Electronic Supplementary Information

Synthesis and reactivity of a μ-1,2-dinitrogen dinickel(II) complex with C-H activated silaamidinate pincer ligand

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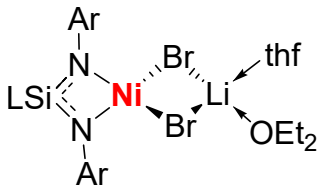
Table of Contents

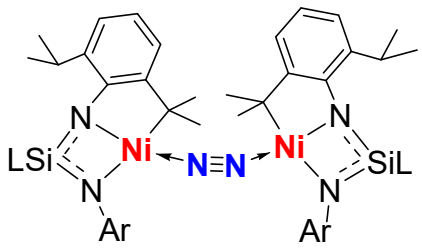
1. Experimental Section

General Information. All reactions were carried out under an atmosphere of nitrogen using standard Schlenk line and glovebox techniques. Solvents were dried over Na/K and degassed before use. ^{1}H, ^{13}C, ^{29}Si NMR spectra were obtained with Bruker 400 or 600 (^{1}H: 600 MHz) NMR spectrometer at 298 K, usually in C_6D_6 with Me_4Si (^{1}H, ^{13}C, and ^{29}Si) as internal standards. NMR multiplicities are abbreviated (s = singlet, d = doublet, t = triplet, m = multiplet). Coupling constants J are given in Hz. Melting points were measured with a capillary melting point apparatus (Melting Point M-560, BUCHI). Elemental analyses were carried out on an Elementar Vario EL analyzer. IR spectra were recorded in the range of 500−4000 cm^{-1} on a Bruker Alpha II spectrophotometer in a glovebox filled with argon gas. The generated H_2 was analyzed by injection of 1 mL aliquots from reaction vial headspace into gas chromatography (GC, FuLi 97902II) equipped with TCD detector. The $NaHBEt_3$ (1 M in THF), EtMgBr (1 M in THF), and 2,6-dimethylphenyl isocyanide were purchased from Aladdin or J&K Scientific Ltd and diluted to 0.1 M in THF before use. The gases of CO (purity ≥ 99.99%), Argon (purity ≥ 99.99%), and H_2 (purity ≥ 99.99%) were purchased from Tianjin HAOLUN. The gas of N_2 (purity ≥ 99.99%) was supplied by Liquefied Air (Tianjin). The silaamidinate ligand was prepared according to the literature procedures.[1]



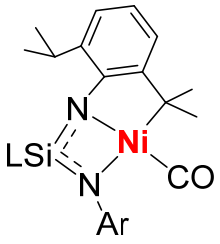
L = PhC(N*t*Bu)$_2$,
Ar = 2,6-*i*Pr$_2$C$_6$H$_3$

Synthesis of LSi(NAr)$_2$NiBr$_2$(thf)(Et$_2$O) [1, L = PhC(N*t*Bu)$_2$, Ar = 2,6-*i*Pr$_2$C$_6$H$_3$). A solution of PhC(N*t*Bu)$_2$Si(N(2,6-*i*Pr$_2$C$_6$H$_3$))$_2$Li(thf)$_2$ (2.00 g, 2.62 mmol) and $NiBr_2$·DME (0.85 g, 2.76 mmol) in degassed tetrahydrofuran was refluxed at 80 °C for 2 days. Solvent was removed under vacuum and the remaining solid was washed with *n*-hexane (30 mL). The residuals were extracted with diethyl ether (50 mL). It was filtered off and subsequent recrystallization from hexane at −40 °C gave **1** as red solid (1.18 g, 46%). Single crystals were obtained by slow evaporation of a concentrated diethyl ether solution of **1**. Mp: 118 °C(dec). Anal. Calcd for $C_{47}H_{75}Br_2LiN_4NiO_2Si$ (978.35): C, 57.51 ; H, 7.70 ; N, 5.71 ; Found: C, 57.42 ; H, 7.77 ; N, 5.84 ; Magnetic Susceptibility (MSB, 300 K): μ_{eff} = 3.08 μ_B.



L = PhC(N*t*Bu)$_2$
Ar = 2,6-*i*Pr$_2$C$_6$H$_3$

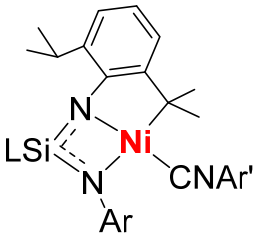
Synthesis of [LSi(NAr)(N*Ar*)Ni]$_2$(μ-1,2-N$_2$) (2, *Ar* = 2-C(CH$_3$)$_2$-6-*i*PrC$_6$H$_3$). A solution of **2** (0.20 g, 0.20 mmol) and NaHBEt$_3$ in degassed THF (5 mL) was stirred at room temperature for 2 hours under nitrogen atmosphere. Solvent was removed under vacuum and the remaining solid was washed with *n*-hexane (10 mL). Diethyl ether (30 mL) and toluene (5 mL) were transferred to the remaining residual. It was filtered off and concentrated. Crystallization from diethyl ether and toluene at −40 °C gave **2** as red solid (0.03 g, 21%). Mp: 89-91 ℃ (decomposed to black oil). ^{1}H NMR (600 MHz, C$_6$D$_6$) δ 7.25 (d, J = 7.6 Hz, 4H), 7.21 (d, J = 7.4 Hz, 6H), 7.11 (d, J = 8.9 Hz, 2H), 7.06 (t, J = 7.6 Hz, 2H), 6.96 – 6.82 (m, 8H), 4.66 (hept, J = 6.6 Hz, 4H, *Me* in *i*Pr group for the side non-C-H bond activation), 3.31 (hept, J = 6.4 Hz, 2H, *Me* in *i*Pr group for the side C-H bond activation), 1.64 (d, J = 6.7 Hz, 12H, *Me* in *i*Pr group), 1.60 (s, 12H, *Me* in NiC(C*H*$_3$)$_2$ group), 1.49 (d, J = 7.0 Hz, 12H, *Me* in *i*Pr group), 1.35 (d, J = 6.8 Hz, 12H, *Me* in *i*Pr group), 1.04 (s, 36H, *tBu*) ppm. Satisfactory ^{13}C NMR spectrum,^{29}Si NMR spectrum, and elemental analysis cannot be obtained due to the easy decompose of **2**. IR (cm^{-1}): ṽ (s, N≡N) 2101. After many attempts, we are very unfortunately failed to synthesize the ^{15}N-labeled **2**, mainly due to the poor stability of the nickel(II) dinitrogen compound and the difficulty in realizing the strictly anaerobic ^{15}N$_2$ gas under our conditions.



L = PhC(N*t*Bu)$_2$,
Ar = 2,6-*i*Pr$_2$C$_6$H$_3$

Synthesis of LSi(NAr)(N*Ar*)NiCO (3). A solution of **2** (0.06 g, 0.04 mmol) in degassed tetrahydrofuran was exposed to an atmosphere of carbon monoxide (CO) for 0.5 hour, which led to a color change to brownish red. Solvent was removed under vacuum and hexane (30 mL) was transferred to the remaining residual. It was filtered off. Evaporation of hexane and subsequent recrystallization from hexane at −10 °C gave **3** as orange solid (0.05 g, 82%). Mp: 196-198 ℃ (turns to a brown powder). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 7.24 (d, *J* = 8.0 Hz, 2H), 7.20-7.14 (m, 4H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.96 (t, *J* = 8.0 Hz, 1H), 6.91-6.82 (m, 3H), 4.57-4.54 (m, 2H, C*H*(CH$_3$)$_2$ in Ar group), 3.33-3.30 (m, 1H, C*H*(CH$_3$)$_2$ in Ni−Ar), 1.89 (s, 6H, Ni−C(C*H*$_3$)$_2$), 1.64 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 1.48 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 1.36 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 0.99 (s, 18H, C(C*H*$_3$)$_3$) ppm. ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 191.0(*C*O), 178.5 (N*C*N), 153.9 (Ar-*C*), 152.3 (Ar-*C*), 148.0 (Ar-*C*), 143.2 (Ar-*C*), 135.7 (Ar-*C*), 131.0 (*C*H), 129.6 (Ar-*C*), 129.3 (Ar-*C*), 128.4 (*C*H), 128.3 (*C*H), 127.8 (*C*H), 123.3 (*C*H), 122.7 (*C*H), 122.2 (*C*H), 120.8 (*C*H), 118.8 (*C*H), 55.7 (Ni-*C*), 54.9 (*C*(CH$_3$)$_3$), 34.4 ((CH$_3$)$_2$*C*H), 30.9 (C(*C*H$_3$)$_3$), 28.3 ((CH$_3$)$_2$*C*H), 27.6 ((CH$_3$)$_2$*C*H in Ni−Ar), 25.8 ((*C*H$_3$)$_2$CH), 24.2

((*C*H$_3$)$_2$CH), 24.1 ((*C*H$_3$)$_2$CH) ppm. ^{29}Si NMR (79 MHz, C$_6$D$_6$) δ −87.1 ppm. Anal. Calcd for C$_{40}$H$_{56}$N$_4$NiOSi (694.36): C, 69.06; H, 8.11; N, 8.05; Found: C, 69.34; H, 8.03; N, 8.32. IR (cm^{-1}): ṽ (s, C≡O) 2009.



L = PhC(N*t*Bu)$_2$
Ar = 2,6-*i*Pr$_2$C$_6$H$_3$
Ar' = 2,6-Me$_2$C$_6$H$_3$

Synthesis of LSi(NAr)(N*Ar*)NiCNAr' (4). The 2,6-dimethylphenyl isocyanide (0.80 mL, 0.1 M in THF, 0.08 mmol) was added to a solution of **2** (0.06 g, 0.04 mmol) in degassed tetrahydrofuran and stirred for 1 hours, which led to a color change to brownish red. Solvent was removed under vacuum and hexane (30 mL) was transferred to the remaining residual. It was filtered off. Evaporation of hexane and subsequent recrystallization from hexane at −10 °C gave **4** as orange solid (0.05 g, 78%). Mp: 195-198 °C (turns to a brownish red powder). ^{1}H NMR (400 MHz, C$_6$D$_6$) δ 7.35 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.20 – 7.18 (m, 3H), 7.01 (t, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.84 (m, 1H), 6.71 (t, *J* = 8.0 Hz, 1H), 6.59 (d, *J* = 8.0 Hz, 2H), 4.75 – 4.68 (m, 2H, C*H*(CH$_3$)$_2$ in Ar group), 3.53 – 3.46 (m, 1H, C*H*(CH$_3$)$_2$ in Ni−Ar), 2.00 (s, 6H, C*H*$_3$ in Ar' group), 1.95 (s, 6H, NiC(C*H*$_3$)$_2$ in Ni−Ar), 1.65 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 1.52 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 1.45 (d, *J* = 8.0 Hz, 6H, CH(C*H*$_3$)$_2$ in Ar group), 1.11 (s, 18H, C(C*H*$_3$)$_3$). ^{13}C NMR (101 MHz, C$_6$D$_6$) δ 177.5 (N*C*N), 162.6 (Ni−*C*NAr'), 155.7 (Ar-*C*), 153.1 (Ar-*C*), 149.8 (Ar-*C*), 143.3 (Ar-*C*), 135.6 (Ar-*C*), 135.1 (Ar-*C*), 130.7 (Ar-*C*), 130.3 (*C*H), 129.1 (Ar-*C*), 128.2 (*C*H), 128.0 (*C*H), 127.9 (*C*H), 127.9 (*C*H), 127.3 (*C*H), 123.1 (*C*H), 122.1 (*C*H), 122.0 (*C*H), 119.6 (*C*H), 117.9 (*C*H), 54.7 (*C*(CH$_3$)$_3$), 46.3 (Ni-*C*), 34.8 ((CH$_3$)$_2$*C*H), 31.1 (C(*C*H$_3$)$_3$), 28.3 ((CH$_3$)$_2$*C*H), 27.6 ((CH$_3$)$_2$*C*H in Ni−Ar), 25.8 ((*C*H$_3$)$_2$CH), 24.4 ((*C*H$_3$)$_2$CH), 24.3 ((*C*H$_3$)$_2$CH), 18.9 (*C*H$_3$ in Ar'). Anal. Calcd for C$_{46}$H$_{65}$N$_5$NiSi (797.44): C, 72.17; H, 8.20; N, 8.77; Found: C, 72.29; H, 8.61; N, 8.52. IR (cm^{-1}): ṽ (s, C≡N) 2101.

2. Crystallographic Data

All intensity data were collected with a Rigaku Saturn 724 CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 113 K. The structures were resolved by direct methods and refined by full-matrix least-squares on F^2.[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were considered in calculated positions. Crystallographic data and CCDC numbers were listed in Table S1.

Table S1. Crystallographic Data for Compounds **1 - 4**

	1	**2**	**3**	**4**
formula	$C_{47}H_{75}Br_2LiN_4NiO_2Si$	$C_{78}H_{112}N_{10}Ni_2Si_2$	$C_{40}H_{57}LiN_4NiOSi$	$C_{48}H_{65}N_5NiSi$
fw	981.67	1360.73	703.63	798.85
T(K)	113.15	113.15	293(2)	113.15
space group	$P2_1/n$	P-1	P-1	P21/c
a (Å)	17.4789(11)	15.2773(9)	11.4166(3)	24.045(2)
b (Å)	16.6281(8)	16.5998(8)	12.1080(5)	12.0991(16)
c (Å)	21.2921(10)	18.2805(10)	16.0882(6)	15.7064(15)
α (deg.)	90	103.515(5)	73.179(3)	90
β (deg.)	104.114(6)	111.529(5)	73.148(3)	100.380(9)
γ (deg.)	90	96.493(4)	67.295(3)	90
V (Å3)	6001.5(6)	4090.5(4)	1923.38(13)	4494.6(9)
Z	4	2	2	4
ρ_{calc} g/cm3	1.086	1.161	1.215	1.181
F(000)	2064.0	1536.0	756.0	1720.0
GOF	1.000	1.005	1.015	1.047
R1	0.0639	0.0682	0.0701	0.0810
wR2 (all data)	0.1528	0.1615	0.2131	0.1669
CCDC	2108050	2108053	2108055	2108056

3. Computational Details

All stationary points were fully optimized at the density functional theory level with the Gaussian 09 E01 suit of program,[3] using the pbe1pbe functional without symmetry constraints.[4] The basis set of def2-TZVP was used for Ni, Si, and Br, and the def2-SVP basis set was used for H, C, O, N, and Li.[5] All optimized species were verified as minima by the presence of zero imaginary vibrational frequency. Natural bond orbital (NBO) and natural localized molecular orbital (NLMO) calculations were carried out using NBO 6.0 program.[6] Optimized structures were visualized by the Chemcraft program.[7]

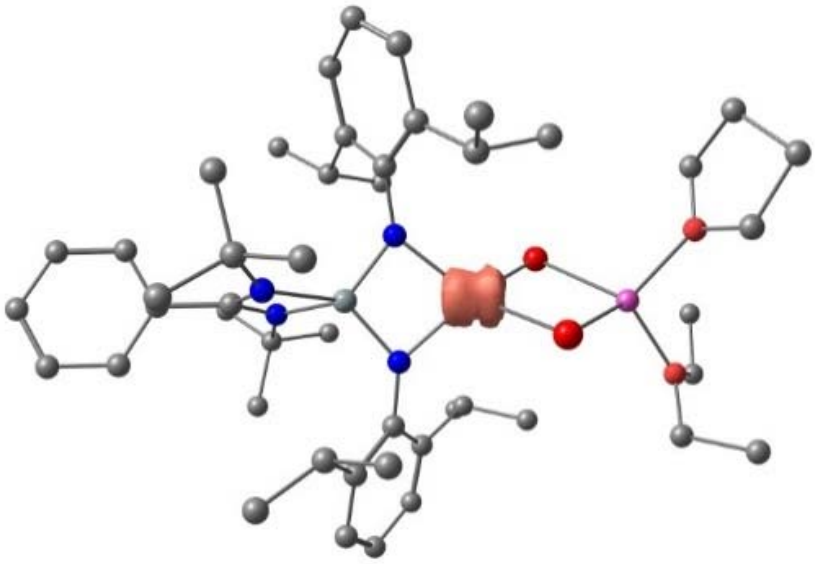


Figure S1. Calculated spin density map of **1** (isovalue=0.05)

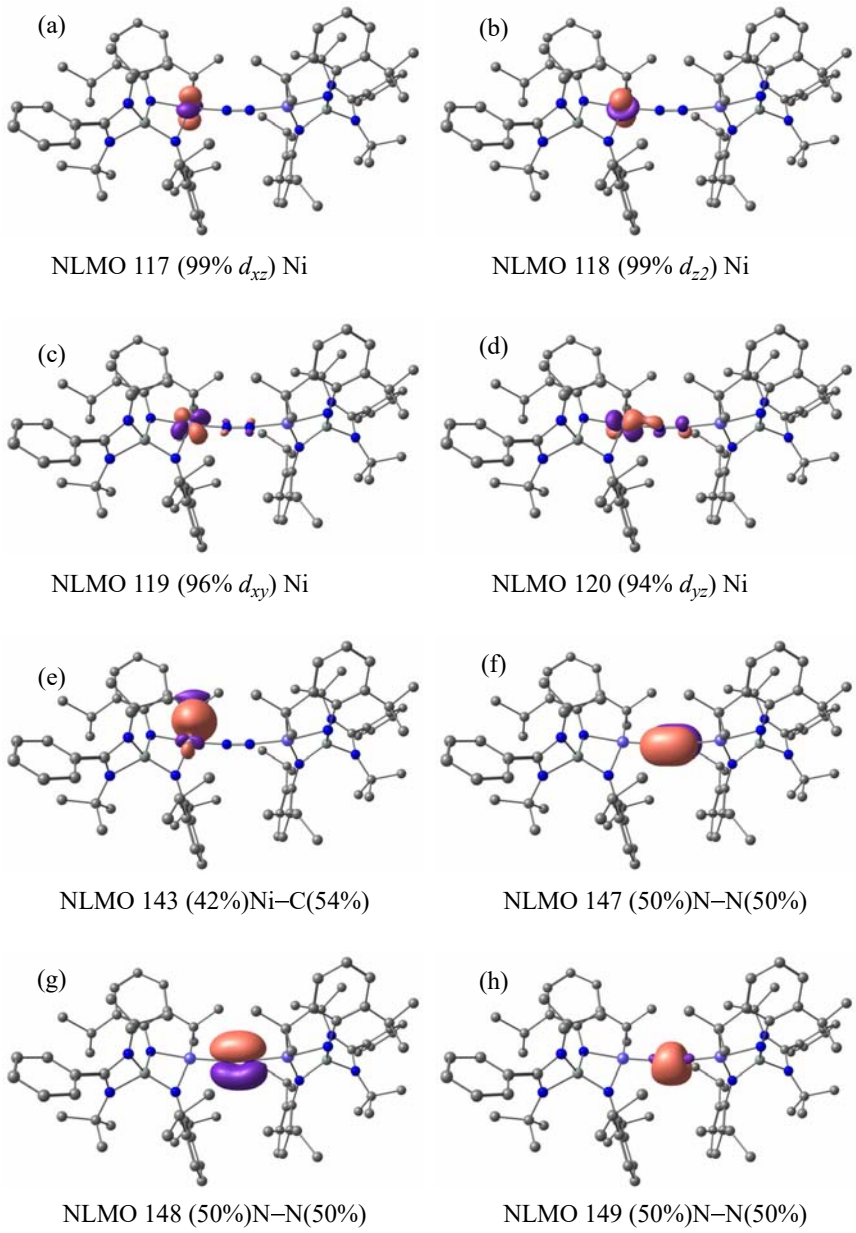


Figure S2. Selected NLMOs of **2** (isovalue=0.05). (a-d) Four d-type nonbonding electron pairs at Ni1. (e) Ni1−C1 σ-bond. (f) N1−N2 π-bond. (g) N1−N2 π-bond. (h) N1−N2 σ-bond.

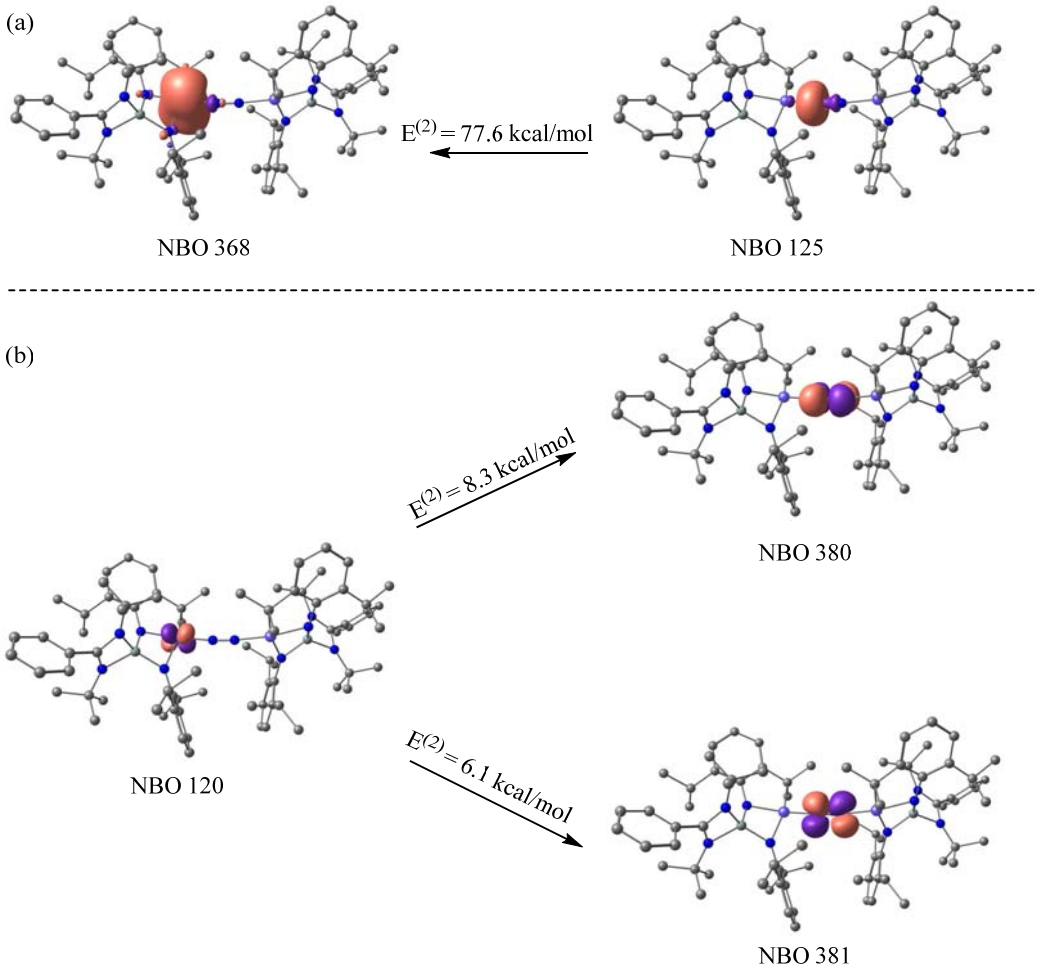


Figure S3. Selected NBOs of **2** for the second-order perturbation theory analysis. (a) LP (N1) to LV (Ni1). (b) d-type nonbonding electron (Ni) to π*-bond (N1–N2). (isovalue=0.05)

Table S2. Wiberg Bond Index Matrix in the NAO Basis

Atom	Ni1	Ni2	Si3	Si4	N5	N6
Ni1	0.0000	0.0159	0.0492	0.0003	**0.4209**	0.1624
Ni2	0.0159	0.0000	0.0003	0.0492	0.1624	**0.4209**
Si3	0.0492	0.0003	0.0000	0.0000	0.0034	0.0021
Si4	0.0003	0.0492	0.0000	0.0000	0.0021	0.0034
N5	**0.4209**	0.1624	0.0034	0.0021	0.0000	**2.5903**
N6	0.1624	**0.4209**	0.0021	0.0034	**2.5903**	0.0000

4. NMR Spectra

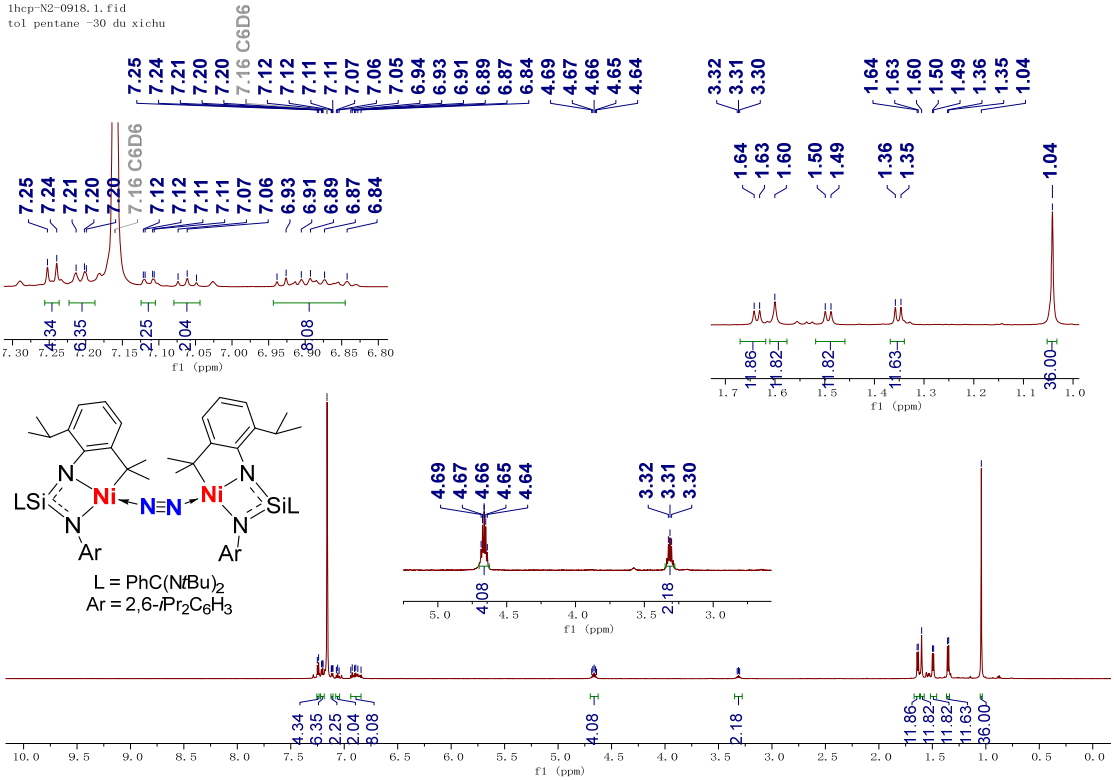


Figure S4. ^{1}H NMR spectrum of **2** in C_6D_6

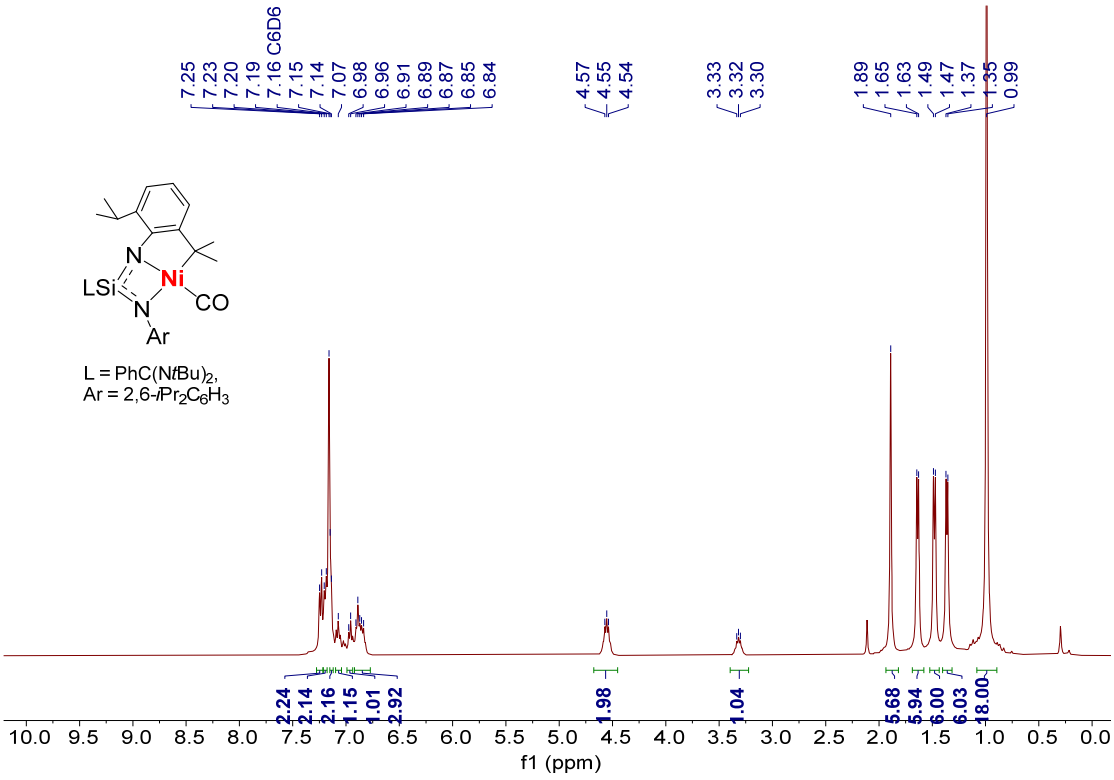


Figure S5. ^{1}H NMR spectrum of **3** in C_6D_6.

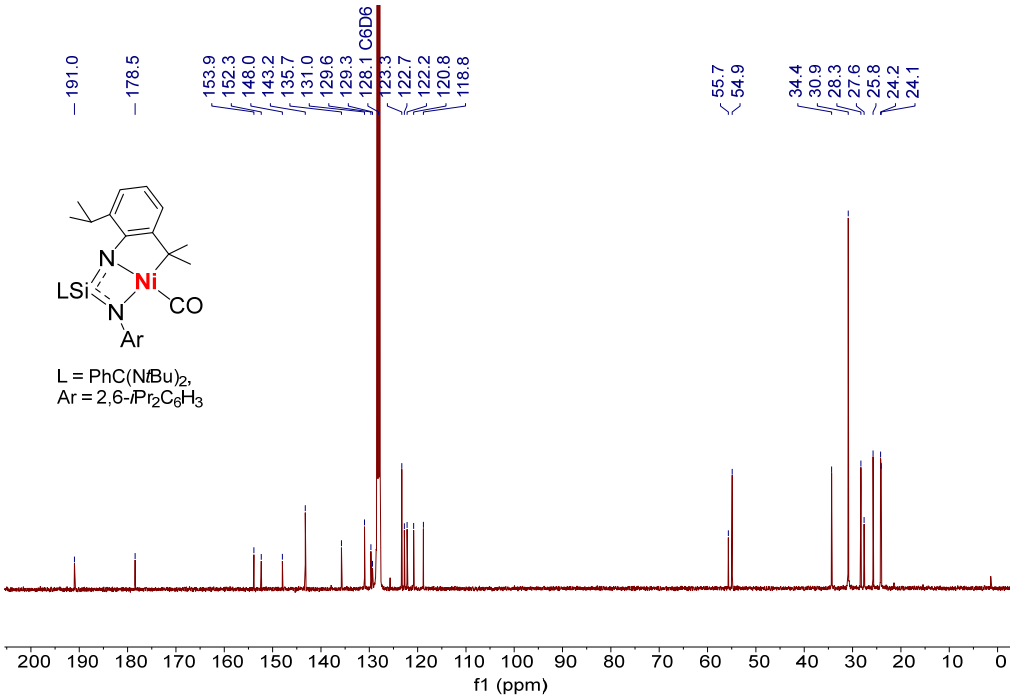


Figure S6. ^{13}C NMR spectrum of **3** in C_6D_6.

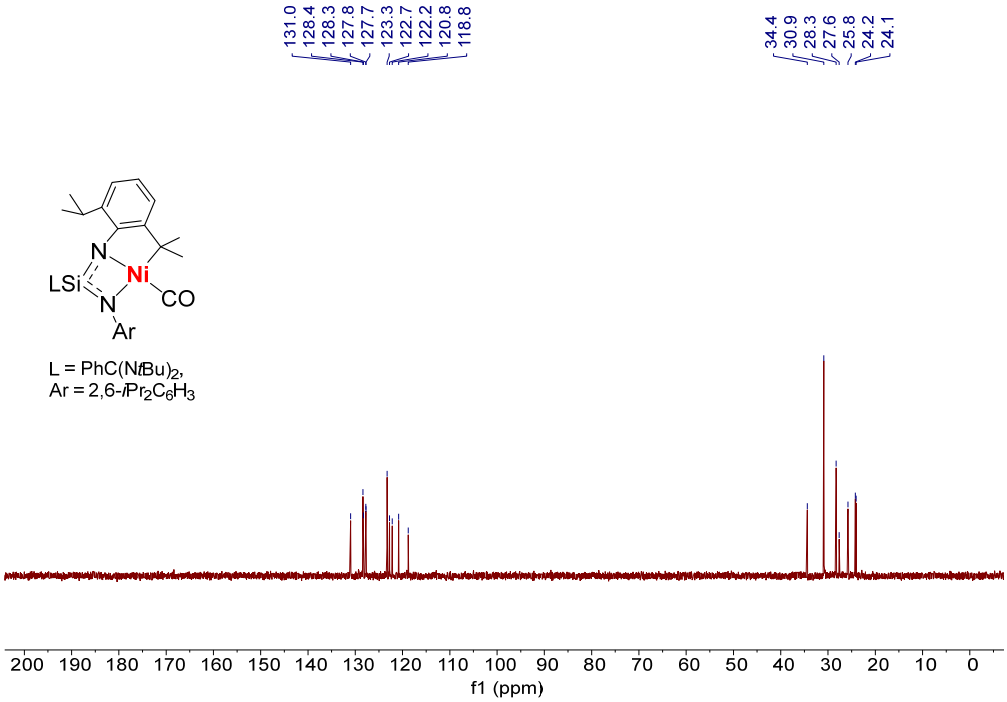


Figure S7. DEPT135 NMR spectrum of **3** in C_6D_6.

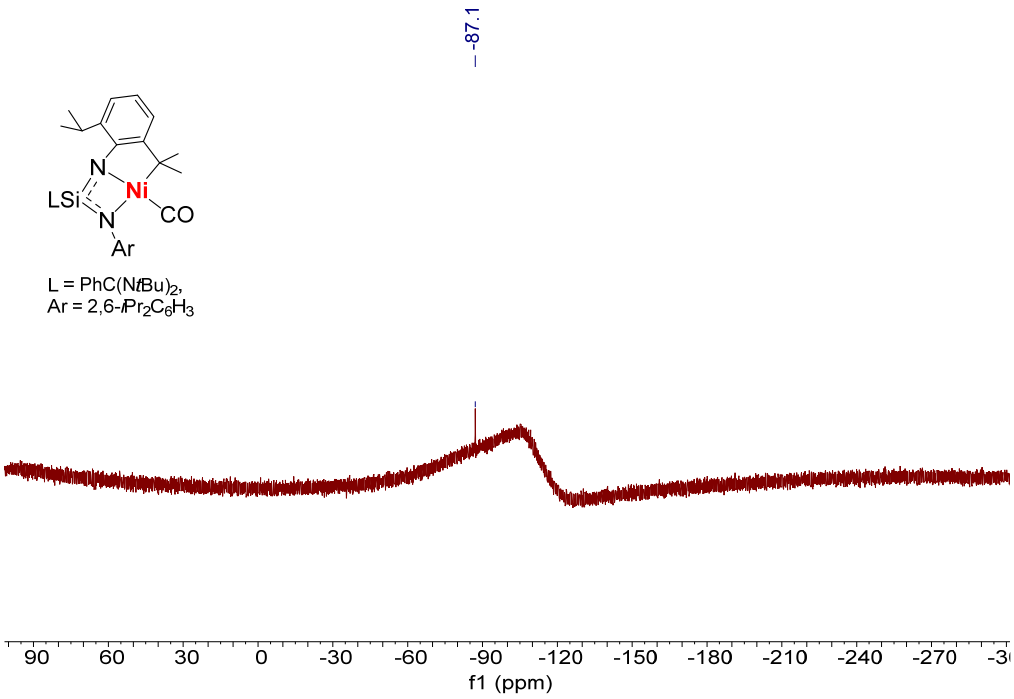


Figure S8. ^{29}Si NMR spectrum of **3** in C_6D_6.

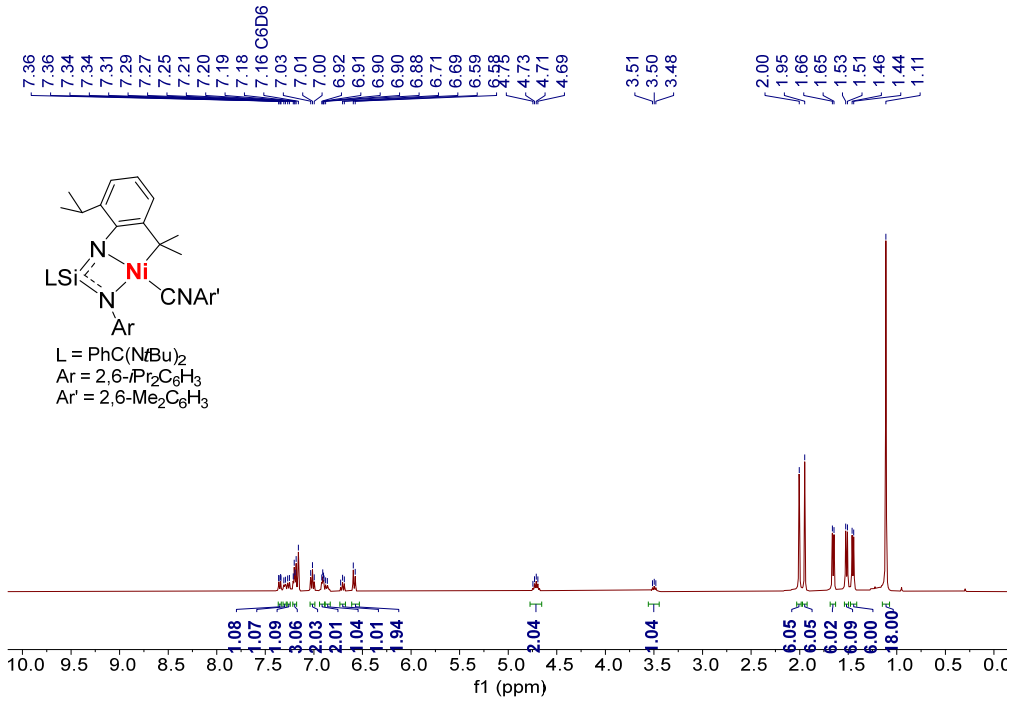


Figure S9. ^{1}H NMR spectrum of **4** in C_6D_6.

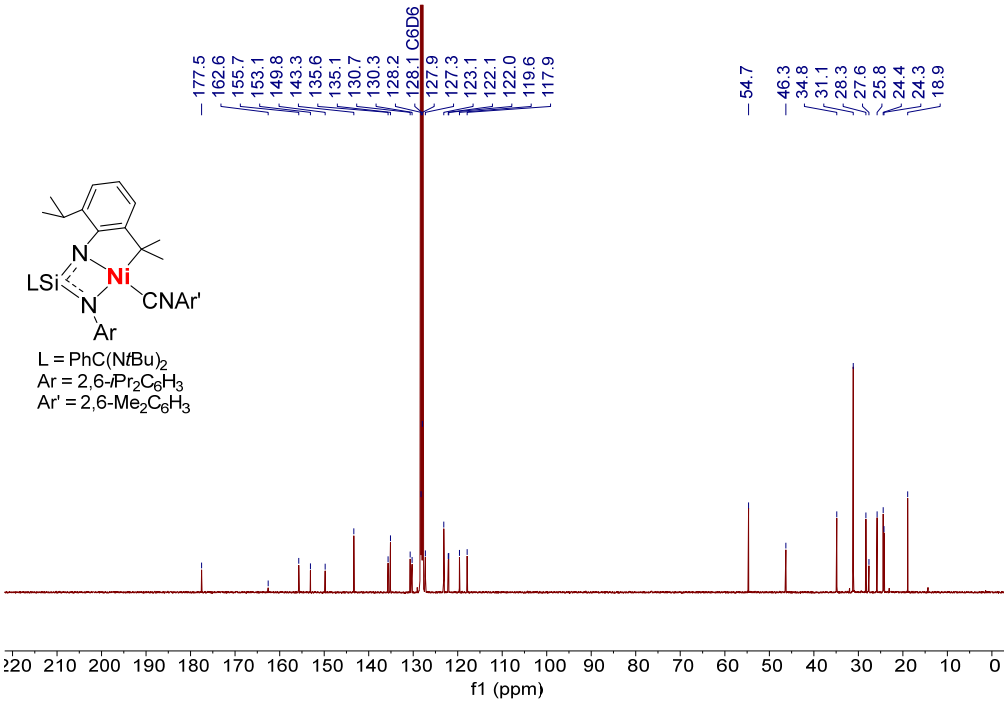


Figure S10. ^{13}C NMR spectrum of **4** in C_6D_6.

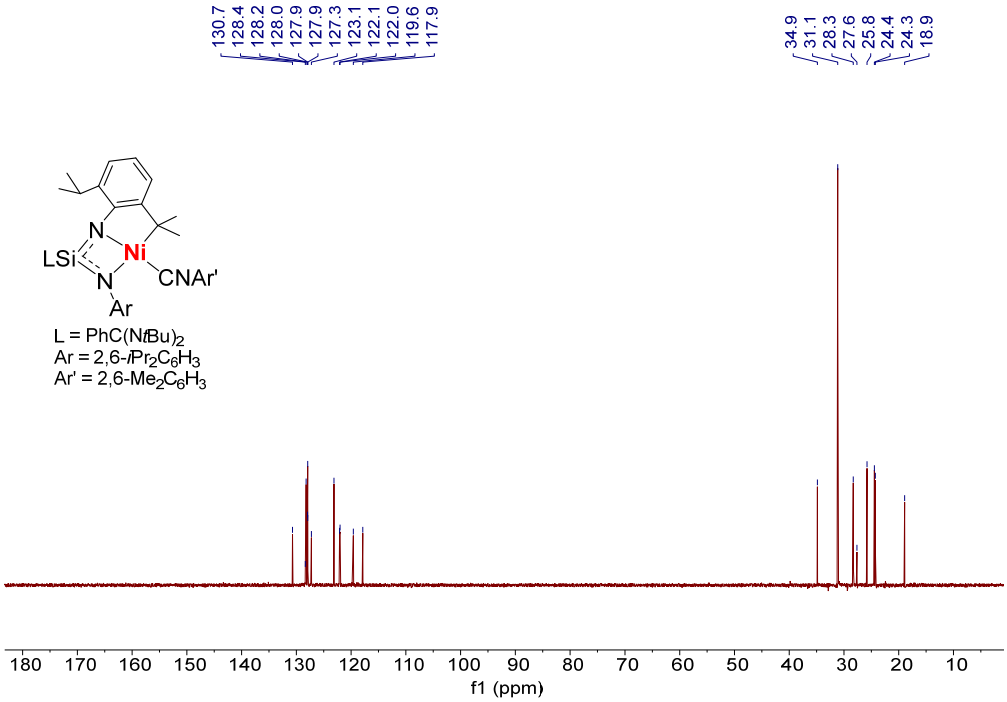


Figure S11. DEPT135 NMR spectrum of **4** in C_6D_6.

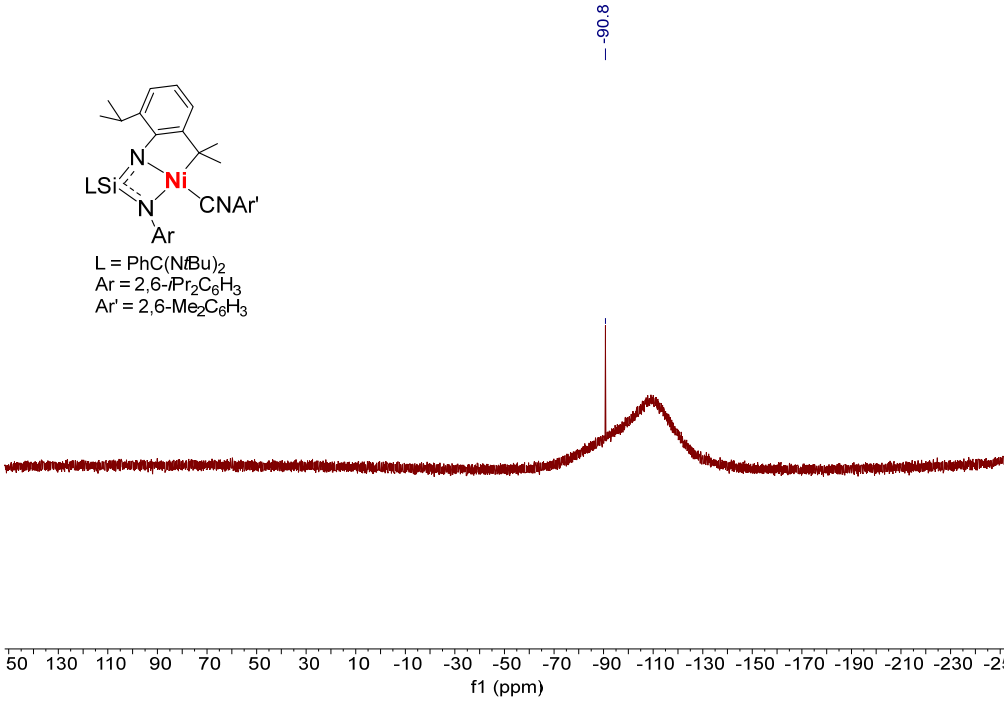


Figure S12. ^{29}Si NMR spectrum of **4** in C_6D_6.

5. IR Spectra

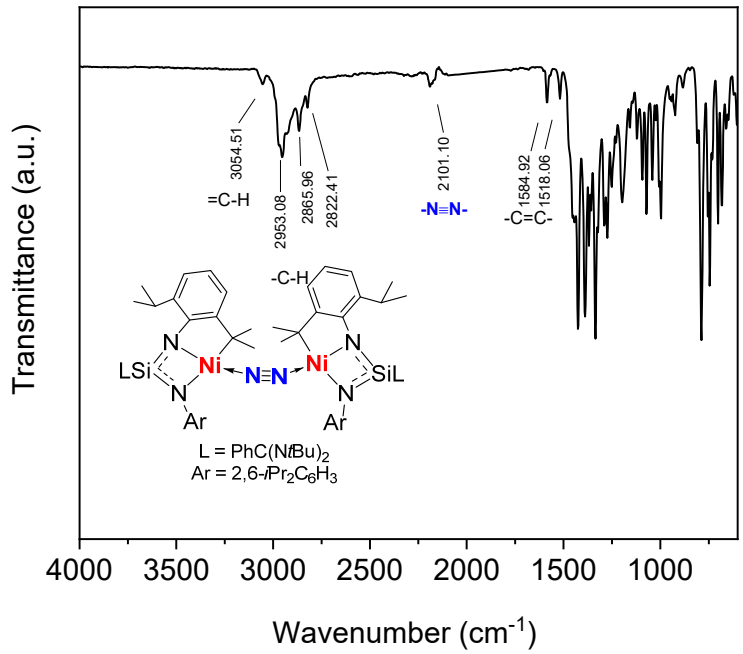


Figure S13. IR spectrum of **2**

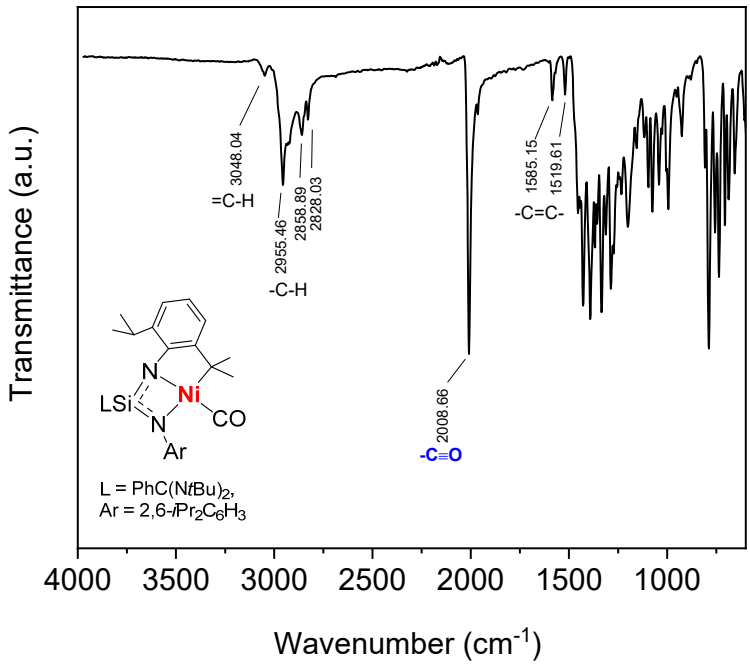


Figure S14. IR spectrum of reaction of **3**.

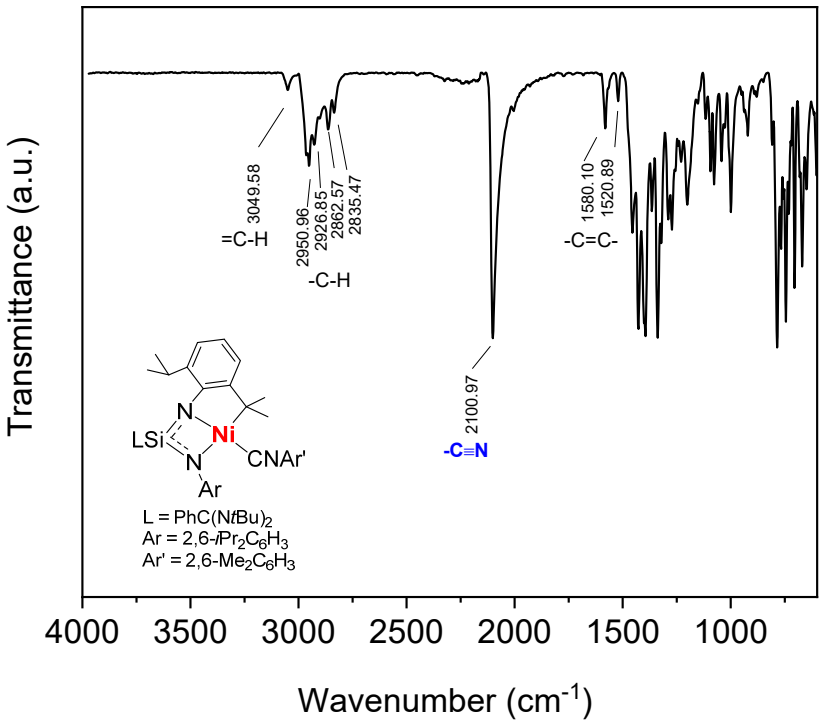


Figure S15. IR spectrum of reaction of **4**.

6. Mechanistic Studies

6.1 Detection of the Nickel Hydride Species by NMR Spectroscopy

1a) Reaction of **1** with $NaHBEt_3$ under Ar.

In an argon-filled glove box, a *d*8-THF (0.6 mL), **1** (10 mg, 0.010 mmol) and $NaHBEt_3$ (10 µL, 0.010 mmol) were loaded in a dried J-Young-Tube at room temperature, the tube was sealed and the reaction was monitored by NMR spectroscopy. The ^1H NMR spectrum was detected after 20 minutes.

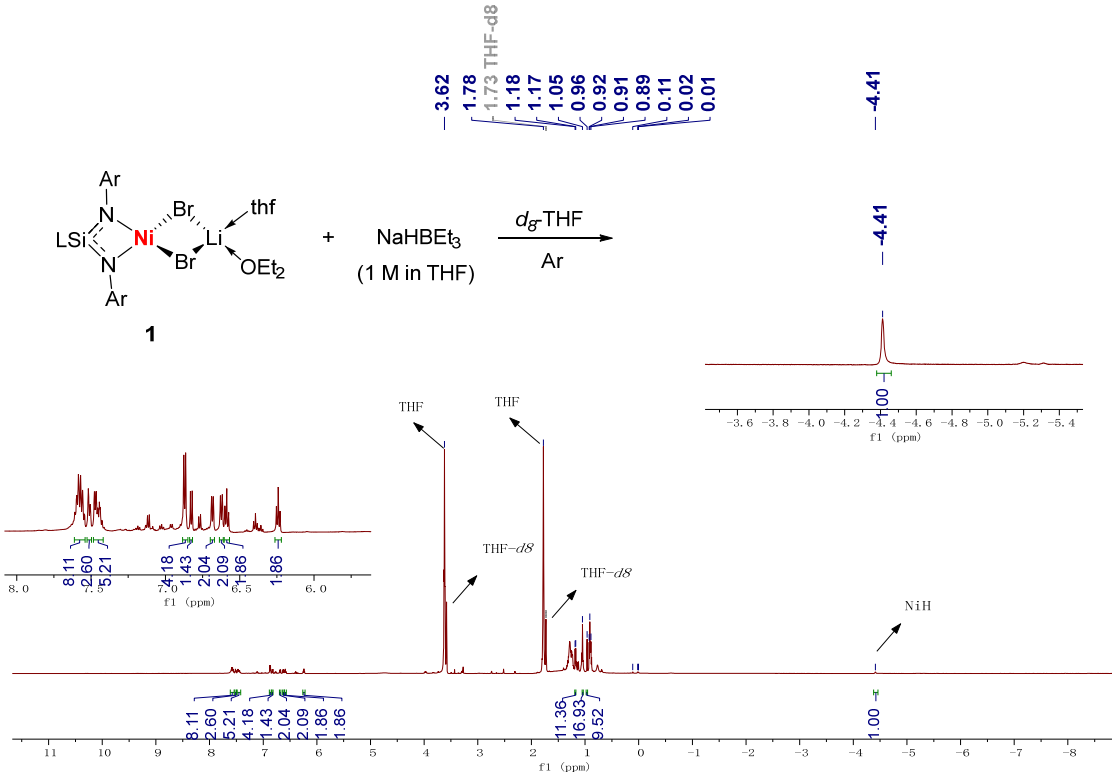


Figure S16. ^1H NMR spectrum of the reaction of **1** with $NaHBEt_3$ in D_8-THF

1b) Reaction of **1** with $NaHBEt_3$ under Ar.

In an argon-filled glove box, the C_6D_6 (0.4 mL), **1** (20 mg, 0.02 mmol), $NaHBEt_3$ (20 µL, 0.02 mmol, 1 M in THF) were loaded in a dried J-Young-Tube at room temperature, the tube was sealed immediately and the reaction was monitored by NMR spectroscopy. The ^1H NMR spectrum was detected after 20 minutes.

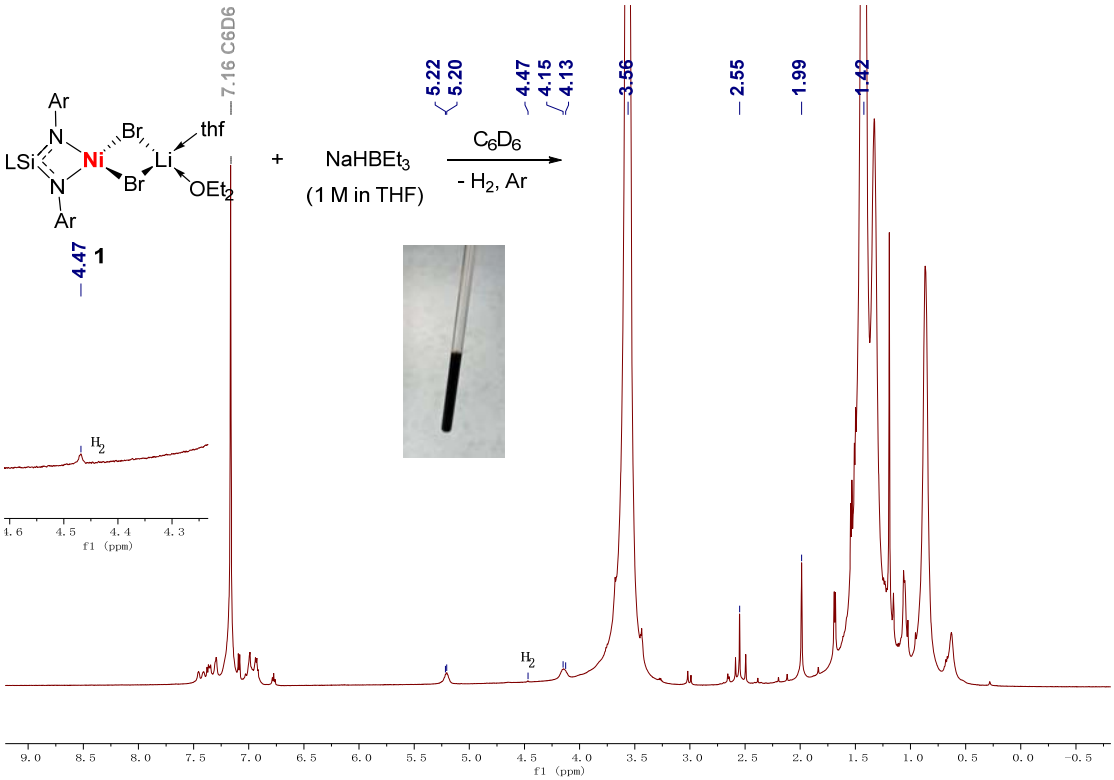


Figure S17. ^{1}H NMR spectrum of the reaction of **1** with $NaHBEt_3$ (600MHz, C_6D_6). * marks solvent residue of THF in $NaHBEt_3$.

6.2 Detection of the H_2 Gas by GC Spectroscopy.

2a) The GC spectrum for H_2 gas.

The purchased H_2 was analyzed by injection of 0.1 mL aliquots into GC.

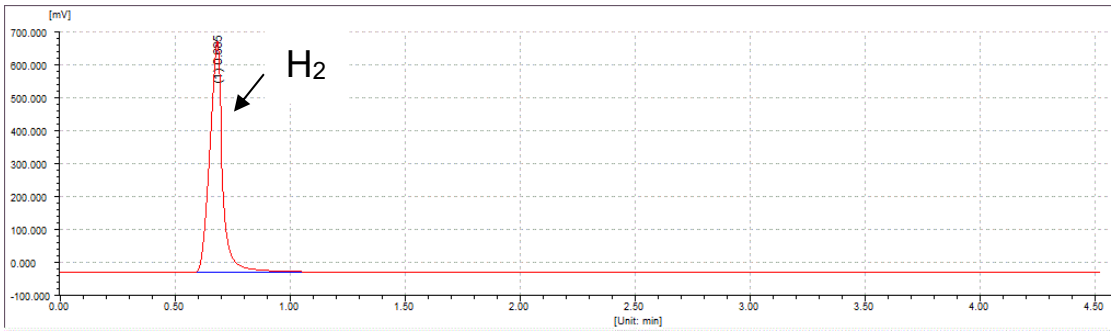


Figure S18. GC spectrum for H_2 gas (Retention time: 0.685 min).

2b) Reaction of **1** with $NaHBEt_3$ under Ar.

In an argon-filled glove box, the THF (1.0 mL), **1** (50 mg, 0.05 mmol), $NaHBEt_3$ (0.5 mL, 0.05 mmol) were loaded in a dried schlenk tube at room temperature, the tube was sealed. After 2 hours, the reaction was analyzed by injection of 1 mL gaseous aliquots into GC.

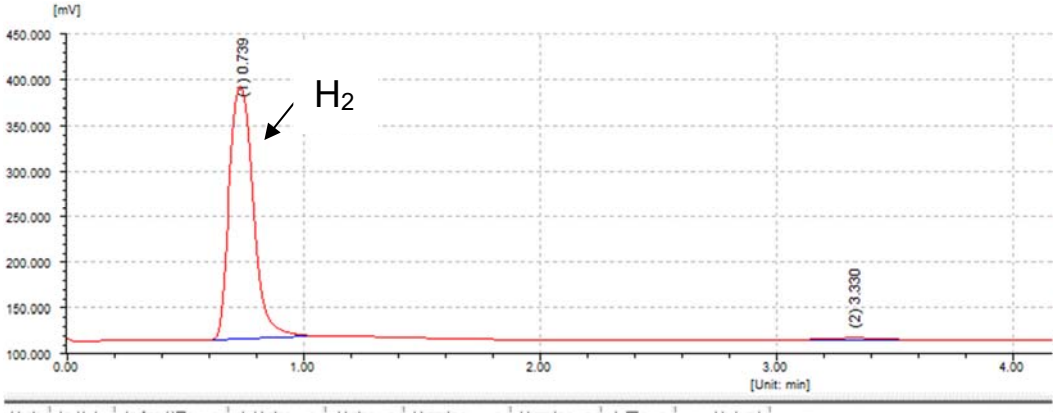


Figure S19. GC spectrum for this reaction.

2c) Reaction of **1** with $NaHBEt_3$ under N_2.

In a nitrogen-filled glove box, the THF (1.0 mL), **1** (50 mg, 0.05 mmol), $NaHBEt_3$ (0.5 mL, 0.05 mmol) were loaded in a dried schlenk tube at room temperature, the tube was sealed. After 2 hours, the reaction was analyzed by injection of 1 mL gaseous aliquots into GC.

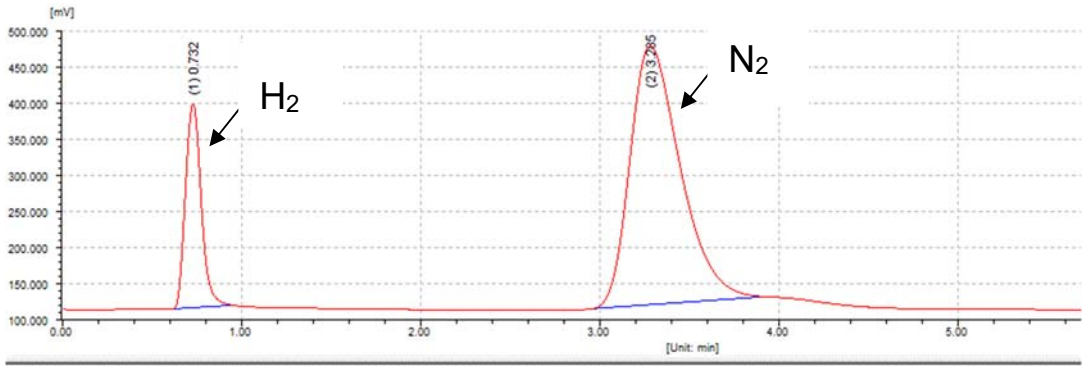


Figure S20. GC spectrum for this reaction.

2d) Reaction of **1**, $NaHBEt_3$ with isocyanide under Ar.

In an argon-filled glove box, the THF (1.0 mL), **1** (50 mg, 0.05 mmol), $NaHBEt_3$ (0.5 mL, 0.05 mmol) and 2,6-$Me_2C_6H_3NC$ (0.5 mL, 0.05 mmol) were loaded in a dried schlenk tube at room temperature. The tube was sealed. After 2 hours, the reaction was analyzed by injection of 1 mL gaseous aliquots into GC.

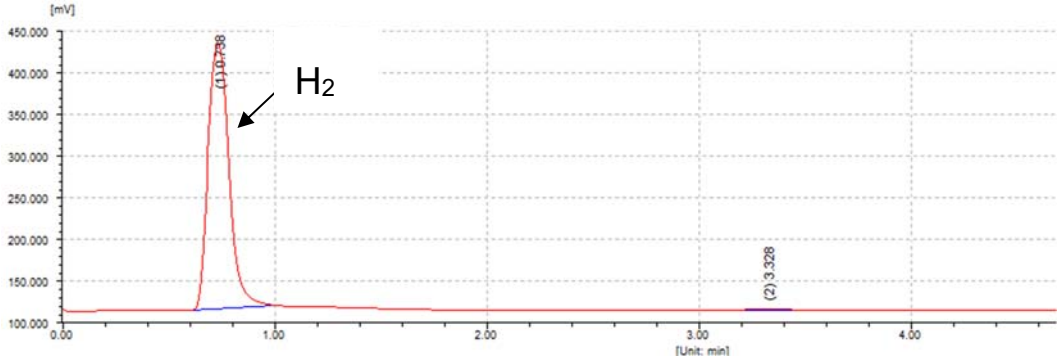


Figure S21. GC spectrum for this reaction.

Reference

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Coordinates of the Studied Molecules

1

Atom	x	y	z
Br	-2.560994	0.37476	1.91174
Br	-2.614225	-0.412904	-1.749823
Ni	-0.996124	-0.021107	0.062199
Si	1.597575	-0.000456	0.003434
O	-5.421743	1.236365	-0.118903
O	-5.294421	-1.860702	0.228836
N	0.550261	1.243572	0.313686
N	0.559283	-1.26685	-0.237763
N	3.046014	0.490154	-1.017356
N	3.127774	-0.447965	0.916245
C	0.691153	2.622234	0.398215
C	0.727922	-2.643904	-0.299879
C	3.874042	0.038441	-0.076007
C	0.047309	3.488986	-0.529692
C	0.309098	4.86109	-0.48906
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2

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H	3.25984200	-2.65165200	0.23364100
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H	10.68334800	-1.83697400	0.98754400
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H	-0.31171900	-0.20468700	3.41794800
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H	3.84849400	-5.53601700	-3.94726900
C	7.81547900	0.21107800	2.62193100
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C	5.06220000	-3.84272700	-3.38560800
H	5.98832800	-4.33264200	-3.69471700
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C	2.85595300	2.24587900	0.43488400
C	10.06066100	-0.67702200	2.70112600

H	11.01132700	-0.79634800	3.22570700
C	2.35575900	3.25770900	-0.43099900
C	2.59848000	4.02247700	-2.84174700
H	2.06884800	4.98215800	-2.73169300
H	2.46468600	3.69849200	-3.88589900
H	3.66948300	4.21250600	-2.67867700
C	2.14091400	4.54301900	0.07263700
H	1.74503900	5.31351900	-0.59378600
C	7.67045600	-2.58117900	-2.79177200
H	7.67425200	-3.34092600	-1.99500100
H	8.55257000	-1.93422400	-2.65813300
H	7.80352600	-3.10342000	-3.75210700
C	5.90221800	2.57117900	-1.74963800
H	5.91110200	1.88610600	-2.60934700
H	6.32176500	3.53642800	-2.06628000
H	4.85907300	2.73755800	-1.44466100
C	2.43039700	4.86765000	1.39282300
H	2.26337000	5.88166800	1.76352000
C	2.93321800	3.88263700	2.23873000
H	3.15808000	4.13559200	3.27707700
C	3.14407900	2.57908000	1.78881700
C	-2.05185300	2.96200600	1.88677900
H	-2.55060100	2.00839700	2.12538800
C	8.66798300	-1.10899000	0.77594000
H	8.52239200	-1.55557300	-0.20971400
C	8.15468900	1.76325300	-1.02482900
H	8.79121000	1.43497100	-0.19212000
H	8.57522100	2.70024000	-1.41874500
H	8.19938200	1.00568600	-1.82150100
C	-3.62574800	1.49460800	-2.73158800
H	-4.27780500	0.82733300	-2.14739700
C	-7.67050800	-2.58078200	2.79195600
H	-7.67435800	-3.34060800	1.99526000
H	-8.55259100	-1.93379500	2.65826400
H	-7.80358700	-3.10292100	3.75234600
C	-0.55322800	2.77676800	2.11816300
H	-0.12897400	2.00078800	1.46914500
H	-0.35200300	2.49019900	3.16238600
H	0.00151900	3.70332600	1.90818400
C	-2.59862100	4.02253900	2.84152500
H	-2.06899900	4.98222800	2.73149200
H	-2.46491300	3.69858000	3.88569600
H	-3.66961400	4.21254300	2.67836000
C	-4.43958400	2.00247400	-3.91534100
H	-5.27442200	2.64325100	-3.59049800
H	-4.85349600	1.15490500	-4.48537900

H	-3.82651300	2.58704600	-4.61926200
C	-2.44260900	0.64787100	-3.20131000
H	-1.74810800	1.25478300	-3.80226500
H	-2.76998000	-0.20431300	-3.81895500
H	-1.88666600	0.25429600	-2.33932100
C	-2.66769700	-2.61286900	2.64883300
C	-2.65714700	-3.89858100	3.18727100
H	-1.70981300	-4.41946300	3.34400900
C	-3.85584700	-4.52321600	3.53721600
H	-3.84869200	-5.53578400	3.94751400
C	-5.06231500	-3.84245300	3.38579700
H	-5.98846600	-4.33231200	3.69492700
C	-5.11480700	-2.55384500	2.84249300
C	-3.90152500	-1.97121900	2.41426100
C	-2.85590500	2.24582500	-0.43502600
C	-2.35572600	3.25769200	0.43081800
C	-2.14087700	4.54298100	-0.07287300
H	-1.74499400	5.31350700	0.59351400
C	-2.43037800	4.86755900	-1.39306700
H	-2.26336500	5.88156500	-1.76380500
C	-2.93324200	3.88252200	-2.23892300
H	-3.15816200	4.13544900	-3.27726400
C	-3.14408300	2.57897900	-1.78896100