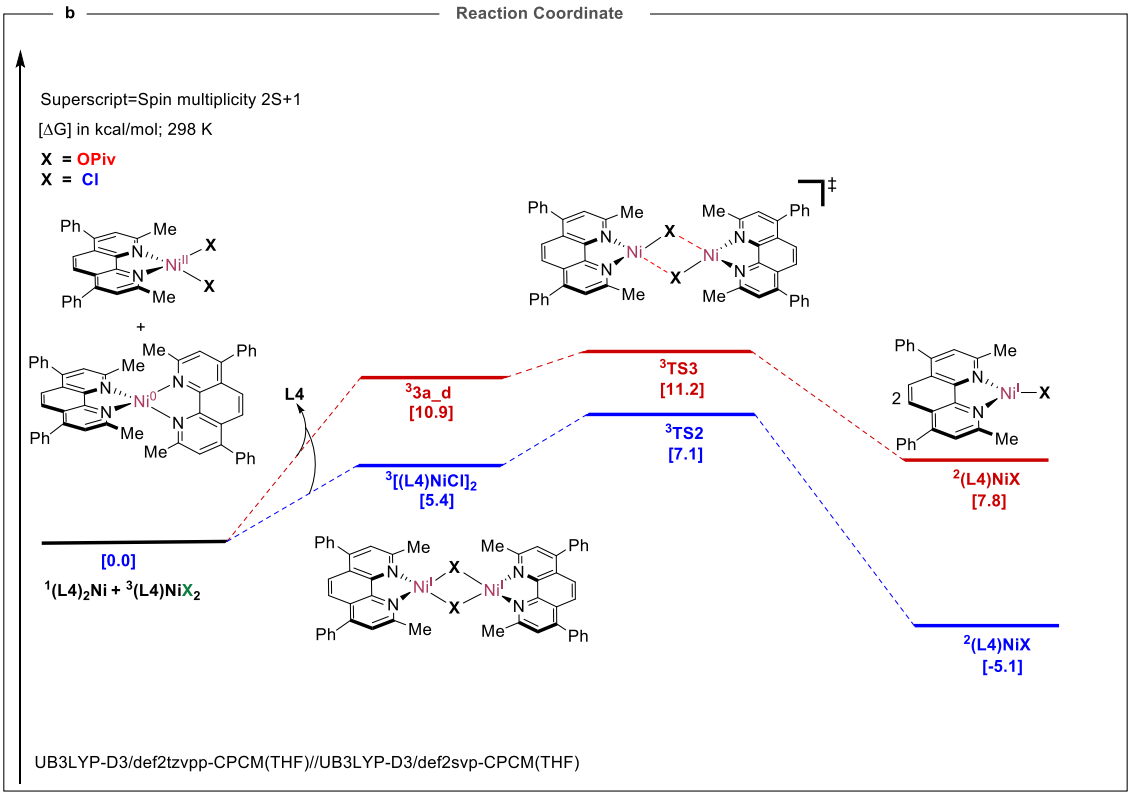
Supplementary Figure 71. Calculated energetics of the comproportionation step of Ni-Chlorides. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2tzvpp-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF) (in blue), and UPBE1PBE-D3/def2tzvpp-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF) (in dark red) levels of theory.

The comproportionation pathway for Ni-Chlorides starts by dissociation of ^{1}**(L4)$_2$Ni** which results in a monomeric **(L4)Ni^0** complex. The coordinating solvent THF can bind to the coordinatively unsaturated Ni center and stabilize the monomeric **(L4)Ni^0** species. This THF bound **(L4)Ni^0** combines with **(L4)NiCl$_2$** to form **int1**. In the next step, **int1** forms **int2** via **TS1**.The energy

barrier for **TS1** is about ~17 kcal and can easily be surmounted at room temperature. Apart from stabilizing the monomeric **(L4)Ni^0** species, THF also prevents the 2 Ni centers from coming together and forming a Ni-Ni bond, thus favoring the formation of **int2** via **TS1.** Once **int2** is formed, the THF molecule leaves and forms a Ni^I dimeric species bridged by two chloride ligands (**int3**). The fact that both the Ni centers in **int3** have the exact same Mulliken charge and spin density, indicates that both of them are having the same oxidation state i.e. +1. The conversion of Ni^I dimeric species to Ni^I monomeric species has a very low barrier (about ~2 kcal/mol) and the monomeric Ni^I species is thermodynamically more stable as compared to its dimeric counterpart. Thus, dissociation of **int3** occurs via **TS2** and finally results in the monomeric Ni^I chloride (**L4**)NiCl.

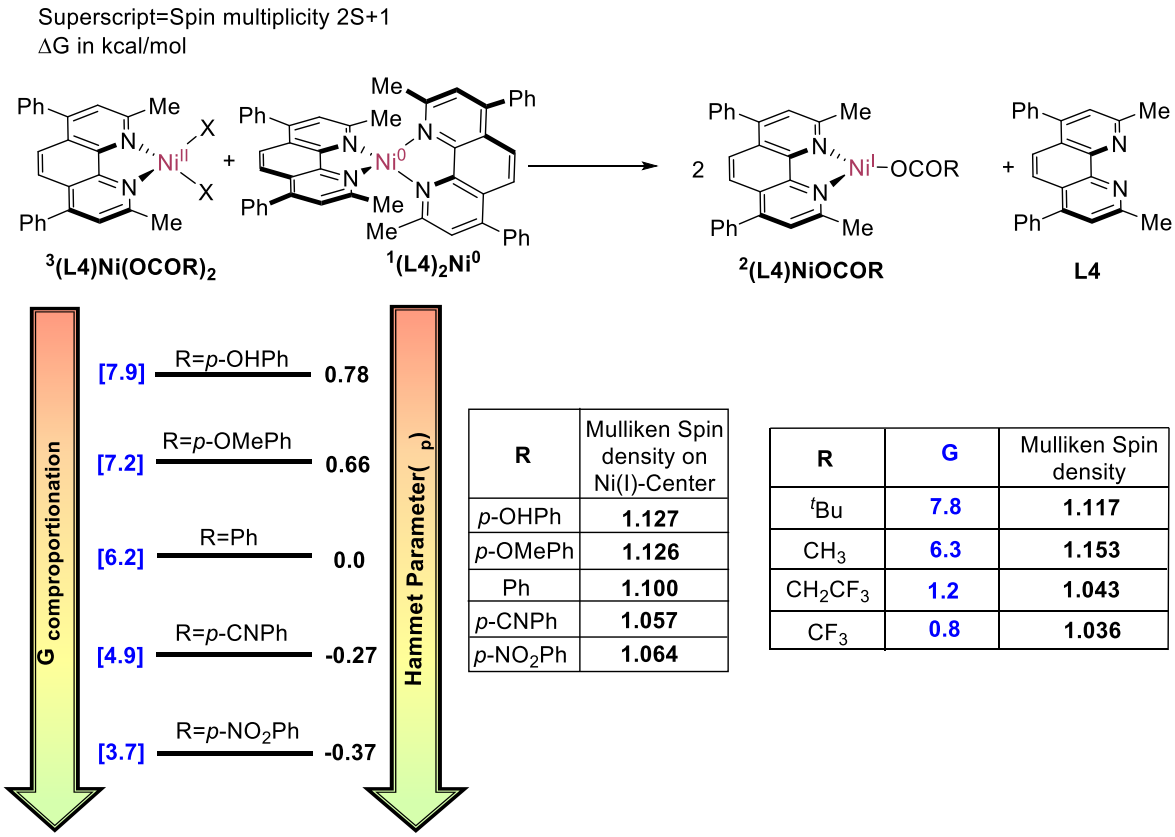


Supplementary Figure 72. Calculated energetics of the comproportionation step of Ni-Pivalates. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2tzvpp-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF) (in blue) level of theory.



Supplementary Figure 73. Calculated energetics of the comproportionation step of Ni-Pivalates (in dark red) and Ni-Chlorides (in blue). Free energies (kcal/mol) were computed at the UB3LYP-D3/def2tzvpp-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF) level of theory.

Electronic Effects on stability of Ni-pseudohalides



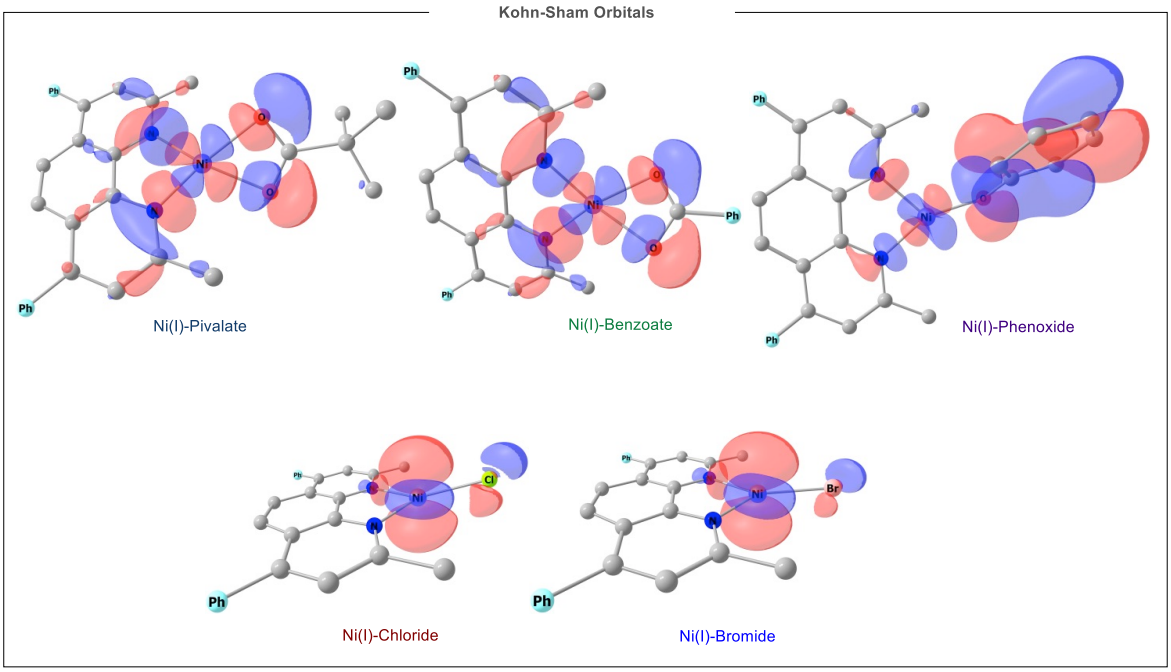
R	Mulliken Spin density on Ni(I)-Center
p-OHPh	**1.127**
p-OMePh	**1.126**
Ph	**1.100**
p-CNPh	**1.057**
p-NO_2Ph	**1.064**

R	G	Mulliken Spin density
^{t}Bu	7.8	**1.117**
CH_3	6.3	**1.153**
CH_2CF_3	1.2	**1.043**
CF_3	0.8	**1.036**

Supplementary Figure 74. Electronic Effect on stability of Ni pseudohalides. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2tzvpp-CPCM(THF)//UB3LYP-D3/def2svp-CPCM(THF) levels of theory.

To explore the electronic effects on stability of pseudohalides, the energetics for a number of different pseudohalides were computed by varying the substituents. From the computations, it has been observed that it is possible to modulate the reactivity patter of pseudohalides by changing electronic properties of the substituents. The more electron withdrawing substituents are observed to have more favorable Gibbs free energy of comproportionation ($\Delta G_{comproportionation}$), whereas the electron donating groups show the opposite effect. It has also been observed that the Ni centers containing electron withdrawing groups have smaller Mulliken spin density as compared to those containing electron donating groups. This trend seems to correlate well with Hammett parameter of the substituents. The substituents having smaller Hammett parameter are more electron withdrawing in nature and thus have more favorable Gibbs free energy of comproportionation ($\Delta G_{comproportionation}$). For example, the pseudohalide having -OH as substituent (Hammett parameter: 0.78, electron donating in nature) has higher spin density on its Ni center as compared to that of the pseudohalide having -NO_2 as substituent (Hammett parameter: -0.37, electron withdrawing in nature. As shown in **Supplementary Figure 74**, the Gibbs free energy of comproportionation ($\Delta G_{comproportionation}$) for these species also vary accordingly. Although an exact correlation between spin density and $\Delta G_{comproportionation}$ is difficult to establish, but our hypothesis is that electron withdrawing groups reduce spin density on the Ni center and thus stabilizes the Ni^I species. This in turn results in a more favorable Gibbs free energy of comproportionation ($\Delta G_{comproportionation}$) for Ni-pseudohalides having electron withdrawing substituents.

Kohn-Sham molecular orbitals (KS MO) of Ni(I) species



Supplementary Figure 75. Kohn-Sham orbitals (Contour Value= 0.025) depicting the SOMO of Ni(I)-halides and Ni(I)-Pseudohalides.

KS MO pictures of SOMO of these Ni(I) species points toward a molecular origin for the observed divergent reactivity pattern. In case of halides, the unpaired e^- is primarily located in the d_z^2 orbital which is aligned with p_z orbital of Cl or Br in such a way that the overlapping lobes are in the same phase, thus facilitating effective delocalization of the unpaired electron. However, in the case of Ni(I)-pivalate, the unpaired e^- is located in d_{xy} orbital and the adjacent p orbitals on the O atoms are oriented in such a way that the overlapping lobes between these 2 orbitals are in opposite phases thus preventing electron delocalization. Similar picture was seen in Ni(I)-phenoxide, where the key orbitals on Ni(I) and O atoms are oriented in a way that leads to overlap of lobes having opposite phases, thus preventing effective delocalization of the unpaired e^-. An effective delocalization of unpaired e^- results in reduced spin density on the Ni center for halides which is not case for pseudohalides and this in turn gives rise to the observed divergent reactivity.

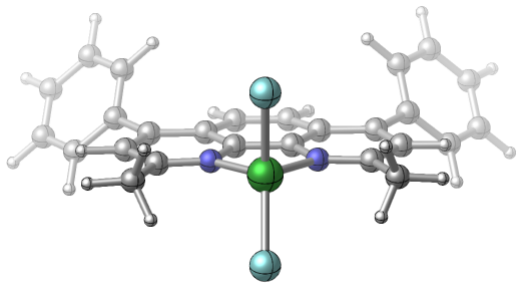
Supplementary Table 4. Cartesian coordinates (xyz format) and energies of all the structures involved in each reaction mechanism studied calculated at the UB3LYP-D3/def2-SVP-CPCM(THF) level of theory.

^{1}(L4)NiCl$_2$
E(scf) = -3540.09855978 a.u.

ν_{min} = 27.02 cm^{-1}

Ni	27.546214	10.221762	1.788963
N	28.904518	8.788784	2.250413
N	26.897105	9.789285	3.660797
C	27.576819	8.762580	4.223354
C	28.668079	8.216044	3.454185
C	28.102840	7.190630	6.017611
H	27.921582	6.821001	7.026608
C	29.436129	7.141865	3.962005
C	29.135964	6.669680	5.286377
H	29.762377	5.892339	5.723355
C	25.499707	9.890621	5.579676
H	24.648212	10.357532	6.076706
C	27.262936	8.235504	5.498333
C	26.153776	8.822406	6.187793
C	25.681393	8.329566	7.507257
C	29.898963	8.354209	1.479605
C	25.883834	10.362513	4.306205
C	30.704524	7.276431	1.905748
H	31.493599	6.917791	1.243286
C	30.484522	6.641243	3.125221
C	25.482419	9.232470	8.567664
H	25.719680	10.289486	8.425855
C	25.377333	6.969730	7.706989
H	25.500749	6.261435	6.884788
C	24.707945	7.430142	9.990661
H	24.331405	7.080465	10.955035
C	25.182190	11.481142	3.596966
H	24.397325	11.939458	4.211454
H	24.741001	11.090187	2.664477
H	25.921469	12.241974	3.297826
C	30.074407	9.041679	0.158918
H	30.947456	8.671668	-0.392948
H	30.164723	10.127783	0.323491
H	29.163656	8.890585	-0.444906
C	25.005172	8.784122	9.801697
H	24.866159	9.495689	10.619206
C	24.891172	6.525695	8.938885
H	24.649652	5.468822	9.075500
C	31.323637	5.476742	3.508412
C	32.927369	3.254778	4.152674
H	33.549747	2.392605	4.404424
C	30.735829	4.257326	3.894667
H	29.647782	4.167177	3.925055
C	31.532932	3.154765	4.210754
H	31.061733	2.211935	4.498928

C	32.726228	5.563098	3.441866
H	33.194025	6.505870	3.148528
C	33.521364	4.461629	3.767931
H	34.609732	4.547295	3.722314
Cl	26.092657	9.071067	0.512466
Cl	28.543525	12.232038	1.856174



Zero-point correction= 0.392871 (Hartree/Particle)
Thermal correction to Energy= 0.420055
Thermal correction to Enthalpy= 0.420999
Thermal correction to Gibbs Free Energy= 0.333804
Sum of electronic and zero-point Energies= -3539.705689
Sum of electronic and thermal Energies= -3539.678505
Sum of electronic and thermal Enthalpies= -3539.677561
Sum of electronic and thermal Free Energies= -3539.764756

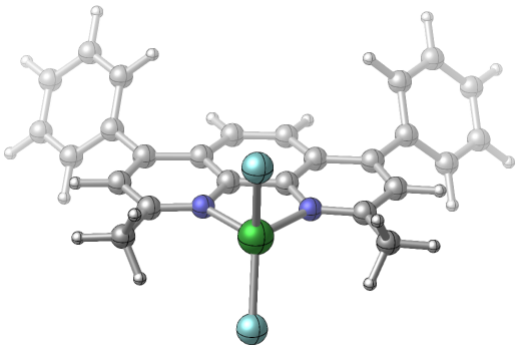
^{3}(L4)NiCl$_2$

E(scf) = -3540.12158529 a.u.

ν_{min} = 32.49 cm^{-1}

Ni	27.541061	10.223592	1.781686
N	28.906071	8.789517	2.248416
N	26.896287	9.791969	3.661677
C	27.577495	8.765337	4.223000
C	28.669039	8.218422	3.453152
C	28.104673	7.193493	6.017858
H	27.923715	6.824297	7.027052
C	29.436957	7.144409	3.961977
C	29.137592	6.672605	5.286554
H	29.764414	5.895603	5.723505
C	25.501022	9.892613	5.582647
H	24.649917	10.359004	6.080782
C	27.264649	8.237955	5.498278
C	26.155629	8.823821	6.188938
C	25.683422	8.328765	7.507644
C	29.900954	8.353331	1.478696
C	25.884011	10.364931	4.309200
C	30.706173	7.275978	1.906016
H	31.495253	6.916198	1.244205
C	30.485294	6.642290	3.125976
C	25.484371	9.229741	8.569654
H	25.721927	10.286963	8.429905

C	25.378873	6.968638	7.704672
H	25.502403	6.261873	6.881171
C	24.708723	7.424964	9.988915
H	24.331619	7.073598	10.952453
C	25.181346	11.483780	3.601243
H	24.399892	11.944568	4.218176
H	24.735012	11.092075	2.671410
H	25.920506	12.242997	3.297489
C	30.076819	9.038126	0.156558
H	30.951783	8.669390	-0.393061
H	30.163692	10.125006	0.318344
H	29.167615	8.882734	-0.448589
C	25.006534	8.779191	9.802659
H	24.867429	9.489241	10.621467
C	24.892052	6.522437	8.935511
H	24.650070	5.465399	9.070003
C	31.323243	5.477329	3.510370
C	32.924618	3.254218	4.156332
H	33.546088	2.391583	4.408734
C	30.734097	4.258339	3.895931
H	29.645943	4.169016	3.925171
C	31.530045	3.155185	4.212828
H	31.057845	2.212678	4.500411
C	32.725952	5.562705	3.445360
H	33.194745	6.505130	3.152496
C	33.519921	4.460656	3.772327
H	34.608400	4.545531	3.727951
Cl	26.083572	9.069717	0.501381
Cl	28.534803	12.243706	1.834715



Zero-point correction= 0.393077 (Hartree/Particle)
Thermal correction to Energy= 0.420142
Thermal correction to Enthalpy= 0.421086
Thermal correction to Gibbs Free Energy= 0.333472
Sum of electronic and zero-point Energies= -3539.728508
Sum of electronic and thermal Energies= -3539.701443
Sum of electronic and thermal Enthalpies= -3539.700499
Sum of electronic and thermal Free Energies= -3539.788113

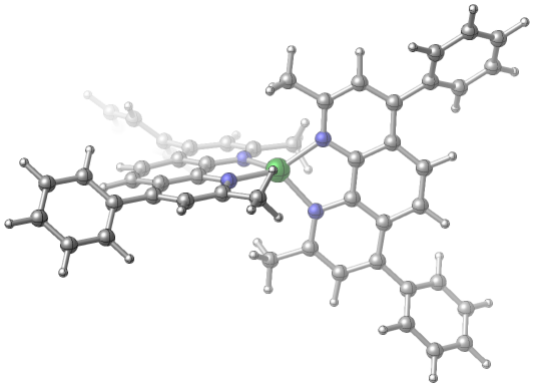
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3541.852976 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3539.908122 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3540.096927 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3534.517825 a.u.

^{1}(L4)$_2$Ni
E(scf) = -3731.51663406 a.u.
ν_{min} = 5.59 cm^{-1}

N	25.673614	10.186670	-0.102440
N	26.825346	12.386071	0.710000
C	25.901158	12.535109	-0.300111
C	25.273083	11.339416	-0.740031
C	24.513001	13.803046	-1.855457
H	24.171667	14.758522	-2.254463
C	24.281547	11.358846	-1.762953
C	23.906059	12.651722	-2.277081
H	23.094709	12.714839	-3.002643
C	27.161144	14.755716	0.676880
H	27.700325	15.615126	1.078793
C	25.565595	13.796552	-0.870441
C	26.239255	14.945915	-0.379957
C	26.017105	16.311509	-0.912967
C	25.079683	9.022003	-0.438382
C	27.434961	13.490871	1.194457
C	24.109290	8.966363	-1.439516
H	23.681781	7.997571	-1.703078
C	23.699681	10.121667	-2.143939
C	25.819986	17.395264	-0.032663
H	25.789310	17.210595	1.043924
C	26.044967	16.578940	-2.297346
H	26.232896	15.762465	-2.997906
C	25.660763	18.940048	-1.895145
H	25.520995	19.955198	-2.275001
C	28.425960	13.264691	2.300355
H	28.857850	14.204126	2.670763
H	29.239659	12.608088	1.948117
H	27.943495	12.729573	3.134460
C	25.535217	7.805553	0.316297
H	24.991884	6.901282	0.010952
H	25.397970	7.964560	1.398687
H	26.615582	7.647292	0.167118
C	25.640435	18.692692	-0.517702
H	25.478822	19.514978	0.184236
C	25.866899	17.877127	-2.781786

H	25.899297	18.060625	-3.858926
C	22.690814	9.995223	-3.223853
C	20.780909	9.679806	-5.284663
H	20.041761	9.559890	-6.080671
C	22.892961	10.572745	-4.494051
H	23.812154	11.128811	-4.690592
C	21.948118	10.417700	-5.511423
H	22.129584	10.868983	-6.490355
C	21.515666	9.245106	-3.015011
H	21.336505	8.793324	-2.036300
C	20.570278	9.092459	-4.031886
H	19.661400	8.515149	-3.843250
Ni	27.016870	10.503828	1.336576
N	28.503230	9.223967	1.642754
N	26.675923	10.135420	3.273110
C	27.545270	9.213691	3.809410
C	28.539229	8.717345	2.923762
C	28.504404	7.868424	5.605004
H	28.534945	7.576479	6.655006
C	29.500385	7.760959	3.358974
C	29.462106	7.391582	4.752255
H	30.236227	6.730195	5.142128
C	25.567999	10.246408	5.389766
H	24.751047	10.662776	5.981240
C	27.473481	8.772186	5.162455
C	26.435080	9.297675	5.974348
C	26.225103	8.897066	7.387689
C	29.433972	8.798174	0.756371
C	25.701288	10.639555	4.055852
C	30.396548	7.857143	1.112146
H	31.107179	7.522302	0.354610
C	30.449543	7.294849	2.411080
C	26.031303	9.877619	8.381276
H	26.078793	10.934132	8.106303
C	26.164124	7.541661	7.769661
H	26.276511	6.764346	7.010817
C	25.753999	8.166827	10.076963
H	25.574083	7.884212	11.117208
C	24.772722	11.629022	3.410691
H	23.957748	11.928859	4.082989
H	24.347505	11.198834	2.489342
H	25.329758	12.527187	3.098955
C	29.350578	9.395171	-0.619171
H	30.102863	8.977190	-1.301563
H	29.484360	10.489008	-0.561886
H	28.344297	9.234267	-1.040190

C	25.802544	9.516833	9.711181
H	25.665563	10.294612	10.466927
C	25.932333	7.181463	9.099528
H	25.882320	6.124030	9.371842
C	31.472330	6.266361	2.716238
C	33.435224	4.291316	3.218918
H	34.193625	3.529302	3.415185
C	31.136295	5.053821	3.353770
H	30.097604	4.864163	3.632812
C	32.106369	4.080114	3.603656
H	31.819663	3.145699	4.093239
C	32.813576	6.458131	2.324612
H	33.098752	7.391959	1.833951
C	33.783190	5.484733	2.575697
H	34.818250	5.661494	2.271629



Zero-point correction= 0.775533 (Hartree/Particle)
Thermal correction to Energy= 0.822860
Thermal correction to Enthalpy= 0.823804
Thermal correction to Gibbs Free Energy= 0.690134
Sum of electronic and zero-point Energies= -3730.741101
Sum of electronic and thermal Energies= -3730.693774
Sum of electronic and thermal Enthalpies= -3730.692830
Sum of electronic and thermal Free Energies= -3730.826500

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3734.107978 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3731.15489 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3731.506936 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3723.686706 a.u.

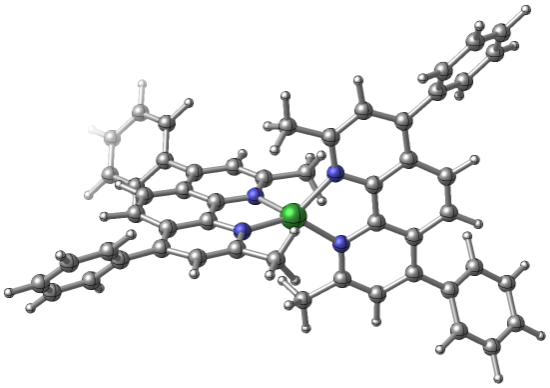
^{3}(L4)$_2$Ni
E(scf) = -3731.50878151 a.u.
ν_{min} = 6.25 cm^{-1}

N	28.930303	9.048355	2.247679
N	27.034847	10.121382	3.766058
C	27.541476	8.901183	4.176470

C	28.553206	8.329285	3.367267
C	27.753268	7.021847	5.722751
H	27.496551	6.539709	6.666454
C	29.146178	7.069225	3.697358
C	28.730262	6.470126	4.941524
H	29.228431	5.561574	5.281122
C	25.553717	10.112290	5.643672
H	24.742486	10.605569	6.180683
C	27.072781	8.239730	5.355658
C	26.033960	8.851301	6.097106
C	25.432812	8.247292	7.309359
C	29.879374	8.551064	1.434618
C	26.065010	10.707754	4.492597
C	30.489344	7.323734	1.690550
H	31.228798	6.941400	0.985688
C	30.126001	6.542716	2.822560
C	25.216228	9.031450	8.462315
H	25.536956	10.076066	8.464963
C	25.010197	6.901276	7.339017
H	25.127712	6.282931	6.446600
C	24.221124	7.146732	9.620192
H	23.755524	6.721156	10.512669
C	25.551944	12.019911	3.966614
H	24.784893	12.458818	4.618927
H	25.131519	11.880632	2.956810
H	26.385397	12.733028	3.855848
C	30.215903	9.383356	0.227838
H	31.004252	8.926354	-0.385411
H	30.538096	10.389939	0.540790
H	29.314775	9.528714	-0.390448
C	24.622967	8.487631	9.603628
H	24.477351	9.113837	10.487884
C	24.415106	6.358228	8.480260
H	24.090818	5.314189	8.474825
C	30.783839	5.230917	3.031170
C	32.068493	2.728435	3.351680
H	32.564368	1.762696	3.477654
C	30.043223	4.063779	3.313800
H	28.954977	4.123163	3.382891
C	30.678045	2.829751	3.474458
H	30.080607	1.939126	3.686654
C	32.182848	5.107965	2.896520
H	32.778246	5.998309	2.680017
C	32.817262	3.874527	3.059277
H	33.904116	3.808378	2.961393
N	26.691287	10.796415	0.518570

N	28.480896	12.537143	1.325534
C	27.802875	12.860802	0.170764
C	26.831504	11.912286	-0.263813
C	27.315737	14.209177	-1.804854
H	27.537495	15.069228	-2.436871
C	26.074311	12.127088	-1.451275
C	26.382410	13.300396	-2.223161
H	25.877603	13.453875	-3.177105
C	29.714739	14.579928	1.095060
H	30.471402	15.249375	1.508243
C	28.041507	14.050824	-0.570122
C	29.017977	14.961259	-0.075194
C	29.329992	16.258868	-0.718643
C	25.812691	9.849386	0.156667
C	29.438672	13.394733	1.767443
C	25.021801	10.000425	-0.992677
H	24.296727	9.222646	-1.237132
C	25.117791	11.138683	-1.807971
C	28.314562	17.162742	-1.095650
H	27.269575	16.903067	-0.912931
C	30.670297	16.647429	-0.924089
H	31.474332	15.961452	-0.646391
C	29.962680	18.763251	-1.874859
H	30.206659	19.729493	-2.323378
C	30.153651	12.985341	3.021598
H	30.905682	13.721936	3.333933
H	30.648734	12.009715	2.873984
H	29.427877	12.844029	3.841620
C	25.707512	8.638377	1.038285
H	24.986659	7.909404	0.645520
H	25.408181	8.935822	2.055056
H	26.694235	8.160940	1.138312
C	28.627596	18.397837	-1.668259
H	27.822759	19.083750	-1.945324
C	30.982533	17.882263	-1.497136
H	32.029091	18.155878	-1.654897
C	24.232226	11.262088	-2.994264
C	22.503577	11.442032	-5.217189
H	21.835587	11.512807	-6.079208
C	24.113106	10.193270	-3.903199
H	24.708704	9.290206	-3.749252
C	23.260746	10.284356	-5.006338
H	23.190142	9.447993	-5.706378
C	23.459912	12.419135	-3.214638
H	23.516693	13.246998	-2.504557
C	22.603813	12.507088	-4.315248

H	22.007032	13.410392	-4.465004
Ni	27.955690	10.818158	2.106802

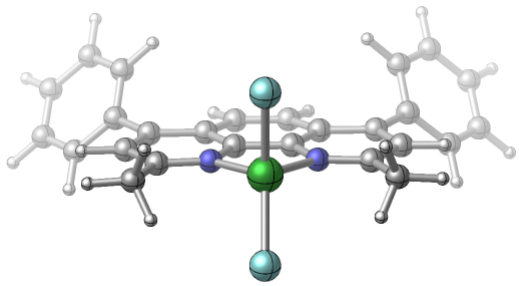


Zero-point correction= 0.775223 (Hartree/Particle)
Thermal correction to Energy= 0.822472
Thermal correction to Enthalpy= 0.823416
Thermal correction to Gibbs Free Energy= 0.689557
Sum of electronic and zero-point Energies= -3730.733558
Sum of electronic and thermal Energies= -3730.686310
Sum of electronic and thermal Enthalpies= -3730.685365
Sum of electronic and thermal Free Energies= -3730.819225

^{1}(L4)NiCl$_2$
E(scf) = -3540.09855978 a.u.
ν_{min} = 27.02 cm^{-1}

Ni	27.546214	10.221762	1.788963
N	28.904518	8.788784	2.250413
N	26.897105	9.789285	3.660797
C	27.576819	8.762580	4.223354
C	28.668079	8.216044	3.454185
C	28.102840	7.190630	6.017611
H	27.921582	6.821001	7.026608
C	29.436129	7.141865	3.962005
C	29.135964	6.669680	5.286377
H	29.762377	5.892339	5.723355
C	25.499707	9.890621	5.579676
H	24.648212	10.357532	6.076706
C	27.262936	8.235504	5.498333
C	26.153776	8.822406	6.187793
C	25.681393	8.329566	7.507257
C	29.898963	8.354209	1.479605
C	25.883834	10.362513	4.306205
C	30.704524	7.276431	1.905748
H	31.493599	6.917791	1.243286
C	30.484522	6.641243	3.125221
C	25.482419	9.232470	8.567664
H	25.719680	10.289486	8.425855
C	25.377333	6.969730	7.706989
H	25.500749	6.261435	6.884788

C	24.707945	7.430142	9.990661
H	24.331405	7.080465	10.955035
C	25.182190	11.481142	3.596966
H	24.397325	11.939458	4.211454
H	24.741001	11.090187	2.664477
H	25.921469	12.241974	3.297826
C	30.074407	9.041679	0.158918
H	30.947456	8.671668	-0.392948
H	30.164723	10.127783	0.323491
H	29.163656	8.890585	-0.444906
C	25.005172	8.784122	9.801697
H	24.866159	9.495689	10.619206
C	24.891172	6.525695	8.938885
H	24.649652	5.468822	9.075500
C	31.323637	5.476742	3.508412
C	32.927369	3.254778	4.152674
H	33.549747	2.392605	4.404424
C	30.735829	4.257326	3.894667
H	29.647782	4.167177	3.925055
C	31.532932	3.154765	4.210754
H	31.061733	2.211935	4.498928
C	32.726228	5.563098	3.441866
H	33.194025	6.505870	3.148528
C	33.521364	4.461629	3.767931
H	34.609732	4.547295	3.722314
Cl	26.092657	9.071067	0.512466
Cl	28.543525	12.232038	1.856174



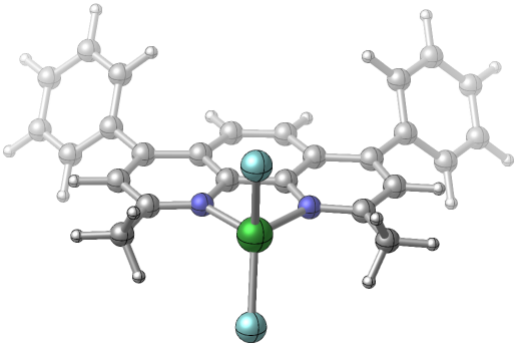
Zero-point correction= 0.392871 (Hartree/Particle)
Thermal correction to Energy= 0.420055
Thermal correction to Enthalpy= 0.420999
Thermal correction to Gibbs Free Energy= 0.333804
Sum of electronic and zero-point Energies= -3539.705689
Sum of electronic and thermal Energies= -3539.678505
Sum of electronic and thermal Enthalpies= -3539.677561
Sum of electronic and thermal Free Energies= -3539.764756

^{3}(L4)NiCl$_2$
E(scf) = -3540.12158529 a.u.
ν_{min} = 32.49 cm^{-1}

Ni	27.541061	10.223592	1.781686

N	28.906071	8.789517	2.248416
N	26.896287	9.791969	3.661677
C	27.577495	8.765337	4.223000
C	28.669039	8.218422	3.453152
C	28.104673	7.193493	6.017858
H	27.923715	6.824297	7.027052
C	29.436957	7.144409	3.961977
C	29.137592	6.672605	5.286554
H	29.764414	5.895603	5.723505
C	25.501022	9.892613	5.582647
H	24.649917	10.359004	6.080782
C	27.264649	8.237955	5.498278
C	26.155629	8.823821	6.188938
C	25.683422	8.328765	7.507644
C	29.900954	8.353331	1.478696
C	25.884011	10.364931	4.309200
C	30.706173	7.275978	1.906016
H	31.495253	6.916198	1.244205
C	30.485294	6.642290	3.125976
C	25.484371	9.229741	8.569654
H	25.721927	10.286963	8.429905
C	25.378873	6.968638	7.704672
H	25.502403	6.261873	6.881171
C	24.708723	7.424964	9.988915
H	24.331619	7.073598	10.952453
C	25.181346	11.483780	3.601243
H	24.399892	11.944568	4.218176
H	24.735012	11.092075	2.671410
H	25.920506	12.242997	3.297489
C	30.076819	9.038126	0.156558
H	30.951783	8.669390	-0.393061
H	30.163692	10.125006	0.318344
H	29.167615	8.882734	-0.448589
C	25.006534	8.779191	9.802659
H	24.867429	9.489241	10.621467
C	24.892052	6.522437	8.935511
H	24.650070	5.465399	9.070003
C	31.323243	5.477329	3.510370
C	32.924618	3.254218	4.156332
H	33.546088	2.391583	4.408734
C	30.734097	4.258339	3.895931
H	29.645943	4.169016	3.925171
C	31.530045	3.155185	4.212828
H	31.057845	2.212678	4.500411
C	32.725952	5.562705	3.445360
H	33.194745	6.505130	3.152496

C	33.519921	4.460656	3.772327
H	34.608400	4.545531	3.727951
Cl	26.083572	9.069717	0.501381
Cl	28.534803	12.243706	1.834715

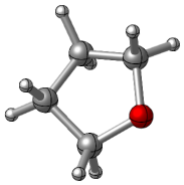


Zero-point correction= 0.393077 (Hartree/Particle)
Thermal correction to Energy= 0.420142
Thermal correction to Enthalpy= 0.421086
Thermal correction to Gibbs Free Energy= 0.333472
Sum of electronic and zero-point Energies= -3539.728508
Sum of electronic and thermal Energies= -3539.701443
Sum of electronic and thermal Enthalpies= -3539.700499
Sum of electronic and thermal Free Energies= -3539.788113

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3541.852976 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3539.908122 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3540.096927 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3534.517825 a.u.

THF
E(scf) = -232.288794659 a.u.
ν_{min} = 86.91 cm^{-1}

C	28.768646	13.937104	1.535776
O	28.112432	12.758656	1.063704
C	27.237256	13.081196	-0.018945
C	27.119529	14.608006	-0.029330
C	28.503951	15.020095	0.485850
H	28.350240	14.230595	2.519136
H	29.841901	13.724043	1.677561
H	27.667535	12.712451	-0.971367
H	26.269608	12.572879	0.131473
H	26.877572	15.012047	-1.023566
H	26.336722	14.938184	0.673954
H	29.247386	14.958219	-0.326486
H	28.537678	16.037688	0.902574



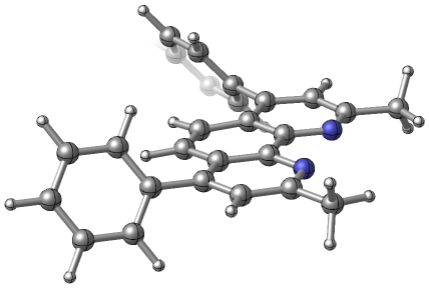
Zero-point correction= 0.116134 (Hartree/Particle)
Thermal correction to Energy= 0.120986
Thermal correction to Enthalpy= 0.121930
Thermal correction to Gibbs Free Energy= 0.088164
Sum of electronic and zero-point Energies= -232.172661
Sum of electronic and thermal Energies= -232.167809
Sum of electronic and thermal Enthalpies= -232.166865
Sum of electronic and thermal Free Energies= -232.200631

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -232.556107 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -232.280495 a.u.

L4
E(scf) = -1111.61693113 a.u.
ν_{min} = 27.57 cm^{-1}

N	28.789699	8.668626	2.120143
N	26.797167	9.772033	3.628736
C	27.518743	8.764566	4.169765
C	28.586550	8.174480	3.362340
C	28.147992	7.254635	6.017801
H	28.015595	6.931355	7.050463
C	29.374643	7.118106	3.909653
C	29.145910	6.704636	5.264425
H	29.796887	5.949688	5.705715
C	25.512601	9.900576	5.648523
H	24.688151	10.374190	6.186394
C	27.284584	8.270826	5.488109
C	26.214706	8.860098	6.236366
C	25.835824	8.397814	7.599907
C	29.757457	8.166738	1.370652
C	25.833183	10.335687	4.338111
C	30.580799	7.103916	1.819983
H	31.348630	6.700089	1.156131
C	30.396304	6.554346	3.078949
C	25.737418	9.321285	8.656330
H	25.983578	10.370334	8.474828
C	25.519753	7.049598	7.851646
H	25.571195	6.323687	7.036958
C	25.037209	7.563620	10.171456
H	24.729592	7.239428	11.168760
C	25.052637	11.462558	3.710727

H	23.982754	11.205766	3.636100
H	25.439198	11.674412	2.705126
H	25.121379	12.377240	4.322662
C	29.965236	8.744946	-0.006036
H	29.824718	7.973611	-0.781577
H	30.991760	9.131173	-0.119634
H	29.253516	9.562063	-0.183116
C	25.345603	8.906959	9.932362
H	25.283287	9.636870	10.743441
C	25.122373	6.637234	9.126072
H	24.873561	5.587645	9.301942
C	31.249863	5.414877	3.514461
C	32.887044	3.242208	4.252936
H	33.521461	2.400394	4.541385
C	30.681836	4.205201	3.955960
H	29.594886	4.105159	3.998471
C	31.493916	3.128137	4.320069
H	31.035689	2.193673	4.653648
C	32.651046	5.514291	3.442092
H	33.104559	6.449353	3.104414
C	33.462899	4.438525	3.812429
H	34.550066	4.536709	3.758454



Zero-point correction= 0.386779 (Hartree/Particle)
Thermal correction to Energy= 0.409160
Thermal correction to Enthalpy= 0.410105
Thermal correction to Gibbs Free Energy= 0.333393
Sum of electronic and zero-point Energies= -1111.230152
Sum of electronic and thermal Energies= -1111.207771
Sum of electronic and thermal Enthalpies= -1111.206827
Sum of electronic and thermal Free Energies= -1111.283538

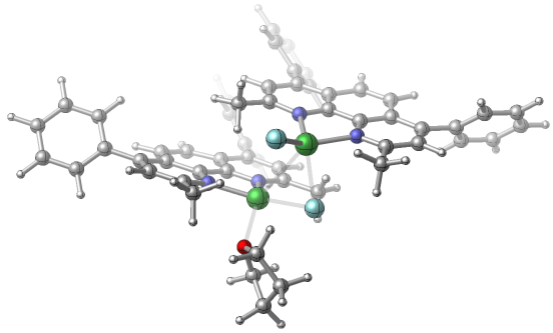
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -1112.814451 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -1111.48404 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -1111.606662
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -1108.331152

^{1}int1
E(scf) = -6392.32663920 a.u.
ν_{min} = 11.88 cm^{-1}

C	1.744642	4.438051	-0.815577
C	0.842654	4.664842	-1.872178
C	-0.541204	4.643631	-1.671835
N	1.299717	4.209286	0.424124
C	-1.015108	4.440327	-0.343168
C	-0.041478	4.229310	0.668854
C	-0.424415	4.027729	2.033576
N	0.606965	3.859160	2.920435
C	-1.794207	4.013395	2.403757
C	-2.106244	3.795751	3.778472
C	0.303433	3.760611	4.234811
C	-1.023017	3.712096	4.670523
Ni	2.362123	3.603692	2.043428
H	1.239646	4.825963	-2.876069
H	-1.213599	3.574268	5.736161
Cl	3.079260	1.540768	0.876492
Cl	4.375589	4.315403	2.899506
C	4.153381	1.048948	5.848087
C	4.141837	0.937879	7.253589
C	2.983141	0.625612	7.954497
N	3.043232	0.833938	5.130408
C	1.794215	0.410552	7.193985
C	1.882659	0.543740	5.783547
C	0.697257	0.432116	4.967221
N	0.863195	0.594826	3.621457
C	-0.559977	0.185154	5.580384
C	-1.713833	0.152657	4.741467
C	-0.223390	0.515879	2.834383
C	-1.505586	0.304932	3.375163
Ni	2.801495	0.898997	3.128814
H	5.064033	1.140102	7.800827
H	-2.359488	0.296943	2.696666
C	5.410444	1.436893	5.131030
H	5.894775	0.538465	4.723591
H	5.183208	2.112908	4.293609
H	6.114896	1.932316	5.813475
C	-0.043567	0.683841	1.358385
H	0.489776	1.619621	1.157860
H	0.600257	-0.112391	0.954115
H	-1.006766	0.679430	0.831681
C	1.466768	3.741173	5.177072
H	2.235342	3.061674	4.789724
H	1.931450	4.740536	5.217979
H	1.177713	3.433955	6.190852
C	3.229631	4.400291	-1.039518
H	3.762028	4.710085	-0.128176

H	3.545290	3.365166	-1.246965
H	3.525476	5.036066	-1.886114
O	4.666311	-0.310059	2.768810
C	4.249749	-1.551209	2.167599
C	5.804855	0.229262	2.056475
C	5.400621	-1.971321	1.257654
H	4.021269	-2.267309	2.971855
H	3.331203	-1.367205	1.583575
C	5.926428	-0.608289	0.787764
H	5.612051	1.293922	1.869151
H	6.699261	0.126136	2.695713
H	5.069490	-2.623672	0.436177
H	6.173776	-2.507607	1.832668
H	5.265495	-0.193069	0.011596
H	6.955132	-0.642602	0.399794
C	-2.392521	4.484060	0.065797
H	-3.158633	4.711394	-0.675686
C	-2.759433	4.278489	1.368388
H	-3.813202	4.346779	1.638560
C	0.528387	0.050681	7.766509
H	0.468861	-0.150635	8.835852
C	-0.594139	-0.053908	6.995974
H	-1.538081	-0.339978	7.458932
C	-1.452159	4.834175	-2.830350
C	-2.490988	3.922439	-3.099531
C	-1.260624	5.914144	-3.712556
C	-3.317995	4.091961	-4.212766
H	-2.636675	3.063321	-2.441017
C	-2.091905	6.085907	-4.822334
H	-0.461651	6.632673	-3.514282
C	-3.124111	5.176005	-5.076017
H	-4.114244	3.369681	-4.409767
H	-1.934171	6.936402	-5.490387
H	-3.773439	5.309483	-5.944850
C	-3.494006	3.672810	4.282314
C	-3.899568	4.369042	5.438026
C	-4.432240	2.831008	3.650941
C	-5.201217	4.246642	5.929927
H	-3.190126	5.030068	5.941657
C	-5.732042	2.709078	4.142916
H	-4.127434	2.245255	2.781850
C	-6.124716	3.420211	5.281491
H	-5.496590	4.803957	6.822699
H	-6.436086	2.036721	3.647017
H	-7.141226	3.319532	5.669514
C	-3.090779	-0.020153	5.267596

C	-3.576007	0.782750	6.317074
C	-3.957443	-0.963497	4.685905
C	-4.883209	0.633823	6.780973
H	-2.934445	1.553522	6.747270
C	-5.265633	-1.113722	5.153717
H	-3.594461	-1.594952	3.871393
C	-5.731229	-0.318149	6.205558
H	-5.247430	1.280422	7.582032
H	-5.922100	-1.858407	4.696501
H	-6.755479	-0.432179	6.569109
C	3.019455	0.557807	9.438901
C	2.136183	1.319081	10.227697
C	3.985042	-0.237259	10.083375
C	2.212610	1.278225	11.622059
H	1.398749	1.962769	9.743034
C	4.055750	-0.282405	11.478144
H	4.675135	-0.834443	9.482449
C	3.169458	0.474551	12.251897
H	1.524713	1.882036	12.219159
H	4.805638	-0.913064	11.962166
H	3.225971	0.440940	13.342723



Zero-point correction= 0.901231 (Hartree/Particle)
Thermal correction to Energy= 0.959704
Thermal correction to Enthalpy= 0.960648
Thermal correction to Gibbs Free Energy= 0.804260
Sum of electronic and zero-point Energies= -6391.425409
Sum of electronic and thermal Energies= -6391.366935
Sum of electronic and thermal Enthalpies= -6391.365991
Sum of electronic and thermal Free Energies= -6391.522380

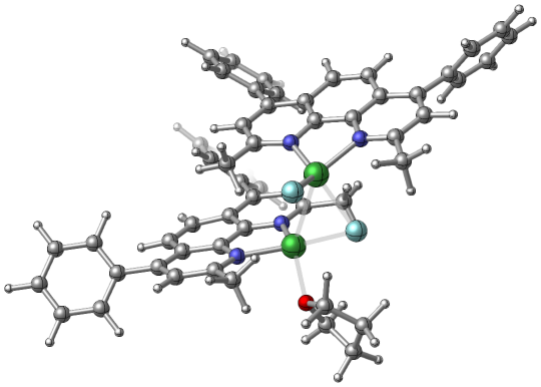
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.714068 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.864264 a.u.
^{3}int1
E(scf) = -6392.32671282 a.u.
ν_{min} = 11.36 cm^{-1}

C	1.762166	4.422991	-0.818740
C	0.860714	4.659081	-1.873904

C	-0.523154	4.647851	-1.672147
N	1.316796	4.198368	0.421508
C	-0.997370	4.445563	-0.343620
C	-0.024024	4.227529	0.667444
C	-0.407324	4.023398	2.031343
N	0.623743	3.844739	2.917188
C	-1.776898	4.010772	2.402040
C	-2.089273	3.784982	3.775449
C	0.320099	3.750402	4.232266
C	-1.005775	3.702208	4.668164
Ni	2.370548	3.557818	2.036472
H	1.257737	4.817581	-2.878185
H	-1.196463	3.563632	5.733706
Cl	2.999173	1.477413	0.843722
Cl	4.435679	4.276383	2.757161
C	4.111997	1.066883	5.843295
C	4.102145	0.944510	7.248308
C	2.949419	0.610646	7.947045
N	3.006342	0.837369	5.122633
C	1.763118	0.386192	7.184541
C	1.849160	0.529329	5.774700
C	0.661145	0.412125	4.960556
N	0.817571	0.584098	3.615436
C	-0.591700	0.152545	5.578283
C	-1.749968	0.119742	4.745263
C	-0.271545	0.504419	2.834162
C	-1.550924	0.282735	3.380449
Ni	2.767027	0.901994	3.119231
H	5.021186	1.157813	7.796689
H	-2.408398	0.274068	2.706652
C	5.364360	1.490543	5.138546
H	5.894421	0.605247	4.760030
H	5.127212	2.137960	4.282252
H	6.033916	2.029010	5.823798
C	-0.107756	0.679677	1.357228
H	0.428548	1.612554	1.153565
H	0.526039	-0.118289	0.941220
H	-1.077703	0.683004	0.843094
C	1.483890	3.738434	5.174518
H	2.256479	3.063556	4.787347
H	1.937875	4.742897	5.219069
H	1.198201	3.427063	6.188039
C	3.245978	4.366436	-1.044394
H	3.783003	4.688185	-0.139837
H	3.549069	3.323037	-1.228655
H	3.547031	4.979942	-1.905361

O	4.697868	-0.207219	2.777425
C	4.356694	-1.478960	2.195297
C	5.805357	0.388076	2.059800
C	5.531857	-1.843934	1.292084
H	4.171085	-2.195810	3.010032
H	3.429185	-1.358580	1.609019
C	5.979773	-0.459464	0.803983
H	5.552892	1.438355	1.861107
H	6.702105	0.344503	2.702677
H	5.240602	-2.525559	0.479271
H	6.333442	-2.327061	1.875295
H	5.299390	-0.094963	0.019476
H	7.010495	-0.440312	0.420183
C	-2.374376	4.493507	0.066220
H	-3.139976	4.726442	-0.674074
C	-2.741607	4.283415	1.368087
H	-3.795123	4.353565	1.638976
C	0.503137	0.010147	7.758713
H	0.449346	-0.199199	8.826770
C	-0.620948	-0.097567	6.991451
H	-1.561716	-0.393637	7.454585
C	-1.433526	4.844666	-2.830140
C	-2.476916	3.938440	-3.100297
C	-1.236318	5.924331	-3.711442
C	-3.302813	4.113041	-4.213585
H	-2.626954	3.079408	-2.442651
C	-2.066482	6.101215	-4.821262
H	-0.433519	6.638417	-3.512551
C	-3.103233	5.196765	-5.075930
H	-4.102588	3.394884	-4.411409
H	-1.904203	6.951362	-5.488674
H	-3.751585	5.334149	-5.944887
C	-3.476461	3.650804	4.277455
C	-3.886784	4.332497	5.440310
C	-4.409795	2.810018	3.637233
C	-5.187634	4.196731	5.930699
H	-3.181839	4.992944	5.950953
C	-5.708707	2.674349	4.127997
H	-4.101625	2.236225	2.761389
C	-6.105827	3.370829	5.274026
H	-5.486575	4.742896	6.829156
H	-6.408453	2.002661	3.625063
H	-7.121455	3.259165	5.661285
C	-3.123352	-0.063326	5.277858
C	-3.609170	0.737690	6.328133
C	-3.985309	-1.013205	4.700167

C	-4.914104	0.581407	6.796236
H	-2.970356	1.512471	6.755349
C	-5.290860	-1.171183	5.172757
H	-3.620946	-1.642835	3.884861
C	-5.757907	-0.376745	6.224873
H	-5.279663	1.226463	7.597946
H	-5.944118	-1.920756	4.718985
H	-6.780127	-0.496930	6.592141
C	2.986936	0.534438	9.431079
C	2.096926	1.282901	10.224544
C	3.961043	-0.254246	10.070410
C	2.175132	1.235659	11.618587
H	1.352632	1.921718	9.743921
C	4.033551	-0.305835	11.464893
H	4.656612	-0.841156	9.465691
C	3.140556	0.438285	12.243343
H	1.481888	1.829562	12.219426
H	4.790224	-0.931363	11.944982
H	3.198508	0.399673	13.333926



Zero-point correction= 0.901478 (Hartree/Particle)
Thermal correction to Energy= 0.959827
Thermal correction to Enthalpy= 0.960771
Thermal correction to Gibbs Free Energy= 0.804246
Sum of electronic and zero-point Energies= -6391.425234
Sum of electronic and thermal Energies= -6391.366886
Sum of electronic and thermal Enthalpies= -6391.365941
Sum of electronic and thermal Free Energies= -6391.522467

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.713532 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.86343 a.u.

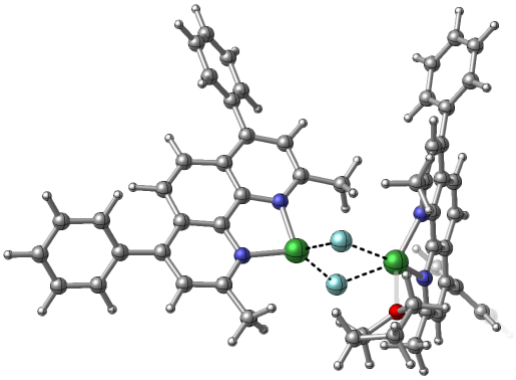
^{1}TS1
E(scf) = -6392.31187881 a.u.
ν_{min} = -43.72 cm^{-1}

C	1.652010	4.388435	-0.713710
C	1.239349	5.255919	-1.725041

C	-0.071664	5.771662	-1.779861
N	0.806025	4.009119	0.272815
C	-0.961061	5.398313	-0.729765
C	-0.473771	4.505044	0.260301
C	-1.313313	4.072918	1.333415
N	-0.738367	3.215757	2.227707
C	-2.656189	4.526851	1.442615
C	-3.426844	4.030706	2.532298
C	-1.457807	2.770780	3.267040
C	-2.795757	3.165670	3.436098
Ni	1.158820	2.766779	1.737951
H	1.949259	5.514678	-2.512868
H	-3.359145	2.761073	4.278537
Cl	1.433221	0.453449	1.325007
Cl	2.623750	2.864437	3.552500
C	4.439805	1.050975	5.861328
C	4.583203	1.539955	7.174759
C	3.553686	1.434285	8.108351
N	3.314969	0.445849	5.469412
C	2.365402	0.757932	7.706733
C	2.300865	0.284204	6.365888
C	1.142270	-0.426065	5.898161
N	1.184128	-0.867971	4.598380
C	0.044937	-0.654127	6.769968
C	-1.070520	-1.383992	6.260297
C	0.185536	-1.679399	4.176230
C	-0.932696	-1.931997	4.978620
Ni	2.587222	0.082935	3.566152
H	5.509432	2.048148	7.447907
H	-1.736202	-2.546930	4.568647
C	5.522890	1.250519	4.844239
H	5.663765	0.339407	4.248439
H	5.202638	2.038750	4.144084
H	6.470294	1.548585	5.313017
C	0.307123	-2.296515	2.814444
H	0.028660	-1.578203	2.029690
H	1.355648	-2.572619	2.624106
H	-0.327580	-3.189537	2.726346
C	-0.762812	1.843067	4.216574
H	-0.250410	1.050548	3.653540
H	0.038146	2.380300	4.748805
H	-1.450825	1.394655	4.944815
C	3.032569	3.803365	-0.642054
H	3.505486	4.080970	0.315871
H	2.968618	2.701756	-0.644640
H	3.673711	4.131682	-1.470675

O	4.323417	-0.192944	2.372916
C	4.331418	-1.462783	1.684477
C	4.778809	0.860817	1.485418
C	5.175686	-1.235624	0.434797
H	4.729142	-2.222773	2.373356
H	3.292879	-1.719884	1.419762
C	4.837891	0.224073	0.102078
H	4.072027	1.694804	1.568401
H	5.773023	1.191510	1.830333
H	4.924792	-1.940181	-0.371586
H	6.248310	-1.343296	0.665835
H	3.845248	0.282957	-0.370079
H	5.575090	0.709306	-0.554009
C	-2.300519	5.900466	-0.556505
H	-2.674552	6.650304	-1.253814
C	-3.104977	5.488433	0.471669
H	-4.102854	5.915754	0.572453
C	1.257921	0.477147	8.575323
H	1.313849	0.780725	9.620620
C	0.153432	-0.192042	8.126740
H	-0.656220	-0.412567	8.822577
C	-0.462144	6.657783	-2.902696
C	-1.640613	6.434418	-3.644122
C	0.372367	7.726337	-3.288987
C	-1.977406	7.257282	-4.721583
H	-2.285526	5.591381	-3.386867
C	0.034207	8.549557	-4.365619
H	1.287273	7.921532	-2.724208
C	-1.143678	8.320602	-5.085859
H	-2.892659	7.060378	-5.285878
H	0.692090	9.378199	-4.640307
H	-1.408596	8.964627	-5.928105
C	-4.853242	4.389614	2.742299
C	-5.292491	4.830594	4.005218
C	-5.802618	4.254328	1.710960
C	-6.636513	5.141202	4.226217
H	-4.567329	4.945074	4.814526
C	-7.147469	4.559983	1.934668
H	-5.485853	3.885808	0.732872
C	-7.568935	5.007944	3.191476
H	-6.956309	5.491847	5.210764
H	-7.870842	4.441215	1.124033
H	-8.620633	5.249328	3.364613
C	-2.327833	-1.583256	7.019746
C	-2.992584	-0.496726	7.624382
C	-2.920867	-2.858459	7.105830

C	-4.202315	-0.681779	8.297693
H	-2.565285	0.505508	7.544693
C	-4.129148	-3.043037	7.782190
H	-2.417664	-3.715130	6.650951
C	-4.774932	-1.956021	8.382102
H	-4.704509	0.176155	8.752095
H	-4.566573	-4.042796	7.844926
H	-5.720546	-2.100595	8.910493
C	3.731527	2.019118	9.463335
C	2.790008	2.918388	9.998982
C	4.880684	1.718493	10.217873
C	2.989703	3.493142	11.256655
H	1.905643	3.182832	9.415047
C	5.076010	2.288861	11.478386
H	5.618003	1.019488	9.815719
C	4.130995	3.177672	12.002274
H	2.252350	4.195506	11.653394
H	5.969587	2.035955	12.054598
H	4.284573	3.625431	12.987268



Zero-point correction= 0.899826 (Hartree/Particle)
Thermal correction to Energy= 0.957880
Thermal correction to Enthalpy= 0.958824
Thermal correction to Gibbs Free Energy= 0.801954
Sum of electronic and zero-point Energies= -6391.412052
Sum of electronic and thermal Energies= -6391.353999
Sum of electronic and thermal Enthalpies= -6391.353055
Sum of electronic and thermal Free Energies= -6391.509924

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.698063 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.850749 a.u.

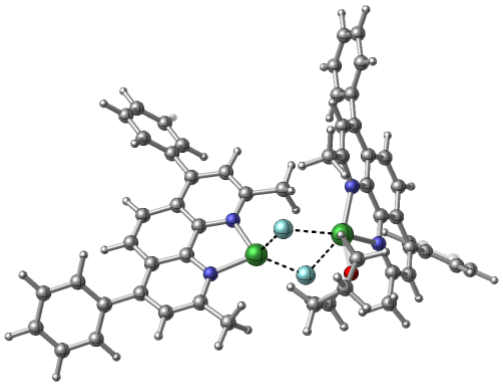
^{3}TS1
E(scf) = -6392.31198339 a.u.
ν_{min} = -45.94 cm^{-1}

C	1.653828	4.390680	-0.710912
C	1.240827	5.257004	-1.723036
C	-0.070713	5.771410	-1.778920

N	0.807735	4.011241	0.275554
C	-0.960269	5.397884	-0.729024
C	-0.472603	4.505819	0.261968
C	-1.312359	4.073609	1.334868
N	-0.737178	3.217523	2.230042
C	-2.655778	4.526310	1.443035
C	-3.426532	4.030184	2.532621
C	-1.456758	2.772546	3.269258
C	-2.795140	3.166355	3.437380
Ni	1.160591	2.769536	1.741483
H	1.950906	5.515959	-2.510646
H	-3.358595	2.761832	4.279807
Cl	1.432050	0.456398	1.330201
Cl	2.625580	2.868180	3.554943
C	4.439953	1.049771	5.860799
C	4.583736	1.538428	7.174308
C	3.554340	1.432959	8.108042
N	3.314847	0.445115	5.468905
C	2.365782	0.757048	7.706496
C	2.300866	0.283551	6.365583
C	1.141962	-0.426273	5.897980
N	1.183440	-0.867995	4.598123
C	0.044614	-0.653913	6.769877
C	-1.071369	-1.382952	6.260158
C	0.184174	-1.678494	4.175790
C	-0.934108	-1.930595	4.978267
Ni	2.586939	0.082094	3.565951
H	5.510192	2.046238	7.447396
H	-1.738113	-2.544815	4.568195
C	5.523018	1.249185	4.843674
H	5.663178	0.338349	4.247297
H	5.203214	2.038117	4.144105
H	6.470691	1.546306	5.312512
C	0.304815	-2.295249	2.813695
H	0.023360	-1.577559	2.029442
H	1.353521	-2.569271	2.621531
H	-0.328301	-3.189518	2.726657
C	-0.761467	1.845864	4.219600
H	-0.250201	1.052128	3.657252
H	0.040391	2.383387	4.750158
H	-1.449102	1.398975	4.949127
C	3.034874	3.806917	-0.638291
H	3.506547	4.084239	0.320334
H	2.972005	2.705235	-0.641796
H	3.676514	4.136406	-1.466060
O	4.322720	-0.192732	2.372030

C	4.330321	-1.461812	1.682140
C	4.777736	0.861984	1.485470
C	5.173254	-1.233107	0.431832
H	4.728884	-2.222514	2.369746
H	3.291580	-1.718869	1.418207
C	4.835102	0.226994	0.101275
H	4.071486	1.696243	1.570280
H	5.772477	1.191736	1.829763
H	4.921489	-1.936687	-0.375128
H	6.246131	-1.341041	0.661560
H	3.841889	0.286498	-0.369624
H	5.571510	0.713024	-0.555106
C	-2.300316	5.898846	-0.556822
H	-2.674694	6.647830	-1.254863
C	-3.104957	5.486780	0.471197
H	-4.103297	5.913217	0.571125
C	1.258360	0.476511	8.575233
H	1.314590	0.779886	9.620573
C	0.153523	-0.192152	8.126718
H	-0.656116	-0.412453	8.822640
C	-0.461452	6.656380	-2.902557
C	-1.639391	6.431498	-3.644383
C	0.372314	7.725383	-3.289250
C	-1.976402	7.253317	-4.722572
H	-2.283700	5.588085	-3.386848
C	0.033945	8.547551	-4.366617
H	1.286795	7.921772	-2.724196
C	-1.143422	8.317095	-5.087230
H	-2.891232	7.055230	-5.287140
H	0.691249	9.376559	-4.641589
H	-1.408510	8.960301	-5.930048
C	-4.853383	4.387889	2.741616
C	-5.293715	4.829328	4.003997
C	-5.802085	4.250978	1.709873
C	-6.638147	5.138814	4.224071
H	-4.569089	4.945053	4.813608
C	-7.147344	4.555510	1.932661
H	-5.484449	3.882076	0.732213
C	-7.569896	5.003949	3.188933
H	-6.958795	5.489840	5.208206
H	-7.870177	4.435488	1.121729
H	-8.621915	5.244452	3.361347
C	-2.328698	-1.581651	7.019723
C	-2.992707	-0.494883	7.624751
C	-2.922512	-2.856512	7.105518
C	-4.202464	-0.679382	8.298166

H	-2.564816	0.507117	7.545267
C	-4.130819	-3.040538	7.781982
H	-2.419897	-3.713361	6.650325
C	-4.775854	-1.953296	8.382290
H	-4.704074	0.178734	8.752870
H	-4.568853	-4.040045	7.844489
H	-5.721488	-2.097437	8.910765
C	3.732578	2.017535	9.463083
C	2.791439	2.917046	9.998992
C	4.881751	1.716431	10.217404
C	2.991516	3.491568	11.256710
H	1.907074	3.181859	9.415225
C	5.077458	2.286568	11.477963
H	5.618779	1.017238	9.815044
C	4.132817	3.175622	12.002113
H	2.254456	4.194125	11.653654
H	5.971040	2.033291	12.054005
H	4.286695	3.623201	12.987142



Zero-point correction= 0.899827 (Hartree/Particle)
Thermal correction to Energy= 0.957880
Thermal correction to Enthalpy= 0.958824
Thermal correction to Gibbs Free Energy= 0.800889
Sum of electronic and zero-point Energies= -6391.412156
Sum of electronic and thermal Energies= -6391.354104
Sum of electronic and thermal Enthalpies= -6391.353160
Sum of electronic and thermal Free Energies= -6391.511094

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.698187 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.850882 a.u.

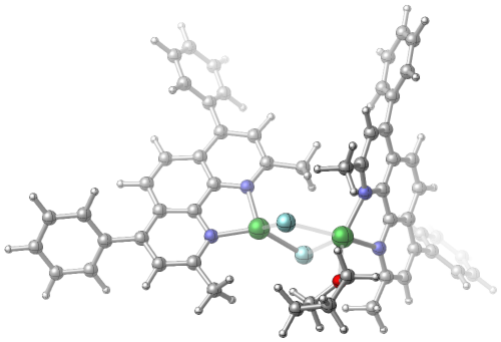
^{1}Int2
E(scf) = -6392.31201368 a.u.
ν_{min} = 7.20 cm^{-1}

C	1.594413	4.301028	-0.782392
C	1.193632	5.178465	-1.791074
C	-0.101907	5.730951	-1.829553

N	0.749603	3.947906	0.213237
C	-0.989253	5.384055	-0.768382
C	-0.514992	4.478085	0.215886
C	-1.352831	4.066578	1.298902
N	-0.790422	3.191055	2.183522
C	-2.680973	4.556694	1.423418
C	-3.452902	4.079218	2.520893
C	-1.511693	2.761114	3.228382
C	-2.836070	3.193312	3.413657
Ni	1.089205	2.701126	1.673239
H	1.900246	5.415269	-2.588690
H	-3.401299	2.801175	4.260759
Cl	1.494191	0.417476	1.236243
Cl	2.536918	2.771524	3.523995
C	4.451074	1.107353	5.907309
C	4.593738	1.564939	7.231501
C	3.567682	1.422387	8.165703
N	3.334125	0.494147	5.505399
C	2.385842	0.744780	7.751020
C	2.322036	0.299714	6.398748
C	1.169765	-0.406310	5.914033
N	1.213122	-0.820260	4.601539
C	0.073036	-0.658712	6.781246
C	-1.038936	-1.385257	6.260241
C	0.220398	-1.640849	4.171598
C	-0.892902	-1.915431	4.969536
Ni	2.596275	0.183115	3.585753
H	5.513876	2.078700	7.514416
H	-1.688265	-2.535483	4.551321
C	5.526013	1.348968	4.889707
H	5.715263	0.439069	4.305092
H	5.170041	2.110191	4.177208
H	6.456098	1.698996	5.356970
C	0.346491	-2.247089	2.805439
H	0.035110	-1.538265	2.024516
H	1.400990	-2.486570	2.600704
H	-0.259104	-3.160806	2.722573
C	-0.834551	1.810009	4.167984
H	-0.311154	1.030644	3.597078
H	-0.045762	2.333943	4.730761
H	-1.536330	1.344358	4.872066
C	2.958755	3.678160	-0.721656
H	3.468940	3.988040	0.206798
H	2.859916	2.580692	-0.665697
H	3.584710	3.947103	-1.582662
O	4.355300	-0.108693	2.429534

C	4.422133	-1.408654	1.804539
C	4.806735	0.915678	1.507404
C	5.314915	-1.217977	0.583073
H	4.807203	-2.124353	2.546005
H	3.402227	-1.704075	1.508846
C	4.951016	0.212539	0.162559
H	4.062928	1.720988	1.514500
H	5.770042	1.305875	1.876712
H	5.120812	-1.968572	-0.197007
H	6.378492	-1.281557	0.866459
H	3.981054	0.217031	-0.357909
H	5.704309	0.687741	-0.482482
C	-2.312227	5.922492	-0.579405
H	-2.674297	6.682330	-1.272195
C	-3.114698	5.531515	0.458551
H	-4.099370	5.985479	0.571752
C	1.281965	0.435821	8.613814
H	1.336680	0.713613	9.666320
C	0.181324	-0.228328	8.148672
H	-0.626265	-0.470814	8.839635
C	-0.481805	6.626445	-2.948946
C	-1.673347	6.431972	-3.677140
C	0.375296	7.673218	-3.344548
C	-2.000599	7.262090	-4.751983
H	-2.336545	5.605809	-3.411755
C	0.046500	8.503919	-4.418375
H	1.300786	7.845447	-2.789630
C	-1.144199	8.303776	-5.125937
H	-2.926380	7.087900	-5.306443
H	0.721962	9.315584	-4.700889
H	-1.401672	8.953545	-5.966073
C	-4.865932	4.477912	2.748612
C	-5.276836	4.929810	4.017155
C	-5.831137	4.370993	1.728729
C	-6.608613	5.278651	4.254697
H	-4.538867	5.022527	4.817625
C	-7.163850	4.714770	1.969070
H	-5.536998	3.994743	0.746524
C	-7.556933	5.173257	3.231272
H	-6.906243	5.637252	5.243311
H	-7.900151	4.617687	1.167242
H	-8.599083	5.444546	3.417364
C	-2.295621	-1.603729	7.013770
C	-2.960941	-0.533630	7.647603
C	-2.890957	-2.880303	7.066569
C	-4.170468	-0.735660	8.316277

H	-2.533821	0.470389	7.593901
C	-4.099453	-3.081839	7.737495
H	-2.388708	-3.725644	6.589950
C	-4.744653	-2.011067	8.366791
H	-4.671824	0.110445	8.793368
H	-4.537501	-4.082709	7.773399
H	-5.690372	-2.168975	8.891184
C	3.744415	1.974594	9.534577
C	2.796298	2.850544	10.096668
C	4.899396	1.666479	10.277234
C	2.994844	3.394510	11.368167
H	1.907263	3.121242	9.522814
C	5.093761	2.205971	11.551422
H	5.642233	0.985677	9.854514
C	4.141888	3.071338	12.101543
H	2.251994	4.078978	11.785442
H	5.991997	1.947283	12.117769
H	4.294632	3.494977	13.097284



Zero-point correction= 0.899827 (Hartree/Particle)
Thermal correction to Energy= 0.958684
Thermal correction to Enthalpy= 0.959629
Thermal correction to Gibbs Free Energy= 0.800461
Sum of electronic and zero-point Energies= -6391.412187
Sum of electronic and thermal Energies= -6391.353329
Sum of electronic and thermal Enthalpies= -6391.352385
Sum of electronic and thermal Free Energies= -6391.511553

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.697015 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.850176 a.u.

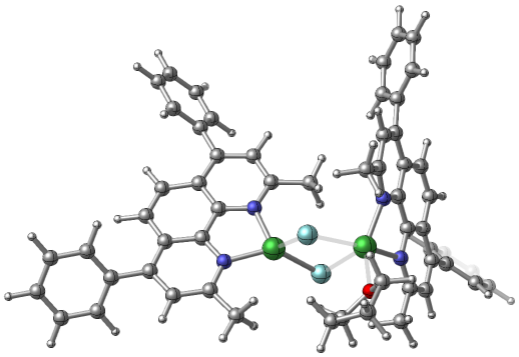
^{3}Int2
E(scf) = -6392.31213725 a.u.
ν_{min} = 7.23 cm^{-1}

C	1.593618	4.301239	-0.782393
C	1.193251	5.177921	-1.791885
C	-0.102319	5.730235	-1.831374
N	0.748365	3.948812	0.213112
C	-0.990218	5.383864	-0.770469

C	-0.516353	4.478605	0.214642
C	-1.354871	4.067427	1.297293
N	-0.792997	3.192275	2.182612
C	-2.683224	4.557325	1.420622
C	-3.455867	4.080106	2.517693
C	-1.515032	2.762405	3.226960
C	-2.839595	3.194549	3.411160
Ni	1.086941	2.702234	1.673620
H	1.900237	5.414258	-2.589310
H	-3.405409	2.802564	4.257938
Cl	1.493712	0.419671	1.237975
Cl	2.532730	2.769670	3.525645
C	4.452068	1.107904	5.908225
C	4.596067	1.563105	7.233036
C	3.570811	1.418963	8.167989
N	3.334801	0.495222	5.506269
C	2.388568	0.742278	7.753240
C	2.323378	0.299281	6.400234
C	1.170520	-0.405433	5.915340
N	1.212443	-0.817360	4.601947
C	0.074265	-0.658514	6.783082
C	-1.038671	-1.383503	6.262063
C	0.218608	-1.636812	4.171829
C	-0.893934	-1.911984	4.970348
Ni	2.595224	0.187329	3.586499
H	5.516462	2.076392	7.515957
H	-1.689905	-2.531162	4.551983
C	5.526037	1.351659	4.890075
H	5.716666	0.442264	4.305115
H	5.168446	2.112436	4.177916
H	6.455755	1.703146	5.356965
C	0.342414	-2.241460	2.804673
H	0.024304	-1.533927	2.025307
H	1.397140	-2.475733	2.595502
H	-0.259257	-3.157973	2.723724
C	-0.838633	1.811377	4.167216
H	-0.314625	1.032075	3.596808
H	-0.050551	2.335448	4.730828
H	-1.541044	1.345582	4.870578
C	2.957853	3.678332	-0.720573
H	3.467705	3.988940	0.207825
H	2.858763	2.580923	-0.663704
H	3.584204	3.946450	-1.581548
O	4.354347	-0.103851	2.430684
C	4.423734	-1.404447	1.807259
C	4.805100	0.920136	1.507858

C	5.316906	-1.213692	0.586082
H	4.809565	-2.118631	2.549789
H	3.404510	-1.701967	1.511340
C	4.951041	0.215810	0.163837
H	4.060278	1.724501	1.513641
H	5.767693	1.311907	1.877353
H	5.124389	-1.965431	-0.193282
H	6.380421	-1.275322	0.870119
H	3.981306	0.218305	-0.357084
H	5.703898	0.691464	-0.481374
C	-2.313409	5.922158	-0.582631
H	-2.675179	6.681534	-1.276083
C	-3.116483	5.531592	0.455015
H	-4.101318	5.985418	0.567333
C	1.285410	0.432246	8.616515
H	1.341189	0.708154	9.669461
C	0.184073	-0.230584	8.151164
H	-0.622989	-0.473928	8.842442
C	-0.481750	6.624933	-2.951564
C	-1.672844	6.429765	-3.680303
C	0.375405	7.671579	-3.347383
C	-1.999615	7.259093	-4.755900
H	-2.336059	5.603676	-3.414735
C	0.047085	8.501494	-4.421963
H	1.300551	7.844334	-2.792057
C	-1.143173	8.300669	-5.130071
H	-2.925048	7.084371	-5.310772
H	0.722572	9.313081	-4.704643
H	-1.400275	8.949821	-5.970796
C	-4.869131	4.478655	2.744241
C	-5.280986	4.931046	4.012293
C	-5.833592	4.371086	1.723731
C	-6.612990	5.279762	4.248745
H	-4.543590	5.024246	4.813237
C	-7.166536	4.714724	1.962991
H	-5.538697	3.994444	0.741904
C	-7.560574	5.173722	3.224708
H	-6.911375	5.638757	5.236987
H	-7.902263	4.617139	1.160696
H	-8.602903	5.444907	3.409951
C	-2.294814	-1.602362	7.016277
C	-2.958628	-0.533037	7.653064
C	-2.891387	-2.878490	7.066931
C	-4.167687	-0.735382	8.322478
H	-2.530695	0.470725	7.601049
C	-4.099437	-3.080340	7.738551

H	-2.390405	-3.723311	6.588064
C	-4.743052	-2.010349	8.370809
H	-4.667792	0.110176	8.801855
H	-4.538378	-4.080885	7.772704
H	-5.688418	-2.168504	8.895765
C	3.748919	1.968847	9.537622
C	2.801456	2.843948	10.102147
C	4.904622	1.659422	10.278623
C	3.001302	3.385749	11.374367
H	1.911884	3.115701	9.529627
C	5.100302	2.196753	11.553522
H	5.646995	0.979286	9.854015
C	4.149044	3.061258	12.106062
H	2.258917	4.069571	11.793528
H	5.999087	1.937047	12.118534
H	4.302813	3.483208	13.102363



Zero-point correction= 0.899838 (Hartree/Particle)
Thermal correction to Energy= 0.958679
Thermal correction to Enthalpy= 0.959623
Thermal correction to Gibbs Free Energy= 0.799521
Sum of electronic and zero-point Energies= -6391.412299
Sum of electronic and thermal Energies= -6391.353458
Sum of electronic and thermal Enthalpies= -6391.352514
Sum of electronic and thermal Free Energies= -6391.512616

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6395.697091 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6391.850302 a.u.

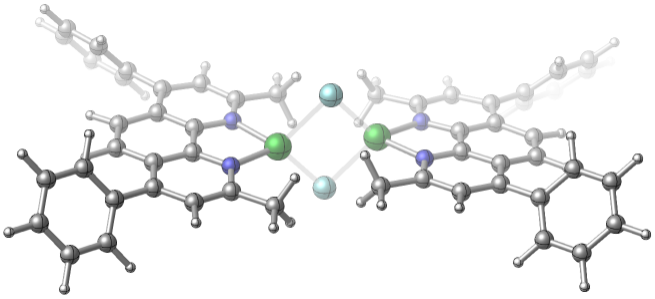
^{1}[(L4)NiCl]$_2$
E(scf) = -6160.00149650 a.u.
n_{min} = 7.08 cm^{-1}

Ni	15.907727	7.659116	6.340609
N	17.224805	6.136083	6.246963
N	16.192984	7.445491	8.265972
C	17.062499	6.434996	8.590283
C	17.622651	5.720838	7.483822
C	18.407059	5.066605	10.101566

H	18.755566	4.842544	11.109783
C	18.545979	4.660353	7.690242
C	18.941317	4.382033	9.044143
H	19.703603	3.624716	9.227541
C	15.957390	7.893946	10.609463
H	15.478156	8.492600	11.386218
C	17.419335	6.099008	9.922686
C	16.819568	6.846908	10.978731
C	17.727745	5.533455	5.162016
C	15.659341	8.173113	9.273840
C	18.634172	4.465731	5.283850
H	18.998235	3.980223	4.377017
C	19.047608	3.995026	6.534652
C	14.728519	9.271936	8.860199
H	15.249286	9.956742	8.171042
H	14.342145	9.842452	9.714868
H	13.881474	8.848966	8.295502
C	17.259583	6.048801	3.835732
H	17.430067	7.134964	3.785465
H	16.169202	5.917810	3.753729
H	17.758364	5.552438	2.993220
Cl	16.531313	9.548637	4.970365
Cl	13.993379	7.184246	4.954751
N	14.422396	9.363946	1.657679
N	13.177624	10.476438	3.675465
C	12.779452	10.888466	2.437612
C	13.456810	10.282788	1.331924
C	11.505978	12.266861	0.874006
H	10.790314	13.067918	0.688565
C	13.132645	10.647016	-0.001433
C	12.153816	11.687426	-0.182761
H	11.942814	12.039428	-1.192594
C	11.594003	11.984267	4.636058
H	11.134664	12.381858	5.542451
C	11.770536	11.867599	2.229458
C	11.141233	12.414840	3.384488
C	15.118311	8.788890	0.650051
C	12.608773	11.019159	4.759487
C	14.846565	9.090279	-0.686344
H	15.416250	8.575924	-1.462423
C	13.841266	10.000260	-1.056895
C	13.101999	10.530253	6.086597
H	12.627948	11.051627	6.928258
H	14.194706	10.652264	6.137623
H	12.922164	9.446952	6.168755
C	16.173885	7.809520	1.064463

H	16.879869	8.298933	1.755404
H	16.727650	7.398451	0.210308
H	15.712893	6.981757	1.627759
Ni	14.616538	9.068487	3.584133
C	13.568145	10.245303	-2.493975
C	14.630548	10.489698	-3.387161
C	12.259329	10.191643	-3.014893
C	14.392006	10.687730	-4.749183
H	15.651964	10.541813	-3.002372
C	12.021959	10.387714	-4.377517
H	11.423686	9.970031	-2.347468
C	13.086327	10.639697	-5.250398
H	15.230422	10.885521	-5.422021
H	10.999707	10.334473	-4.760802
H	12.899461	10.794410	-6.315965
C	10.041814	13.411344	3.307054
C	10.105767	14.595711	4.065045
C	8.898842	13.178014	2.518416
C	9.064480	15.526290	4.024236
H	10.988640	14.792995	4.677864
C	7.855370	14.106340	2.483659
H	8.820313	12.251707	1.945106
C	7.935936	15.285231	3.233058
H	9.136474	16.445347	4.611258
H	6.972407	13.904514	1.872061
H	7.120675	16.012339	3.202502
C	19.979819	2.840510	6.610747
C	21.158346	2.830684	5.841039
C	19.688846	1.718157	7.409884
C	22.027696	1.737715	5.880569
H	21.400270	3.696449	5.219892
C	20.555898	0.623202	7.443595
H	18.765216	1.696726	7.992394
C	21.729952	0.630414	6.682400
H	22.943394	1.752553	5.284160
H	20.309581	-0.242454	8.063575
H	22.409068	-0.225259	6.712058
C	17.065996	6.573039	12.415514
C	16.948891	5.273624	12.949248
C	17.377833	7.628673	13.295596
C	17.148702	5.038152	14.311687
H	16.675032	4.445139	12.292353
C	17.579690	7.391895	14.657371
H	17.479724	8.642359	12.900445
C	17.468083	6.095126	15.171398
H	17.045686	4.023643	14.705255

H	17.830421	8.224401	15.319824
H	17.625841	5.909611	16.236754



Zero-point correction= 0.781378 (Hartree/Particle)
Thermal correction to Energy= 0.834313
Thermal correction to Enthalpy= 0.835257
Thermal correction to Gibbs Free Energy= 0.688603
Sum of electronic and zero-point Energies= -6159.220119
Sum of electronic and thermal Energies= -6159.167183
Sum of electronic and thermal Enthalpies= -6159.166239
Sum of electronic and thermal Free Energies= -6159.312893

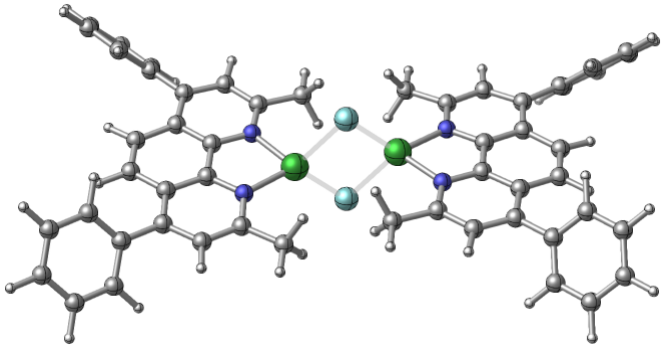
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6163.135134 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6159.568689 a.u.

^{3}[(L4)NiCl]$_2$
E(scf) = -6160.00164312 a.u.
ν_{min} = 6.93 cm^{-1}

Ni	15.902646	7.658390	6.340179
N	17.218515	6.133985	6.246083
N	16.188104	7.443513	8.266239
C	17.057298	6.432431	8.589702
C	17.616671	5.718352	7.482812
C	18.401891	5.062984	10.100151
H	18.750702	4.838518	11.108171
C	18.539683	4.657425	7.688663
C	18.935493	4.378586	9.042324
H	19.697621	3.620981	9.225175
C	15.953677	7.891088	10.610045
H	15.475000	8.489627	11.387227
C	17.414487	6.095782	9.921908
C	16.815452	6.843422	10.978492
C	17.720888	5.531146	5.160925
C	15.655345	8.170956	9.274640
C	18.626980	4.463160	5.282262
H	18.990562	3.977686	4.375219
C	19.040758	3.992121	6.532864
C	14.725005	9.270563	8.862090
H	15.245839	9.955274	8.172910
H	14.339629	9.841003	9.717257

H	13.877263	8.848429	8.297832
C	17.252581	6.046497	3.834717
H	17.422940	7.132654	3.784548
H	16.162234	5.915300	3.752627
H	17.751464	5.550264	2.992189
Cl	16.532888	9.545846	4.971630
Cl	13.989370	7.185714	4.954277
N	14.425628	9.364711	1.658204
N	13.180772	10.476628	3.676789
C	12.782615	10.888972	2.438941
C	13.460032	10.283799	1.333020
C	11.509026	12.267925	0.875777
H	10.793291	13.068998	0.690685
C	13.135920	10.648735	-0.000223
C	12.157027	11.689124	-0.181194
H	11.946123	12.041602	-1.190880
C	11.596847	11.984108	4.637625
H	11.137412	12.381396	5.544102
C	11.773541	11.868054	2.231061
C	11.143962	12.414848	3.386114
C	15.121558	8.790362	0.650243
C	12.611731	11.019186	4.760861
C	14.849972	9.092580	-0.685999
H	15.419775	8.578779	-1.462354
C	13.844619	10.002710	-1.056016
C	13.104624	10.530196	6.088042
H	12.631635	11.052767	6.929559
H	14.197521	10.650483	6.138679
H	12.922978	9.447263	6.170853
C	16.177154	7.810627	1.063705
H	16.882646	8.299156	1.755759
H	16.731467	7.401091	0.209173
H	15.716103	6.981782	1.625325
Ni	14.619103	9.067799	3.585411
C	13.571626	10.248666	-2.492968
C	14.634112	10.493926	-3.385818
C	12.262904	10.195036	-3.014118
C	14.395730	10.692854	-4.747737
H	15.655455	10.546008	-3.000833
C	12.025699	10.391984	-4.376644
H	11.427216	9.972769	-2.346967
C	13.090139	10.644842	-5.249184
H	15.234200	10.891321	-5.420308
H	11.003520	10.338751	-4.760126
H	12.903398	10.800247	-6.314672
C	10.044164	13.410929	3.308889

C	10.107400	14.594975	4.067458
C	8.901414	13.177453	2.519953
C	9.065674	15.525074	4.026924
H	10.990067	14.792396	4.680529
C	7.857512	14.105303	2.485450
H	8.823393	12.251369	1.946215
C	7.937377	15.283871	3.235434
H	9.137129	16.443878	4.614409
H	6.974748	13.903342	1.873608
H	7.121772	16.010602	3.205094
C	19.972793	2.837438	6.608395
C	21.151024	2.827595	5.838215
C	19.682018	1.714950	7.407424
C	22.020270	1.734525	5.877202
H	21.392807	3.693447	5.217135
C	20.548972	0.619900	7.440608
H	18.758605	1.693497	7.990278
C	21.722731	0.627113	6.678958
H	22.935735	1.749376	5.280434
H	20.302802	-0.245841	8.060530
H	22.401771	-0.228636	6.708202
C	17.062175	6.568700	12.415060
C	16.944587	5.269065	12.948158
C	17.374728	7.623737	13.295606
C	17.144631	5.032799	14.310424
H	16.670169	4.441049	12.290906
C	17.576827	7.386160	14.657204
H	17.476987	8.637580	12.900955
C	17.464733	6.089180	15.170596
H	17.041230	4.018138	14.703497
H	17.828122	8.218206	15.320023
H	17.622669	5.903044	16.235818



Zero-point correction= 0.781349 (Hartree/Particle)
Thermal correction to Energy= 0.834303
Thermal correction to Enthalpy= 0.835247
Thermal correction to Gibbs Free Energy= 0.687356
Sum of electronic and zero-point Energies= -6159.220294

Sum of electronic and thermal Energies= -6159.167341
Sum of electronic and thermal Enthalpies= -6159.166396
Sum of electronic and thermal Free Energies= -6159.314287

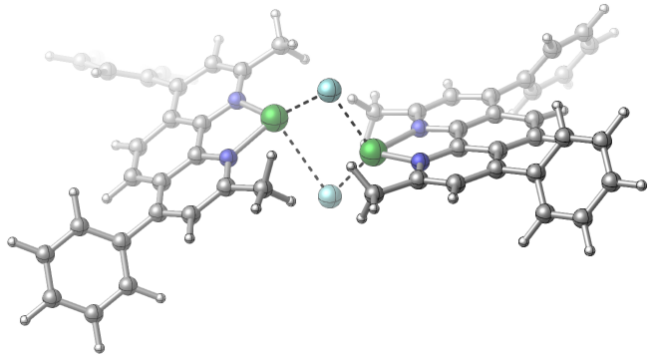
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6163.135266 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6159.568861 a.u.

^{1}TS2
E(scf) = -6159.99593760 a.u.
ν_{min} = -34.60 cm^{-1}

Ni	16.438860	7.843578	6.406707
N	17.309283	6.068954	6.436999
N	16.426466	7.618651	8.365159
C	16.912050	6.401881	8.750674
C	17.391810	5.552214	7.691030
C	17.434708	4.629637	10.349561
H	17.408815	4.247274	11.369867
C	17.918727	4.268876	7.975919
C	17.884943	3.821110	9.341233
H	18.210369	2.807082	9.573452
C	16.029469	8.112054	10.671828
H	15.690956	8.842525	11.408860
C	16.969833	5.966772	10.096526
C	16.518781	6.880726	11.100469
C	17.745384	5.348069	5.398988
C	15.990215	8.464941	9.307458
C	18.293122	4.063913	5.598124
H	18.663656	3.512499	4.732362
C	18.404580	3.503983	6.869287
C	15.461594	9.797998	8.862712
H	15.913666	10.086254	7.902305
H	15.655242	10.577689	9.613160
H	14.371159	9.744688	8.710227
C	17.610214	5.968914	4.042718
H	17.934554	7.020590	4.079292
H	16.542092	5.991486	3.772488
H	18.177633	5.425724	3.275484
Cl	16.359524	9.549314	4.900361
Cl	14.164387	6.481305	4.768536
N	14.378673	9.051964	1.810237
N	12.992348	9.790631	3.902803
C	12.655309	10.398065	2.728248
C	13.414034	10.000863	1.583058
C	11.317815	11.863994	1.306959
H	10.476197	12.545026	1.179068
C	13.151771	10.566068	0.307200

C	12.045353	11.484139	0.211429
H	11.766643	11.869969	-0.769301
C	11.301161	11.066083	5.000467
H	10.800516	11.321151	5.935895
C	11.617798	11.364080	2.621705
C	10.930876	11.718827	3.817458
C	15.135878	8.644348	0.765812
C	12.331717	10.110460	5.022189
C	14.941481	9.162212	-0.515010
H	15.589944	8.816651	-1.322255
C	13.963747	10.140539	-0.784992
C	12.752849	9.401791	6.275548
H	12.257978	9.808550	7.167506
H	13.845579	9.466714	6.387475
H	12.535863	8.325480	6.186067
C	16.185821	7.623477	1.091655
H	16.854901	8.017901	1.874650
H	16.782521	7.336861	0.215633
H	15.710096	6.723314	1.516747
Ni	14.514438	8.491226	3.682053
C	9.854482	12.742473	3.855608
C	8.626913	12.454372	4.481772
C	10.047383	14.028493	3.315188
C	7.617341	13.417509	4.552294
H	8.460357	11.459446	4.901711
C	9.039188	14.992737	3.391508
H	11.003547	14.279210	2.850753
C	7.819490	14.690057	4.006804
H	6.667215	13.171586	5.033246
H	9.210235	15.987879	2.973264
H	7.030502	15.444121	4.063321
C	13.826557	10.675493	-2.161206
C	13.781569	9.797038	-3.262814
C	13.787263	12.061855	-2.415253
C	13.685521	10.285280	-4.567993
H	13.804425	8.718620	-3.087833
C	13.692883	12.549401	-3.721015
H	13.856486	12.763256	-1.580947
C	13.638315	11.664011	-4.803385
H	13.642087	9.584480	-5.405782
H	13.671112	13.628466	-3.894216
H	13.563066	12.046404	-5.824384
C	16.564335	6.572312	12.553004
C	15.420548	6.762865	13.350733
C	17.751621	6.134301	13.170425
C	15.458783	6.509690	14.724189

H	14.490810	7.097075	12.884057
C	17.789824	5.887615	14.544938
H	18.656165	6.007643	12.571516
C	16.643148	6.070646	15.325740
H	14.558242	6.653538	15.326393
H	18.722165	5.556355	15.008952
H	16.673451	5.874040	16.400273
C	19.019422	2.160564	7.028801
C	20.081380	1.945876	7.927893
C	18.574736	1.083106	6.240271
C	20.676031	0.686600	8.038775
H	20.456802	2.777744	8.527923
C	19.166063	-0.177322	6.357356
H	17.747854	1.234675	5.542299
C	20.218089	-0.379832	7.257144
H	21.505016	0.539670	8.735549
H	18.801333	-1.005375	5.744502
H	20.681645	-1.365313	7.347456



Zero-point correction= 0.781635 (Hartree/Particle)
Thermal correction to Energy= 0.833681
Thermal correction to Enthalpy= 0.834625
Thermal correction to Gibbs Free Energy= 0.689658
Sum of electronic and zero-point Energies= -6159.214303
Sum of electronic and thermal Energies= -6159.162257
Sum of electronic and thermal Enthalpies= -6159.161313
Sum of electronic and thermal Free Energies= -6159.306279

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6163.133609 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6159.56622 a.u.

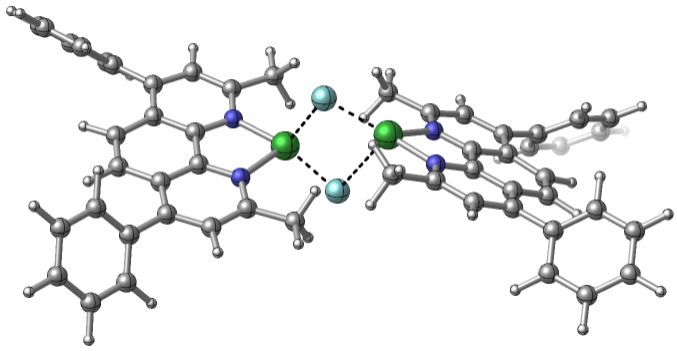
^{3}TS2
E(scf) = -6159.99605127 a.u.
ν_{min} = -37.52 cm^{-1}

Ni	16.444228	7.842578	6.387154
N	17.312298	6.068034	6.425837
N	16.430292	7.625886	8.348226
C	16.912308	6.408939	8.737872

C	17.391661	5.554920	7.681496
C	17.428484	4.639990	10.342652
H	17.400146	4.260706	11.364039
C	17.915331	4.271254	7.970890
C	17.878373	3.827466	9.337393
H	18.201097	2.813367	9.573054
C	16.031673	8.126675	10.653046
H	15.694107	8.860148	11.387545
C	16.967203	5.977462	10.084996
C	16.517100	6.895407	11.085759
C	17.748587	5.343306	5.390609
C	15.995208	8.475930	9.287489
C	18.293348	4.058659	5.594294
H	18.664204	3.503997	4.730750
C	18.401391	3.502127	6.867258
C	15.471233	9.809978	8.840022
H	15.913660	10.088931	7.872578
H	15.680165	10.592695	9.583289
H	14.378534	9.764367	8.702001
C	17.616435	5.960597	4.032418
H	17.940969	7.012325	4.066852
H	16.548879	5.982282	3.759964
H	18.185379	5.415383	3.267750
Cl	16.357606	9.551472	4.887467
Cl	14.170536	6.463673	4.764820
N	14.378704	9.041166	1.810600
N	12.990941	9.771491	3.905645
C	12.655786	10.384721	2.733455
C	13.415332	9.992256	1.587218
C	11.321412	11.858993	1.317766
H	10.480643	12.541514	1.192242
C	13.155133	10.564032	0.313779
C	12.049762	11.483709	0.221228
H	11.772526	11.874579	-0.757921
C	11.299919	11.043689	5.007432
H	10.798553	11.294956	5.943499
C	11.619417	11.352446	2.630431
C	10.931549	11.702331	3.826995
C	15.136877	8.638230	0.765151
C	12.329507	10.087069	5.025805
C	14.944447	9.162460	-0.513350
H	15.593390	8.820171	-1.321598
C	13.967819	10.143039	-0.779555
C	12.748519	9.372463	6.276517
H	12.255228	9.777695	7.170048
H	13.841396	9.433409	6.388443

H	12.527956	8.297216	6.183463
C	16.185750	7.615028	1.087252
H	16.854560	8.005782	1.872304
H	16.782820	7.331696	0.210416
H	15.709022	6.713494	1.508238
Ni	14.515636	8.475534	3.681867
C	9.856212	12.726928	3.868880
C	8.627751	12.437228	4.492577
C	10.050966	14.015303	3.334748
C	7.619157	13.401111	4.566763
H	8.459742	11.440513	4.907672
C	9.043741	14.980268	3.414724
H	11.007833	14.267202	2.872406
C	7.823162	14.676015	4.027493
H	6.668338	13.153944	5.045709
H	9.216252	15.977197	3.001364
H	7.034945	15.430665	4.086896
C	13.832473	10.684733	-2.153312
C	13.787697	9.811624	-3.259179
C	13.794660	12.072335	-2.400754
C	13.693193	10.306210	-4.562079
H	13.809458	8.732358	-3.089353
C	13.701820	12.566230	-3.704237
H	13.863798	12.769659	-1.563032
C	13.647382	11.686098	-4.790894
H	13.649856	9.609485	-5.403264
H	13.681147	13.646135	-3.872268
H	13.573324	12.073459	-5.810106
C	16.559976	6.590881	12.539216
C	15.415475	6.785960	13.334788
C	17.745520	6.152123	13.159420
C	15.451294	6.536401	14.708975
H	14.487096	7.120842	12.865898
C	17.781323	5.909100	14.534649
H	18.650602	6.021937	12.562082
C	16.633931	6.096575	15.313341
H	14.550223	6.683713	15.309543
H	18.712337	5.577190	15.000855
H	16.662347	5.902805	16.388441
C	19.013028	2.157834	7.031597
C	20.072986	1.943318	7.933089
C	18.567379	1.079181	6.245238
C	20.664738	0.683074	8.048410
H	20.449200	2.776011	8.531476
C	19.155798	-0.182184	6.366756
H	17.742021	1.230620	5.545436

C	20.205854	-0.384496	7.268890
H	21.492223	0.536268	8.746990
H	18.790344	-1.011116	5.755524
H	20.667150	-1.370714	7.362660



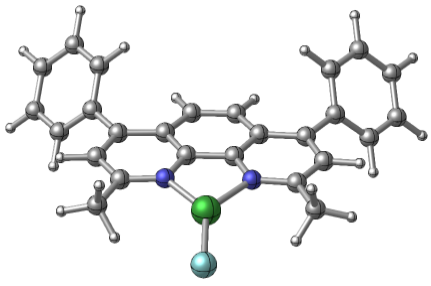
Zero-point correction= 0.781629 (Hartree/Particle)
Thermal correction to Energy= 0.833683
Thermal correction to Enthalpy= 0.834627
Thermal correction to Gibbs Free Energy= 0.688458
Sum of electronic and zero-point Energies= -6159.214423
Sum of electronic and thermal Energies= -6159.162369
Sum of electronic and thermal Enthalpies= -6159.161424
Sum of electronic and thermal Free Energies= -6159.307593

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6163.133654 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -6159.566302 a.u.

^{2}(L4)NiCl
E(scf) = -3079.98247907 a.u.
ν_{min} = 30.28 cm^{-1}

Ni	27.585046	10.193442	1.881795
N	28.852243	8.734961	2.264916
N	26.924784	9.766906	3.692962
C	27.559492	8.699459	4.249448
C	28.622119	8.131025	3.462829
C	27.924283	6.967638	5.929831
H	27.629850	6.481468	6.859867
C	29.345946	7.008865	3.931547
C	28.935645	6.427229	5.181707
H	29.429625	5.519614	5.528538
C	25.518372	9.860396	5.620374
H	24.707231	10.369714	6.143531
C	27.217182	8.146661	5.506481
C	26.156115	8.778956	6.227826
C	25.720179	8.330001	7.575175
C	29.815294	8.254716	1.468712
C	25.914667	10.341991	4.356377
C	30.591399	7.147777	1.866343

H	31.384536	6.799522	1.202564
C	30.393765	6.513880	3.093077
C	24.356676	8.097869	7.835718
H	23.629221	8.211032	7.028338
C	26.644258	8.171472	8.625640
H	27.702787	8.373873	8.448150
C	24.858729	7.546880	10.142015
H	24.525241	7.241125	11.136744
C	25.269952	11.531690	3.706511
H	24.312306	11.791243	4.177505
H	25.125508	11.342254	2.631705
H	25.942872	12.403384	3.775647
C	30.041402	8.977246	0.172514
H	30.667771	8.398723	-0.519751
H	30.534068	9.945091	0.367311
H	29.075806	9.215804	-0.299685
C	23.930760	7.705041	9.106978
H	22.869315	7.519094	9.288753
C	26.215786	7.785049	9.897915
H	26.945586	7.675058	10.703865
C	31.260044	5.370143	3.478088
C	32.955070	3.222263	4.155224
H	33.610479	2.388544	4.418898
C	31.929805	5.346330	4.716455
H	31.806546	6.178825	5.412646
C	32.771074	4.282102	5.050098
H	33.289725	4.284023	6.012002
C	31.461662	4.303630	2.582013
H	30.943670	4.305801	1.619961
C	32.298143	3.236947	2.920054
H	32.434870	2.412238	2.216183
Cl	26.949925	11.433088	0.180223



Zero-point correction= 0.390107 (Hartree/Particle)
Thermal correction to Energy= 0.415940
Thermal correction to Enthalpy= 0.416885
Thermal correction to Gibbs Free Energy= 0.331159
Sum of electronic and zero-point Energies= -3079.592372
Sum of electronic and thermal Energies= -3079.566539
Sum of electronic and thermal Enthalpies= -3079.565595

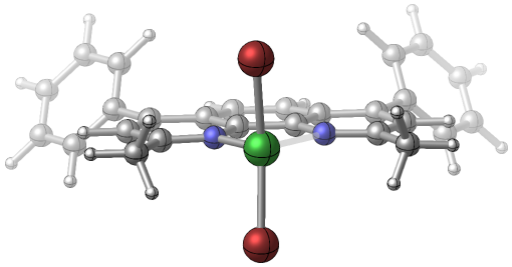
Sum of electronic and thermal Free Energies= -3079.651320

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3081.563192 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3079.779317 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3079.966271 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3074.925397 a.u.

^{1}(L4)NiBr$_2$
E(scf) = -7767.67679001 a.u.
ν_{min} = 22.86 cm^{-1}

Ni	27.370711	10.395564	1.886649
N	28.912855	8.742738	2.161381
N	26.854951	9.801888	3.593164
C	27.561509	8.767386	4.131079
C	28.660652	8.203406	3.367788
C	28.092656	7.212537	5.952874
H	27.906828	6.863122	6.967832
C	29.425313	7.134229	3.908383
C	29.127812	6.681327	5.236953
H	29.755143	5.913699	5.689628
C	25.482208	9.884731	5.529779
H	24.635769	10.345662	6.039951
C	27.253532	8.247396	5.414956
C	26.150930	8.821218	6.122138
C	25.702216	8.327274	7.449796
C	29.912408	8.290715	1.418322
C	25.844044	10.370804	4.258440
C	30.717579	7.218654	1.864384
H	31.515645	6.844747	1.220569
C	30.482693	6.614355	3.095409
C	25.535909	9.230538	8.515395
H	25.780039	10.285433	8.369446
C	25.389309	6.970232	7.653889
H	25.489399	6.262027	6.828440
C	24.777498	7.433398	9.953238
H	24.420690	7.085552	10.925744
C	25.115365	11.507333	3.611761
H	24.310049	11.885311	4.254510
H	24.694776	11.175376	2.649451
H	25.824623	12.320611	3.391715
C	30.112310	8.968438	0.092702
H	30.981585	8.578569	-0.453239
H	30.234928	10.051759	0.252955
H	29.208476	8.839525	-0.525038
C	25.083074	8.784755	9.759565

H	24.970072	9.496285	10.581101
C	24.927377	6.529018	8.896040
H	24.679499	5.474199	9.036970
C	31.324249	5.464020	3.519549
C	32.940084	3.273838	4.243196
H	33.566814	2.424468	4.525924
C	30.743227	4.243477	3.911573
H	29.655791	4.140517	3.917561
C	31.545928	3.157061	4.267964
H	31.079516	2.213486	4.561681
C	32.726850	5.566919	3.487886
H	33.189500	6.510821	3.189810
C	33.527919	4.481603	3.852149
H	34.615976	4.581005	3.831977
Br	28.678224	12.200833	2.613111
Br	25.753739	9.203003	0.681897

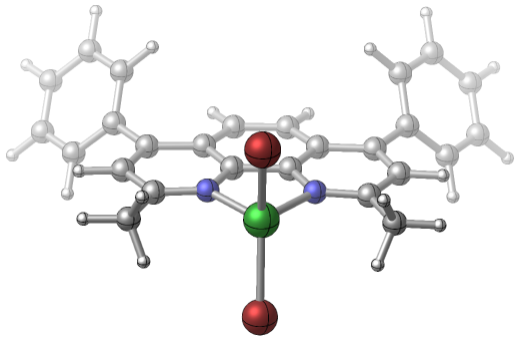


Zero-point correction= 0.391432 (Hartree/Particle)
Thermal correction to Energy= 0.419395
Thermal correction to Enthalpy= 0.420339
Thermal correction to Gibbs Free Energy= 0.329411
Sum of electronic and zero-point Energies= -7767.285358
Sum of electronic and thermal Energies= -7767.257395
Sum of electronic and thermal Enthalpies= -7767.256451
Sum of electronic and thermal Free Energies= -7767.347379

^{3}(L4)NiBr$_2$
E(scf) = -7767.73765086 a.u.
ν_{min} = 26.65 cm^{-1}

Ni	27.496236	10.234627	1.799066
N	28.823895	8.751625	2.205490
N	26.848885	9.771686	3.664389
C	27.553141	8.756857	4.220762
C	28.623452	8.201110	3.427625
C	28.151894	7.229817	6.032669
H	28.007657	6.882792	7.055437
C	29.417694	7.146200	3.937121
C	29.163988	6.700084	5.279558
H	29.811400	5.938168	5.712840
C	25.526316	9.910699	5.633767
H	24.695756	10.388711	6.154929
C	27.288980	8.257672	5.518576

C	26.207089	8.858207	6.238882
C	25.797826	8.402571	7.592359
C	29.809754	8.315610	1.423024
C	25.861332	10.358349	4.338239
C	30.634841	7.253454	1.849974
H	31.413823	6.892765	1.176917
C	30.451220	6.639819	3.085576
C	25.506040	7.049381	7.847240
H	25.588026	6.317090	7.041025
C	25.653076	9.336473	8.634637
H	25.882200	10.388649	8.449887
C	24.956887	7.576983	10.148526
H	24.632719	7.255782	11.141408
C	25.143714	11.478205	3.648317
H	24.712940	11.107946	2.703045
H	25.869811	12.262890	3.378156
H	24.349293	11.909023	4.270462
C	29.972303	8.989451	0.094375
H	30.825079	8.592573	-0.470422
H	30.101207	10.073416	0.248952
H	29.049397	8.861179	-0.495852
C	25.085694	6.641996	9.115516
H	24.853575	5.589607	9.295931
C	25.241656	8.924799	9.904574
H	25.145115	9.660166	10.707010
C	31.318429	5.497854	3.473511
C	32.977754	3.320821	4.129459
H	33.621789	2.476171	4.386057
C	32.717195	5.607020	3.368849
H	33.160408	6.550509	3.041619
C	33.540063	4.527971	3.700631
H	34.625195	4.631577	3.625119
C	30.762502	4.278258	3.903638
H	29.677371	4.169933	3.964128
C	31.587240	3.197909	4.225582
H	31.140694	2.254367	4.548510
Br	28.777319	12.241704	2.129229
Br	25.877757	9.201171	0.355687



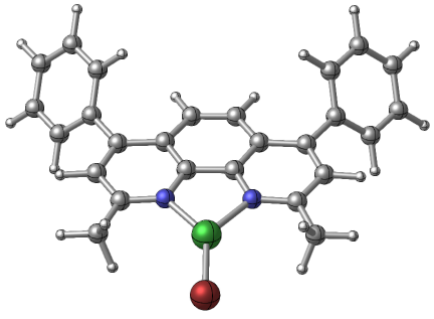
Zero-point correction= 0.392079 (Hartree/Particle)
Thermal correction to Energy= 0.419830
Thermal correction to Enthalpy= 0.420774
Thermal correction to Gibbs Free Energy= 0.329817
Sum of electronic and zero-point Energies= -7767.345571
Sum of electronic and thermal Energies= -7767.317821
Sum of electronic and thermal Enthalpies= -7767.316876
Sum of electronic and thermal Free Energies= -7767.407834

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -7769.773103 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -7767.509433 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -7767.71368 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -7760.204379 a.u.

^{2}(L4)NiBr
E(scf) = -5193.79191586 a.u.
ν_{min} = 18.37 cm^{-1}

Ni	27.538852	10.163840	1.849508
N	28.793847	8.683345	2.230043
N	26.857663	9.717211	3.649340
C	27.541094	8.700839	4.240557
C	28.608239	8.131777	3.458795
C	28.120989	7.188439	6.066734
H	27.971256	6.850004	7.091913
C	29.398155	7.077655	3.976208
C	29.135877	6.647961	5.323767
H	29.777652	5.888039	5.769462
C	25.509639	9.876769	5.613896
H	24.674299	10.364136	6.119349
C	27.262206	8.215548	5.540334
C	26.176745	8.826559	6.243844
C	25.746421	8.387318	7.596126
C	29.776788	8.220501	1.449690
C	25.861908	10.308498	4.319412
C	30.601364	7.162697	1.882840
H	31.375482	6.792402	1.208784

C	30.428890	6.561367	3.129130
C	25.573075	9.332972	8.623989
H	25.796638	10.384596	8.429207
C	25.460945	7.035493	7.867471
H	25.563594	6.292357	7.073641
C	24.863428	7.589491	10.150798
H	24.523284	7.279487	11.141945
C	25.146813	11.419898	3.609119
H	24.387228	11.898076	4.241393
H	24.668234	11.030209	2.695810
H	25.875047	12.172727	3.268059
C	29.928231	8.873952	0.107863
H	30.768972	8.460202	-0.464289
H	30.064364	9.959601	0.236012
H	28.997327	8.757344	-0.470095
C	25.139966	8.936239	9.891605
H	25.020855	9.682513	10.680998
C	25.021425	6.641640	9.133660
H	24.796168	5.589486	9.324634
C	31.303893	5.428404	3.526178
C	32.982644	3.268882	4.204634
H	33.633470	2.432083	4.469876
C	32.701519	5.538618	3.402345
H	33.137008	6.477253	3.051407
C	33.533520	4.469423	3.743506
H	34.617192	4.575946	3.651074
C	30.760722	4.214094	3.987492
H	29.676942	4.102007	4.063472
C	31.593903	3.143687	4.321556
H	31.155162	2.205320	4.669687
Br	27.178973	11.710738	0.135571



Zero-point correction= 0.389910 (Hartree/Particle)
Thermal correction to Energy= 0.415911
Thermal correction to Enthalpy= 0.416856
Thermal correction to Gibbs Free Energy= 0.330136
Sum of electronic and zero-point Energies= -5193.402006
Sum of electronic and thermal Energies= -5193.376004
Sum of electronic and thermal Enthalpies= -5193.375060

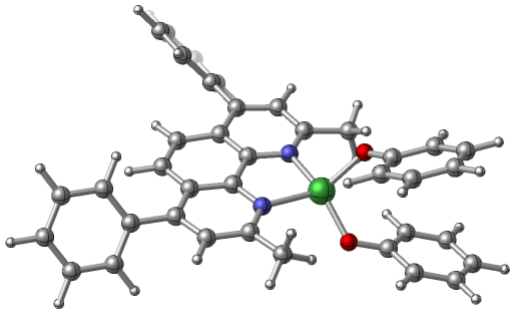
Sum of electronic and thermal Free Energies= -5193.461780

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5195.523826 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5193.580919 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5193.775502 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5187.771603 a.u.

^{1}(L4)Ni(OPh)$_2$
E(scf) = -3233.22788598 a.u.
ν_{min} = 4.34 cm^{-1}

Ni	28.766125	10.399728	2.552010
O	28.159381	9.974819	0.800521
O	28.911392	12.282368	2.432083
N	29.555240	8.578378	2.973474
N	28.108118	10.236960	4.506820
C	28.507675	9.060795	5.069710
C	29.290891	8.168784	4.243896
C	28.739246	7.471319	6.924535
H	28.566109	7.221627	7.970794
C	29.763072	6.940323	4.772555
C	29.490269	6.635725	6.147234
H	29.910603	5.729007	6.581157
C	26.974787	10.763003	6.543046
H	26.335534	11.464277	7.081506
C	28.192098	8.690104	6.401659
C	27.376331	9.588551	7.159726
C	26.947170	9.306291	8.554324
C	30.336524	7.832793	2.185157
C	27.339503	11.073331	5.212061
C	30.822035	6.585123	2.636670
H	31.418517	5.981116	1.951536
C	30.532382	6.102266	3.904821
C	27.159815	10.265619	9.561017
H	27.677348	11.196149	9.315953
C	26.283051	8.110294	8.885225
H	26.087553	7.367313	8.108853
C	26.077232	8.834285	11.189494
H	25.741541	8.649643	12.212872
C	26.804688	12.314645	4.564038
H	26.601046	13.092573	5.313025
H	25.846773	12.073387	4.070040
H	27.495971	12.678272	3.792675
C	30.716241	8.354543	0.831787
H	31.093991	7.550845	0.186081
H	31.520159	9.102250	0.947799

H	29.859349	8.862609	0.368714
C	26.733388	10.027786	10.870042
H	26.915881	10.777766	11.643506
C	25.849347	7.878985	10.192771
H	25.327008	6.949684	10.432686
C	31.027992	4.762363	4.312832
C	31.974673	2.201763	5.000311
H	32.342203	1.208381	5.269016
C	32.383945	4.429715	4.139256
H	33.075423	5.178141	3.745084
C	32.854035	3.160782	4.486369
H	33.912158	2.921251	4.355990
C	30.151196	3.789626	4.829066
H	29.091085	4.024992	4.946294
C	30.621896	2.518559	5.166504
H	29.927244	1.770910	5.556951
C	27.331278	10.744177	0.112385
C	27.516741	10.925978	-1.280275
C	26.222425	11.390559	0.713455
C	26.641511	11.717283	-2.026030
H	28.374602	10.440500	-1.752334
C	25.354582	12.182505	-0.038980
H	26.073212	11.266368	1.788214
C	25.552842	12.355212	-1.415650
H	26.814938	11.843629	-3.099211
H	24.510838	12.673035	0.456369
H	24.872220	12.977416	-2.002149
C	29.342913	12.900047	1.343400
C	28.756601	14.125240	0.942135
C	30.403561	12.392296	0.552338
C	29.205483	14.800354	-0.193991
H	27.930637	14.519285	1.539580
C	30.841842	13.070104	-0.585677
H	30.859654	11.444027	0.846174
C	30.249692	14.280501	-0.971221
H	28.728831	15.742366	-0.482177
H	31.658230	12.648623	-1.180274
H	30.595321	14.809210	-1.863062



Zero-point correction= 0.578550 (Hartree/Particle)
Thermal correction to Energy= 0.615030
Thermal correction to Enthalpy= 0.615974
Thermal correction to Gibbs Free Energy= 0.505399
Sum of electronic and zero-point Energies= -3232.649336
Sum of electronic and thermal Energies= -3232.612856
Sum of electronic and thermal Enthalpies= -3232.611912
Sum of electronic and thermal Free Energies= -3232.722487

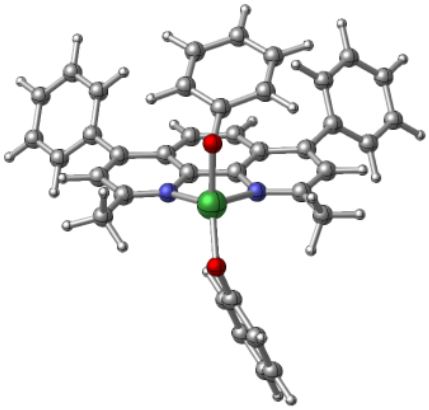
^{3}(L4)Ni(OPh)$_2$

E(scf) = -3233.25145697 a.u.

ν_{min} = 13.83 cm^{-1}

Ni	27.457082	10.410047	2.094302
O	25.990076	9.175942	1.849071
O	28.296844	11.916814	1.296661
N	28.888308	8.980109	2.456479
N	27.446134	10.460041	4.134058
C	28.079221	9.385953	4.662141
C	28.846251	8.573185	3.747646
C	28.732452	7.892961	6.484421
H	28.735752	7.652912	7.547356
C	29.485445	7.399235	4.208000
C	29.434490	7.105986	5.613632
H	29.985663	6.244834	5.991323
C	26.586552	10.991350	6.285648
H	25.961042	11.646886	6.893355
C	27.994743	9.039886	6.031603
C	27.183732	9.873748	6.863305
C	26.938103	9.570150	8.296481
C	29.575250	8.280644	1.555984
C	26.722581	11.264676	4.908957
C	30.224132	7.084398	1.928889
H	30.736368	6.502448	1.161308
C	30.158803	6.601751	3.231595
C	27.137031	10.558625	9.276959
H	27.517922	11.539492	8.982510
C	26.450469	8.309570	8.690205
H	26.265784	7.542591	7.934577
C	26.389084	9.030752	11.003371
H	26.177797	8.820594	12.054709

C	26.028778	12.408297	4.230869
H	25.148990	12.026262	3.684897
H	26.698390	12.859432	3.482522
H	25.692939	13.172355	4.943951
C	29.580043	8.794938	0.146972
H	30.195090	8.171627	-0.514482
H	29.954778	9.830453	0.125845
H	28.548684	8.815980	-0.241806
C	26.870419	10.287690	10.621455
H	27.040419	11.061713	11.373809
C	26.175585	8.044596	10.033742
H	25.788187	7.064781	10.323393
C	30.737093	5.274243	3.558482
C	31.788649	2.721138	4.093931
H	32.197961	1.729776	4.303373
C	32.061063	4.959780	3.205302
H	32.685567	5.718959	2.728249
C	32.584499	3.693118	3.477838
H	33.618629	3.464900	3.208407
C	29.941936	4.289084	4.174891
H	28.902124	4.516429	4.421676
C	30.465326	3.021040	4.437054
H	29.834639	2.262040	4.906408
C	25.963725	8.010141	2.469266
C	25.423761	7.874558	3.775046
C	26.512821	6.844467	1.874136
C	25.461043	6.654353	4.452721
H	25.003418	8.765053	4.249783
C	26.550349	5.629246	2.558884
H	26.932894	6.934016	0.869096
C	26.030514	5.520774	3.856679
H	25.049818	6.590393	5.465081
H	27.002105	4.755579	2.079248
H	26.066830	4.568758	4.392230
C	29.568596	12.255280	1.388795
C	30.227302	12.874971	0.295258
C	30.334305	12.024273	2.562228
C	31.573489	13.237742	0.374872
H	29.648134	13.055839	-0.614426
C	31.679528	12.389287	2.629676
H	29.840401	11.548519	3.412145
C	32.315947	12.999035	1.539603
H	32.052004	13.711945	-0.487785
H	32.240570	12.194395	3.549152
H	33.369891	13.282170	1.596404



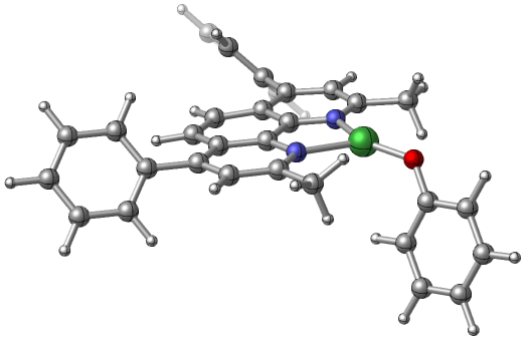
Zero-point correction= 0.578358 (Hartree/Particle)
Thermal correction to Energy= 0.614962
Thermal correction to Enthalpy= 0.615907
Thermal correction to Gibbs Free Energy= 0.504718
Sum of electronic and zero-point Energies= -3232.673099
Sum of electronic and thermal Energies= -3232.636495
Sum of electronic and thermal Enthalpies= -3232.635550
Sum of electronic and thermal Free Energies= -3232.746739

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3235.331037 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3232.996685 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3233.228882 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3227.028927 a.u.

^{2}(L4)NiOPh
E(scf) = -2926.54224132 a.u.
ν_{min} = 10.41 cm^{-1}

Ni	-1.709606	6.421999	7.999223
N	-1.221997	5.991795	9.909291
N	0.040975	7.253462	7.996570
C	0.628380	7.892727	6.972781
C	-0.132175	7.912789	5.679290
H	0.403117	8.451512	4.886451
H	-1.117473	8.382201	5.837737
H	-0.330407	6.880071	5.347673
C	1.890605	8.493065	7.125177
H	2.345512	8.980414	6.261210
C	2.585432	8.450157	8.335760
C	3.931114	9.070815	8.433248
C	4.137741	10.385665	7.974617
H	3.291470	10.957645	7.586596
C	5.405340	10.970258	8.031023
H	5.544490	11.995755	7.679834
C	6.491110	10.248357	8.538450
H	7.482879	10.705207	8.581517

C	6.300946	8.936818	8.987528
H	7.145971	8.361580	9.373989
C	5.032929	8.352750	8.937117
H	4.897929	7.321523	9.270708
C	1.950036	7.794622	9.436148
C	2.473230	7.728056	10.774559
H	3.408191	8.240417	11.001004
C	1.816155	7.060137	11.772443
H	2.238923	7.049572	12.777056
C	0.564973	6.392243	11.536244
C	-0.172662	5.651546	12.512104
C	0.334043	5.405967	13.887226
C	1.612499	4.858371	14.106252
H	2.249943	4.617476	13.252693
C	2.060822	4.595178	15.402915
H	3.052473	4.161715	15.554518
C	1.242488	4.878031	16.502089
H	1.595803	4.675048	17.516067
C	-0.031333	5.418803	16.296369
H	-0.675975	5.644096	17.149553
C	-0.484077	5.676115	14.999938
H	-1.476386	6.106255	14.844659
C	-1.412951	5.142920	12.132976
H	-1.999550	4.565348	12.849473
C	-1.924856	5.324756	10.830023
C	-3.270656	4.799400	10.426634
H	-4.016718	5.610869	10.473960
H	-3.603192	3.983524	11.082678
H	-3.250700	4.467654	9.379136
C	-0.009930	6.508706	10.247552
C	0.684876	7.205123	9.197497
O	-3.389998	5.955475	7.292606
C	-4.576948	6.429962	7.588969
C	-4.778850	7.464813	8.544995
C	-5.738663	5.910578	6.954264
C	-6.056921	7.941036	8.842794
H	-3.896314	7.875301	9.045272
C	-7.011252	6.395655	7.257875
H	-5.601698	5.113082	6.218354
C	-7.188868	7.415346	8.204760
H	-6.170866	8.737234	9.585628
H	-7.881712	5.970469	6.747796
H	-8.187637	7.791743	8.439474



Zero-point correction= 0.483119 (Hartree/Particle)
Thermal correction to Energy= 0.513320
Thermal correction to Enthalpy= 0.514264
Thermal correction to Gibbs Free Energy= 0.418242
Sum of electronic and zero-point Energies= -2926.059123
Sum of electronic and thermal Energies= -2926.028922
Sum of electronic and thermal Enthalpies= -2926.027977
Sum of electronic and thermal Free Energies= -2926.123999

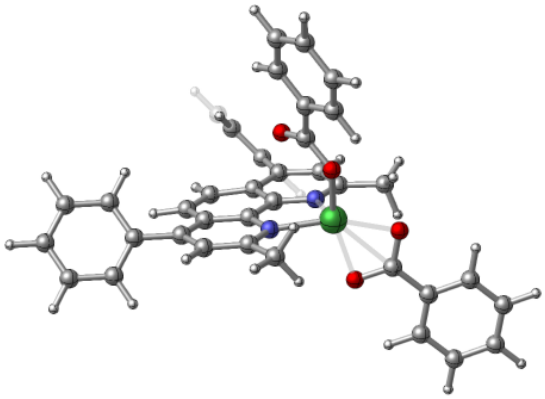
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2928.295229 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2926.315358 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2926.526268 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2921.173711 a.u.

^{1}(L4)Ni(OCOPh)$_2$
E(scf) = -3459.80161236 a.u.
ν_{min} = 9.97 cm^{-1}

Ni	27.633444	10.654379	2.088851
O	29.170309	12.128296	2.064745
O	26.078090	7.940618	2.710161
O	25.898415	9.911501	1.639556
O	28.082334	11.578934	0.240122
N	29.024445	8.983040	2.373335
N	27.432132	10.332842	4.077956
C	28.134813	9.288250	4.575538
C	28.994235	8.564544	3.660683
C	28.888568	7.827070	6.392217
H	28.888831	7.570154	7.451125
C	25.439109	8.782975	2.076998
C	29.753188	7.464260	4.132797
C	29.703147	7.145465	5.532809
H	30.344203	6.352187	5.916616
C	26.448642	10.691896	6.213130
H	25.744929	11.261656	6.821460
C	28.045591	8.896794	5.935224
C	27.142434	9.624347	6.772864

C	26.915274	9.274765	8.199486
C	29.793857	8.357601	1.488433
C	26.606273	11.031814	4.854513
C	30.567639	7.237794	1.871688
H	31.162206	6.723659	1.114730
C	30.554140	6.762904	3.176414
C	27.014115	10.266567	9.192195
H	27.300560	11.282577	8.910317
C	29.005002	12.242274	0.811200
C	26.549953	7.969267	8.578178
H	26.444008	7.195111	7.815008
C	26.409670	8.655661	10.898817
H	26.215387	8.414515	11.946787
C	25.846654	12.152574	4.206734
H	25.190091	12.671982	4.916066
H	25.246603	11.749589	3.374795
H	26.552998	12.878533	3.771770
C	29.827598	8.878360	0.080350
H	30.135148	8.098324	-0.629410
H	30.552705	9.707153	0.008589
H	28.850751	9.287730	-0.206715
C	26.769169	9.957053	10.532416
H	26.860858	10.735880	11.293407
C	26.296486	7.664480	9.917599
H	26.004644	6.648630	10.194957
C	31.351540	5.558233	3.527435
C	32.864273	3.255859	4.110074
H	33.451586	2.363020	4.338270
C	32.715942	5.493618	3.191324
H	33.191709	6.351210	2.709644
C	33.467350	4.353045	3.485907
H	34.528806	4.322486	3.227978
C	30.753816	4.447736	4.152376
H	29.689571	4.473826	4.396815
C	31.504921	3.305157	4.438333
H	31.024298	2.447732	4.915766
C	23.976784	8.538133	1.758634
C	23.217170	9.468198	1.031435
C	23.367474	7.354818	2.204201
C	21.869413	9.219096	0.756227
H	23.699226	10.384475	0.686950
C	22.020549	7.104503	1.930949
H	23.972673	6.641469	2.767114
C	21.268378	8.037152	1.205751
H	21.284707	9.948277	0.189032
H	21.553978	6.180564	2.283015

H	20.214216	7.842553	0.990798
C	29.902628	13.123582	0.008666
C	29.748612	13.204344	-1.384655
C	30.909231	13.868961	0.643234
C	30.594006	14.023649	-2.135718
H	28.962155	12.617371	-1.862326
C	31.752730	14.688799	-0.109173
H	31.016485	13.793316	1.726806
C	31.595896	14.766599	-1.498792
H	30.473290	14.084521	-3.220146
H	32.535204	15.268704	0.386543
H	32.257013	15.408027	-2.087350



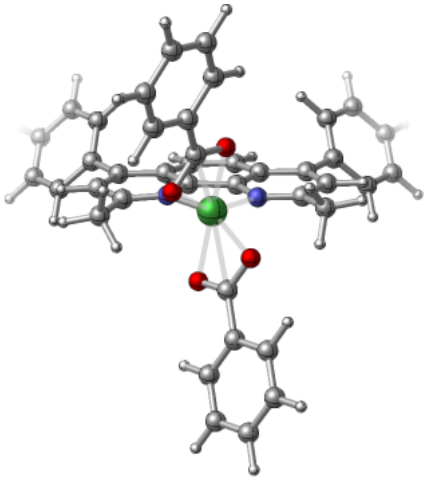
Zero-point correction= 0.601455 (Hartree/Particle)
Thermal correction to Energy= 0.641446
Thermal correction to Enthalpy= 0.642390
Thermal correction to Gibbs Free Energy= 0.522765
Sum of electronic and zero-point Energies= -3459.200158
Sum of electronic and thermal Energies= -3459.160166
Sum of electronic and thermal Enthalpies= -3459.159222
Sum of electronic and thermal Free Energies= -3459.278847

^{3}(L4)Ni(OCOPh)$_2$
E(scf) = -3459.82740075 a.u.
ν_{min} = 6.84 cm^{-1}

Ni	27.901795	10.558482	1.723359
O	29.023926	12.264842	2.203791
O	26.605306	9.317307	0.641543
O	26.090822	11.435987	0.908484
O	28.989797	11.542689	0.129863
N	29.141080	8.936589	2.196794
N	27.356556	10.253356	3.716516
C	28.004338	9.207468	4.288374
C	28.955979	8.489028	3.464426
C	28.580249	7.735122	6.165265
H	28.480832	7.476835	7.219193
C	25.828276	10.298659	0.422562
C	29.645433	7.367961	3.995816

C	29.454360	7.038075	5.379995
H	30.039820	6.228761	5.815310
C	26.288824	10.692213	5.801944
H	25.589985	11.312560	6.365011
C	27.804126	8.822197	5.639224
C	26.870795	9.586584	6.407928
C	26.521347	9.248883	7.812475
C	29.953490	8.275711	1.370760
C	26.549848	11.019194	4.452618
C	30.660427	7.138024	1.819384
H	31.303955	6.609488	1.114664
C	30.526251	6.662760	3.117222
C	26.588100	10.235164	8.813339
H	26.939959	11.237505	8.557915
C	29.366603	12.392618	0.986522
C	26.073000	7.960331	8.158628
H	25.993382	7.190909	7.387443
C	25.786311	8.652135	10.464033
H	25.502920	8.419730	11.493504
C	25.942605	12.232253	3.814299
H	25.430959	12.860188	4.555247
H	25.236999	11.940154	3.023425
H	26.733842	12.809728	3.312602
C	30.061566	8.745082	-0.049227
H	30.632135	8.035269	-0.662074
H	30.535254	9.736015	-0.094857
H	29.052117	8.875742	-0.466871
C	26.228802	9.936587	10.130063
H	26.296529	10.710637	10.898398
C	25.705594	7.666658	9.473923
H	25.350556	6.664205	9.725156
C	31.278088	5.449985	3.534079
C	32.717058	3.135153	4.239529
H	33.275578	2.237335	4.515400
C	30.618144	4.338957	4.091751
H	29.535708	4.369086	4.234621
C	31.333103	3.190075	4.438644
H	30.805277	2.332113	4.862160
C	32.667686	5.379573	3.326718
H	33.190983	6.237318	2.897478
C	33.382029	4.232824	3.682744
H	34.462803	4.197667	3.525351
C	24.599330	10.101961	-0.409657
C	23.744297	11.184418	-0.670337
C	24.295566	8.835873	-0.934450
C	22.597262	11.002200	-1.446161

H	23.996046	12.162922	-0.257200
C	23.148081	8.654065	-1.709820
H	24.970900	8.004501	-0.724493
C	22.297756	9.736841	-1.966326
H	21.934184	11.847418	-1.647438
H	22.914588	7.666750	-2.116402
H	21.399934	9.594399	-2.573516
C	30.220817	13.550061	0.571884
C	30.602070	13.698251	-0.771083
C	30.644769	14.493013	1.521484
C	31.399337	14.777146	-1.159811
H	30.262452	12.957575	-1.497368
C	31.441904	15.571915	1.132170
H	30.339742	14.364842	2.561577
C	31.820161	15.714991	-0.208625
H	31.693896	14.889315	-2.206340
H	31.770009	16.304167	1.874294
H	32.443922	16.559571	-0.513021



Zero-point correction= 0.600606 (Hartree/Particle)
Thermal correction to Energy= 0.640562
Thermal correction to Enthalpy= 0.641506
Thermal correction to Gibbs Free Energy= 0.521562
Sum of electronic and zero-point Energies= -3459.226795
Sum of electronic and thermal Energies= -3459.186839
Sum of electronic and thermal Enthalpies= -3459.185894
Sum of electronic and thermal Free Energies= -3459.305839

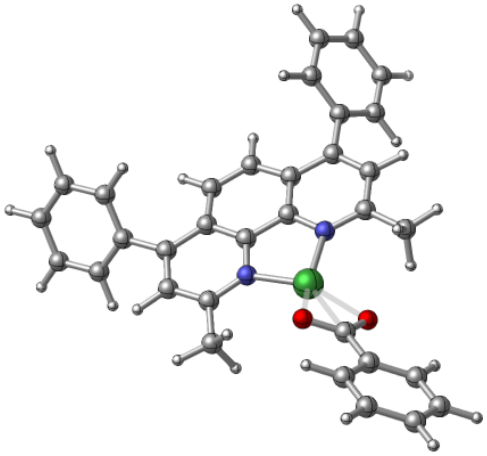
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3462.16232 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3459.588565 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3459.808254 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3453.043998 a.u.

^{2}(L4)NiOCOPh

E(scf) = -3039.82963458 a.u.
ν_{min} = 9.58 cm^{-1}

Ni	28.901699	10.207493	2.124374
O	30.272463	11.462533	1.032586
O	28.097780	11.786663	0.971025
N	29.703318	8.428346	2.510697
N	27.785337	9.771525	3.703900
C	28.144488	8.595025	4.294135
C	29.191257	7.856975	3.636844
C	27.960233	6.793886	5.937701
H	27.457840	6.355536	6.799940
C	29.621238	6.605749	4.146927
C	28.946582	6.087390	5.305986
H	29.214113	5.096760	5.673555
C	26.177407	10.078402	5.448922
H	25.408447	10.716326	5.887977
C	27.543175	8.090113	5.474826
C	26.527429	8.886794	6.086069
C	25.847578	8.501702	7.349337
C	30.639356	7.766942	1.815712
C	26.811536	10.504095	4.267555
C	31.129440	6.525821	2.264550
H	31.918416	6.036602	1.690867
C	30.660777	5.931191	3.436494
C	24.442317	8.523192	7.430748
H	23.857955	8.783968	6.545063
C	29.269480	12.109491	0.610996
C	26.582682	8.156127	8.499853
H	27.674315	8.161497	8.463833
C	24.532474	7.848943	9.757296
H	24.023120	7.593894	10.689891
C	26.452926	11.794145	3.591562
H	25.660848	12.332128	4.129062
H	26.138952	11.604222	2.554596
H	27.344933	12.434401	3.508180
C	29.465098	13.268213	-0.320611
C	31.121749	8.405080	0.546468
H	31.963861	7.855868	0.104724
H	31.400294	9.452932	0.727555
H	30.296046	8.436305	-0.184636
C	23.791017	8.195500	8.622510
H	22.698975	8.208041	8.663674
C	25.930174	7.834093	9.692429
H	26.517485	7.576381	10.577326
C	28.539362	15.071654	-1.658334
H	27.674038	15.632453	-2.020997

C	30.938111	14.715833	-1.598579
H	31.945507	14.998851	-1.914587
C	31.244615	4.643289	3.892007
C	28.357752	13.992770	-0.789891
H	27.360382	13.694582	-0.461738
C	29.829826	15.434491	-2.063979
H	29.972012	16.278777	-2.743750
C	32.418072	2.214080	4.711511
H	32.870989	1.271946	5.030039
C	30.756403	13.636960	-0.730053
H	31.607394	13.064870	-0.356117
C	31.366133	3.564862	2.995646
H	30.988649	3.669845	1.975665
C	31.943445	2.359719	3.403468
H	32.020075	1.529740	2.696629
C	31.730026	4.485987	5.204495
H	31.668723	5.321357	5.905467
C	32.312631	3.282430	5.608989
H	32.691426	3.181181	6.629092



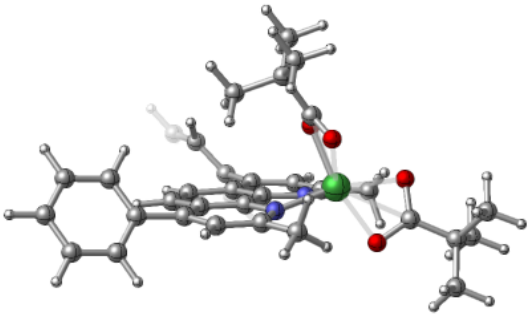
Zero-point correction= 0.493529 (Hartree/Particle)
Thermal correction to Energy= 0.525787
Thermal correction to Enthalpy= 0.526732
Thermal correction to Gibbs Free Energy= 0.425175
Sum of electronic and zero-point Energies= -3039.336105
Sum of electronic and thermal Energies= -3039.303847
Sum of electronic and thermal Enthalpies= -3039.302903
Sum of electronic and thermal Free Energies= -3039.404459

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3041.708996 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3039.609392 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3039.81703 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3034.180815 a.u.

^{1}(L4)Ni(OPiv)$_2$
E(scf) -3312.31321831 a.u.
ν_{min} = 6.65cm^{-1}

Ni	28.338035	11.001336	1.702438
O	29.404960	12.825196	1.816956
O	27.163064	9.436201	1.124986
O	25.958685	11.282085	1.145155
O	29.063112	11.862625	-0.120447
N	29.751949	9.451583	2.373265
N	27.734787	10.700492	3.652756
C	28.127911	9.495328	4.136061
C	29.210020	8.821903	3.443698
C	28.070464	7.661561	5.761378
H	27.666754	7.232759	6.678296
C	26.033270	10.035983	1.081645
C	29.673924	7.566863	3.916332
C	29.084482	7.020395	5.106470
H	29.476833	6.086974	5.509274
C	26.200890	10.911826	5.458544
H	25.429491	11.508932	5.947395
C	27.546737	8.912091	5.288898
C	26.502918	9.644710	5.939836
C	25.745314	9.097111	7.094388
C	30.775607	8.903675	1.725686
C	26.832027	11.430744	4.306057
C	24.773044	9.155943	1.074172
C	31.288876	7.647409	2.122122
H	32.107645	7.207738	1.550363
C	30.744202	6.950215	3.193067
C	25.598229	9.852754	8.271458
H	26.085251	10.827711	8.349179
C	29.541467	12.825052	0.554616
C	25.117361	7.840119	7.010694
H	25.203438	7.254417	6.092642
C	24.234450	8.105698	9.252305
H	23.649426	7.719893	10.090775
C	26.481934	12.782820	3.760103
H	26.073497	13.435155	4.543912
H	25.738452	12.664553	2.956871
H	27.369907	13.246320	3.306549
C	30.291846	13.951200	-0.160423
C	31.360094	9.664285	0.571400
H	32.031255	9.039152	-0.032109
H	31.936115	10.525251	0.950485
H	30.559658	10.078532	-0.057391
C	24.853134	9.357113	9.344447
H	24.756769	9.950864	10.256732

C	24.365243	7.350942	8.081202
H	23.875503	6.377655	7.998062
C	31.281426	5.609440	3.544800
C	32.331101	3.063450	4.132256
H	32.737936	2.075658	4.362247
C	30.432077	4.492480	3.654860
H	29.358512	4.612383	3.493157
C	30.954571	3.229536	3.943560
H	30.283203	2.370474	4.016808
C	32.664822	5.429128	3.725176
H	33.333468	6.289681	3.646684
C	33.184381	4.166587	4.022276
H	34.260257	4.044995	4.170003
C	30.659858	15.068152	0.824668
H	31.205056	15.869469	0.300573
H	29.759417	15.504421	1.283253
H	31.296581	14.686653	1.636500
C	31.568009	13.336636	-0.773384
H	32.228202	12.929644	0.009551
H	31.315642	12.522189	-1.468407
H	32.130087	14.106810	-1.325666
C	29.386833	14.497183	-1.282038
H	28.463117	14.932982	-0.868085
H	29.913878	15.284382	-1.844742
H	29.104163	13.695042	-1.978953
C	24.957289	7.980343	0.100529
H	25.855486	7.400759	0.356525
H	24.082240	7.311037	0.138356
H	25.067055	8.338506	-0.936119
C	24.632088	8.623290	2.519232
H	25.517054	8.035815	2.807619
H	24.527264	9.452485	3.237650
H	23.740826	7.980553	2.605922
C	23.537827	9.981699	0.694782
H	23.636167	10.397612	-0.320409
H	22.633896	9.351620	0.722591
H	23.399007	10.823661	1.388045



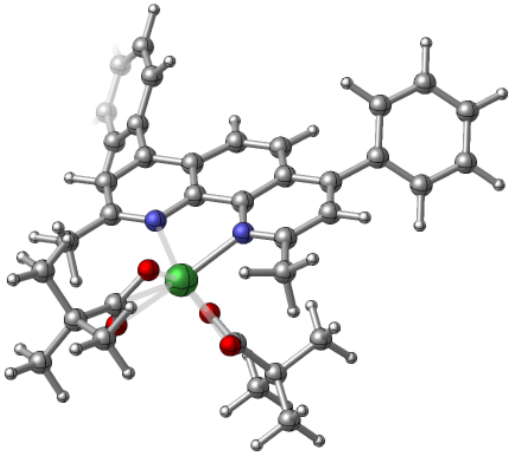
Zero-point correction= 0.662136 (Hartree/Particle)
Thermal correction to Energy= 0.704223
Thermal correction to Enthalpy= 0.705167
Thermal correction to Gibbs Free Energy= 0.582238
Sum of electronic and zero-point Energies= -3311.651082
Sum of electronic and thermal Energies= -3311.608995
Sum of electronic and thermal Enthalpies= -3311.608051
Sum of electronic and thermal Free Energies= -3311.730980

^{3}(L4)Ni(OPiv)$_2$
E(scf) -3312.33654687 a.u.
ν_{min} = 9.85 cm^{-1}

Ni	27.203311	10.275234	1.625312
O	28.550085	11.594648	2.536029
O	25.841311	9.447199	0.274204
O	25.659597	11.549050	0.865136
O	28.677520	11.284869	0.368861
N	28.529986	8.713351	1.953800
N	26.592263	9.650694	3.560266
C	27.612217	8.969250	4.145192
C	28.661048	8.467353	3.279573
C	28.841768	8.061643	6.065578
H	28.940757	7.948912	7.144866
C	25.256625	10.571130	0.172386
C	29.744723	7.731378	3.819899
C	29.829315	7.591265	5.246292
H	30.704273	7.108271	5.680496
C	25.558726	9.860426	5.700991
H	24.701925	10.211675	6.277776
C	27.677691	8.719344	5.540082
C	26.585732	9.179559	6.341073
C	26.509968	8.949671	7.807746
C	29.396771	8.200047	1.083364
C	25.578546	10.088771	4.306622
C	24.066882	10.709777	-0.783293
C	30.498834	7.443278	1.542055
H	31.190862	7.025358	0.809219
C	30.702180	7.204937	2.895088
C	26.266999	10.029317	8.676268

H	26.177593	11.038318	8.266787
C	29.151841	11.773526	1.432156
C	26.628099	7.656205	8.349930
H	26.791614	6.804728	7.685685
C	26.282161	8.533634	10.583047
H	26.196029	8.372088	11.660362
C	24.446230	10.797409	3.624120
H	23.736872	11.216567	4.349310
H	23.906297	10.089558	2.973319
H	24.827240	11.588294	2.964361
C	30.516369	12.473224	1.428110
C	29.169890	8.440293	-0.380185
H	29.573392	7.612850	-0.980629
H	29.661384	9.377363	-0.682930
H	28.096978	8.567761	-0.578988
C	26.160123	9.822931	10.053959
H	25.982159	10.673471	10.716530
C	26.511920	7.451017	9.726814
H	26.596923	6.439694	10.131873
C	31.883499	6.412841	3.327821
C	34.137592	4.897641	4.067655
H	35.012552	4.310370	4.356979
C	31.741638	5.262494	4.125787
H	30.746420	4.945596	4.445447
C	32.861038	4.510026	4.489767
H	32.734387	3.614102	5.102451
C	33.169848	6.787190	2.898945
H	33.290707	7.681288	2.282505
C	34.288851	6.037976	3.271476
H	35.282820	6.347508	2.939301
C	30.545442	13.584449	2.488896
H	31.544762	14.047385	2.529353
H	29.812881	14.373795	2.254813
H	30.303066	13.182123	3.482608
C	31.540677	11.372446	1.791927
H	31.314346	10.936944	2.777639
H	31.527836	10.559088	1.048819
H	32.558671	11.793753	1.822326
C	30.829955	13.044649	0.038688
H	30.092210	13.810225	-0.250144
H	31.827911	13.512348	0.035979
H	30.811578	12.255329	-0.726230
C	22.977266	9.721181	-0.320164
H	22.623091	9.969221	0.693933
H	22.111862	9.761926	-1.001247
H	23.365708	8.692326	-0.305997

C	23.524438	12.144262	-0.770297
H	23.186267	12.430578	0.236904
H	24.298464	12.862978	-1.078542
H	22.671154	12.233064	-1.461959
C	24.547711	10.329597	-2.197971
H	24.949240	9.305870	-2.210444
H	23.710782	10.387881	-2.912609
H	25.339907	11.013529	-2.543594



Zero-point correction= 0.661116 (Hartree/Particle)
Thermal correction to Energy= 0.703206
Thermal correction to Enthalpy= 0.704150
Thermal correction to Gibbs Free Energy= 0.581160
Sum of electronic and zero-point Energies= -3311.675430
Sum of electronic and thermal Energies= -3311.633341
Sum of electronic and thermal Enthalpies= -3311.632397
Sum of electronic and thermal Free Energies= -3311.755387

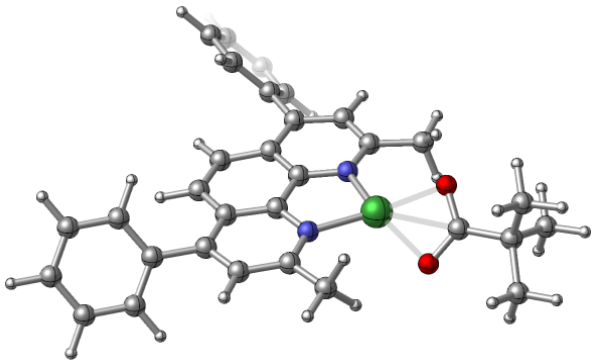
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3314.524524 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3312.104744 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3312.318693 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3305.974303 a.u.

^{2}(L4)NiOPiv
E(scf) = -2966.08358777 a.u.
ν_{min} = 12.42 cm^{-1}

Ni	28.664629	10.436752	2.608230
O	28.799298	12.545255	2.389891
O	28.756263	11.240073	0.625613
N	29.415052	8.608052	2.738129
N	27.744566	9.910054	4.290176
C	28.079106	8.653740	4.701184
C	28.998688	7.942144	3.853919
C	27.946593	6.688653	6.149476
H	27.504839	6.178559	7.005461

C	29.417452	6.629494	4.189505
C	28.829928	6.016260	5.350255
H	29.079118	4.980887	5.582459
C	26.302000	10.080307	6.189576
H	25.606361	10.695131	6.763261
C	27.560738	8.046041	5.872972
C	26.652445	8.814527	6.662595
C	26.077645	8.322049	7.940794
C	30.281492	8.001653	1.910773
C	26.851273	10.608699	5.006661
C	30.753392	6.704775	2.181763
H	31.473692	6.256750	1.495112
C	30.353369	5.996170	3.316522
C	26.901821	7.823638	8.968186
H	27.983664	7.788601	8.821981
C	28.808330	12.398008	1.130668
C	24.689706	8.390484	8.165418
H	24.036652	8.769180	7.375486
C	24.969433	7.463212	10.387447
H	24.539990	7.128247	11.334868
C	26.465915	11.960375	4.481634
H	25.828768	12.508645	5.188335
H	25.920589	11.843077	3.529744
H	27.363106	12.547071	4.239149
C	28.859484	13.645587	0.236522
C	30.742740	8.785271	0.717541
H	31.384641	8.187265	0.057050
H	31.301545	9.674963	1.052637
H	29.879990	9.175083	0.159262
C	26.351873	7.399811	10.180433
H	27.007842	7.023603	10.969449
C	24.140523	7.960646	9.376026
H	23.059540	8.011833	9.528481
C	30.908779	4.642084	3.570250
C	32.024884	2.087815	3.999599
H	32.455458	1.097449	4.166962
C	30.899527	3.671743	2.550336
H	30.442339	3.910865	1.587151
C	31.448455	2.405047	2.764818
H	31.422918	1.661449	1.964297
C	31.496800	4.312294	4.806760
H	31.539175	5.061602	5.600285
C	32.050271	3.047089	5.017982
H	32.509527	2.811997	5.981431
C	27.548255	14.426450	0.463670
C	30.058821	14.507773	0.674097

C	28.994300	13.252604	-1.239798
H	26.673337	13.824095	0.168982
H	27.436244	14.698026	1.523834
H	27.544023	15.350222	-0.137833
H	29.979771	14.767986	1.739485
H	30.097516	15.438367	0.084552
H	31.009017	13.969594	0.523073
H	28.148129	12.627607	-1.561239
H	29.024010	14.153969	-1.873629
H	29.916397	12.676757	-1.412605



Zero-point correction= 0.523732 (Hartree/Particle)
Thermal correction to Energy= 0.557062
Thermal correction to Enthalpy= 0.558006
Thermal correction to Gibbs Free Energy= 0.455093
Sum of electronic and zero-point Energies= -2965.559855
Sum of electronic and thermal Energies= -2965.526526
Sum of electronic and thermal Enthalpies= -2965.525582
Sum of electronic and thermal Free Energies= -2965.628495

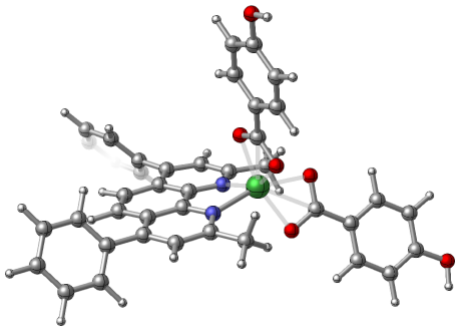
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2967.888984 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2965.866383 a.u.
uB3LYP-d3/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2966.07232 a.u.
DLPNO-CCSD(T)/def2-svp(Gas)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2960.645927 a.u.

^{3}(L4)Ni(OCO-*p*-OHPh)$_2$
E(scf) = -3610.16954552 a.u.
ν_{min} = 6.08 cm^{-1}

Ni	28.290787	10.664182	1.671710
O	29.507813	12.368102	1.747440
O	26.880351	9.273492	1.003275
O	26.373431	11.411571	0.962333
O	29.167237	11.339112	-0.162670
N	29.518756	9.072038	2.354698
N	27.698389	10.563050	3.653896
C	28.063339	9.394789	4.235612
C	29.036633	8.585614	3.528830
C	28.072918	7.759710	6.062772

H	27.744744	7.461599	7.058186
C	26.054567	10.205673	0.745383
C	29.471788	7.359614	4.096171
C	28.973513	6.983502	5.389211
H	29.351104	6.073635	5.854875
C	26.384742	11.083420	5.569614
H	25.714794	11.789315	6.063077
C	27.576355	8.984015	5.502419
C	26.662368	9.861783	6.168809
C	26.026380	9.518194	7.467445
C	30.456372	8.391272	1.695266
C	26.916949	11.423330	4.305213
C	30.922819	7.149331	2.182534
H	31.663576	6.602304	1.597558
C	30.434836	6.600164	3.360052
C	26.078565	10.424215	8.542293
H	26.627212	11.362202	8.428774
C	29.695777	12.287283	0.491085
C	25.322396	8.310484	7.632019
H	25.253406	7.607805	6.798591
C	24.757978	8.920365	9.909167
H	24.267192	8.687270	10.857291
C	26.612775	12.741191	3.656898
H	26.271937	13.478068	4.396701
H	25.837425	12.606974	2.887606
H	27.505573	13.111961	3.132829
C	31.007068	8.972011	0.426652
H	31.648082	8.251796	-0.098147
H	31.604379	9.869535	0.657551
H	30.195463	9.309988	-0.230570
C	25.453683	10.124322	9.755406
H	25.512369	10.833867	10.584390
C	24.690951	8.016700	8.842887
H	24.140317	7.079163	8.951988
C	30.923201	5.269958	3.808336
C	31.872325	2.733108	4.577413
H	32.240357	1.749049	4.877962
C	30.023855	4.231307	4.114314
H	28.948725	4.406980	4.035150
C	30.496247	2.972456	4.492896
H	29.785520	2.173687	4.718496
C	32.304563	5.015145	3.885458
H	33.012332	5.814984	3.655080
C	32.774732	3.757781	4.272771
H	33.850730	3.578797	4.338267
C	24.708162	9.871197	0.198733

C	24.327260	8.532519	0.000447
C	23.798463	10.888998	-0.127929
C	23.071287	8.215115	-0.507331
C	22.538271	10.583859	-0.638617
C	22.166775	9.241788	-0.831222
H	22.765950	7.178351	-0.663797
H	21.834740	11.382225	-0.892160
C	30.542845	13.296348	-0.202903
C	30.780539	13.199111	-1.585417
C	31.121440	14.357618	0.511165
C	31.575418	14.134254	-2.240126
C	31.918315	15.301200	-0.133978
C	32.150834	15.193836	-1.516431
H	31.766680	14.067132	-3.313149
H	32.365200	16.126501	0.428025
O	20.958300	8.880998	-1.322892
O	32.915990	16.076200	-2.199606
H	25.037008	7.742773	0.253537
H	24.095935	11.928374	0.022611
H	30.937081	14.432932	1.584284
H	30.328797	12.373371	-2.138087
H	20.425386	9.667417	-1.509407
H	33.257598	16.755953	-1.600907



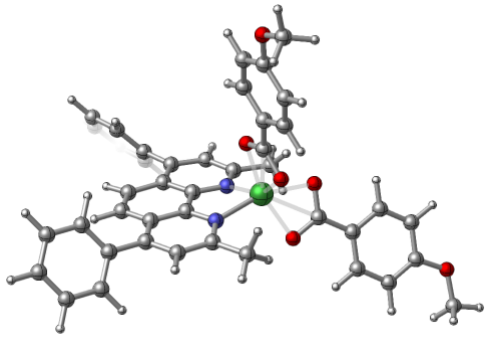
Zero-point correction= 0.608915 (Hartree/Particle)
Thermal correction to Energy= 0.651240
Thermal correction to Enthalpy= 0.652185
Thermal correction to Gibbs Free Energy= 0.526768
Sum of electronic and zero-point Energies= -3609.560631
Sum of electronic and thermal Energies= -3609.518305
Sum of electronic and thermal Enthalpies= -3609.517361
Sum of electronic and thermal Free Energies= -3609.642777

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3612.688186 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3609.985964 a.u.

^{3}(L4)Ni(OCO-*p*-OMePh)$_2$
E(scf) = -3688.71747657 a.u.
ν_{min} = 6.54 cm^{-1}

Ni	28.294932	10.668829	1.675936
O	29.513196	12.371225	1.755725
O	26.885517	9.278919	1.005649
O	26.376769	11.416575	0.965883
O	29.173100	11.346790	-0.156871
N	29.520563	9.074492	2.357852
N	27.701038	10.566008	3.657489
C	28.064161	9.396640	4.238055
C	29.036625	8.586948	3.530738
C	28.070224	7.759096	6.062983
H	27.741197	7.460198	7.057881
C	26.058901	10.210606	0.748374
C	29.469050	7.359174	4.096287
C	28.969519	6.982103	5.388575
H	29.345164	6.070810	5.853031
C	26.387470	11.086183	5.573267
H	25.718392	11.792497	6.067305
C	27.575999	8.985048	5.504139
C	26.663236	9.863523	6.171265
C	26.026589	9.519660	7.469515
C	30.457249	8.393071	1.697819
C	26.920429	11.426639	4.309334
C	30.920629	7.149160	2.183000
H	31.660432	6.601534	1.597375
C	30.430717	6.598889	3.359220
C	26.080348	10.424504	8.545278
H	26.630614	11.361654	8.432686
C	29.701628	12.293325	0.499275
C	25.320521	8.313008	7.632879
H	25.250297	7.611295	6.798740
C	24.757184	8.921567	9.910657
H	24.266006	8.688365	10.858552
C	26.618109	12.745356	3.661931
H	26.275712	13.481509	4.401719
H	25.844655	12.612113	2.890552
H	27.512293	13.116465	3.140425
C	31.010080	8.975342	0.430829
H	31.649780	8.254855	-0.095200
H	31.609316	9.870959	0.664167
H	30.199677	9.316681	-0.226158
C	25.454956	10.124479	9.758096
H	25.514875	10.833094	10.587788
C	24.688588	8.019096	8.843465
H	24.136335	7.082402	8.951629
C	30.915425	5.266548	3.805119
C	31.857302	2.725562	4.569477

H	32.222526	1.739896	4.868186
C	30.013128	4.229799	4.108879
H	28.938509	4.408620	4.029804
C	30.481915	2.968905	4.485124
H	29.768908	2.171686	4.709009
C	32.296052	5.007739	3.882062
H	33.006102	5.806044	3.653391
C	32.762624	3.748314	4.267030
H	33.838103	3.566198	4.332413
C	24.712905	9.873798	0.201863
C	24.333962	8.532858	0.004071
C	23.801692	10.886512	-0.125483
C	23.080101	8.217745	-0.502841
C	22.537587	10.586167	-0.637742
C	22.168761	9.242189	-0.829465
H	22.772591	7.181762	-0.660221
H	21.853176	11.397809	-0.883446
C	30.548576	13.303933	-0.192797
C	30.782576	13.212619	-1.577905
C	31.130318	14.360057	0.521366
C	31.575149	14.150527	-2.225785
C	31.929037	15.311665	-0.116105
C	32.156589	15.210532	-1.500832
H	31.765323	14.092020	-3.299506
H	32.366330	16.121066	0.467930
O	20.973414	8.838938	-1.317396
O	32.911465	16.074072	-2.216674
C	33.530374	17.169202	-1.562899
H	34.080984	17.721793	-2.335262
H	32.786020	17.841082	-1.100968
H	34.239417	16.832224	-0.786626
C	20.001399	9.807682	-1.672245
H	20.365039	10.475432	-2.472766
H	19.127882	9.252608	-2.038320
H	19.700856	10.420120	-0.804145
H	25.044041	7.743475	0.257250
H	24.097859	11.926460	0.024712
H	30.948999	14.430102	1.595487
H	30.329186	12.390335	-2.134323



Zero-point correction= 0.665275 (Hartree/Particle)
Thermal correction to Energy= 0.710426
Thermal correction to Enthalpy= 0.711370
Thermal correction to Gibbs Free Energy= 0.579549
Sum of electronic and zero-point Energies= -3688.052201
Sum of electronic and thermal Energies= -3688.007051
Sum of electronic and thermal Enthalpies= -3688.006107
Sum of electronic and thermal Free Energies= -3688.137928

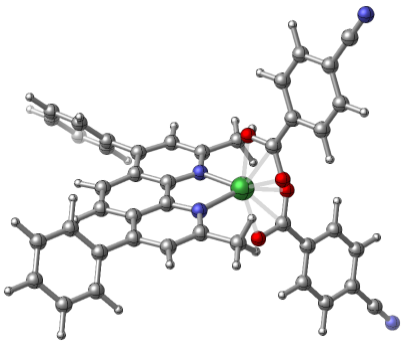
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3691.318509 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3688.494744 a.u.

^{3}(L4)Ni(OCO-*p*-CNPh)$_2$
E(scf) = -3644.18076190 a.u.
ν_{min} = 6.04 cm^{-1}

Ni	27.904666	10.539544	1.742665
O	29.057073	12.238568	2.192939
O	26.573784	9.321887	0.668728
O	26.100133	11.452672	0.932595
O	28.978934	11.508852	0.120558
N	29.127625	8.910447	2.204508
N	27.372302	10.253657	3.735672
C	28.014501	9.202890	4.306080
C	28.950368	8.470983	3.476608
C	28.593219	7.733800	6.184130
H	28.501386	7.481534	7.240164
C	25.820374	10.319435	0.453229
C	29.634010	7.345989	4.006545
C	29.453005	7.024561	5.393968
H	30.034801	6.211742	5.827569
C	26.327558	10.711588	5.828411
H	25.639975	11.341239	6.394920
C	27.822904	8.825953	5.660296
C	26.904493	9.603261	6.434289
C	26.565434	9.276041	7.843683
C	29.927657	8.239151	1.374529
C	26.578950	11.030092	4.475419
C	30.627447	7.096862	1.822173

H	31.259792	6.559317	1.114213
C	30.499752	6.628070	3.123043
C	26.650202	10.267242	8.838348
H	27.008348	11.265106	8.574293
C	29.375921	12.353034	0.970228
C	26.109259	7.993256	8.200911
H	26.015356	7.220410	7.434778
C	25.850569	8.700054	10.505039
H	25.575006	8.475662	11.538390
C	25.973011	12.244315	3.837592
H	25.493399	12.889682	4.584930
H	25.236388	11.953136	3.074999
H	26.756165	12.803844	3.304509
C	30.032177	8.703026	-0.047699
H	30.577218	7.976866	-0.664554
H	30.535499	9.679074	-0.100645
H	29.023351	8.860464	-0.456880
C	26.301003	9.978806	10.159991
H	26.382821	10.756280	10.923457
C	25.751797	7.709972	9.521186
H	25.390369	6.712092	9.781266
C	31.242659	5.409506	3.538399
C	32.663685	3.083176	4.241236
H	33.215321	2.180833	4.516138
C	30.576314	4.308491	4.108256
H	29.495727	4.350769	4.261664
C	31.282436	3.153766	4.453722
H	30.749786	2.303567	4.886698
C	32.629288	5.323325	3.317457
H	33.157489	6.173245	2.878774
C	33.334834	4.170845	3.672358
H	34.413552	4.123316	3.504586
C	24.583940	10.144503	-0.379241
C	23.747018	11.242104	-0.631141
C	24.263192	8.885317	-0.908482
C	22.598051	11.088914	-1.402700
C	23.117291	8.717920	-1.681773
C	22.279067	9.822482	-1.931439
H	21.945457	11.941111	-1.600460
H	22.865290	7.739545	-2.094801
C	30.236468	13.502961	0.535469
C	30.593834	13.639847	-0.814437
C	30.685241	14.442587	1.475789
C	31.392969	14.702928	-1.226895
C	31.484914	15.510598	1.077066
C	31.842210	15.643801	-0.279250

H	31.672303	14.811933	-2.276316
H	31.835610	16.243002	1.806330
C	32.667353	16.742512	-0.697151
N	33.334999	17.631036	-1.034764
C	21.095448	9.656728	-2.727830
N	20.137990	9.522421	-3.371609
H	30.234216	12.900833	-1.531795
H	30.397420	14.321765	2.521013
H	24.013433	12.214176	-0.213673
H	24.925733	8.043109	-0.704258



Zero-point correction= 0.597935 (Hartree/Particle)
Thermal correction to Energy= 0.641534
Thermal correction to Enthalpy= 0.642478
Thermal correction to Gibbs Free Energy= 0.513653
Sum of electronic and zero-point Energies= -3643.582827
Sum of electronic and thermal Energies= -3643.539228
Sum of electronic and thermal Enthalpies= -3643.538284
Sum of electronic and thermal Free Energies= -3643.667109

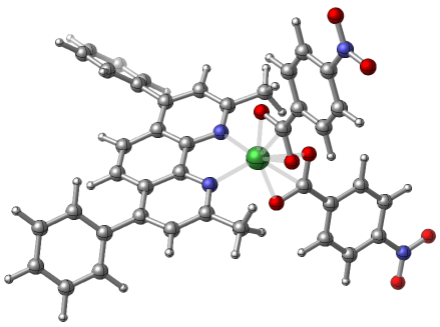
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3646.726652 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3643.942127 a.u.

^{3}(L4)Ni(OCO-*p*-NO$_2$Ph)$_2$
E(scf) = -3868.53376672 a.u.
ν_{min} = 6.55 cm^{-1}

Ni	27.889479	10.500454	1.674501
O	29.140954	12.193797	2.052870
O	26.476581	9.295165	0.618701
O	26.080597	11.456938	0.777441
O	29.060689	11.396123	0.000513
N	29.035838	8.824170	2.220856
N	27.360083	10.325832	3.698867
C	27.969329	9.282853	4.317652
C	28.860949	8.466612	3.518334
C	28.517862	7.898641	6.267115
H	28.433394	7.710081	7.336947
C	25.764298	10.311547	0.354421

C	29.506468	7.345412	4.100606
C	29.335496	7.111092	5.506733
H	29.891053	6.300936	5.978061
C	26.361402	10.939424	5.772981
H	25.705515	11.624919	6.311520
C	27.782971	8.990233	5.693028
C	26.906404	9.845505	6.433098
C	26.576670	9.611171	7.862975
C	29.792782	8.075861	1.417126
C	26.605454	11.171790	4.401546
C	30.452233	6.932163	1.918178
H	31.049461	6.329322	1.232747
C	30.326513	6.543256	3.245784
C	26.712689	10.653073	8.798386
H	27.103201	11.620333	8.473408
C	29.483287	12.245272	0.832015
C	26.079319	8.368449	8.298389
H	25.945334	7.557733	7.578771
C	25.881715	9.213176	10.561738
H	25.613867	9.057803	11.609686
C	26.040183	12.367862	3.696210
H	25.555539	13.057207	4.399442
H	25.319990	12.057199	2.925549
H	26.850052	12.887072	3.160928
C	29.883690	8.460695	-0.029075
H	30.414714	7.699348	-0.614668
H	30.388673	9.431059	-0.139860
H	28.868665	8.601255	-0.431338
C	26.373305	10.452766	10.138724
H	26.495147	11.268371	10.855629
C	25.731845	8.173608	9.637187
H	25.338118	7.206213	9.958325
C	31.024360	5.319182	3.718708
C	32.357320	2.976745	4.531427
H	32.874860	2.068220	4.848927
C	30.322301	4.282953	4.362453
H	29.247630	4.381204	4.530919
C	30.984698	3.119962	4.762385
H	30.424443	2.320060	5.252565
C	32.401538	5.159685	3.479998
H	32.957242	5.959082	2.984065
C	33.063594	3.999531	3.889387
H	34.135866	3.895092	3.706805
C	24.522584	10.140535	-0.474201
C	24.159029	8.868565	-0.943092
C	23.726496	11.255217	-0.780310

C	23.008536	8.704173	-1.711523
C	22.573205	11.107123	-1.547722
C	22.233080	9.829891	-2.001156
H	22.705609	7.727467	-2.086513
H	21.939683	11.956870	-1.798568
C	30.411624	13.335186	0.376246
C	30.801507	13.404704	-0.970276
C	30.889082	14.282911	1.294819
C	31.663704	14.410051	-1.402478
C	31.751356	15.294758	0.877878
C	32.125297	15.340480	-0.467693
H	31.980625	14.484226	-2.441888
H	32.135316	16.041420	1.571713
N	33.040309	16.408618	-0.917116
O	33.428789	17.216480	-0.086429
O	33.361437	16.428671	-2.096092
N	21.011995	9.664062	-2.814552
O	20.730090	8.539460	-3.201132
O	20.347182	10.660064	-3.058469
H	24.790706	8.014293	-0.696595
H	24.026783	12.235727	-0.408590
H	30.574475	14.213662	2.336823
H	30.418226	12.660425	-1.669414



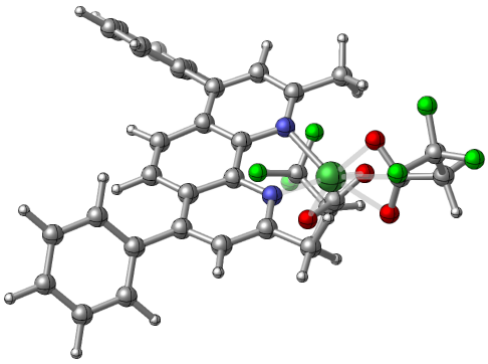
Zero-point correction= 0.607200 (Hartree/Particle)
Thermal correction to Energy= 0.652255
Thermal correction to Enthalpy= 0.653199
Thermal correction to Gibbs Free Energy= 0.519129
Sum of electronic and zero-point Energies= -3867.926566
Sum of electronic and thermal Energies= -3867.881512
Sum of electronic and thermal Enthalpies= -3867.880568
Sum of electronic and thermal Free Energies= -3868.014638

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3871.353416 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3868.371495 a.u.

^{3}(L4)Ni(OCOCH$_2$CF$_3$)$_2$
E(scf) = -3750.18941882 a.u.
n_{min} = 15.42 cm^{-1}

Ni	27.202747	10.241369	1.637697
O	28.623304	11.513333	2.532688
O	25.777609	9.458366	0.309546
O	25.711045	11.580954	0.872162
O	28.740432	11.175404	0.360299
N	28.482071	8.650091	1.964087
N	26.567716	9.649399	3.560511
C	27.571501	8.948055	4.152260
C	28.616731	8.428471	3.295115
C	28.782962	8.040256	6.083066
H	28.871272	7.925786	7.163081
C	25.244445	10.601967	0.231909
C	29.704967	7.710261	3.845872
C	29.780838	7.575374	5.272602
H	30.654475	7.096284	5.713870
C	25.514779	9.861350	5.690424
H	24.655732	10.218931	6.259766
C	27.624630	8.700055	5.547691
C	26.528155	9.167518	6.338589
C	26.435039	8.932673	7.803210
C	29.347204	8.122397	1.101527
C	25.553044	10.100720	4.298340
C	24.017239	10.802831	-0.642451
C	30.464175	7.397256	1.573794
H	31.172165	6.993273	0.848683
C	30.679490	7.201753	2.929598
C	26.185872	10.009667	8.673344
H	26.104663	11.020720	8.267271
C	29.229022	11.620878	1.429050
C	26.542967	7.636541	8.341283
H	26.711123	6.787226	7.675462
C	26.174582	8.506049	10.573841
H	26.075741	8.340376	11.649430
C	24.446099	10.845323	3.612350
H	23.709858	11.222666	4.333603
H	23.932058	10.185197	2.895775
H	24.852269	11.679339	3.023780
C	30.633654	12.210695	1.424230
C	29.124295	8.328311	-0.367206
H	29.429003	7.435353	-0.932178
H	29.724514	9.184031	-0.709812
H	28.069882	8.559409	-0.567122
C	26.062897	9.797957	10.048831
H	25.880462	10.646343	10.712925
C	26.410399	7.426139	9.715844
H	26.487418	6.412897	10.117647

C	31.913193	6.504184	3.377283
C	34.284391	5.202603	4.146235
H	35.205410	4.696826	4.446424
C	31.863685	5.338845	4.162599
H	30.896384	4.928953	4.462123
C	33.042863	4.691386	4.540680
H	32.991084	3.781206	5.143204
C	33.164979	7.006991	2.978689
H	33.206441	7.919361	2.378812
C	34.342616	6.362139	3.365432
H	35.309045	6.768463	3.057097
C	31.670758	11.122390	1.610785
C	22.968217	9.729647	-0.459356
F	32.910009	11.636044	1.689734
F	31.672668	10.239832	0.589171
F	31.462491	10.408277	2.736355
F	21.837311	10.053161	-1.115918
F	23.358793	8.530146	-0.912269
F	22.635567	9.576928	0.843476
H	23.558772	11.773880	-0.419101
H	30.750582	12.922258	2.251571
H	24.320178	10.794353	-1.700398
H	30.842453	12.707210	0.467784



Zero-point correction= 0.505059 (Hartree/Particle)
Thermal correction to Energy= 0.545287
Thermal correction to Enthalpy= 0.546231
Thermal correction to Gibbs Free Energy= 0.426753
Sum of electronic and zero-point Energies= -3749.684360
Sum of electronic and thermal Energies= -3749.644132
Sum of electronic and thermal Enthalpies= -3749.643188
Sum of electronic and thermal Free Energies= -3749.762666

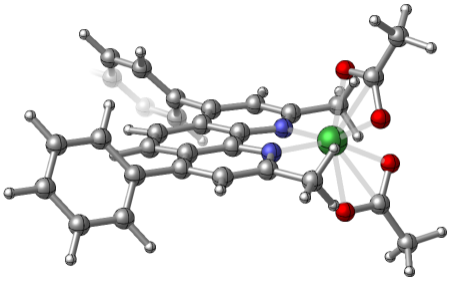
uB3LYP-d3/def2-tzvpp-CPCM(THF) //uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3752.928807 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF) //uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3750.18753 a.u.

^{3}(L4)Ni(OCOCH$_3$)$_2$
E(scf) = -3076.59768213 a.u.

ν_{min} = 11.78 cm^{-1}

Ni	27.451853	10.419779	1.658181
O	28.205297	12.312254	2.155464
O	26.442178	8.931642	0.580982
O	25.495509	10.891529	0.855765
O	28.334789	11.615154	0.079237
N	28.998735	9.080422	2.131905
N	27.004378	10.022204	3.668598
C	27.871407	9.152264	4.244170
C	28.937323	8.632148	3.410596
C	28.784140	7.877509	6.132873
H	28.763438	7.628929	7.193639
C	25.471891	9.723317	0.375119
C	29.856236	7.690806	3.943933
C	29.768488	7.361053	5.338611
H	30.520128	6.702944	5.773638
C	25.910157	10.272497	5.772148
H	25.106931	10.743281	6.340945
C	27.784854	8.763872	5.606489
C	26.725813	9.329504	6.383732
C	26.483529	8.956837	7.802045
C	29.907822	8.578316	1.294749
C	26.069779	10.617294	4.411462
C	30.845787	7.622647	1.744602
H	31.567116	7.220022	1.032020
C	30.843906	7.162521	3.054959
C	26.357937	9.956920	8.783427
H	26.483870	11.005130	8.502098
C	28.534383	12.512232	0.946036
C	26.326346	7.610624	8.181773
H	26.397880	6.824600	7.426696
C	25.942318	8.277297	10.480464
H	25.734219	8.013199	11.520219
C	25.218157	11.670702	3.769756
H	24.538563	12.136256	4.495162
H	24.646797	11.250912	2.930215
H	25.875542	12.435520	3.327042
C	29.865506	9.011621	-0.139680
H	30.614449	8.482420	-0.742813
H	30.010433	10.097500	-0.223467
H	28.857687	8.816600	-0.539170
C	26.095122	9.618548	10.113276
H	26.011160	10.406415	10.865818
C	26.054725	7.275215	9.510303
H	25.926104	6.226105	9.787654
C	31.839387	6.140816	3.473580

C	33.740632	4.188649	4.182217
H	34.478434	3.431695	4.459355
C	31.435909	4.931775	4.070612
H	30.374167	4.742304	4.243299
C	32.380131	3.963072	4.419132
H	32.050452	3.025611	4.873645
C	33.208379	6.352020	3.228412
H	33.533317	7.288050	2.767881
C	34.151860	5.385508	3.585963
H	35.212678	5.569161	3.398737
C	29.201529	13.811855	0.559650
H	30.276092	13.740173	0.796428
H	29.094528	14.002423	-0.516358
H	28.785649	14.645087	1.143284
C	24.273560	9.247335	-0.412829
H	23.604735	8.690987	0.264722
H	23.716674	10.097077	-0.829415
H	24.586986	8.560978	-1.211827



Zero-point correction= 0.492208 (Hartree/Particle)
Thermal correction to Energy= 0.526748
Thermal correction to Enthalpy= 0.527692
Thermal correction to Gibbs Free Energy= 0.421467
Sum of electronic and zero-point Energies= -3076.105475
Sum of electronic and thermal Energies= -3076.070934
Sum of electronic and thermal Enthalpies= -3076.069990
Sum of electronic and thermal Free Energies= -3076.176215

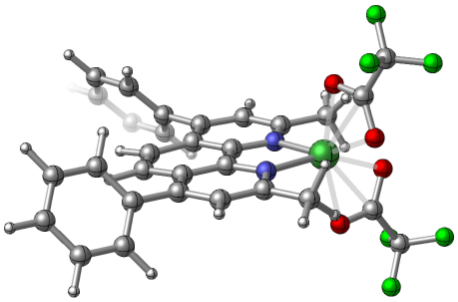
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3078.530914 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3076.415625 a.u.

^{3}(L4)Ni(OCOCF$_3$)$_2$
E(scf) = -3671.57856784 a.u.
ν_{min} = 5.01 cm^{-1}

Ni	27.445938	10.404309	1.675092
O	28.376331	12.269888	2.088310
O	26.258264	8.951067	0.679363
O	25.499785	11.016399	0.886714
O	28.300960	11.531906	0.006463
N	28.985606	9.087095	2.111372

N	26.978812	10.022893	3.655044
C	27.851366	9.150532	4.225654
C	28.925835	8.644508	3.395482
C	28.767650	7.878642	6.114345
H	28.741784	7.624814	7.173563
C	25.379073	9.829982	0.511218
C	29.859921	7.722591	3.934866
C	29.769108	7.386389	5.326846
H	30.530903	6.742464	5.764966
C	25.852492	10.217684	5.747109
H	25.032604	10.663746	6.311739
C	27.758220	8.749080	5.583203
C	26.682164	9.287496	6.357239
C	26.436829	8.899011	7.770244
C	29.924956	8.617253	1.287582
C	26.018538	10.583627	4.393202
C	24.033214	9.434723	-0.133006
C	30.878554	7.683333	1.749016
H	31.619726	7.302393	1.045257
C	30.868351	7.216199	3.055749
C	26.285528	9.889828	8.757384
H	26.393495	10.942285	8.484657
C	28.641549	12.372928	0.866465
C	26.302529	7.547067	8.138211
H	26.393277	6.768054	7.377970
C	25.891095	8.189816	10.438845
H	25.681379	7.914117	11.475224
C	25.118730	11.604009	3.760993
H	24.559672	12.160777	4.524273
H	24.405013	11.121975	3.076482
H	25.710349	12.300774	3.151076
C	29.503590	13.558325	0.382598
C	29.934653	9.074648	-0.141252
H	30.571011	8.425497	-0.756646
H	30.304621	10.108120	-0.215125
H	28.912111	9.082325	-0.543043
C	26.020950	9.536490	10.082858
H	25.917442	10.316877	10.840657
C	26.028225	7.197048	9.462312
H	25.917121	6.143799	9.731173
C	31.878992	6.213650	3.482430
C	33.811004	4.298673	4.204885
H	34.560981	3.555884	4.487478
C	31.492980	4.994881	4.071177
H	30.433562	4.782952	4.231478
C	32.452959	4.044346	4.426223

H	32.137638	3.098667	4.873699
C	33.245821	6.454029	3.252316
H	33.556919	7.398129	2.798805
C	34.204592	5.505718	3.617326
H	35.263412	5.711554	3.442626
F	28.969930	14.134000	-0.702396
F	29.654839	14.496357	1.320917
F	30.727543	13.104133	0.048427
F	23.066482	9.471728	0.804204
F	24.057392	8.204283	-0.651506
F	23.694417	10.291570	-1.105384



Zero-point correction= 0.448131 (Hartree/Particle)
Thermal correction to Energy= 0.486067
Thermal correction to Enthalpy= 0.487011
Thermal correction to Gibbs Free Energy= 0.369887
Sum of electronic and zero-point Energies= -3671.130437
Sum of electronic and thermal Energies= -3671.092501
Sum of electronic and thermal Enthalpies= -3671.091556
Sum of electronic and thermal Free Energies= -3671.208681

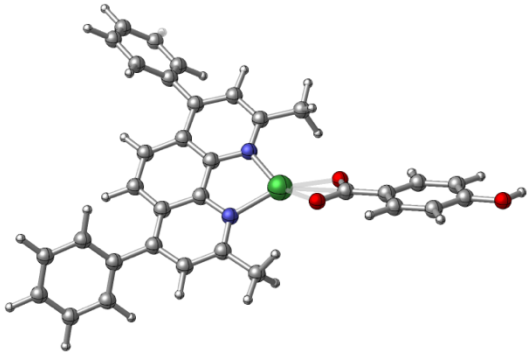
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3674.236744 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3671.589829 a.u.

^{2}(L4)NiOCO-*p*-OHPh
E(scf) = -3115.00073138 a.u.
ν_{min} = 9.94 cm^{-1}

Ni	28.958279	10.124626	2.006238
O	30.360096	11.457682	1.080349
O	28.196752	11.617350	0.716430
N	29.857545	8.425155	2.546330
N	27.721851	9.646099	3.469736
C	28.120760	8.537514	4.160775
C	29.286399	7.866215	3.650146
C	27.929858	6.810773	5.881472
H	27.383687	6.371566	6.716243
C	29.769990	6.685659	4.269984
C	29.031218	6.166401	5.388614
H	29.345258	5.223988	5.837248

C	25.923624	9.886445	5.031120
H	25.060000	10.469866	5.355004
C	27.450082	8.038934	5.306505
C	26.312400	8.766703	5.770644
C	25.546610	8.385237	6.984503
C	30.909063	7.817478	1.980448
C	26.632159	10.309851	3.893619
C	31.457314	6.649688	2.544596
H	32.337720	6.205990	2.076720
C	30.928125	6.074490	3.700488
C	24.143102	8.285217	6.933541
H	23.628272	8.448925	5.983747
C	29.380558	12.024333	0.507514
C	26.191281	8.163262	8.217037
H	27.276753	8.264910	8.283288
C	24.060919	7.735754	9.293122
H	23.485837	7.481924	10.187039
C	26.227255	11.520960	3.106945
H	25.341063	12.009503	3.533280
H	26.032860	11.243862	2.059976
H	27.061787	12.237796	3.062686
C	29.618829	13.173197	-0.414688
C	31.454841	8.427306	0.722600
H	32.410755	7.973897	0.427897
H	31.565964	9.514440	0.842576
H	30.731171	8.282748	-0.098082
C	23.407955	7.959459	8.076034
H	22.319938	7.876680	8.014138
C	25.454554	7.842448	9.359828
H	25.972019	7.681552	10.308931
C	28.759976	14.877514	-1.924534
H	27.917570	15.363382	-2.425611
C	31.150410	14.714361	-1.511209
H	32.159289	15.086732	-1.701424
C	31.573111	4.869631	4.283303
C	28.544597	13.804640	-1.061375
C	30.067653	15.339437	-2.154646
C	32.865981	2.602448	5.349962
H	33.365301	1.723010	5.764078
C	30.922274	13.643750	-0.652164
C	31.874203	3.763060	3.467192
H	31.590797	3.781643	2.412103
C	32.510657	2.637889	3.997197
H	32.727429	1.783842	3.350684
C	31.939414	4.823723	5.642203
H	31.737758	5.684110	6.284079

C	32.581428	3.700511	6.169265
H	32.865923	3.685915	7.224345
O	30.342943	16.376333	-2.980572
H	27.533037	13.439256	-0.875688
H	31.755811	13.151658	-0.147675
H	29.524898	16.724738	-3.363330



Zero-point correction= 0.497781 (Hartree/Particle)
Thermal correction to Energy= 0.531124
Thermal correction to Enthalpy= 0.532068
Thermal correction to Gibbs Free Energy= 0.428705
Sum of electronic and zero-point Energies= -3114.502951
Sum of electronic and thermal Energies= -3114.469608
Sum of electronic and thermal Enthalpies= -3114.468663
Sum of electronic and thermal Free Energies= -3114.572027

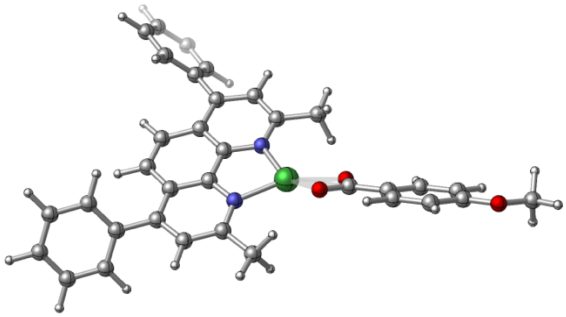
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3116.971515 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3114.80757 a.u.

^{2}(L4)NiOCO-*p*-OMePh
E(scf) = -3154.27467658 a.u.
ν_{min} = 8.13 cm^{-1}

Ni	28.956738	10.122859	2.007464
O	30.357024	11.456370	1.077082
O	28.192520	11.614258	0.719458
N	29.856799	8.424411	2.548143
N	27.720907	9.644603	3.472210
C	28.120249	8.536068	4.162966
C	29.286068	7.865220	3.652067
C	27.930095	6.808997	5.883454
H	27.384154	6.369480	6.718211
C	29.770136	6.684799	4.271767
C	29.031660	6.165131	5.390409
H	29.346101	5.222779	5.838887
C	25.922832	9.884149	5.033845
H	25.059088	10.467266	5.357948
C	27.449857	8.037050	5.308681
C	26.311964	8.764368	5.773013

C	25.546254	8.382320	6.986756
C	30.908480	7.817062	1.982113
C	26.631171	10.307997	3.896315
C	31.457240	6.649490	2.546186
H	32.337737	6.206126	2.078162
C	30.928441	6.074054	3.702133
C	24.142811	8.281607	6.935589
H	23.628026	8.445219	5.985756
C	29.375439	12.022021	0.506932
C	26.190907	8.160480	8.219313
H	27.276323	8.262638	8.285691
C	24.060625	7.731754	9.295072
H	23.485562	7.477507	10.188884
C	26.225665	11.519152	3.110027
H	25.340028	12.007854	3.537329
H	26.030038	11.242057	2.063294
H	27.060304	12.235774	3.064758
C	29.610655	13.170874	-0.416265
C	31.453863	8.427133	0.724233
H	32.408961	7.972792	0.428335
H	31.566398	9.514048	0.844848
H	30.729207	8.284226	-0.095855
C	23.407689	7.955302	8.077943
H	22.319721	7.871989	8.015903
C	25.454198	7.839137	9.361969
H	25.971624	7.678357	10.311112
C	28.741867	14.879270	-1.924482
H	27.884803	15.348373	-2.407168
C	31.135120	14.709863	-1.519016
H	32.141715	15.084526	-1.716673
C	31.573920	4.869417	4.284852
C	28.537168	13.803481	-1.057558
C	30.049825	15.340091	-2.160559
C	32.867621	2.602630	5.351381
H	33.367249	1.723343	5.765447
C	30.914755	13.641058	-0.659987
C	31.875376	3.762980	3.468691
H	31.591917	3.781499	2.413615
C	32.512245	2.638011	3.998628
H	32.729290	1.784066	3.352071
C	31.940299	4.823575	5.643738
H	31.738368	5.683864	6.285659
C	32.582714	3.700563	6.170736
H	32.867242	3.686022	7.225808
O	30.361736	16.371521	-2.978658
C	29.326688	17.058380	-3.661069

H	28.616597	17.528011	-2.957982
H	29.812814	17.842596	-4.255946
H	28.769098	16.387079	-4.337487
H	27.526265	13.438510	-0.866828
H	31.751246	13.149270	-0.160153



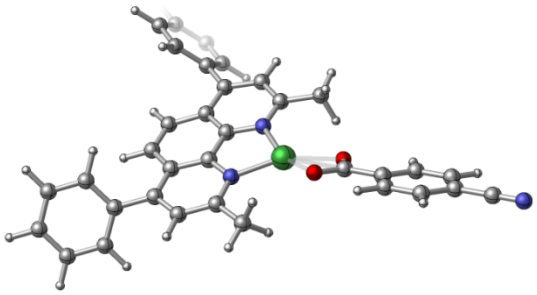
Zero-point correction= 0.525843 (Hartree/Particle)
Thermal correction to Energy= 0.560639
Thermal correction to Enthalpy= 0.561583
Thermal correction to Gibbs Free Energy= 0.454519
Sum of electronic and zero-point Energies= -3153.748833
Sum of electronic and thermal Energies= -3153.714038
Sum of electronic and thermal Enthalpies= -3153.713093
Sum of electronic and thermal Free Energies= -3153.820157

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3156.286652 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3154.062022 a.u.

^{2}(L4)NiOCO-*p*-CNPh
E(scf) = -3132.00678353 a.u.
ν_{min} = 7.42 cm^{-1}

Ni	29.013828	10.295156	2.243682
O	30.288074	11.460947	0.971809
O	28.124820	11.856020	1.082074
N	29.847302	8.536258	2.652675
N	27.863884	9.834375	3.803439
C	28.191192	8.632688	4.356563
C	29.273211	7.920197	3.724151
C	27.917615	6.763124	5.910531
H	27.368854	6.290444	6.724999
C	29.673723	6.648620	4.206892
C	28.935722	6.081796	5.302607
H	29.182462	5.075285	5.640212
C	26.175942	10.075686	5.480743
H	25.390990	10.699596	5.911396
C	27.529914	8.079488	5.482218
C	26.488189	8.855348	6.077564
C	25.746156	8.418018	7.288126
C	30.831429	7.906360	1.995455

C	26.869803	10.548536	4.349955
C	31.293061	6.645233	2.419253
H	32.116736	6.180227	1.874914
C	30.752990	6.000481	3.530917
C	24.338820	8.436414	7.298826
H	23.799432	8.733811	6.396319
C	29.269779	12.118930	0.615377
C	26.423937	8.025417	8.458288
H	27.515999	8.031229	8.476651
C	24.313826	7.667635	9.597367
H	23.758839	7.374740	10.492021
C	26.544513	11.868299	3.715487
H	25.787997	12.421272	4.287839
H	26.191233	11.716769	2.684628
H	27.458314	12.474079	3.620863
C	29.422158	13.234556	-0.380875
C	31.423071	8.609969	0.810245
H	32.147276	7.977759	0.279640
H	31.909209	9.544794	1.127000
H	30.622470	8.920430	0.122171
C	23.629274	8.059857	8.441952
H	22.536555	8.070529	8.428795
C	25.713049	7.655431	9.602564
H	26.255605	7.361685	10.504598
C	28.437866	15.021862	-1.694997
H	27.569114	15.607669	-2.000838
C	30.832080	14.561148	-1.844636
H	31.812341	14.790889	-2.266260
C	31.305239	4.690280	3.961583
C	28.304140	13.986563	-0.773477
C	29.706295	15.313346	-2.235217
C	32.421581	2.220038	4.735697
H	32.852398	1.261880	5.036572
C	30.683160	13.528982	-0.921922
C	31.470678	3.651479	3.026400
H	31.150083	3.803993	1.993034
C	32.019524	2.425745	3.411520
H	32.130978	1.626956	2.674056
C	31.717436	4.472765	5.290339
H	31.621416	5.276946	6.023219
C	32.272062	3.248803	5.672348
H	32.594312	3.100435	6.706012
C	29.851941	16.379458	-3.186002
N	29.969868	17.241891	-3.955356
H	27.331636	13.744536	-0.342624
H	31.541237	12.934158	-0.605970



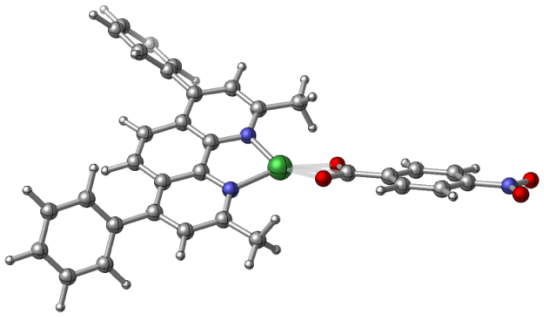
Zero-point correction= 0.492309 (Hartree/Particle)
Thermal correction to Energy= 0.526366
Thermal correction to Enthalpy= 0.527311
Thermal correction to Gibbs Free Energy= 0.421351
Sum of electronic and zero-point Energies= -3131.514475
Sum of electronic and thermal Energies= -3131.480417
Sum of electronic and thermal Enthalpies= -3131.479473
Sum of electronic and thermal Free Energies= -3131.585433

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3133.992348 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3131.787245 a.u.

^{2}(L4)NiOCO-*p*-NO_2Ph
E(scf) = -3244.18347501 a.u.
ν_{min} = 6.73 cm^{-1}

Ni	28.922110	10.197231	2.127154
O	30.272957	11.459546	0.996647
O	28.090602	11.750450	0.948148
N	29.787574	8.468222	2.581176
N	27.750157	9.732559	3.668246
C	28.133971	8.578935	4.284532
C	29.246179	7.884320	3.686342
C	27.950635	6.782959	5.935031
H	27.426521	6.329089	6.776015
C	29.705210	6.658378	4.230441
C	28.998167	6.117988	5.359497
H	29.292314	5.143594	5.749316
C	26.046913	9.977486	5.329671
H	25.229600	10.582740	5.725338
C	27.499400	8.054754	5.438824
C	26.419912	8.809289	5.993079
C	25.699273	8.402514	7.226855
C	30.787839	7.845559	1.942771
C	26.718138	10.422739	4.174574
C	31.309096	6.630585	2.427851
H	32.146798	6.172699	1.899161
C	30.808409	6.024792	3.579550
C	24.292601	8.354329	7.240005

H	23.739680	8.576823	6.324217
C	29.255402	12.079139	0.579897
C	26.394668	8.105724	8.414822
H	27.485185	8.164826	8.430497
C	24.303821	7.709053	9.576367
H	23.763251	7.438218	10.486657
C	26.327926	11.686501	3.467045
H	25.511330	12.208848	3.982713
H	26.030388	11.463629	2.431477
H	27.199898	12.352171	3.378728
C	29.426866	13.231244	-0.371466
C	31.317435	8.502975	0.702856
H	32.121659	7.916558	0.239293
H	31.673729	9.517794	0.931352
H	30.498183	8.635220	-0.022370
C	23.601617	8.006041	8.403259
H	22.509630	7.963965	8.392107
C	25.702031	7.763803	9.578851
H	26.257851	7.544858	10.493974
C	28.453788	14.998410	-1.722142
H	27.596574	15.555208	-2.098462
C	30.879178	14.675063	-1.675309
H	31.865911	14.985921	-2.016170
C	31.423425	4.766832	4.075891
C	28.303208	13.930958	-0.839921
C	29.743692	15.353762	-2.126824
C	32.657351	2.397098	4.975163
H	33.133774	1.477780	5.324554
C	30.711378	13.609831	-0.793532
C	31.631883	3.686946	3.197598
H	31.298883	3.767207	2.160042
C	32.239107	2.510884	3.644926
H	32.383537	1.678686	2.951457
C	31.852253	4.641960	5.411308
H	31.722722	5.479926	6.099819
C	32.465238	3.467803	5.855328
H	32.799498	3.391536	6.892995
N	29.912311	16.482382	-3.061136
O	31.048053	16.778773	-3.403496
O	28.907607	17.063610	-3.445486
H	27.313463	13.623532	-0.500149
H	31.572549	13.055204	-0.418953



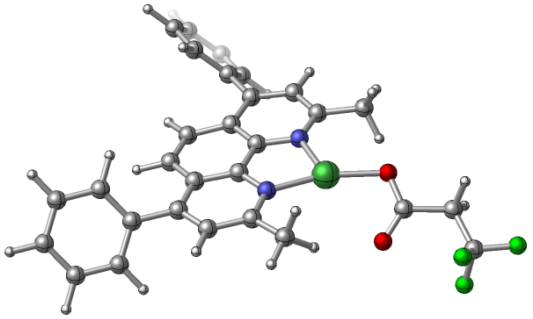
Zero-point correction= 0.496265 (Hartree/Particle)
Thermal correction to Energy= 0.531136
Thermal correction to Enthalpy= 0.532080
Thermal correction to Gibbs Free Energy= 0.423115
Sum of electronic and zero-point Energies= -3243.687210
Sum of electronic and thermal Energies= -3243.652339
Sum of electronic and thermal Enthalpies= -3243.651395
Sum of electronic and thermal Free Energies= -3243.760360

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3246.305699 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3244.002198 a.u.

^{2}(L4)NiOCOCH$_2$CF$_3$
E(scf) = -3185.00760139 a.u.
ν_{min} = 13.20 cm^{-1}

Ni	29.048556	10.415757	2.672516
O	28.650663	12.179670	1.943809
O	29.032602	11.198331	-0.033851
N	29.760060	8.620935	2.892449
N	28.030667	9.957794	4.348102
C	28.267494	8.676879	4.738922
C	29.213349	7.940580	3.938881
C	27.917075	6.675627	6.097326
H	27.385040	6.164800	6.899801
C	29.521934	6.593554	4.245956
C	28.812824	5.976716	5.334561
H	28.979759	4.919658	5.540949
C	26.494454	10.167387	6.164745
H	25.807870	10.809506	6.718948
C	27.635395	8.063305	5.848236
C	26.723104	8.864963	6.603231
C	26.026607	8.364819	7.816709
C	30.644711	7.997641	2.100402
C	27.156036	10.697154	5.036956
C	31.007682	6.658721	2.343501
H	31.746434	6.191325	1.690257
C	30.479108	5.934850	3.411542
C	26.742098	7.780365	8.879103

H	27.827621	7.681970	8.808979
C	28.743913	12.174886	0.666245
C	24.632810	8.513014	7.942311
H	24.064562	8.959612	7.122884
C	24.691740	7.494044	10.140607
H	24.174097	7.154450	11.041097
C	26.938711	12.106179	4.570476
H	26.140949	12.607421	5.134171
H	26.709476	12.115067	3.495057
H	27.872918	12.681373	4.673813
C	28.442923	13.537678	0.030641
C	31.248049	8.809905	0.992893
H	31.814950	8.187852	0.287190
H	31.930929	9.563840	1.421508
H	30.465658	9.372086	0.458236
C	26.079407	7.351109	10.031560
H	26.651153	6.907688	10.850527
C	23.970813	8.076516	9.092585
H	22.886607	8.189956	9.169156
C	30.920685	4.535193	3.641187
C	31.820521	1.892208	4.029734
H	32.167210	0.867011	4.181265
C	30.911961	3.609683	2.580759
H	30.539572	3.919483	1.601355
C	31.353599	2.298546	2.775023
H	31.329940	1.590556	1.942861
C	31.397149	4.115861	4.898136
H	31.437117	4.828290	5.725068
C	31.844325	2.806199	5.088985
H	32.218687	2.500202	6.069039
C	28.729013	13.643821	-1.445685
F	27.972249	12.815232	-2.185799
F	28.473367	14.898769	-1.885650
F	30.017247	13.387654	-1.739840
H	29.024791	14.314265	0.547260
H	27.380106	13.776652	0.187535



Zero-point correction= 0.445838 (Hartree/Particle)

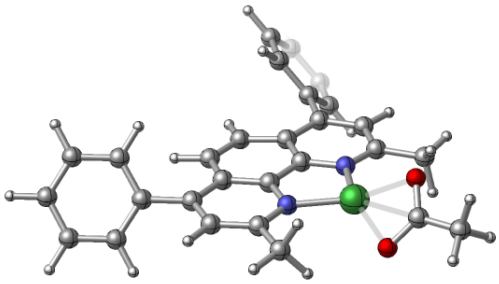
Thermal correction to Energy= 0.478350
Thermal correction to Enthalpy= 0.479294
Thermal correction to Gibbs Free Energy= 0.376515
Sum of electronic and zero-point Energies= -3184.561764
Sum of electronic and thermal Energies= -3184.529252
Sum of electronic and thermal Enthalpies= -3184.528308
Sum of electronic and thermal Free Energies= -3184.631087

uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3187.09496 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3184.911103 a.u.

^{2}(L4)NiOCOCH$_3$
E(scf) = -2848.21418274 a.u.
ν_{min} = 14.44 cm^{-1}

Ni	28.633316	10.413049	2.575055
O	28.903632	12.521964	2.458871
O	28.776065	11.293078	0.641571
N	29.359292	8.585609	2.699941
N	27.694064	9.886266	4.256883
C	28.045841	8.638256	4.678299
C	28.963556	7.927564	3.830277
C	27.948797	6.691459	6.153004
H	27.522079	6.187028	7.019917
C	29.400631	6.623780	4.177379
C	28.831828	6.019786	5.352664
H	29.095151	4.990315	5.595397
C	26.265533	10.065202	6.164555
H	25.567998	10.679339	6.736635
C	27.544349	8.040330	5.862848
C	26.635126	8.809520	6.649941
C	26.077433	8.327081	7.939721
C	30.220729	7.972644	1.868089
C	26.798696	10.583940	4.969460
C	30.708280	6.686087	2.150680
H	31.423153	6.235693	1.459829
C	30.332405	5.987922	3.302177
C	26.916831	7.853651	8.966475
H	27.997729	7.830714	8.811243
C	28.900238	12.423282	1.195628
C	24.690673	8.380246	8.174978
H	24.026184	8.739697	7.385591
C	25.001289	7.486994	10.406783
H	24.584262	7.159272	11.362253
C	26.383494	11.919620	4.425024
H	25.826750	12.509260	5.165852
H	25.736264	11.769913	3.543342
H	27.260850	12.478337	4.069171

C	30.654816	8.743731	0.656868
H	31.284664	8.140245	-0.010296
H	31.216029	9.640311	0.968649
H	29.778981	9.123584	0.111773
C	26.382691	7.439179	10.188996
H	27.050140	7.082432	10.977412
C	24.157348	7.959491	9.395838
H	23.077087	7.998330	9.556775
C	30.907864	4.644934	3.567290
C	32.064045	2.110859	4.017669
H	32.510052	1.128738	4.193066
C	30.906207	3.662375	2.558673
H	30.438982	3.883511	1.595989
C	31.475050	2.406318	2.783352
H	31.455008	1.653605	1.991193
C	31.509256	4.336688	4.803263
H	31.547287	5.095504	5.587923
C	32.081967	3.081903	5.025017
H	32.550976	2.864461	5.987954
C	29.011945	13.674474	0.351619
H	28.029801	14.175214	0.329569
H	29.729389	14.375728	0.801330
H	29.304826	13.431312	-0.678185



Zero-point correction= 0.439098 (Hartree/Particle)
Thermal correction to Energy= 0.468731
Thermal correction to Enthalpy= 0.469675
Thermal correction to Gibbs Free Energy= 0.374431
Sum of electronic and zero-point Energies= -2847.775085
Sum of electronic and thermal Energies= -2847.745452
Sum of electronic and thermal Enthalpies= -2847.744508
Sum of electronic and thermal Free Energies= -2847.839752

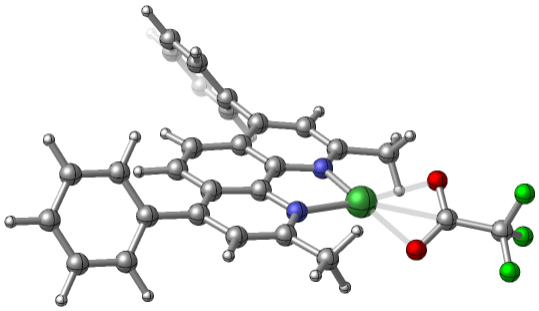
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2849.892529 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -2848.022398 a.u.

^{2}(L4)NiOCOCF$_3$
E(scf) = -3145.70657490 a.u.
ν_{min} = 9.44 cm^{-1}

Ni	28.647004	10.430908	2.605116

O	28.678512	12.610001	2.384585
O	28.925960	11.283117	0.626901
N	29.400742	8.595733	2.723531
N	27.722022	9.903195	4.281009
C	28.067572	8.651976	4.693349
C	28.988292	7.937966	3.843129
C	27.949493	6.690788	6.150506
H	27.513500	6.184022	7.011282
C	29.409123	6.628160	4.184353
C	28.831110	6.017673	5.350399
H	29.086108	4.984551	5.585934
C	26.288388	10.071546	6.186710
H	25.591001	10.683932	6.760718
C	27.557966	8.044765	5.868318
C	26.647532	8.811261	6.660186
C	26.081096	8.317522	7.941839
C	30.256225	7.985450	1.892194
C	26.831135	10.600025	4.998739
C	30.734157	6.689506	2.169446
H	31.450412	6.237889	1.481085
C	30.343455	5.991070	3.310043
C	26.914279	7.834634	8.969098
H	27.996103	7.811799	8.820251
C	28.842226	12.410720	1.160410
C	24.693020	8.369946	8.168132
H	24.033904	8.736834	7.377689
C	24.989448	7.457437	10.393959
H	24.566258	7.121819	11.343939
C	26.449879	11.956300	4.483753
H	25.690437	12.435551	5.115422
H	26.066760	11.867089	3.454656
H	27.337535	12.601321	4.411313
C	30.689017	8.748068	0.675314
H	31.437518	8.196642	0.091281
H	31.096540	9.726545	0.972020
H	29.819327	8.975645	0.041051
C	26.372206	7.410478	10.184716
H	27.034358	7.046577	10.974273
C	24.151936	7.938938	9.381985
H	23.070771	7.977067	9.536596
C	30.903851	4.640425	3.572821
C	32.029304	2.094842	4.018308
H	32.463825	1.107319	4.192024
C	30.882271	3.658683	2.564560
H	30.412369	3.885758	1.604613
C	31.435852	2.395452	2.787527

H	31.401022	1.641949	1.996756
C	31.507676	4.327662	4.805801
H	31.557683	5.086433	5.589853
C	32.066708	3.066267	5.024729
H	32.539001	2.843491	5.984732
C	28.924273	13.666888	0.263107
F	27.754346	14.331349	0.287232
F	29.877371	14.505580	0.703453
F	29.198373	13.370717	-1.012495



Zero-point correction= 0.417237 (Hartree/Particle)
Thermal correction to Energy= 0.448649
Thermal correction to Enthalpy= 0.449593
Thermal correction to Gibbs Free Energy= 0.348627
Sum of electronic and zero-point Energies= -3145.289338
Sum of electronic and thermal Energies= -3145.257926
Sum of electronic and thermal Enthalpies= -3145.256982
Sum of electronic and thermal Free Energies= -3145.357948
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3147.749835 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -3145.612842 a.u.

^{3}TS3

E(scf) = -5932.22058798 a.u.

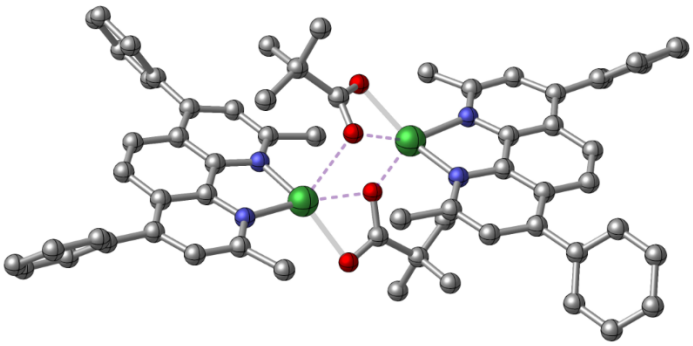
ν_{min} = -62.04 cm^{-1}

Ni	27.351093	10.310588	1.772894
O	28.054476	13.430539	3.687060
O	25.776588	10.389964	0.234526
O	25.947022	11.930865	1.776266
O	28.761968	12.871076	1.690311
N	28.743372	8.947633	1.307021
N	27.692635	9.661990	3.620879
C	28.664072	8.703561	3.671700
C	29.221190	8.299145	2.407184
C	30.149008	7.110630	4.787861
H	30.507489	6.641197	5.703722
C	25.276383	11.370188	0.833156
C	30.220643	7.295193	2.348722

C	30.671322	6.720196	3.585777
H	31.452262	5.960612	3.562869
C	27.483528	9.477009	5.998304
H	26.990695	9.828756	6.906151
C	29.128893	8.118911	4.876846
C	28.529285	8.559935	6.095980
C	29.256229	8.655823	0.106429
C	27.080855	10.017783	4.763824
C	23.861389	11.845277	0.479993
C	30.242397	7.659042	-0.036297
H	30.610638	7.425684	-1.036703
C	30.728885	6.949659	1.058788
C	28.955801	12.957696	2.938817
C	25.993952	11.041655	4.667193
H	25.529920	11.236888	5.643108
H	25.225723	10.713352	3.950943
H	26.413083	11.972539	4.260505
C	30.324795	12.569331	3.517759
C	28.762974	9.447308	-1.068068
H	28.961834	8.933928	-2.018701
H	29.278062	10.421886	-1.092173
H	27.688907	9.654950	-0.966595
C	30.173022	12.012147	4.940923
H	31.164476	11.829237	5.386141
H	29.624358	12.717127	5.581100
H	29.623373	11.061145	4.938934
C	31.001378	11.535410	2.606421
H	30.355445	10.657027	2.482066
H	31.186444	11.950769	1.605759
H	31.961976	11.210559	3.037829
C	31.155324	13.871562	3.554594
H	30.682157	14.620310	4.209160
H	32.168154	13.666493	3.938481
H	31.250585	14.305159	2.546350
C	22.937289	10.611201	0.539641
H	22.922633	10.176972	1.552680
H	21.906923	10.899773	0.277196
H	23.277008	9.835026	-0.160774
C	23.376024	12.915925	1.463786
H	23.348725	12.525631	2.492718
H	24.043927	13.784444	1.460463
H	22.362391	13.249619	1.190769
C	23.881651	12.404748	-0.957319
H	24.288566	11.661703	-1.659375
H	22.858283	12.661753	-1.274273
H	24.495573	13.313680	-1.022102

Ni	26.841045	13.818611	1.874082
N	26.605011	14.600222	0.005541
N	25.698892	15.393381	2.366899
C	25.313222	16.143423	1.276833
C	25.792820	15.706684	0.003975
C	24.042488	17.907243	0.147537
H	23.324205	18.725860	0.193929
C	25.413583	16.386583	-1.191781
C	24.493185	17.483708	-1.070550
H	24.128572	17.970752	-1.974931
C	24.369277	16.839259	3.744496
H	24.022890	17.086028	4.749500
C	24.455163	17.277049	1.373814
C	24.002345	17.665344	2.663959
C	27.053933	14.122404	-1.169528
C	25.187535	15.722109	3.578324
C	26.729585	14.749335	-2.379585
H	27.136465	14.342067	-3.306378
C	25.922726	15.896349	-2.423346
C	25.518434	14.82067	4.729857
H	25.103035	13.817685	4.538228
H	25.104285	15.199828	5.673699
H	26.604182	14.681364	4.819723
C	27.919767	12.898664	-1.144604
H	28.044294	12.476303	-2.150468
H	27.493973	12.139495	-0.477701
H	28.90691	13.135766	-0.721027
C	25.627377	16.527973	-3.734614
C	25.836243	17.903767	-3.953168
C	25.172519	15.740875	-4.81033
C	25.587044	18.474431	-5.203918
H	26.216921	18.525381	-3.139795
C	24.919254	16.313188	-6.059337
H	25.001038	14.672699	-4.656357
C	25.124464	17.682673	-6.260898
H	25.7621	19.54267	-5.355123
H	24.556545	15.686811	-6.878348
H	24.927782	18.130497	-7.238193
C	23.162343	18.862045	2.910034
C	23.505163	20.125016	2.384784
C	22.016771	18.772145	3.72688
C	22.724681	21.251322	2.65625
H	24.406693	20.22642	1.776589
C	21.235654	19.898341	3.9962
H	21.728338	17.802001	4.138773
C	21.584702	21.143439	3.460852

H	23.014415	22.221253	2.243679
H	20.346047	19.801875	4.624091
H	20.974017	22.02483	3.671945
C	31.743556	5.883805	0.850112
C	31.543852	4.579285	1.340161
C	32.909058	6.155757	0.110108
C	32.488305	3.577816	1.101905
H	30.632108	4.34486	1.894061
C	33.855981	5.154701	-0.121369
H	33.078231	7.165338	-0.272044
C	33.648971	3.862857	0.374091
H	32.313635	2.56841	1.48252
H	34.76045	5.38603	-0.689463
H	34.388697	3.079449	0.191666
C	28.977118	8.094583	7.433114
C	28.042599	7.605716	8.364944
C	30.328931	8.183573	7.817728
C	28.449994	7.20315	9.639417
H	26.990814	7.528143	8.079059
C	30.733846	7.785809	9.094187
H	31.062216	8.588994	7.116867
C	29.796832	7.290718	10.008098
H	27.711898	6.816898	10.346853
H	31.785815	7.869644	9.378323
H	30.115028	6.977238	11.005461



Zero-point correction= 1.051082 (Hartree/Particle)
Thermal correction to Energy= 1.117469
Thermal correction to Enthalpy= 1.118414
Thermal correction to Gibbs Free Energy= 0.944756
Sum of electronic and zero-point Energies= -5931.169506
Sum of electronic and thermal Energies= -5931.103119
Sum of electronic and thermal Enthalpies= -5931.102174
Sum of electronic and thermal Free Energies= -5931.275832
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5935.807074 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)

E(scf) = -5931.757066 a.u.

^{3}3a_d

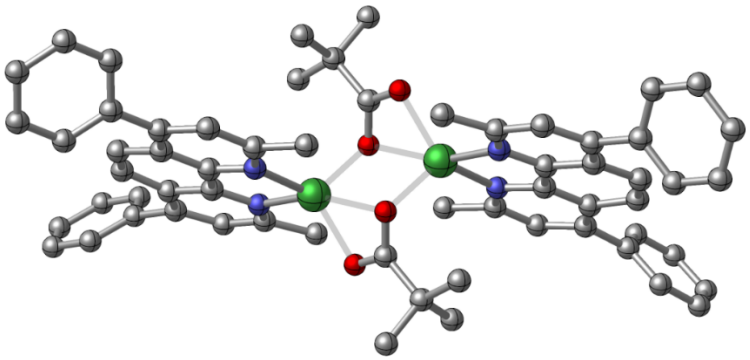
E(scf) = -5932.22581891 a.u.

ν_{min} = 7.83 cm^{-1}

Ni	27.660078	10.591774	2.152287
O	28.349117	13.971521	3.067584
O	26.113701	10.514189	0.725552
O	25.840457	12.116018	2.205216
O	28.621215	12.383915	1.572715
N	28.846555	9.037405	1.608808
N	27.953087	9.821684	3.959335
C	28.771964	8.716508	3.956843
C	29.247783	8.288649	2.676552
C	29.945813	6.824368	4.969353
H	30.174318	6.222001	5.848656
C	25.407374	11.435110	1.213731
C	30.102188	7.157642	2.550894
C	30.397208	6.414888	3.745194
H	30.978295	5.495896	3.668143
C	27.823057	9.621148	6.347131
H	27.440808	10.032640	7.282921
C	29.152034	8.014475	5.133051
C	28.676793	8.503675	6.383643
C	29.284028	8.723496	0.382832
C	27.481766	10.258630	5.153828
C	24.006056	11.685466	0.638194
C	30.130758	7.621300	0.179126
H	30.482126	7.406674	-0.831317
C	30.565532	6.826599	1.246503
C	29.055753	13.056071	2.570627
C	26.614162	11.478568	5.123795
H	26.297002	11.781898	6.130528
H	25.728741	11.303413	4.494056
H	27.149783	12.312912	4.646209
C	30.458973	12.802743	3.139998
C	28.859470	9.628697	-0.734778
H	29.266447	9.309268	-1.703103
H	29.196906	10.652880	-0.513397
H	27.761759	9.674429	-0.785484
C	31.121357	11.601433	2.456209
H	32.125022	11.431067	2.877025
H	30.521173	10.694586	2.601044
H	31.218506	11.763440	1.372565
C	31.280769	14.084268	2.884312

H	31.358912	14.295707	1.805327
H	30.811910	14.951444	3.372153
H	32.300989	13.964625	3.283244
C	30.341651	12.553805	4.655797
H	29.774775	11.633628	4.859184
H	31.344113	12.442982	5.099400
H	29.829271	13.391165	5.151147
C	23.342646	12.891116	1.313308
H	23.943752	13.796618	1.164234
H	22.339943	13.059398	0.889414
H	23.243507	12.736003	2.397810
C	24.129396	11.927193	-0.878366
H	24.698698	12.845494	-1.083875
H	24.641909	11.086653	-1.368213
H	23.128751	12.038054	-1.326047
C	23.182281	10.406012	0.897004
H	23.099402	10.200289	1.976751
H	22.163833	10.524204	0.493136
H	23.652614	9.535942	0.415780
Ni	26.813830	13.897036	1.621911
N	26.531642	14.668314	-0.186627
N	25.616358	15.443856	2.157767
C	25.226056	16.197757	1.089425
C	25.718086	15.777912	-0.187155
C	23.944562	17.970148	-0.001843
H	23.221409	18.783911	0.053450
C	25.344645	16.480789	-1.365174
C	24.414845	17.570860	-1.222358
H	24.055857	18.074409	-2.119940
C	24.292800	16.833012	3.577469
H	23.954693	17.058818	4.590007
C	24.353217	17.315054	1.209981
C	23.899595	17.656286	2.515494
C	26.987991	14.216495	-1.381371
C	25.140597	15.731241	3.375759
C	26.670781	14.867529	-2.573903
H	27.087433	14.478169	-3.504479
C	25.865086	16.020263	-2.608732
C	25.548129	14.813567	4.489426
H	25.228083	13.789742	4.242146
H	25.113903	15.112905	5.452334
H	26.644841	14.77884	4.566912
C	27.840046	12.985595	-1.349441
H	28.143191	12.670011	-2.356725
H	27.297648	12.162466	-0.86043
H	28.73383	13.153206	-0.72941

C	25.591853	16.682993	-3.906795
C	25.771761	18.070481	-4.080651
C	25.189309	15.920101	-5.02165
C	25.54472	18.673162	-5.320333
H	26.116141	18.677118	-3.240224
C	24.960552	16.523828	-6.260355
H	25.037817	14.844014	-4.906601
C	25.135191	17.9037	-6.415183
H	25.697489	19.749574	-5.433592
H	24.639219	15.913585	-7.108414
H	24.956448	18.37629	-7.384214
C	23.027195	18.828622	2.784004
C	23.367389	20.114178	2.320633
C	21.857779	18.679469	3.553435
C	22.557417	21.214638	2.611889
H	24.285083	20.253117	1.744906
C	21.045404	19.779659	3.838902
H	21.577243	17.687393	3.915403
C	21.39189	21.051124	3.368688
H	22.841843	22.206003	2.250258
H	20.135776	19.642314	4.42899
H	20.75736	21.912039	3.593365
C	31.488626	5.692677	0.980966
C	31.183297	4.755212	-0.023768
C	32.701109	5.55441	1.683545
C	32.05602	3.701494	-0.306529
H	30.244525	4.847876	-0.57523
C	33.575922	4.503748	1.395624
H	32.96801	6.288998	2.446446
C	33.255056	3.571443	0.402773
H	31.796809	2.977298	-1.082966
H	34.516125	4.416933	1.946041
H	33.938665	2.748291	0.180515
C	29.043171	7.9054	7.689972
C	30.385808	7.641798	8.030185
C	28.04854	7.635339	8.65149
C	30.718551	7.115561	9.28071
H	31.177248	7.875537	7.314712
C	28.381939	7.10718	9.900924
H	27.001166	7.82722	8.405939
C	29.71844	6.842807	10.220839
H	31.766944	6.926144	9.525306
H	27.59264	6.896592	10.627221
H	29.97958	6.430001	11.198446



Zero-point correction= 1.050982 (Hartree/Particle)
Thermal correction to Energy= 1.118045
Thermal correction to Enthalpy= 1.118989
Thermal correction to Gibbs Free Energy= 0.943236
Sum of electronic and zero-point Energies= -5931.174837
Sum of electronic and thermal Energies= -5931.107774
Sum of electronic and thermal Enthalpies= -5931.106830
Sum of electronic and thermal Free Energies= -5931.282583
uB3LYP-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5935.80595 a.u.
uPBE0-d3/def2-tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)
E(scf) = -5931.756809 a.u.

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