SUPPORTING INFORMATION

Single Electron Oxidation of *N*-Heterocyclic Carbene-Supported Nickel Amides Yielding Benzylic C-H Activation

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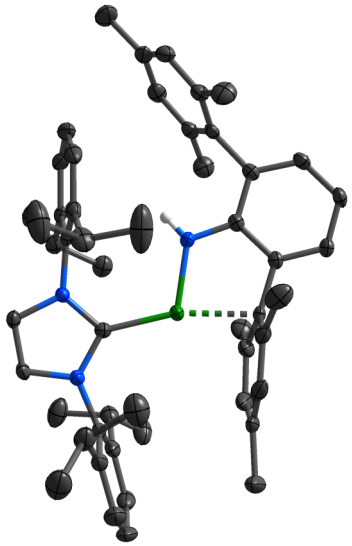
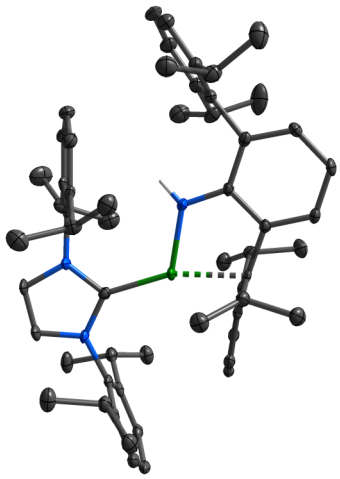
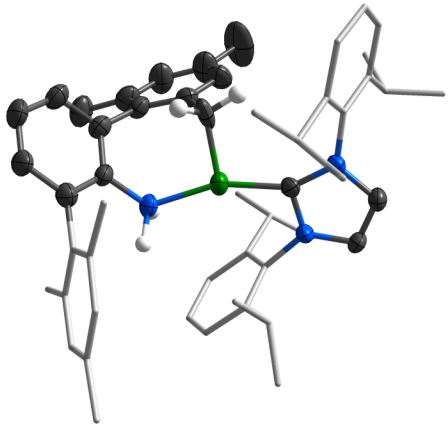
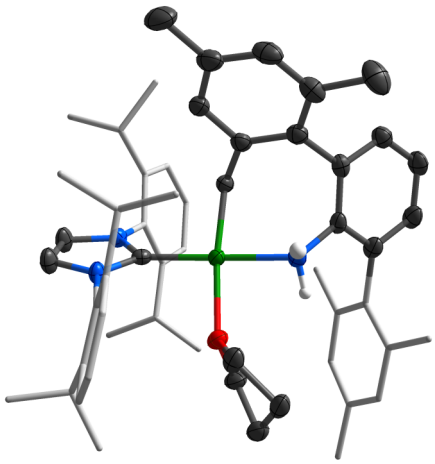
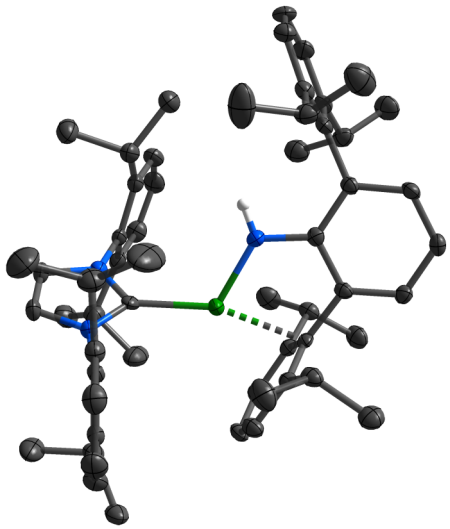










(I) Experimental Procedures

General Considerations

Unless stated otherwise, all operations were performed in a MBraun *Lab Master* dry box under an atmosphere of purified nitrogen. Anhydrous diethyl ether was purchased from Fischer, stirred over sodium metal, and filtered through activated alumina. Pentane was purchased from Sigma Aldrich and dried by passage through activated alumina and Q-5 columns. CD_2Cl_2 and C_6D_6 were purchased from Cambridge Isotope Laboratories, degassed by freeze-pump-thaw cycles, and dried over CaH_2 or activated 4 Å molecular sieves. Celite, alumina, and 4 Å molecular sieves were activated by evacuation overnight at 180°C. {(IPr)Ni(μ-Cl)}$_2$,[1] LiNHdmp,[2] LiNHdippp,[3] [Cp_2Fe][B(Ar^F)$_4$],[4] and KC_8[5] were prepared according to the literature (IPr = 1,3-di(2',6'-diisopropylphenyl)imidazolin-2-ylidene). All other chemicals were used as received. Elemental analyses were performed by Midwest Microlab (Indianapolis, IN). ^{1}H NMR spectra were recorded on a Bruker 500 MHz or 400 MHz NMR spectrometer and reported with reference to solvent resonance (for example, residual C_6D_5H in C_6D_6, 7.16 ppm). Solution magnetic susceptibilities were determined by ^{1}H NMR using the method of Evans.[6] X-ray diffraction data were collected on a Siemens Platform goniometer with a Charged Coupled

Device (CCD) detector. Structures were solved by direct or Patterson methods using the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-ray Systems, Madison, WI).

(IPr)Ni(NHdmp) (**4**)

At -35°C, LiNHdmp (315 mg in 10 mL Et_2O, 0.939 mmol) was added to **3** (450 mg in 4 mL Et_2O, 0.466 mmol), causing an immediate color change from yellow to dark red with concurrent formation of fine white precipitate. The reaction was allowed to warm to room temperature before being stirred an additional 30 minutes. Solvent was then removed under reduced pressure and the resulting red solids extracted with 40 mL Et_2O/pentane (1:1). Removal of solvent afforded a rust-red solid that was then washed with 10 mL cold pentane. 680 mg of **4** (84% yield) was isolated on a porous glass frit. Red blocks of **4** suitable for X-ray were grown from a concentrated Et_2O solution at -35°C. Unlike (IPr)Ni(NHdippp), **4** is not stable in CH_2Cl_2.

For **4**: ^{1}H NMR (22°C, 500 MHz, C_6D_6): δ 21.9 (br, $\Delta_{1/2}$ = 364 Hz), 9.31 (br, $\Delta_{1/2}$ = 728 Hz), 4.77 (br, $\Delta_{1/2}$ = 59 Hz), 4.68 (br, $\Delta_{1/2}$ = 65 Hz), 3.62 (br, $\Delta_{1/2}$ = 57 Hz), 1.91 (br, $\Delta_{1/2}$ = 50 Hz), 0.501 (br, $\Delta_{1/2}$ = 242 Hz). μ_{eff} = 1.8 μ_B (C_6D_6, 20°C, Evans' method). Elemental analysis for $C_{51}H_{62}N_3Ni$: %C = 79.0, %H = 8.06, %N = 5.42%; found: %C = 78.8, %H = 7.85, %N = 5.53.

(IPr)Ni(NHdippp) (**5**).

(*Method A*) Prepared in a similar manner to that described above for **4** with 338 mg (0.806 mmol) LiNHdippp and 385 mg (0.399 mmol) **3**. Isolated 550 mg (79% yield) **5** as a rust-red solid. Single crystals were obtained as red blocks by cooling a concentrated CH_2Cl_2 solution of **5** at -35°C overnight.

(*Method B*) A sample of **9** (100 mg in 5 mL Et_2O, 0.058 mmol) was combined with KC_8 (9 mg suspension in 8 mL Et_2O, 0.067 mmol) at room temperature. The solution was stirred for 2 hours before being filtered through Celite. Removal of solvent under vacuum followed by trituration with 5 mL cold pentane afforded 36 mg **5** (72% yield).

For **5**: ^{1}H NMR (22°C, 500 MHz, C_6D_6): δ 10.2 (br, $\Delta_{1/2}$ = 480 Hz), 3.45 (br, $\Delta_{1/2}$ = 35 Hz), 3.27 (br, $\Delta_{1/2}$ = 30 Hz), 2.39 (br, $\Delta_{1/2}$ = 40 Hz), 0.82 (br, $\Delta_{1/2}$ = 135 Hz). Elemental analysis for $C_{57}H_{74}N_3Ni$: %C = 79.6, %H = 8.67, %N = 4.89; found: %C = 79.3, %H = 8.30, %N = 4.92.

[(IPr)Ni(κ^2-*C*,*N*:NH$_2$C$_6$H$_3$(Mes)C$_{10}$H$_9$)][B(Ar^F)$_4$] (7)

At -35°C, [Cp$_2$Fe][B(Ar^F)$_4$] (270 mg in 10 mL Et$_2$O, 0.258 mmol) was added to **4** (200 mg in 5 mL Et$_2$O, 0.258 mmol). The reaction was allowed to warm to room temperature and stirred for 1.5 hours. Solvent was then removed under reduced pressure and the resulting blue solid washed 2 x 10 mL pentane to remove Cp$_2$Fe. Recrystallization from 5 mL Et$_2$O layered with 15 mL pentane at -35°C afforded **7** in 88% yield (374 mg) as a dark blue crystalline solid. X-ray quality crystals (large dark blue blocks) were collected at -35°C from a concentrated Et$_2$O solution of **7** layered with pentane.

For **7**: ^{1}H-NMR (22°C, 500 MHz, CD$_2$Cl$_2$): δ 7.79 (s, 8H, *m*-Ar^F), 7.61 (s, 4H, *p*-Ar^F), 7.42 (t, 2H, J = 7.8 Hz, *p*-Ar^{IPr}), 7.33 (s, 1H, *m*-Ar^{dmp}), 7.26 (d, 2H, J = 7.80 Hz, *m*-Ar^{IPr}), 7.23 (t, 1H, J = 8.0 Hz, *p*-Ar^{dmp}), 7.19 (s, 1H, *m*-Ar^{dmp}), 7.13 (s, 2H, CH=CH), 7.10 (s, 1H, *m*-Ar^{dmp}), 7.06 (d, 2H, J = 7.80 Hz, Ar^{IPr}), 7.02 (dd, 1H, J = 8.0 Hz, J = 1.4 Hz, *m*-Ar^{dmp}), 6.92 (dd, 1H, J = 8.0 Hz, J = 1.4 Hz, *m*-Ar^{dmp}), 6.76 (s, 1H, *m*-Ar^{dmp}), 3.00 (sept, 2H, J = 6.9 Hz, -CH(CH$_3$)$_2$), 2.61 (d, 1H, J = 3.9 Hz, -CH$_2$-), 2.59 (sept., 2H, J = 6.9 Hz, -CH(CH$_3$)$_2$), 2.49 (s, 3H, dmp-CH$_3$), 2.40 (s, 3H, dmp-CH$_3$), 2.26 (s, 3H, dmp-CH$_3$), 2.04 (s, 3H, dmp-CH$_3$), 1.76 (s, 3H, dmp-CH$_3$), 1.73 (s, br, 2H, -NH$_2$-), 1.50 (d, 6H, J = 6.9 Hz, -CH(CH$_3$)$_2$), 1.42 (d, 6H, J = 6.9 Hz, -CH(CH$_3$)$_2$),), 1.38 (d, 1H, J = 3.9 Hz, -CH$_2$-), 1.21 (d, 6H, J = 6.9 Hz, -CH(CH$_3$)$_2$),), 1.13 (d, 6H, J = 6.9 Hz, -CH(CH$_3$)$_2$)). ^{13}C{^{1}H} NMR (22°C, 126 MHz, CD$_2$Cl$_2$): δ 163.1, 162.7, 162.3, 161.9, 158.9, 140.9, 140.8, 139.7, 139.5, 138.1, 136.1, 135.5, 132.9, 132.5, 132.4, 132.2, 132.1, 131.1, 131.0, 130.7, 130.1, 130.0, 129.7, 129.5, 129.2, 128.5, 127.3, 127.1, 126.4, 125.8, 125.2, 124.2, 122.1, 118.2, 30.0, 29.5, 25.0, 24.7, 24.0, 22.1, 21.4, 20.9, 20.7, 19.8, 15.5, 8.3. Elemental analysis for BC$_{83}$H$_{84}$F$_{24}$N$_3$Ni: %C = 60.5, %H = 5.13, %N = 2.55; found: %C = 60.9, %H = 5.06, %N = 2.35.

[(IPr)Ni(THF)(κ^2-*C*,*N*:NH$_2$C$_6$H$_3$(Mes)C$_{10}$H$_9$)][B(Ar^F)$_4$] (8)

7 (190 mg, 0.115 mmol) was dissolved in a minimal amount of THF (~2 mL) and layered with 18 mL pentane at -35°C. Large, red blocks suitable for X-ray were isolated in 94% yield (186 mg).

For **8**: ^{1}H NMR (22°C, 500 MHz, THF-d$_8$): δ 7.79 (s, 8H, *m*-Ar^F), 7.57 (s, 4H, *p*-Ar^F), 7.53 (d, 2H, J = 8.0 Hz, *m*-Ar^{IPr}), 7.50 (s, 2H, CH=CH), 7.47 (t, 2H, J = 7.8 Hz, *m*-Ar^{IPr}), 7.31 (d,

2H, J = 8.0 Hz, *m*-Ar^{IPr}), 7.20 (t, 1H, J = 7.7 Hz, *p*-Ar^{dmp}), 7.14 (s, 1H, *m*-Ar^{dmp}), 7.11 (s, 1H, *m*-Ar^{dmp}), 6.92 (dd, 1H, J = 7.7 Hz, J = 1.4 Hz, *m*-Ar^{dmp}), 6.91 (s, 1H, *m*-Ar^{dmp}), 6.87 (dd, 1H, J = 7.7 Hz, J = 1.4 Hz, *m*-Ar^{dmp}), 6.54 (s, 1H, *m*-Ar^{dmp}), 3.79 (sept, 2H, J = 6.8 Hz, -CH(CH$_3$)$_2$), 3.58 (sept, 2H, J = 6.8 Hz, -CH(CH$_3$)$_2$), 2.38 (s, 3H, dmp-CH$_3$), 2.26 (s, 3H, dmp-CH$_3$), 2.22 (s, 3H. dmp- CH$_3$), 2.15 (s, 3H, dmp-CH$_3$), 1.83 (s, 3H, dmp-CH$_3$), 1.48 (d, 6H, J = 6.8 Hz, -CH(CH$_3$)$_2$), 1.18 (d, 6H, J = 6.8 Hz, -CH(CH$_3$)$_2$), 1.08 (d, 12H, J = 6.8, -CH(CH$_3$)$_2$). ^{13}C{^{1}H} NMR (22°C, 126 MHz, THF-d$_8$): δ 171.1, 163.6, 163.2, 162.8, 162.4, 146.9, 146.2, 145.7, 139.8, 139.3, 138.8, 138.4, 136.9, 136.9, 135.8, 134.3, 133.8, 132.8, 132.2, 131.0, 131.4, 130.6, 130.3, 130.1, 129.9, 128.9, 128.0, 127.8, 126.8, 126.7, 126.1, 125.3, 124.6, 122.4, 118.3, 30.3, 29.9, 26.5, 26.4, 26.1, 22.9, 22.5, 21.6, 21.3, 21.1, 19.9, 10.7. Elemental analysis for $BC_{87}H_{83}F_{24}N_3NiO$: %C = 61.0, %H = 4.89, %N = 2.45; found: %C = 61.4, %H = 5.25, %N = 2.35.

[(IPr)Ni(NHdippp)][B(Ar^F)$_4$] (9)

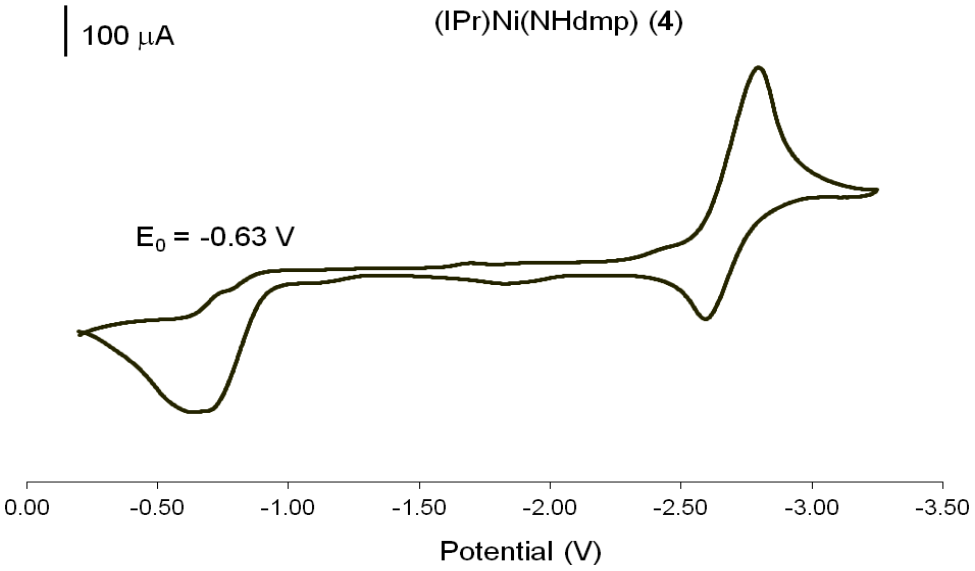
Chilled solutions of **5** (164 mg in 5 mL Et$_2$O at -35°C, 0.190 mmol) and [Cp$_2$Fe][B(Ar^F)$_4$] (198 mg in 12 mL Et$_2$O at -35°C, 0.190 mmol) were combined under vigorous stirring. Upon warming to room temperature, a slight color change from blue to purple/brown occurred. The reaction was stirred at room temperature for 1 hour before solvent was removed under vacuum. After washing with 20 mL pentane to remove Cp$_2$Fe, the purple solid was recrystallized by layering an Et$_2$O solution with pentane. Filtration resulted in isolation of 327 mg (94% yield) crystalline, blue-violet **9**. Single, dichroic blue/red crystals of **9** were collected from a pentane-layered Et$_2$O solution.

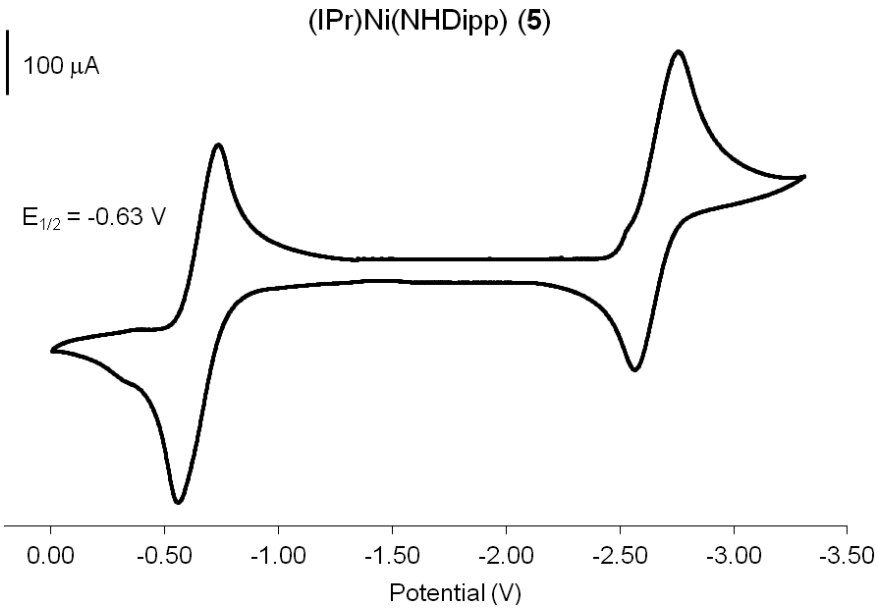
For **9**: ^{1}H NMR (22°C, 500 MHz, CD$_2$Cl$_2$): δ 28.3, 23.6, 20.6, 16.1, 7.75, 7.58, 6.34, 5.94, 5.78, 5.21, 5.16, 2.64, 1.10. μ_{eff} = 3.2 μ_B (CD$_2$Cl$_2$, 20°C, Evans' method). Elemental analysis for $C_{89}BF_{24}H_{86}N_3Ni$: %C = 62.0, %H = 5.03, %N = 2.44; found: %C = 61.8, %H = 4.96, %N = 2.38.

(II) Cyclic Voltammetry

Cyclic voltammetry was performed with solutions of dry THF (0.3-0.4 M solution containing dry, recrystallized tetrabutylammonium hexafluorophosphate, TBAH, Aldrich). A

ceramic patterned electrode with a platinum working electrode and Ag/AgCl reference electrode from Pine Research Instrumentation was used for data collection. Electrochemical response was recorded using an Eco-Chemie Autolab potentiostat (pgstat20) and GPES 4.3 software. The IR correction drop was not utilized as there was no significant resistance in solution. Spectra are recorded at scan rates of 100-500 mV/s, under a N_2 atmosphere. In a typical experiment, 30-40 mg crystalline solid was dissolved in THF with TBAH at 25°C.





The quasi-reversible features near -2.6 V for **4** and **5** are attributed to the reduction of Ni(I) to Ni(0). However, bulk synthetic attempts to reduce the Ni(I) amides reported here with

Na/Hg or KC_8 have resulted in formation of $\{(IPr)Ni\}_2$ as the major Ni-containing product. Further studies were not initiated.

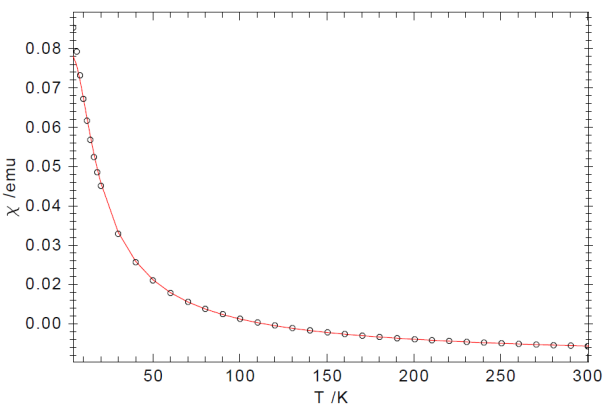
(III) SQUID Measurements

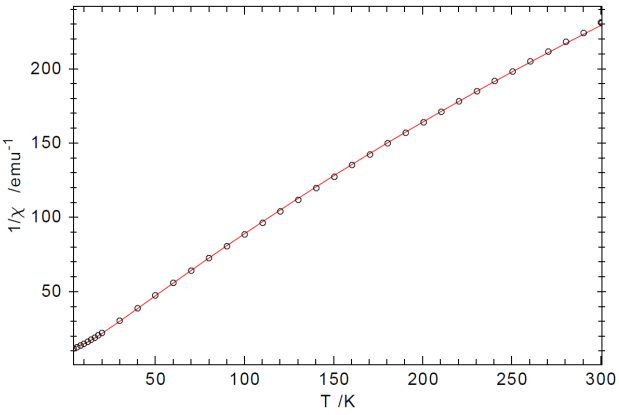
Prior to SQUID sample preparation, crystalline **9** was analyzed by ^1H NMR spectroscopy (CD_2Cl_2, 400 MHz) to ensure purity. The sample was prepared in an N_2-filled glove-box that had just been thoroughly cleaned and purged. Crystalline **9** was ground with a mortar and pestle, and 88.5 mg of the fine powder was transferred to a polycarbonate capsule. The capsule was then wrapped with parafilm, and pierced with a 26.5 G needle. The capsule was then suspended in a plastic straw, placed in two Ziploc bags, and stored at -35 ^oC in the glove-box. A background sample comprised of the polycarbonate capsule and parafilm was prepared analogously (mass of the capsules: 37.2 mg; mass of parafilm: 13.1 +/- 0.1 mg). The sample and blank were then taken to the SQUID magnetometer (separately) in the two plastic bags, and immediately loaded. Upon completion of analysis, the sample of **9** was removed, immediately placed in liquid nitrogen, and brought back into the glove-box. The sample was re-analyzed by ^1H NMR spectroscopy (CD_2Cl_2, 400 MHz) to confirm that no decomposition had occurred during data collection/transport.

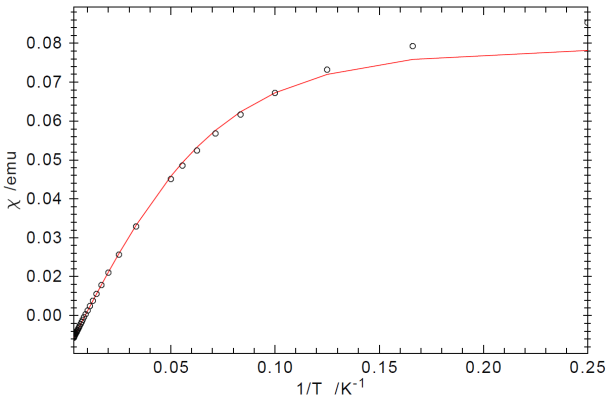
Data were collected on the sample using a Quantum Design Inc. Magnetic Property Measurement System (MPMS-5S) SQUID instrument at 5000G from 4-300K, with data being collected with 2 K increments (4 – 20 K), and 10 K increments (20 – 300 K). Initial cooling of the sample was done in the absence of a magnetic field, and the sample centered using a DC centering scan.

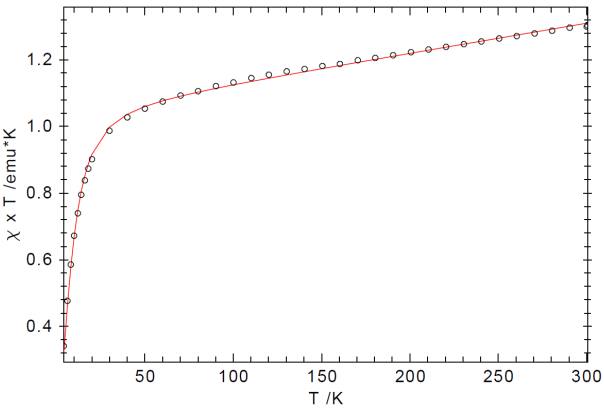
The raw data for **9** were background corrected by subtraction of the contributions of the capsule and straw. Diamagnetic contributions were taken into account using standard Pascal constants (Berry *et al.*, J. Chem. Ed., 2008, 532). The sample exhibits Curie-Weiss behavior, as indicated by the linearity of the X^{-1} vs. T data. Data were fit using the JulX program (v. 1.4.1), written by Eckhard Bill (http://ewww.mpi-muelheim.mpg.de/bac/logins/bill/julX_en.php). Variables used to fit the data were *g*, D, and Temperature-Independent Paramagnetism (TIP). Also, the E/D term was held at 0.33, as the system is rhombic. Simulation of the data provided

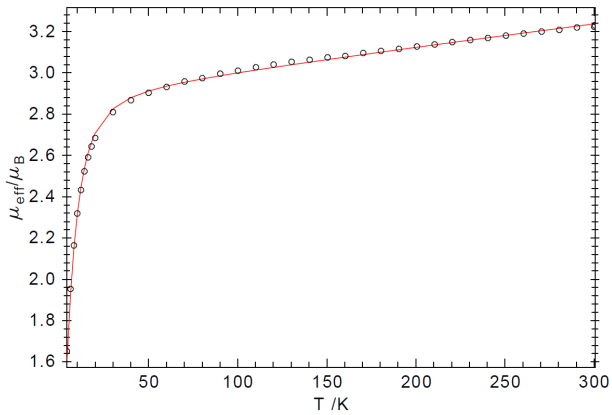
the following values: $g = 2.04$, $D = 22.6\ cm^{-1}$, and $TIP = 895 \times 10^{-6}$ emu. The large TIP term suggests a spin-admixed ground-state. In the plots shown below, data is shown as circles, and fits are shown as red lines.











(III) X-ray Studies

X-Ray Structure Determination. A crystal of suitable size and appearance was selected under a stereo-microscope while immersed in Paratone-N oil to minimize exposure to air. The crystal was extracted from the oil using a tapered glass filament that also held the crystal during data collection. The crystal was mounted and aligned on a Bruker SMART APEX system. All images showed sharp diffractions. Frames separated in reciprocal space were collected and provided an orientation matrix and initial cell parameters. The full data set provided final cell parameters.

A hemisphere of data was obtained at 100 K in reciprocal space to a resolution of 0.84 Å using 0.3° steps in ω using integration times of 10-30 s per frame, depending on the sample. Integration of intensities and refinement of cell parameters were completed with SAINT. Absorption corrections were applied using SADABS or psi-scans and were small. Crystals showed no visual signs of decomposition after data collection.

(IPr)Ni(NHdmp) (4)

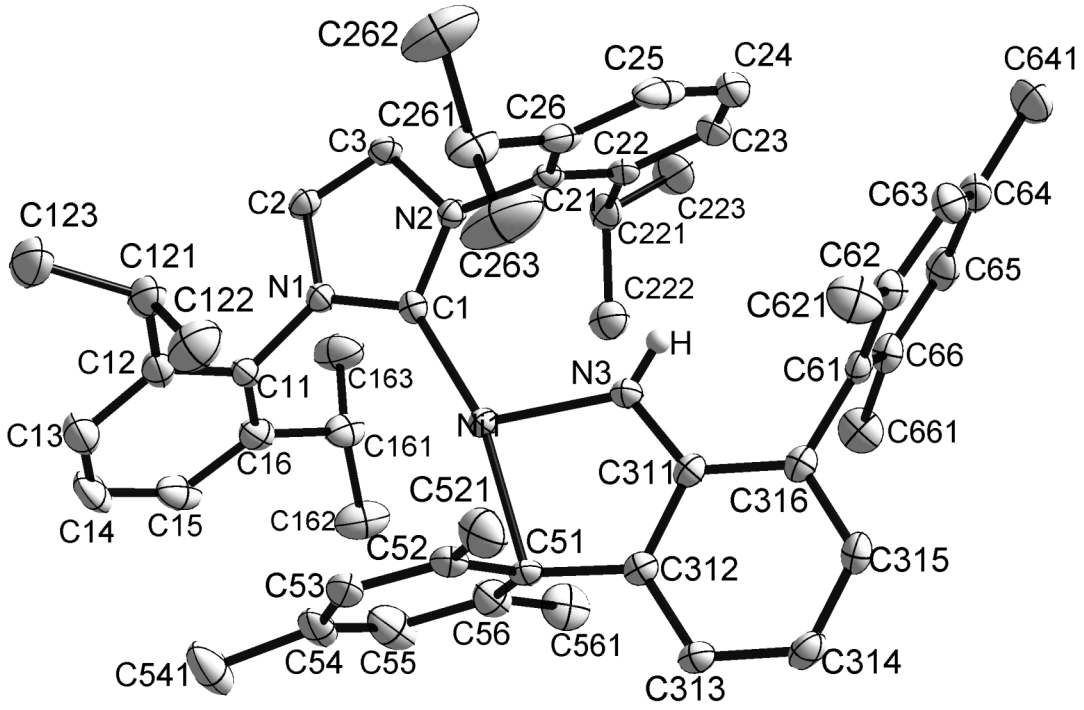
The space group was determined as P2(1)/n based on systematic absences and intensity statistics. Patterson method was used to locate Ni. Direct methods were used to locate C and N atoms. All non-hydrogen atoms were converted to and refined anisotropically. The amide hydrogen was located in the difference map and refined isotropically. All hydrogen atoms were refined isotropically and fixed at calculated positions.

Crystal data and structure refinement for **4**:

Identification code	carl40a		g = 90°
Empirical formula	C_{51} H_{62} N_3 Ni	Volume	4290.8(6) $Å^3$
Formula weight	775.75	Z	4
Temperature	373(2) K	Density (calculated)	1.201 Mg/m^3
Wavelength	0.71073 Å	Absorption coefficient	0.490 mm^{-1}
Crystal system	Monoclinic	F(000)	1668
Space group	P2(1)/n	Crystal size	0.2 x 0.2 x 0.8 mm^3
Unit cell dimensions	a = 12.2859(11) Å	Theta range for data collection	1.55 to 28.30°
	b = 20.3988(17) Å	Index ranges	-16<=h<=13,
	c = 17.3454(15) Å		-27<=k<=16,
	a = 90°		-22<=l<=22
	b = 99.232(2)°		

Reflections collected	27399	Goodness-of-fit on F^2	0.910
Independent reflections	10072 [R(int) =0.0575]	Final R indices [I>2sigma(I)]	R1 = 0.0529
Completeness to theta = 25.00°	100.0 %		wR2 = 0.1090
Absorption correction	Empirical	R indices (all data)	R1 = 0.0862
Max. and min. transmission	0.2900 and 0.2581		wR2 = 0.1182
Refinement method	Full-matrix least-squares on F^2	Largest diff. peak and hole	0.491 and -0.412 e.Å^{-3}
Data / restraints / parameters	10072 / 0 / 500		

Fully labeled ORTEP diagram (50%) for **4**:



Bond Distances (Å) for **4**:

Ni(1)-N(3)	1.935(2)	C(51)-C(56)	1.417(3)	C(313)-C(314)	1.392(3)
Ni(1)-C(1)	1.948(2)	C(51)-C(52)	1.421(3)	C(25)-C(24)	1.369(4)
Ni(1)-C(51)	2.136(2)	C(51)-C(312)	1.492(3)	C(25)-C(26)	1.408(4)
Ni(1)-C(56)	2.395(3)	N(3)-C(311)	1.360(3)	C(16)-C(11)	1.397(4)
Ni(1)-C(52)	2.502(3)	C(316)-C(315)	1.388(3)	C(16)-C(15)	1.402(4)
N(1)-C(1)	1.374(3)	C(316)-C(311)	1.427(3)	C(16)-C(161)	1.515(4)
N(1)-C(2)	1.383(3)	C(316)-C(61)	1.495(3)	C(62)-C(63)	1.390(4)
N(1)-C(11)	1.444(3)	N(2)-C(1)	1.370(3)	C(62)-C(61)	1.396(3)
C(3)-C(2)	1.332(3)	C(52)-C(53)	1.390(4)	C(62)-C(621)	1.515(4)
C(3)-N(2)	1.391(3)	C(52)-C(521)	1.509(4)	C(66)-C(65)	1.389(4)
C(21)-C(26)	1.391(3)	C(312)-C(313)	1.385(3)	C(66)-C(61)	1.402(3)
C(21)-C(22)	1.409(3)	C(312)-C(311)	1.412(3)	C(66)-C(661)	1.505(4)
C(21)-N(2)	1.443(3)	C(315)-C(314)	1.378(4)	C(53)-C(54)	1.385(4)

C(26)-C(261)	1.513(4)	C(221)-C(223)	1.538(3)	C(13)-C(14)	1.366(4)
C(161)-C(163)	1.525(4)	C(63)-C(64)	1.382(4)	C(56)-C(561)	1.512(4)
C(161)-C(162)	1.527(4)	C(23)-C(24)	1.369(4)	C(15)-C(14)	1.382(4)
C(12)-C(13)	1.384(4)	C(23)-C(22)	1.386(3)	C(261)-C(263)	1.508(4)
C(12)-C(11)	1.403(3)	C(64)-C(65)	1.383(4)	C(261)-C(262)	1.538(4)
C(12)-C(121)	1.523(4)	C(64)-C(641)	1.505(4)	C(54)-C(541)	1.512(4)
C(221)-C(22)	1.520(4)	C(55)-C(54)	1.376(4)	C(121)-C(122)	1.530(4)
C(221)-C(222)	1.529(4)	C(55)-C(56)	1.403(4)	C(121)-C(123)	1.534(4)

Bond Angles (°) for **4**:

N(3)-Ni(1)-C(1)	112.17(10)	C(313)-C(312)-C(311)	121.9(2)	C(22)-C(221)-C(222)	112.0(2)
N(3)-Ni(1)-C(51)	81.99(9)	C(313)-C(312)-C(51)	121.6(2)	C(22)-C(221)-C(223)	113.8(2)
C(1)-Ni(1)-C(51)	165.82(10)	C(311)-C(312)-C(51)	116.4(2)	C(222)-C(221)-C(223)	108.6(2)
N(3)-Ni(1)-C(56)	100.52(9)	N(2)-C(1)-N(1)	102.06(19)	C(16)-C(11)-C(12)	123.6(2)
C(1)-Ni(1)-C(56)	134.82(9)	N(2)-C(1)-Ni(1)	125.93(17)	C(16)-C(11)-N(1)	118.5(2)
C(51)-Ni(1)-C(56)	35.88(9)	N(1)-C(1)-Ni(1)	132.02(17)	C(12)-C(11)-N(1)	117.4(2)
N(3)-Ni(1)-C(52)	99.60(9)	C(314)-C(315)-C(316)	123.0(2)	C(64)-C(63)-C(62)	122.1(3)
C(1)-Ni(1)-C(52)	137.43(9)	C(312)-C(313)-C(314)	120.0(2)	C(24)-C(23)-C(22)	120.9(3)
C(51)-Ni(1)-C(52)	34.54(8)	C(3)-C(2)-N(1)	107.7(2)	C(23)-C(22)-C(21)	117.0(2)
C(56)-Ni(1)-C(52)	59.68(9)	N(3)-C(311)-C(312)	116.0(2)	C(23)-C(22)-C(221)	121.6(2)
C(1)-N(1)-C(2)	111.8(2)	N(3)-C(311)-C(316)	126.5(2)	C(21)-C(22)-C(221)	121.5(2)
C(1)-N(1)-C(11)	128.08(19)	C(312)-C(311)-C(316)	117.5(2)	C(63)-C(64)-C(65)	117.5(3)
C(2)-N(1)-C(11)	120.15(19)	C(24)-C(25)-C(26)	121.1(3)	C(63)-C(64)-C(641)	121.2(3)
C(2)-C(3)-N(2)	105.9(2)	C(11)-C(16)-C(15)	116.4(3)	C(65)-C(64)-C(641)	121.3(3)
C(26)-C(21)-C(22)	123.6(2)	C(11)-C(16)-C(161)	121.5(2)	C(64)-C(65)-C(66)	122.4(3)
C(26)-C(21)-N(2)	117.9(2)	C(15)-C(16)-C(161)	122.0(2)	C(54)-C(55)-C(56)	122.6(3)
C(22)-C(21)-N(2)	118.4(2)	C(63)-C(62)-C(61)	119.6(2)	C(14)-C(13)-C(12)	121.4(3)
C(56)-C(51)-C(52)	118.5(2)	C(63)-C(62)-C(621)	120.4(2)	C(55)-C(56)-C(51)	118.7(3)
C(56)-C(51)-C(312)	121.5(2)	C(61)-C(62)-C(621)	120.0(2)	C(55)-C(56)-C(561)	120.4(3)
C(52)-C(51)-C(312)	119.6(2)	C(65)-C(66)-C(61)	119.2(2)	C(51)-C(56)-C(561)	120.2(2)
C(56)-C(51)-Ni(1)	82.07(15)	C(65)-C(66)-C(661)	120.8(2)	C(55)-C(56)-Ni(1)	104.8(2)
C(52)-C(51)-Ni(1)	86.96(15)	C(61)-C(66)-C(661)	120.0(2)	C(51)-C(56)-Ni(1)	62.05(14)
C(312)-C(51)-Ni(1)	106.89(16)	C(62)-C(61)-C(66)	119.2(2)	C(561)-C(56)-Ni(1)	108.99(18)
C(311)-N(3)-Ni(1)	118.70(18)	C(62)-C(61)-C(316)	121.4(2)	C(14)-C(15)-C(16)	120.7(3)
C(315)-C(316)-C(311)	118.8(2)	C(66)-C(61)-C(316)	119.4(2)	C(23)-C(24)-C(25)	121.3(3)
C(315)-C(316)-C(61)	119.7(2)	C(54)-C(53)-C(52)	122.8(3)	C(263)-C(261)-C(26)	111.2(2)
C(311)-C(316)-C(61)	121.5(2)	C(21)-C(26)-C(25)	116.2(3)	C(263)-C(261)-C(262)	108.7(2)
C(1)-N(2)-C(3)	112.6(2)	C(21)-C(26)-C(261)	122.3(2)	C(26)-C(261)-C(262)	112.4(3)
C(1)-N(2)-C(21)	127.00(19)	C(25)-C(26)-C(261)	121.5(2)	C(55)-C(54)-C(53)	117.6(3)
C(3)-N(2)-C(21)	120.2(2)	C(16)-C(161)-C(163)	111.2(2)	C(55)-C(54)-C(541)	121.5(3)
C(53)-C(52)-C(51)	119.0(3)	C(16)-C(161)-C(162)	114.1(2)	C(53)-C(54)-C(541)	120.9(3)
C(53)-C(52)-C(521)	120.3(3)	C(163)-C(161)-C(162)	108.7(2)	C(12)-C(121)-C(122)	110.7(2)
C(51)-C(52)-C(521)	120.2(2)	C(13)-C(12)-C(11)	116.8(3)	C(12)-C(121)-C(123)	113.2(2)
C(53)-C(52)-Ni(1)	102.52(18)	C(13)-C(12)-C(121)	121.3(3)	C(122)-C(121)-C(123)	110.1(2)
C(51)-C(52)-Ni(1)	58.49(13)	C(11)-C(12)-C(121)	121.9(2)	C(13)-C(14)-C(15)	121.0(3)
C(521)-C(52)-Ni(1)	114.07(18)	C(315)-C(314)-C(313)	118.8(2)		

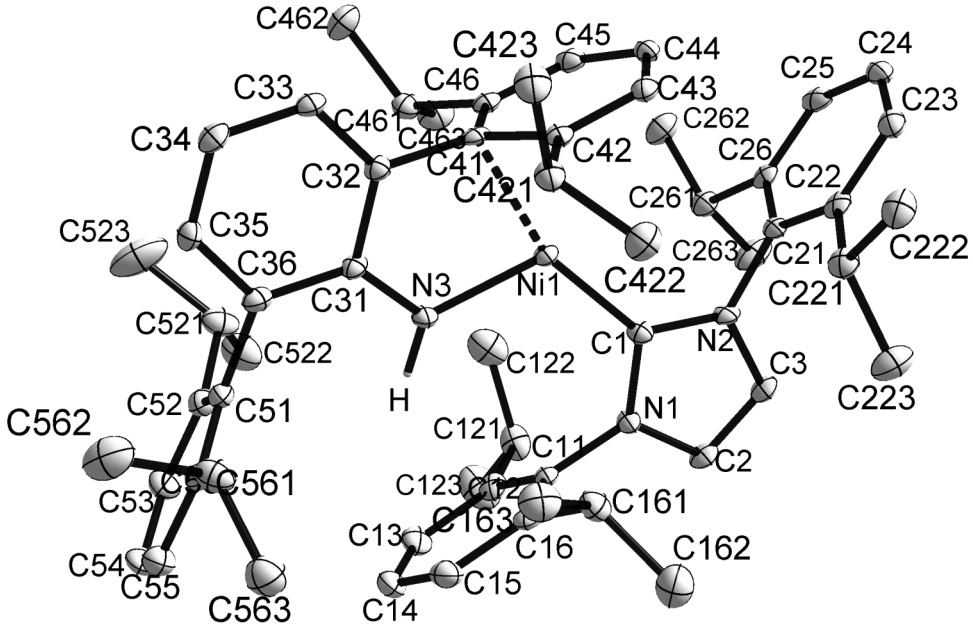
(IPr)Ni(NHdippp) (5)

The space group was determined as P2(1)/c based on systematic absences and intensity statistics. Patterson method was used to locate Ni. Direct methods were used to locate C, N and Cl atoms. All non-hydrogen atoms were converted to and refined anisotropically. The amide hydrogen was located in the difference map and refined isotropically. All other hydrogen atoms were refined isotropically and fixed at calculated positions.

Crystal data and structure refinement for **5**:

Identification code	carl11a	Theta range for data collection	1.68 to 28.29°.
Empirical formula	C_{59} H_{78} Cl_4 N_3 Ni	Index ranges	-27<=h<=28
Formula weight	1029.75		-14<=k<=14
Temperature	100(2) K		-32<=l<=20
Wavelength	0.71073 Å	Reflections collected	34798
Crystal system	Monoclinic	Independent reflections	12904 [R(int) = 0.1440]
Space group	P(2)1/c	Completeness to theta = 25.00°	99.9 %
Unit cell dimensions	a = 21.2763(15) Å	Absorption correction	None
	b = 10.7269(7) Å	Max. and min. transmission	0.3151 and 0.1901
	c = 24.4104(17) Å	Refinement method	Full-matrix least-squares on F^2
	α= 90°		
	β= 97.0530(10)°	Data / restraints / parameters	12904 / 0 / 608
	γ = 90°	Goodness-of-fit on F^2	0.969
Volume	5529.0(7) $Å^3$	Final R indices [I>2sigma(I)]	R1 = 0.0631
Z	4		wR2 = 0.1623
Density (calculated)	1.237 Mg/m^3	R indices (all data)	R1 = 0.0809
Absorption coefficient	0.584 mm^{-1}		wR2 = 0.1733
F(000)	2196	Largest diff. peak and hole	1.397 and -1.166 e.$Å^{-3}$
Crystal size	0.6 x 0.2 x 0.2 mm^3		

Fully labeled ORTEP diagram (50%) for **5**:



Bond Distances (Å) for **5:**

Ni(1)-N(3)	1.953(2)	C(33)-C(34)	1.394(3)	C(24)-C(23)	1.381(4)
Ni(1)-C(1)	1.959(2)	C(11)-C(12)	1.396(4)	C(24)-C(25)	1.387(4)
Ni(1)-C(41)	2.114(2)	C(11)-C(16)	1.400(4)	C(16)-C(15)	1.397(3)
Ni(1)-C(46)	2.380(2)	C(56)-C(55)	1.399(4)	C(461)-C(46)	1.528(3)
Ni(1)-C(42)	2.385(2)	C(56)-C(51)	1.413(3)	C(461)-C(462)	1.528(4)
N(3)-C(31)	1.352(3)	C(56)-C(561)	1.520(4)	C(461)-C(463)	1.530(4)
N(1)-C(1)	1.366(3)	C(22)-C(23)	1.396(3)	C(13)-C(14)	1.385(4)
N(1)-C(2)	1.387(3)	C(22)-C(21)	1.409(3)	C(13)-C(12)	1.396(4)
N(1)-C(11)	1.449(3)	C(22)-C(221)	1.524(4)	C(221)-C(223)	1.539(4)
C(26)-C(25)	1.394(3)	C(43)-C(44)	1.388(4)	C(15)-C(14)	1.388(4)
C(26)-C(21)	1.399(4)	C(43)-C(42)	1.401(3)	C(51)-C(52)	1.417(4)
C(26)-C(261)	1.522(3)	C(44)-C(45)	1.385(3)	C(34)-C(35)	1.384(3)
C(1)-N(2)	1.364(3)	C(41)-C(42)	1.427(3)	C(52)-C(53)	1.389(4)
N(2)-C(3)	1.388(3)	C(41)-C(46)	1.431(3)	C(52)-C(521)	1.519(4)
N(2)-C(21)	1.457(3)	C(41)-C(32)	1.492(3)	C(55)-C(54)	1.380(4)
C(421)-C(422)	1.522(4)	C(161)-C(16)	1.515(3)	C(561)-C(563)	1.530(4)
C(421)-C(423)	1.528(3)	C(161)-C(163)	1.525(4)	C(561)-C(562)	1.536(4)
C(421)-C(42)	1.533(3)	C(161)-C(162)	1.531(4)	C(521)-C(523)	1.522(4)
C(31)-C(32)	1.422(3)	C(261)-C(262)	1.533(4)	C(521)-C(522)	1.530(4)
C(31)-C(36)	1.428(3)	C(261)-C(263)	1.537(4)	C(54)-C(53)	1.380(4)
C(36)-C(35)	1.398(3)	C(3)-C(2)	1.337(3)	C(12)-C(121)	1.528(4)
C(36)-C(51)	1.500(3)	C(45)-C(46)	1.403(3)	C(121)-C(123)	1.520(4)
C(33)-C(32)	1.386(3)	C(222)-C(221)	1.529(3)	C(121)-C(122)	1.536(4)

Bond Angles (°) for **5**:

N(3)-Ni(1)-C(1)	116.41(9)	C(23)-C(22)-C(21)	116.3(2)	C(14)-C(13)-C(12)	121.1(3)
N(3)-Ni(1)-C(41)	81.62(9)	C(23)-C(22)-C(221)	121.4(2)	C(22)-C(221)-C(222)	113.5(2)
C(1)-Ni(1)-C(41)	161.90(9)	C(21)-C(22)-C(221)	122.1(2)	C(22)-C(221)-C(223)	113.8(2)
N(3)-Ni(1)-C(46)	97.89(8)	C(44)-C(43)-C(42)	120.5(2)	C(222)-C(221)-C(223)	108.0(2)
C(1)-Ni(1)-C(46)	134.32(9)	C(45)-C(44)-C(43)	120.4(2)	C(14)-C(15)-C(16)	121.5(2)
C(41)-Ni(1)-C(46)	36.54(9)	C(26)-C(21)-C(22)	123.4(2)	C(56)-C(51)-C(52)	119.7(2)
N(3)-Ni(1)-C(42)	101.93(8)	C(26)-C(21)-N(2)	117.7(2)	C(56)-C(51)-C(36)	121.6(2)
C(1)-Ni(1)-C(42)	130.61(9)	C(22)-C(21)-N(2)	118.6(2)	C(52)-C(51)-C(36)	118.6(2)
C(41)-Ni(1)-C(42)	36.34(9)	C(42)-C(41)-C(46)	119.0(2)	C(24)-C(23)-C(22)	121.5(2)
C(46)-Ni(1)-C(42)	62.21(8)	C(42)-C(41)-C(32)	120.4(2)	C(35)-C(34)-C(33)	118.1(2)
C(31)-N(3)-Ni(1)	118.64(16)	C(46)-C(41)-C(32)	120.6(2)	C(53)-C(52)-C(51)	119.1(2)
C(1)-N(1)-C(2)	112.62(19)	C(42)-C(41)-Ni(1)	82.25(14)	C(53)-C(52)-C(521)	120.3(2)
C(1)-N(1)-C(11)	125.60(19)	C(46)-C(41)-Ni(1)	81.91(14)	C(51)-C(52)-C(521)	120.5(2)
C(2)-N(1)-C(11)	121.8(2)	C(32)-C(41)-Ni(1)	108.02(15)	C(3)-C(2)-N(1)	106.2(2)
C(25)-C(26)-C(21)	117.6(2)	C(16)-C(161)-C(163)	112.9(2)	C(34)-C(35)-C(36)	123.2(2)
C(25)-C(26)-C(261)	120.6(2)	C(16)-C(161)-C(162)	110.8(2)	C(54)-C(55)-C(56)	121.1(3)
C(21)-C(26)-C(261)	121.8(2)	C(163)-C(161)-C(162)	111.0(2)	C(13)-C(14)-C(15)	120.3(2)
N(2)-C(1)-N(1)	102.10(19)	C(26)-C(261)-C(262)	113.2(2)	C(56)-C(561)-C(563)	113.3(2)
N(2)-C(1)-Ni(1)	132.75(17)	C(26)-C(261)-C(263)	111.2(2)	C(56)-C(561)-C(562)	110.8(2)
N(1)-C(1)-Ni(1)	125.15(16)	C(262)-C(261)-C(263)	108.4(2)	C(563)-C(561)-C(562)	108.5(2)
C(1)-N(2)-C(3)	112.3(2)	C(33)-C(32)-C(31)	122.2(2)	C(52)-C(521)-C(523)	111.3(2)
C(1)-N(2)-C(21)	127.69(19)	C(33)-C(32)-C(41)	122.1(2)	C(52)-C(521)-C(522)	113.0(2)
C(3)-N(2)-C(21)	119.9(2)	C(31)-C(32)-C(41)	115.7(2)	C(523)-C(521)-C(522)	109.4(3)
C(422)-C(421)-C(423)	110.3(2)	C(2)-C(3)-N(2)	106.7(2)	C(53)-C(54)-C(55)	119.9(2)
C(422)-C(421)-C(42)	113.3(2)	C(44)-C(45)-C(46)	121.3(2)	C(54)-C(53)-C(52)	121.3(3)
C(423)-C(421)-C(42)	109.8(2)	C(23)-C(24)-C(25)	120.8(2)	C(13)-C(12)-C(11)	116.8(2)
N(3)-C(31)-C(32)	115.8(2)	C(15)-C(16)-C(11)	116.1(2)	C(13)-C(12)-C(121)	121.5(2)
N(3)-C(31)-C(36)	127.3(2)	C(15)-C(16)-C(161)	121.5(2)	C(11)-C(12)-C(121)	121.8(2)
C(32)-C(31)-C(36)	116.8(2)	C(11)-C(16)-C(161)	122.3(2)	C(123)-C(121)-C(12)	113.6(2)
C(35)-C(36)-C(31)	119.1(2)	C(46)-C(461)-C(462)	111.1(2)	C(123)-C(121)-C(122)	110.4(3)
C(35)-C(36)-C(51)	118.6(2)	C(46)-C(461)-C(463)	113.4(2)	C(12)-C(121)-C(122)	111.3(2)
C(31)-C(36)-C(51)	122.1(2)	C(462)-C(461)-C(463)	110.0(2)	C(45)-C(46)-C(41)	118.7(2)
C(32)-C(33)-C(34)	120.5(2)	C(43)-C(42)-C(41)	119.6(2)	C(45)-C(46)-C(461)	121.2(2)
C(12)-C(11)-C(16)	124.3(2)	C(43)-C(42)-C(421)	120.8(2)	C(41)-C(46)-C(461)	119.8(2)
C(12)-C(11)-N(1)	117.7(2)	C(41)-C(42)-C(421)	119.1(2)	C(45)-C(46)-Ni(1)	98.83(16)
C(16)-C(11)-N(1)	118.0(2)	C(43)-C(42)-Ni(1)	99.60(16)	C(41)-C(46)-Ni(1)	61.55(12)
C(55)-C(56)-C(51)	118.9(2)	C(41)-C(42)-Ni(1)	61.41(12)	C(461)-C(46)-Ni(1)	113.15(15)
C(55)-C(56)-C(561)	119.0(2)	C(421)-C(42)-Ni(1)	114.02(15)		
C(51)-C(56)-C(561)	122.0(2)	C(24)-C(25)-C(26)	120.4(2)		

[(IPr)Ni(κ^2-*C*,*N*:NH$_2$C$_6$H$_3$(Mes)C$_{10}$H$_9$)][B(Ar^F)$_4$] (7)

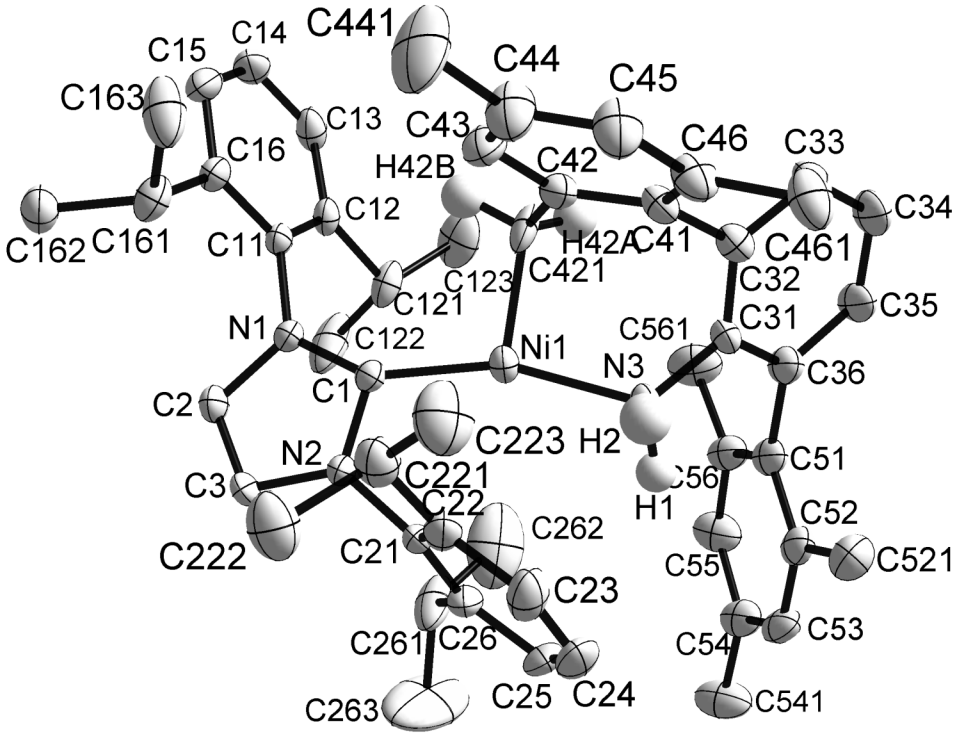
The space group was determined as P2(1)/n based on systematic absences and intensity statistics. Patterson method was used to locate Ni. Direct methods were used to locate B, C, F, N and O atoms. All non-hydrogen atoms were converted to and refined anisotropically. The amine hydrogens were located in the difference map and refined isotropically. All other hydrogen

atoms were refined isotropically and fixed at calculated positions. Two trifluoromethyl groups exhibited typical disorder and were modeled to improve GoF and R1.

Crystal data and structure refinement for **7**:

Identification code	carl129a	Theta range for data collection	1.18 to 25.00°.
Empirical formula	$C_{87} H_{84} B F_{24} N_3 Ni O$	Index ranges	-15<=h<=15
Formula weight	1713.09		-41<=k<=41
Temperature	100(2) K		-23<=l<=23
Wavelength	0.71073 Å	Reflections collected	80470
Crystal system	Monoclinic	Independent reflections	14742 [R(int) = 0.1469]
Space group	P2(1)/n	Completeness to theta = 25.00°	100.0 %
Unit cell dimensions	a = 12.9077(17) Å	Absorption correction	Psi-scan
	b = 34.624(4) Å	Max. and min. transmission	0.9364 and 0.8253
	c = 19.650(3) Å	Refinement method	Full-matrix least-squares on F^2
	α= 90°		
	β= 107.756(2)°	Data / restraints / parameters	14742 / 0 / 1097
	γ = 90°	Goodness-of-fit on F^2	1.004
Volume	8363.8(19) $Å^3$	Final R indices [I>2sigma(I)]	R1 = 0.0889
Z	4		wR2 = 0.2231
Density (calculated)	1.360 Mg/m^3	R indices (all data)	R1 = 0.1426
Absorption coefficient	0.333 mm^{-1}		wR2 = 0.2497
F(000)	3536	Largest diff. peak and hole	2.193 and -0.806 $e.Å^{-3}$
Crystal size	0.60 x 0.20 x 0.20 mm^3		

Fully labeled ORTEP diagram (35%) for **7**:



Bond Distances (Å) for **7:**

Ni(1)-C(1)	1.858(5)	C(93)-C(931)	1.488(7)	C(52)-C(521)	1.507(9)
Ni(1)-C(421)	1.866(6)	C(91)-C(96)	1.381(7)	C(44)-C(45)	1.369(9)
Ni(1)-N(3)	1.972(4)	C(91)-C(92)	1.400(7)	C(222)-C(221)	1.537(9)
C(3)-C(2)	1.349(7)	C(91)-B(1)	1.648(7)	C(25)-C(26)	1.388(8)
C(3)-N(2)	1.383(6)	F(632)-C(631)	1.301(6)	C(221)-C(223)	1.506(9)
F(652)-C(651)	1.338(6)	C(75)-C(74)	1.378(8)	C(53)-C(54)	1.366(9)
C(31)-C(36)	1.381(7)	C(75)-C(76)	1.386(7)	C(54)-C(55)	1.409(9)
C(31)-C(32)	1.394(7)	C(75)-C(751)	1.516(8)	C(54)-C(541)	1.508(9)
C(31)-N(3)	1.463(6)	F(631)-C(631)	1.327(5)	F(852)-C(851)	1.306(6)
N(1)-C(1)	1.366(6)	C(71)-C(76)	1.395(7)	F(931)-C(931)	1.308(7)
N(1)-C(2)	1.391(6)	C(71)-C(72)	1.398(7)	F(831)-C(831)	1.353(8)
N(1)-C(11)	1.439(6)	C(71)-B(1)	1.631(7)	F(832)-C(831)	1.318(7)
F(651)-C(651)	1.343(6)	C(82)-C(81)	1.393(7)	F(951)-C(951)	1.320(7)
N(2)-C(1)	1.355(6)	C(82)-C(83)	1.394(7)	F(951)-F(954)	1.67(4)
N(2)-C(21)	1.465(6)	F(753)-C(751)	1.304(8)	F(952)-C(951)	1.353(7)
C(62)-C(63)	1.389(6)	C(96)-C(95)	1.391(7)	F(833)-F(834)	0.86(9)
C(62)-C(61)	1.401(6)	C(81)-C(86)	1.391(7)	F(833)-C(831)	1.295(12)
C(36)-C(35)	1.387(8)	C(81)-B(1)	1.643(7)	C(94)-C(95)	1.383(7)
C(36)-C(51)	1.494(8)	C(22)-C(23)	1.392(8)	C(86)-C(85)	1.395(7)
C(41)-C(42)	1.390(7)	C(22)-C(221)	1.511(8)	F(851)-C(851)	1.315(7)
C(41)-C(46)	1.408(8)	C(73)-C(74)	1.398(8)	C(85)-C(84)	1.379(7)
C(41)-C(32)	1.481(8)	C(73)-C(72)	1.398(7)	C(85)-C(851)	1.502(7)
C(61)-C(66)	1.389(6)	C(73)-C(731)	1.479(8)	F(953)-F(954)	1.04(6)
C(61)-B(1)	1.638(7)	F(752)-C(751)	1.299(7)	F(953)-C(951)	1.304(10)
C(66)-C(65)	1.382(6)	C(16)-C(15)	1.387(7)	C(26)-C(261)	1.499(9)
C(63)-C(64)	1.379(6)	C(16)-C(161)	1.529(7)	C(831)-F(834)	1.31(2)
C(63)-C(631)	1.495(6)	C(15)-C(14)	1.358(8)	C(831)-C(83)	1.492(8)
C(33)-C(34)	1.384(8)	C(14)-C(13)	1.356(8)	F(732)-C(731)	1.299(8)
C(33)-C(32)	1.398(8)	C(42)-C(43)	1.376(8)	C(851)-F(853)	1.303(7)
C(651)-F(653)	1.334(6)	C(42)-C(421)	1.473(8)	C(84)-C(83)	1.382(7)
C(651)-C(65)	1.494(7)	C(13)-C(12)	1.395(7)	C(46)-C(45)	1.370(8)
C(64)-C(65)	1.386(6)	C(24)-C(25)	1.375(10)	C(46)-C(461)	1.494(8)
C(51)-C(56)	1.391(8)	C(24)-C(23)	1.381(10)	F(731)-C(731)	1.303(8)
C(51)-C(52)	1.407(8)	C(121)-C(122)	1.516(9)	C(95)-C(951)	1.495(8)
C(21)-C(26)	1.383(8)	C(121)-C(12)	1.521(7)	C(951)-F(954)	1.33(3)
C(21)-C(22)	1.418(8)	C(121)-C(123)	1.548(9)	C(731)-F(733)	1.320(8)
C(11)-C(12)	1.390(7)	C(43)-C(44)	1.405(9)	C(931)-F(932)	1.263(7)
C(11)-C(16)	1.406(7)	C(441)-C(44)	1.526(9)	C(931)-F(933)	1.281(8)
C(34)-C(35)	1.367(8)	F(751)-C(751)	1.314(7)	C(561)-C(56)	1.531(8)
F(633)-C(631)	1.313(5)	C(161)-C(162)	1.514(8)	C(56)-C(55)	1.389(8)
C(93)-C(94)	1.371(7)	C(161)-C(163)	1.557(8)	C(261)-C(262)	1.496(13)
C(93)-C(92)	1.403(7)	C(52)-C(53)	1.385(8)	C(261)-C(263)	1.520(11)

Bond Angles (°) for **7**:

C(1)-Ni(1)-C(421)	102.3(2)	C(36)-C(31)-N(3)	119.9(5)	C(1)-N(2)-C(3)	112.8(4)
C(1)-Ni(1)-N(3)	159.8(2)	C(32)-C(31)-N(3)	117.1(5)	C(1)-N(2)-C(21)	117.3(4)
C(421)-Ni(1)-N(3)	97.8(2)	C(1)-N(1)-C(2)	110.5(4)	C(3)-N(2)-C(21)	129.8(4)
C(2)-C(3)-N(2)	105.3(4)	C(1)-N(1)-C(11)	126.6(4)	C(63)-C(62)-C(61)	122.8(4)
C(36)-C(31)-C(32)	123.0(5)	C(2)-N(1)-C(11)	122.9(4)	C(31)-C(36)-C(35)	117.6(5)

C(31)-C(36)-C(51)	121.2(5)	C(91)-C(96)-C(95)	123.5(4)	F(752)-C(751)-C(75)	112.6(5)
C(35)-C(36)-C(51)	121.1(5)	C(86)-C(81)-C(82)	116.2(5)	F(753)-C(751)-C(75)	112.6(5)
C(42)-C(41)-C(46)	120.6(5)	C(86)-C(81)-B(1)	123.5(4)	F(751)-C(751)-C(75)	112.0(6)
C(42)-C(41)-C(32)	119.3(5)	C(82)-C(81)-B(1)	120.1(4)	C(223)-C(221)-C(22)	112.7(6)
C(46)-C(41)-C(32)	120.1(5)	F(632)-C(631)-F(633)	107.4(4)	C(223)-C(221)-C(222)	110.7(6)
C(66)-C(61)-C(62)	115.0(4)	F(632)-C(631)-F(631)	104.7(4)	C(22)-C(221)-C(222)	109.8(5)
C(66)-C(61)-B(1)	122.3(4)	F(633)-C(631)-F(631)	104.2(4)	C(54)-C(53)-C(52)	122.2(6)
C(62)-C(61)-B(1)	122.4(4)	F(632)-C(631)-C(63)	113.1(4)	C(53)-C(54)-C(55)	118.0(6)
C(65)-C(66)-C(61)	122.8(4)	F(633)-C(631)-C(63)	113.3(4)	C(53)-C(54)-C(541)	121.9(6)
C(64)-C(63)-C(62)	120.3(4)	F(631)-C(631)-C(63)	113.4(4)	C(55)-C(54)-C(541)	120.1(6)
C(64)-C(63)-C(631)	119.1(4)	C(23)-C(22)-C(21)	116.5(6)	C(951)-F(951)-F(954)	51(2)
C(62)-C(63)-C(631)	120.6(4)	C(23)-C(22)-C(221)	121.6(6)	F(834)-F(833)-C(831)	71(2)
C(31)-N(3)-Ni(1)	121.5(3)	C(21)-C(22)-C(221)	121.8(5)	C(93)-C(94)-C(95)	118.2(5)
C(34)-C(33)-C(32)	121.6(6)	C(74)-C(73)-C(72)	119.4(5)	C(81)-C(86)-C(85)	121.6(5)
F(653)-C(651)-F(652)	105.1(4)	C(74)-C(73)-C(731)	119.2(5)	C(73)-C(72)-C(71)	122.7(5)
F(653)-C(651)-F(651)	106.4(4)	C(72)-C(73)-C(731)	121.4(6)	C(84)-C(85)-C(86)	121.2(5)
F(652)-C(651)-F(651)	106.1(4)	C(71)-B(1)-C(61)	113.5(4)	C(84)-C(85)-C(851)	119.0(5)
F(653)-C(651)-C(65)	113.7(4)	C(71)-B(1)-C(81)	102.9(4)	C(86)-C(85)-C(851)	119.8(5)
F(652)-C(651)-C(65)	112.0(4)	C(61)-B(1)-C(81)	111.6(4)	C(34)-C(35)-C(36)	121.9(5)
F(651)-C(651)-C(65)	112.9(4)	C(71)-B(1)-C(91)	113.4(4)	F(954)-F(953)-C(951)	68.1(13)
C(63)-C(64)-C(65)	118.2(4)	C(61)-B(1)-C(91)	104.1(4)	C(21)-C(26)-C(25)	116.6(6)
C(56)-C(51)-C(52)	120.1(5)	C(81)-B(1)-C(91)	111.7(4)	C(21)-C(26)-C(261)	120.6(5)
C(56)-C(51)-C(36)	119.4(5)	C(15)-C(16)-C(11)	116.2(5)	C(25)-C(26)-C(261)	122.8(6)
C(52)-C(51)-C(36)	120.5(5)	C(15)-C(16)-C(161)	120.2(5)	F(833)-C(831)-F(834)	39(4)
C(66)-C(65)-C(64)	120.8(4)	C(11)-C(16)-C(161)	123.6(4)	F(833)-C(831)-F(832)	113.5(7)
C(66)-C(65)-C(651)	118.7(4)	C(14)-C(15)-C(16)	121.8(5)	F(834)-C(831)-F(832)	88(3)
C(64)-C(65)-C(651)	120.5(4)	C(13)-C(14)-C(15)	121.0(5)	F(833)-C(831)-F(831)	96.8(8)
C(26)-C(21)-C(22)	123.7(5)	C(43)-C(42)-C(41)	119.9(6)	F(834)-C(831)-F(831)	132(4)
C(26)-C(21)-N(2)	119.1(5)	C(43)-C(42)-C(421)	117.7(5)	F(832)-C(831)-F(831)	101.7(5)
C(22)-C(21)-N(2)	116.9(5)	C(41)-C(42)-C(421)	122.2(5)	F(833)-C(831)-C(83)	118.0(7)
C(31)-C(32)-C(33)	116.7(5)	C(14)-C(13)-C(12)	121.0(5)	F(834)-C(831)-C(83)	106.4(17)
C(31)-C(32)-C(41)	122.3(5)	C(25)-C(24)-C(23)	120.7(6)	F(832)-C(831)-C(83)	112.6(6)
C(33)-C(32)-C(41)	120.8(5)	C(75)-C(74)-C(73)	119.2(5)	F(831)-C(831)-C(83)	111.9(5)
C(3)-C(2)-N(1)	107.8(4)	C(122)-C(121)-C(12)	110.0(5)	F(853)-C(851)-F(852)	105.3(5)
C(12)-C(11)-C(16)	122.9(4)	C(122)-C(121)-C(123)	110.7(6)	F(853)-C(851)-F(851)	105.0(6)
C(12)-C(11)-N(1)	119.5(4)	C(12)-C(121)-C(123)	113.6(5)	F(852)-C(851)-F(851)	105.4(5)
C(16)-C(11)-N(1)	117.6(4)	C(42)-C(43)-C(44)	120.0(6)	F(853)-C(851)-C(85)	112.2(5)
C(35)-C(34)-C(33)	119.2(6)	C(75)-C(76)-C(71)	123.3(5)	F(852)-C(851)-C(85)	114.7(5)
N(2)-C(1)-N(1)	103.6(4)	C(162)-C(161)-C(16)	112.1(5)	F(851)-C(851)-C(85)	113.4(5)
N(2)-C(1)-Ni(1)	107.7(3)	C(162)-C(161)-C(163)	109.0(5)	C(85)-C(84)-C(83)	118.3(5)
N(1)-C(1)-Ni(1)	148.5(4)	C(16)-C(161)-C(163)	111.3(5)	C(45)-C(46)-C(41)	117.6(6)
C(94)-C(93)-C(92)	121.0(5)	C(11)-C(12)-C(13)	117.0(5)	C(45)-C(46)-C(461)	120.2(6)
C(94)-C(93)-C(931)	119.6(5)	C(11)-C(12)-C(121)	122.1(5)	C(41)-C(46)-C(461)	122.3(5)
C(92)-C(93)-C(931)	119.3(4)	C(13)-C(12)-C(121)	120.8(5)	C(84)-C(83)-C(82)	120.2(5)
C(96)-C(91)-C(92)	115.2(4)	C(53)-C(52)-C(51)	119.2(6)	C(84)-C(83)-C(831)	120.0(5)
C(96)-C(91)-B(1)	123.0(4)	C(53)-C(52)-C(521)	119.0(5)	C(82)-C(83)-C(831)	119.8(5)
C(92)-C(91)-B(1)	121.4(4)	C(51)-C(52)-C(521)	121.8(5)	C(44)-C(45)-C(46)	123.1(6)
C(74)-C(75)-C(76)	119.9(5)	C(24)-C(23)-C(22)	120.7(7)	C(94)-C(95)-C(96)	120.2(5)
C(74)-C(75)-C(751)	120.7(5)	C(45)-C(44)-C(43)	118.8(6)	C(94)-C(95)-C(951)	119.6(5)
C(76)-C(75)-C(751)	119.4(5)	C(45)-C(44)-C(441)	121.7(6)	C(96)-C(95)-C(951)	120.2(5)
C(91)-C(92)-C(93)	121.8(4)	C(43)-C(44)-C(441)	119.5(7)	F(953)-C(951)-F(951)	115.6(12)
C(76)-C(71)-C(72)	115.3(4)	C(24)-C(25)-C(26)	121.7(6)	F(953)-C(951)-F(954)	47(3)
C(76)-C(71)-B(1)	121.3(4)	F(752)-C(751)-F(753)	105.3(7)	F(951)-C(951)-F(954)	78(3)
C(72)-C(71)-B(1)	122.7(4)	F(752)-C(751)-F(751)	107.4(5)	F(953)-C(951)-F(952)	98.8(10)
C(81)-C(82)-C(83)	122.6(5)	F(753)-C(751)-F(751)	106.5(6)	F(951)-C(951)-F(952)	100.5(5)

F(954)-C(951)-F(952)	135(3)	F(733)-C(731)-C(73)	112.8(6)	C(56)-C(55)-C(54)	121.6(6)
F(953)-C(951)-C(95)	114.9(6)	F(932)-C(931)-F(933)	105.3(7)	C(262)-C(261)-C(26)	111.8(6)
F(951)-C(951)-C(95)	112.8(5)	F(932)-C(931)-F(931)	104.5(6)	C(262)-C(261)-C(263)	110.9(8)
F(954)-C(951)-C(95)	109.8(16)	F(933)-C(931)-F(931)	103.5(6)	C(26)-C(261)-C(263)	111.9(8)
F(952)-C(951)-C(95)	112.3(5)	F(932)-C(931)-C(93)	115.2(5)	F(953)-F(954)-C(951)	65(3)
F(732)-C(731)-F(731)	104.5(7)	F(933)-C(931)-C(93)	112.8(6)	F(953)-F(954)-F(951)	107(3)
F(732)-C(731)-F(733)	105.6(7)	F(931)-C(931)-C(93)	114.4(5)	C(951)-F(954)-F(951)	50.6(12)
F(731)-C(731)-F(733)	103.0(6)	C(55)-C(56)-C(51)	118.9(5)	F(833)-F(834)-C(831)	70(3)
F(732)-C(731)-C(73)	115.0(5)	C(55)-C(56)-C(561)	119.6(6)	C(42)-C(421)-Ni(1)	102.4(4)
F(731)-C(731)-C(73)	114.7(7)	C(51)-C(56)-C(561)	121.5(5)		

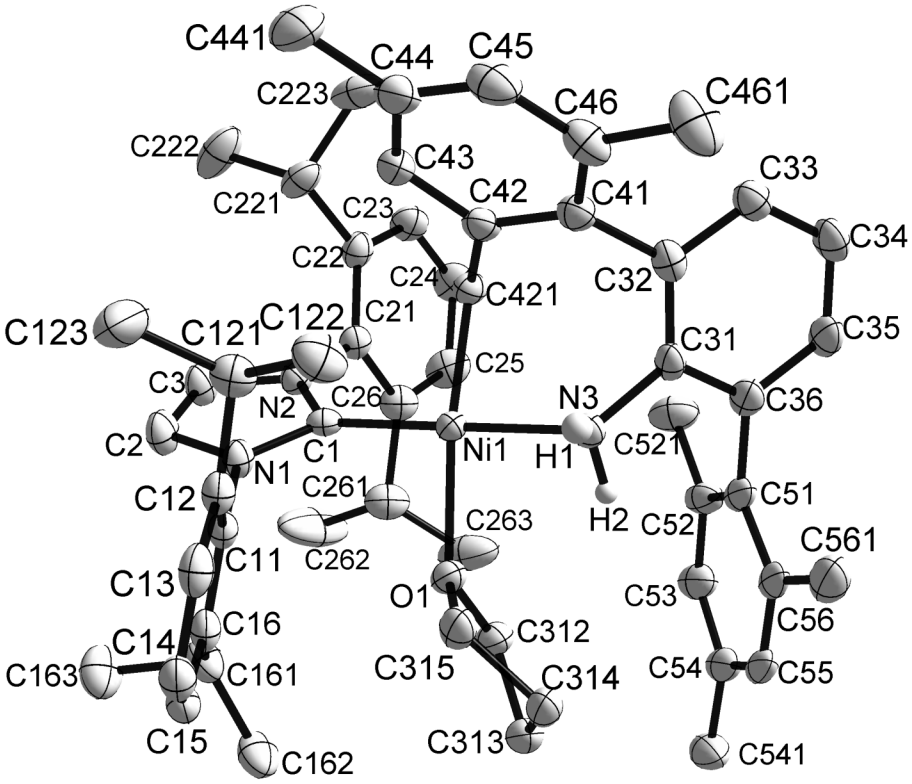
[(IPr)Ni(THF)(κ^2-*C*,*N*:$NH_2C_6H_3(Mes)C_{10}H_9$)][$B(Ar^F)_4$] (8)

The space group was determined as P-1 based on systematic absences and intensity statistics. Patterson method was used to locate Ni. Direct methods were used to locate B, C, F, N and O atoms. All non-hydrogen atoms were converted to and refined anisotropically. The amine and alkyl hydrogens were located in the difference map and refined isotropically. All hydrogen atoms were refined isotropically and fixed at calculated positions. A trifluoromethyl group exhibited typical disorder and was modeled. A co-crystallized molecule of pentane was also modeled to improve GoF and R1.

Crystal data and structure refinement for **8**:

Identification code	carl131a	Crystal size	0.60 x 0.20 x 0.20 mm^3
Empirical formula	C_{197} H_{204} B_2 F_{48} N_6 Ni_2 O_4	Theta range for data collection	1.33 to 25.00°.
		Index ranges	-17<=h<=17
Formula weight	3770.70		-19<=k<=19
Temperature	100(2) K		-25<=l<=25
Wavelength	0.71073 Å	Reflections collected	45508
Crystal system	Triclinic	Independent reflections	16317 [R(int) = 0.1008]
Space group	P-1	Completeness to theta = 25.00°	99.8 %
Unit cell dimensions	a = 14.7621(15) Å	Absorption correction	Psi-scan
	b = 16.7885(17) Å	Max. and min. transmission	0.9411 and 0.8372
	c = 21.465(2) Å	Refinement method	Full-matrix least-squares on F^2
	α= 102.291(2)°		
	β= 106.901(2)°	Data / restraints / parameters	16317 / 0 / 1229
	γ = 105.812(2)°	Goodness-of-fit on F^2	0.973
Volume	4644.3(8) $Å^3$	Final R indices [I>2sigma(I)]	R1 = 0.0601
Z	1		wR2 = 0.1540
Density (calculated)	1.348 Mg/m^3	R indices (all data)	R1 = 0.0807
Absorption coefficient	0.307 mm^{-1}		wR2 = 0.1626
F(000)	1958	Largest diff. peak and hole	0.716 and -0.507 $e.Å^{-3}$

Fully labeled ORTEP diagram (35%) for **8**:



Bond Distances (Å) for **8:**

Ni(1)-C(1)	1.904(3)	C(31)-C(36)	1.398(4)	C(94)-C(95)	1.376(4)
Ni(1)-C(421)	1.931(3)	C(32)-C(33)	1.388(4)	C(94)-C(93)	1.384(4)
Ni(1)-N(3)	2.001(2)	C(32)-C(41)	1.497(4)	C(92)-C(93)	1.381(4)
Ni(1)-O(1)	2.0567(19)	C(41)-C(42)	1.403(4)	C(95)-C(951)	1.490(4)
C(13)-C(14)	1.376(4)	C(41)-C(46)	1.407(4)	C(93)-C(931)	1.492(4)
C(13)-C(12)	1.397(4)	C(42)-C(43)	1.396(4)	C(66)-C(65)	1.393(4)
C(11)-C(16)	1.401(4)	C(42)-C(421)	1.490(4)	C(63)-C(62)	1.378(4)
C(11)-C(12)	1.402(4)	C(46)-C(45)	1.390(4)	C(63)-C(64)	1.387(4)
C(11)-N(1)	1.454(4)	C(46)-C(461)	1.514(4)	C(63)-C(631)	1.503(5)
C(12)-C(121)	1.512(4)	C(45)-C(44)	1.380(5)	C(64)-C(65)	1.388(4)
C(121)-C(122)	1.517(4)	C(61)-C(66)	1.389(4)	C(65)-C(651)	1.499(5)
C(121)-C(123)	1.540(5)	C(61)-C(62)	1.406(4)	C(72)-C(73)	1.391(4)
C(16)-C(15)	1.396(4)	C(61)-B(1)	1.644(4)	C(76)-C(75)	1.391(4)
C(16)-C(161)	1.525(4)	O(1)-C(312)	1.460(3)	C(75)-C(74)	1.378(5)
C(15)-C(14)	1.384(4)	O(1)-C(315)	1.473(3)	C(75)-C(751)	1.482(5)
N(3)-C(31)	1.455(4)	C(71)-C(76)	1.394(4)	C(73)-C(74)	1.394(5)
N(2)-C(1)	1.375(4)	C(71)-C(72)	1.403(4)	C(73)-C(731)	1.491(5)
N(2)-C(3)	1.377(4)	C(71)-B(1)	1.641(5)	C(84)-C(85)	1.380(4)
N(2)-C(21)	1.448(4)	C(81)-C(86)	1.401(4)	C(84)-C(83)	1.391(4)
N(1)-C(1)	1.369(3)	C(81)-C(82)	1.403(4)	C(85)-C(86)	1.400(4)
N(1)-C(2)	1.384(4)	C(81)-B(1)	1.638(4)	C(85)-C(851)	1.498(4)
C(21)-C(26)	1.393(4)	C(91)-C(96)	1.391(4)	C(82)-C(83)	1.379(4)
C(21)-C(22)	1.400(4)	C(91)-C(92)	1.399(4)	C(83)-C(831)	1.494(4)
C(3)-C(2)	1.335(4)	C(91)-B(1)	1.651(4)	C(651)-F(651)	1.324(4)
C(31)-C(32)	1.397(4)	C(96)-C(95)	1.401(4)	C(651)-F(652)	1.333(4)

C(651)-F(653)	1.333(4)	C(44)-C(43)	1.380(4)	C(25)-C(26)	1.398(4)
C(831)-F(831)	1.322(4)	C(44)-C(441)	1.503(4)	C(26)-C(261)	1.516(4)
C(831)-F(833)	1.327(4)	C(34)-C(35)	1.375(4)	C(22)-C(221)	1.527(4)
C(831)-F(832)	1.328(4)	C(34)-C(33)	1.381(4)	C(261)-C(263)	1.511(5)
C(851)-F(852)	1.305(4)	C(35)-C(36)	1.389(4)	C(261)-C(262)	1.530(5)
C(851)-F(853)	1.324(4)	C(36)-C(51)	1.494(4)	C(221)-C(223)	1.535(5)
C(851)-F(851)	1.326(4)	C(51)-C(56)	1.403(4)	C(221)-C(222)	1.538(4)
C(731)-F(731)	1.268(6)	C(51)-C(52)	1.403(5)	C(314)-C(315)	1.516(4)
C(731)-F(733)	1.316(4)	C(54)-C(55)	1.384(5)	C(314)-C(313)	1.521(5)
C(731)-F(732)	1.321(4)	C(54)-C(53)	1.391(5)	C(313)-C(312)	1.521(4)
C(731)-F(734)	1.352(13)	C(54)-C(541)	1.514(5)	C(631)-F(633)	1.301(4)
C(751)-F(753)	1.300(5)	C(52)-C(53)	1.386(4)	C(631)-F(632)	1.327(4)
C(751)-F(752)	1.314(5)	C(52)-C(521)	1.511(4)	C(631)-F(631)	1.340(4)
C(751)-F(751)	1.316(10)	C(55)-C(56)	1.390(5)	C(931)-F(932)	1.324(4)
C(751)-F(754)	1.391(7)	C(56)-C(561)	1.516(5)	C(931)-F(931)	1.336(4)
F(732)-F(734)	1.76(3)	C(161)-C(162)	1.524(4)	C(931)-F(933)	1.342(4)
F(731)-F(734)	0.975(15)	C(161)-C(163)	1.534(4)	F(753)-F(751)	1.669(13)
F(951)-C(951)	1.345(4)	C(23)-C(24)	1.380(4)	F(751)-F(754)	1.178(15)
C(951)-F(952)	1.334(4)	C(23)-C(22)	1.383(4)		
C(951)-F(953)	1.339(4)	C(25)-C(24)	1.380(4)		

Bond Angles (°) for **8**:

C(1)-Ni(1)-C(421)	91.74(12)	C(2)-C(3)-N(2)	107.3(3)	C(86)-C(81)-C(82)	115.5(3)
C(1)-Ni(1)-N(3)	177.44(12)	N(1)-C(1)-N(2)	103.2(2)	C(86)-C(81)-B(1)	126.6(3)
C(421)-Ni(1)-N(3)	88.40(12)	N(1)-C(1)-Ni(1)	126.3(2)	C(82)-C(81)-B(1)	117.7(3)
C(1)-Ni(1)-O(1)	95.05(10)	N(2)-C(1)-Ni(1)	130.2(2)	C(96)-C(91)-C(92)	115.8(3)
C(421)-Ni(1)-O(1)	173.17(11)	C(32)-C(31)-C(36)	121.3(3)	C(96)-C(91)-B(1)	124.5(3)
N(3)-Ni(1)-O(1)	84.86(9)	C(32)-C(31)-N(3)	119.7(3)	C(92)-C(91)-B(1)	119.6(3)
C(14)-C(13)-C(12)	122.0(3)	C(36)-C(31)-N(3)	119.0(3)	C(81)-B(1)-C(71)	116.5(3)
C(16)-C(11)-C(12)	123.0(3)	C(33)-C(32)-C(31)	117.7(3)	C(81)-B(1)-C(61)	102.9(2)
C(16)-C(11)-N(1)	117.7(3)	C(33)-C(32)-C(41)	119.8(3)	C(71)-B(1)-C(61)	111.0(2)
C(12)-C(11)-N(1)	119.1(3)	C(31)-C(32)-C(41)	122.4(2)	C(81)-B(1)-C(91)	111.9(2)
C(13)-C(12)-C(11)	116.8(3)	C(42)-C(41)-C(46)	119.5(3)	C(71)-B(1)-C(91)	103.9(2)
C(13)-C(12)-C(121)	119.6(3)	C(42)-C(41)-C(32)	118.9(3)	C(61)-B(1)-C(91)	110.8(2)
C(11)-C(12)-C(121)	123.6(3)	C(46)-C(41)-C(32)	121.2(3)	C(3)-C(2)-N(1)	107.1(3)
C(12)-C(121)-C(122)	111.4(3)	C(43)-C(42)-C(41)	118.8(3)	C(91)-C(96)-C(95)	121.9(3)
C(12)-C(121)-C(123)	110.0(3)	C(43)-C(42)-C(421)	118.2(3)	C(95)-C(94)-C(93)	118.5(3)
C(122)-C(121)-C(123)	110.8(3)	C(41)-C(42)-C(421)	123.0(3)	C(93)-C(92)-C(91)	122.6(3)
C(15)-C(16)-C(11)	117.1(3)	C(42)-C(421)-Ni(1)	112.7(2)	C(94)-C(95)-C(96)	120.6(3)
C(15)-C(16)-C(161)	119.4(3)	C(45)-C(46)-C(41)	119.0(3)	C(94)-C(95)-C(951)	118.4(3)
C(11)-C(16)-C(161)	123.5(3)	C(45)-C(46)-C(461)	118.1(3)	C(96)-C(95)-C(951)	121.0(3)
C(14)-C(15)-C(16)	121.5(3)	C(41)-C(46)-C(461)	122.9(3)	C(92)-C(93)-C(94)	120.5(3)
C(31)-N(3)-Ni(1)	126.04(19)	C(44)-C(45)-C(46)	122.4(3)	C(92)-C(93)-C(931)	121.2(3)
C(1)-N(2)-C(3)	111.2(2)	C(66)-C(61)-C(62)	116.2(3)	C(94)-C(93)-C(931)	118.3(3)
C(1)-N(2)-C(21)	126.8(2)	C(66)-C(61)-B(1)	123.6(3)	C(61)-C(66)-C(65)	122.2(3)
C(3)-N(2)-C(21)	121.5(2)	C(62)-C(61)-B(1)	119.8(3)	C(62)-C(63)-C(64)	120.7(3)
C(1)-N(1)-C(2)	111.2(2)	C(312)-O(1)-C(315)	108.9(2)	C(62)-C(63)-C(631)	120.5(3)
C(1)-N(1)-C(11)	127.5(2)	C(312)-O(1)-Ni(1)	119.21(17)	C(64)-C(63)-C(631)	118.8(3)
C(2)-N(1)-C(11)	121.1(2)	C(315)-O(1)-Ni(1)	122.82(17)	C(63)-C(62)-C(61)	122.1(3)
C(26)-C(21)-C(22)	122.9(3)	C(76)-C(71)-C(72)	115.4(3)	C(63)-C(64)-C(65)	118.6(3)
C(26)-C(21)-N(2)	117.7(3)	C(76)-C(71)-B(1)	121.0(3)	C(64)-C(65)-C(66)	120.2(3)
C(22)-C(21)-N(2)	119.3(2)	C(72)-C(71)-B(1)	123.1(3)	C(64)-C(65)-C(651)	120.8(3)

C(66)-C(65)-C(651)	118.9(3)	F(733)-C(731)-C(73)	112.8(3)	C(51)-C(56)-C(561)	120.0(3)
C(73)-C(72)-C(71)	122.3(3)	F(732)-C(731)-C(73)	112.8(3)	C(162)-C(161)-C(16)	113.3(3)
C(75)-C(76)-C(71)	123.0(3)	F(734)-C(731)-C(73)	109.3(7)	C(162)-C(161)-C(163)	108.6(3)
C(74)-C(75)-C(76)	120.3(3)	F(753)-C(751)-F(752)	101.2(4)	C(16)-C(161)-C(163)	110.1(2)
C(74)-C(75)-C(751)	120.6(3)	F(753)-C(751)-F(751)	79.3(9)	C(24)-C(23)-C(22)	121.0(3)
C(76)-C(75)-C(751)	119.0(3)	F(752)-C(751)-F(751)	127.8(8)	C(24)-C(25)-C(26)	121.3(3)
C(72)-C(73)-C(74)	120.4(3)	F(753)-C(751)-F(754)	123.1(5)	C(21)-C(26)-C(25)	116.9(3)
C(72)-C(73)-C(731)	120.1(3)	F(752)-C(751)-F(754)	90.7(5)	C(21)-C(26)-C(261)	122.7(3)
C(74)-C(73)-C(731)	119.5(3)	F(751)-C(751)-F(754)	51.5(7)	C(25)-C(26)-C(261)	120.3(3)
C(75)-C(74)-C(73)	118.5(3)	F(753)-C(751)-C(75)	113.2(4)	C(23)-C(24)-C(25)	120.2(3)
C(85)-C(84)-C(83)	118.3(3)	F(752)-C(751)-C(75)	113.9(3)	C(23)-C(22)-C(21)	117.7(3)
C(84)-C(85)-C(86)	121.0(3)	F(751)-C(751)-C(75)	113.4(5)	C(23)-C(22)-C(221)	119.8(3)
C(84)-C(85)-C(851)	118.3(3)	F(754)-C(751)-C(75)	111.7(4)	C(21)-C(22)-C(221)	122.5(3)
C(86)-C(85)-C(851)	120.7(3)	C(731)-F(732)-F(734)	49.6(6)	C(263)-C(261)-C(26)	114.2(3)
C(85)-C(86)-C(81)	121.7(3)	F(734)-F(731)-C(731)	72.8(11)	C(263)-C(261)-C(262)	110.1(3)
C(83)-C(82)-C(81)	123.1(3)	F(952)-C(951)-F(953)	107.5(3)	C(26)-C(261)-C(262)	109.2(3)
C(82)-C(83)-C(84)	120.3(3)	F(952)-C(951)-F(951)	105.1(3)	C(22)-C(221)-C(223)	112.1(3)
C(82)-C(83)-C(831)	120.0(3)	F(953)-C(951)-F(951)	106.2(3)	C(22)-C(221)-C(222)	109.7(3)
C(84)-C(83)-C(831)	119.6(3)	F(952)-C(951)-C(95)	112.3(3)	C(223)-C(221)-C(222)	110.3(3)
F(651)-C(651)-F(652)	105.3(3)	F(953)-C(951)-C(95)	113.4(3)	C(315)-C(314)-C(313)	102.2(3)
F(651)-C(651)-F(653)	105.6(3)	F(951)-C(951)-C(95)	111.7(3)	C(314)-C(313)-C(312)	102.7(3)
F(652)-C(651)-F(653)	106.9(3)	C(43)-C(44)-C(45)	117.8(3)	O(1)-C(312)-C(313)	106.0(3)
F(651)-C(651)-C(65)	112.2(3)	C(43)-C(44)-C(441)	121.4(3)	O(1)-C(315)-C(314)	104.7(2)
F(652)-C(651)-C(65)	112.8(3)	C(45)-C(44)-C(441)	120.8(3)	C(13)-C(14)-C(15)	119.6(3)
F(653)-C(651)-C(65)	113.3(3)	C(44)-C(43)-C(42)	122.5(3)	F(633)-C(631)-F(632)	109.1(3)
F(831)-C(831)-F(833)	104.5(3)	C(35)-C(34)-C(33)	119.4(3)	F(633)-C(631)-F(631)	104.5(3)
F(831)-C(831)-F(832)	106.2(3)	C(34)-C(35)-C(36)	121.1(3)	F(632)-C(631)-F(631)	104.7(3)
F(833)-C(831)-F(832)	105.4(3)	C(34)-C(33)-C(32)	121.8(3)	F(633)-C(631)-C(63)	112.3(3)
F(831)-C(831)-C(83)	112.6(3)	C(35)-C(36)-C(31)	118.5(3)	F(632)-C(631)-C(63)	113.9(3)
F(833)-C(831)-C(83)	114.2(3)	C(35)-C(36)-C(51)	120.4(3)	F(631)-C(631)-C(63)	111.6(3)
F(832)-C(831)-C(83)	113.2(3)	C(31)-C(36)-C(51)	121.0(3)	F(932)-C(931)-F(931)	105.5(3)
F(852)-C(851)-F(853)	106.8(3)	C(56)-C(51)-C(52)	119.8(3)	F(932)-C(931)-F(933)	106.5(3)
F(852)-C(851)-F(851)	106.2(3)	C(56)-C(51)-C(36)	121.0(3)	F(931)-C(931)-F(933)	104.8(3)
F(853)-C(851)-F(851)	103.7(3)	C(52)-C(51)-C(36)	119.2(3)	F(932)-C(931)-C(93)	114.0(3)
F(852)-C(851)-C(85)	114.6(3)	C(55)-C(54)-C(53)	118.6(3)	F(931)-C(931)-C(93)	112.4(3)
F(853)-C(851)-C(85)	112.7(3)	C(55)-C(54)-C(541)	121.8(3)	F(933)-C(931)-C(93)	112.9(3)
F(851)-C(851)-C(85)	112.1(3)	C(53)-C(54)-C(541)	119.7(4)	C(751)-F(753)-F(751)	50.8(7)
F(731)-C(731)-F(733)	96.9(9)	C(53)-C(52)-C(51)	119.3(3)	F(754)-F(751)-C(751)	67.5(10)
F(731)-C(731)-F(732)	115.5(8)	C(53)-C(52)-C(521)	119.8(3)	F(754)-F(751)-F(753)	111.2(9)
F(733)-C(731)-F(732)	100.4(3)	C(51)-C(52)-C(521)	120.9(3)	C(751)-F(751)-F(753)	49.9(4)
F(731)-C(731)-F(734)	43.5(8)	C(52)-C(53)-C(54)	121.5(3)	F(731)-F(734)-C(731)	63.6(7)
F(733)-C(731)-F(734)	132.5(12)	C(54)-C(55)-C(56)	121.7(3)	F(731)-F(734)-F(732)	102.6(13)
F(732)-C(731)-F(734)	82.4(13)	C(55)-C(56)-C(51)	119.1(3)	C(731)-F(734)-F(732)	48.1(8)
F(731)-C(731)-C(73)	116.2(4)	C(55)-C(56)-C(561)	120.8(3)	F(751)-F(754)-C(751)	61.0(5)

[(IPr)Ni(NHdippp)][B(Ar^{F})$_4$] (9)

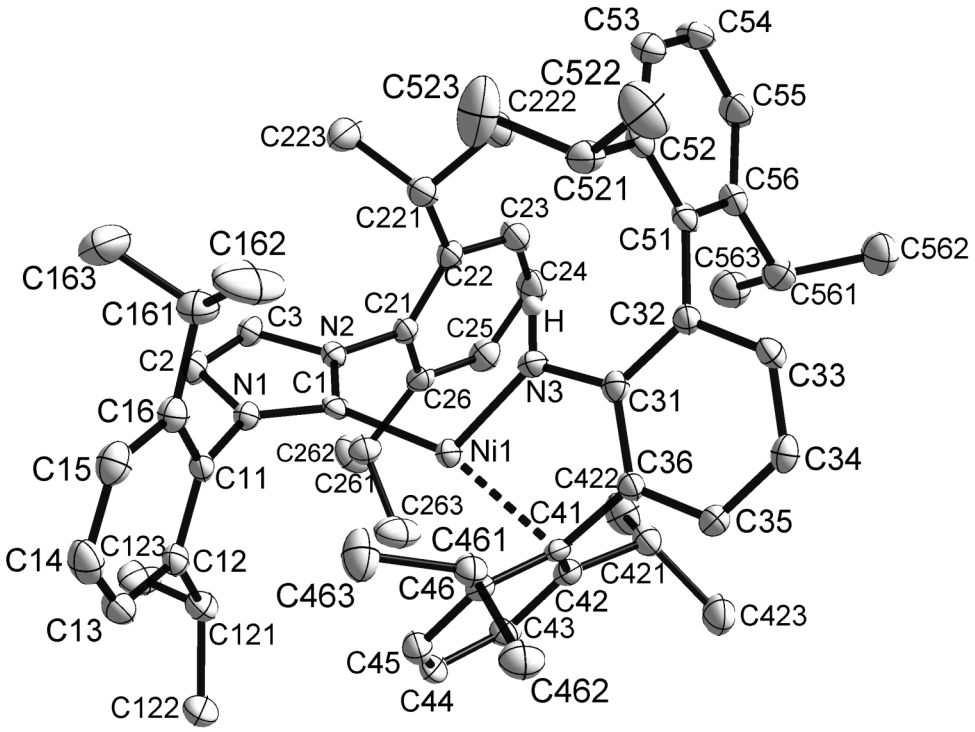
The space group was determined as P(2)1/c based on systematic absences and intensity statistics. Patterson method was used to locate Ni. Direct methods were used to locate B, C, F, N

and O atoms. All non-hydrogen atoms were converted to and refined anisotropically. The amide hydrogen was located in the difference map and refined isotropically.

Crystal data and structure refinement for **9**:

Identification code	carl48a	Theta range for data collection	1.57 to 28.28°.
Empirical formula	C_{93} H_{96} B F_{24} N_3 Ni O	Index ranges	-12<=h<=16
Formula weight	1797.25		-24<=k<=25
Temperature	100(2) K		-45<=l<=45
Wavelength	0.71073 Å	Reflections collected	55707
Crystal system	Monoclinic	Independent reflections	20189 [R(int) = 0.0721]
Space group	P2(1)/c	Completeness to theta = 25.00°	99.7 %
Unit cell dimensions	a = 12.7476(12) Å	Absorption correction	None
	b = 20.1891(19) Å	Max. and min. transmission	0.2793 and 0.2075
	c = 33.921(3) Å	Refinement method	Full-matrix least-squares on F^2
	α= 90°		
	β= 90.696(2)°	Data / restraints / parameters	20189 / 0 / 1112
	γ = 90°	Goodness-of-fit on F^2	0.885
Volume	8729.4(14) $Å^3$	Final R indices [I>2sigma(I)]	R1 = 0.0541
Z	4		wR2 = 0.1104
Density (calculated)	1.368 Mg/m^3	R indices (all data)	R1 = 0.0884
Absorption coefficient	0.322 mm^{-1}		wR2 = 0.1196
F(000)	3728	Largest diff. peak and hole	0.735 and -0.503 $e.Å^{-3}$
Crystal size	0.6 x 0.2 x 0.2 mm^3		

Fully labeled ORTEP diagram (35%) for **9**:



Bond Distances (Å) for **9:**

Ni(1)-N(3)	1.854(2)	C(53)-C(52)	1.392(3)	C(95)-C(96)	1.390(3)
Ni(1)-C(1)	2.003(2)	C(66)-C(65)	1.388(3)	C(95)-C(951)	1.489(3)
Ni(1)-C(41)	2.240(2)	C(66)-C(61)	1.403(3)	C(73)-C(74)	1.386(3)
Ni(1)-C(46)	2.484(2)	C(11)-C(16)	1.399(3)	C(73)-C(731)	1.496(3)
F(853)-C(851)	1.346(3)	C(11)-C(12)	1.406(3)	F(931)-C(931)	1.326(3)
F(633)-C(631)	1.338(3)	C(51)-C(56)	1.407(3)	C(63)-C(64)	1.384(3)
F(632)-C(631)	1.347(3)	C(51)-C(52)	1.408(3)	C(731)-F(731)	1.297(3)
F(852)-C(851)	1.336(3)	C(51)-C(32)	1.494(3)	C(43)-C(44)	1.381(3)
F(851)-C(851)	1.339(3)	C(62)-C(63)	1.391(3)	C(74)-C(75)	1.388(3)
F(631)-C(631)	1.347(3)	C(62)-C(61)	1.398(3)	C(84)-C(83)	1.391(3)
N(1)-C(1)	1.363(3)	C(71)-C(76)	1.397(3)	C(45)-C(44)	1.383(3)
N(1)-C(2)	1.384(3)	C(71)-C(72)	1.400(3)	C(13)-C(14)	1.377(3)
N(1)-C(11)	1.446(3)	C(71)-B(1)	1.650(3)	C(651)-F(651)	1.303(3)
N(3)-C(31)	1.382(3)	C(93)-C(94)	1.390(3)	C(521)-C(522)	1.517(3)
C(81)-C(86)	1.397(3)	C(93)-C(92)	1.396(3)	C(521)-C(523)	1.532(3)
C(81)-C(82)	1.410(3)	C(93)-C(931)	1.491(3)	C(75)-C(76)	1.381(3)
C(81)-B(1)	1.638(3)	C(86)-C(85)	1.385(3)	C(75)-C(751)	1.496(3)
N(2)-C(1)	1.367(3)	C(22)-C(23)	1.393(3)	C(16)-C(15)	1.391(3)
N(2)-C(3)	1.386(3)	C(22)-C(221)	1.529(3)	C(16)-C(161)	1.517(3)
N(2)-C(21)	1.448(3)	C(42)-C(43)	1.402(3)	C(54)-C(55)	1.381(3)
F(733)-C(731)	1.318(3)	C(42)-C(421)	1.515(3)	C(421)-C(422)	1.527(3)
F(933)-C(931)	1.322(3)	C(72)-C(73)	1.387(3)	C(421)-C(423)	1.540(3)
C(46)-C(45)	1.403(3)	F(932)-C(931)	1.331(3)	C(83)-C(831)	1.499(3)
C(46)-C(41)	1.418(3)	C(32)-C(33)	1.399(3)	C(56)-C(55)	1.395(3)
C(46)-C(461)	1.519(3)	C(32)-C(31)	1.414(3)	C(56)-C(561)	1.524(3)
C(21)-C(26)	1.393(3)	C(52)-C(521)	1.515(3)	C(25)-C(24)	1.385(3)
C(21)-C(22)	1.401(3)	C(3)-C(2)	1.333(3)	C(24)-C(23)	1.372(4)
F(953)-C(951)	1.353(3)	C(65)-C(64)	1.385(3)	F(831)-C(831)	1.337(3)
F(653)-C(651)	1.324(3)	C(65)-C(651)	1.496(3)	F(751)-C(751)	1.330(3)
C(91)-C(92)	1.394(3)	C(85)-C(84)	1.380(3)	F(832)-C(831)	1.346(3)
C(91)-C(96)	1.399(3)	C(85)-C(851)	1.504(3)	F(833)-C(831)	1.338(3)
C(91)-B(1)	1.647(3)	C(12)-C(13)	1.389(3)	F(752)-C(751)	1.320(3)
C(35)-C(36)	1.381(3)	C(12)-C(121)	1.526(3)	F(753)-C(751)	1.321(3)
C(35)-C(34)	1.388(3)	C(82)-C(83)	1.381(3)	C(461)-C(463)	1.517(3)
C(36)-C(31)	1.415(3)	F(732)-C(731)	1.300(3)	C(461)-C(462)	1.532(3)
C(36)-C(41)	1.500(3)	C(26)-C(25)	1.389(3)	C(122)-C(121)	1.542(3)
F(952)-C(951)	1.315(3)	C(26)-C(261)	1.528(3)	C(121)-C(123)	1.534(3)
C(41)-C(42)	1.420(3)	C(61)-B(1)	1.639(3)	C(561)-C(563)	1.522(3)
C(34)-C(33)	1.382(3)	C(221)-C(222)	1.514(3)	C(561)-C(562)	1.531(3)
F(951)-C(951)	1.321(3)	C(221)-C(223)	1.544(3)	C(14)-C(15)	1.378(3)
F(652)-C(651)	1.340(3)	C(261)-C(262)	1.516(3)	C(161)-C(162)	1.520(4)
C(631)-C(63)	1.491(3)	C(261)-C(263)	1.527(3)	C(161)-C(163)	1.534(4)
C(53)-C(54)	1.377(4)	C(95)-C(94)	1.387(3)		

Bond Angles (°) for **9**:

N(3)-Ni(1)-C(1)	116.57(9)	C(1)-Ni(1)-C(46)	132.28(9)	C(2)-N(1)-C(11)	119.36(19)
N(3)-Ni(1)-C(41)	81.16(8)	C(41)-Ni(1)-C(46)	34.45(8)	C(31)-N(3)-Ni(1)	121.95(16)
C(1)-Ni(1)-C(41)	162.17(8)	C(1)-N(1)-C(2)	111.5(2)	C(86)-C(81)-C(82)	114.9(2)
N(3)-Ni(1)-C(46)	101.03(8)	C(1)-N(1)-C(11)	129.04(19)	C(86)-C(81)-B(1)	124.05(19)

C(82)-C(81)-B(1)	120.9(2)	C(21)-C(22)-C(221)	121.4(2)	F(931)-C(931)-C(93)	112.3(2)
C(1)-N(2)-C(3)	112.0(2)	C(43)-C(42)-C(41)	117.8(2)	F(932)-C(931)-C(93)	112.1(2)
C(1)-N(2)-C(21)	126.64(18)	C(43)-C(42)-C(421)	120.8(2)	C(64)-C(63)-C(62)	120.8(2)
C(3)-N(2)-C(21)	121.24(19)	C(41)-C(42)-C(421)	121.1(2)	C(64)-C(63)-C(631)	120.5(2)
C(45)-C(46)-C(41)	118.0(2)	C(73)-C(72)-C(71)	122.4(2)	C(62)-C(63)-C(631)	118.8(2)
C(45)-C(46)-C(461)	121.1(2)	C(33)-C(32)-C(31)	118.3(2)	F(731)-C(731)-F(732)	106.2(2)
C(41)-C(46)-C(461)	120.60(19)	C(33)-C(32)-C(51)	118.31(19)	F(731)-C(731)-F(733)	105.6(2)
C(45)-C(46)-Ni(1)	93.67(15)	C(31)-C(32)-C(51)	123.0(2)	F(732)-C(731)-F(733)	104.6(2)
C(41)-C(46)-Ni(1)	63.29(12)	N(3)-C(31)-C(32)	125.0(2)	F(731)-C(731)-C(73)	113.2(2)
C(461)-C(46)-Ni(1)	116.94(14)	N(3)-C(31)-C(36)	115.70(19)	F(732)-C(731)-C(73)	112.7(2)
N(1)-C(1)-N(2)	102.80(18)	C(32)-C(31)-C(36)	119.3(2)	F(733)-C(731)-C(73)	113.8(2)
N(1)-C(1)-Ni(1)	130.47(17)	C(34)-C(33)-C(32)	121.6(2)	C(44)-C(43)-C(42)	121.5(2)
N(2)-C(1)-Ni(1)	126.59(17)	C(53)-C(52)-C(51)	118.1(2)	C(73)-C(74)-C(75)	118.0(2)
C(26)-C(21)-C(22)	123.6(2)	C(53)-C(52)-C(521)	120.3(2)	C(95)-C(96)-C(91)	122.8(2)
C(26)-C(21)-N(2)	118.0(2)	C(51)-C(52)-C(521)	121.5(2)	C(63)-C(64)-C(65)	117.7(2)
C(22)-C(21)-N(2)	118.2(2)	C(2)-C(3)-N(2)	106.2(2)	C(95)-C(94)-C(93)	117.8(2)
C(92)-C(91)-C(96)	115.5(2)	C(64)-C(65)-C(66)	121.3(2)	C(85)-C(84)-C(83)	117.9(2)
C(92)-C(91)-B(1)	122.2(2)	C(64)-C(65)-C(651)	120.2(2)	F(852)-C(851)-F(851)	107.0(2)
C(96)-C(91)-B(1)	122.23(19)	C(66)-C(65)-C(651)	118.5(2)	F(852)-C(851)-F(853)	106.26(19)
C(36)-C(35)-C(34)	119.8(2)	C(84)-C(85)-C(86)	121.1(2)	F(851)-C(851)-F(853)	105.33(19)
C(35)-C(36)-C(31)	120.7(2)	C(84)-C(85)-C(851)	120.1(2)	F(852)-C(851)-C(85)	113.2(2)
C(35)-C(36)-C(41)	123.08(19)	C(86)-C(85)-C(851)	118.8(2)	F(851)-C(851)-C(85)	112.66(19)
C(31)-C(36)-C(41)	116.18(19)	C(13)-C(12)-C(11)	116.4(2)	F(853)-C(851)-C(85)	111.8(2)
C(46)-C(41)-C(42)	121.1(2)	C(13)-C(12)-C(121)	121.3(2)	F(952)-C(951)-F(951)	108.0(2)
C(46)-C(41)-C(36)	119.8(2)	C(11)-C(12)-C(121)	122.3(2)	F(952)-C(951)-F(953)	104.3(2)
C(42)-C(41)-C(36)	119.1(2)	C(83)-C(82)-C(81)	122.7(2)	F(951)-C(951)-F(953)	103.7(2)
C(46)-C(41)-Ni(1)	82.26(13)	C(25)-C(26)-C(21)	116.8(2)	F(952)-C(951)-C(95)	113.7(2)
C(42)-C(41)-Ni(1)	84.20(13)	C(25)-C(26)-C(261)	121.9(2)	F(951)-C(951)-C(95)	114.1(2)
C(36)-C(41)-Ni(1)	104.55(13)	C(21)-C(26)-C(261)	121.3(2)	F(953)-C(951)-C(95)	112.1(2)
C(33)-C(34)-C(35)	120.2(2)	C(62)-C(61)-C(66)	115.4(2)	C(44)-C(45)-C(46)	121.3(2)
F(633)-C(631)-F(632)	106.8(2)	C(62)-C(61)-B(1)	122.05(19)	C(43)-C(44)-C(45)	120.2(2)
F(633)-C(631)-F(631)	106.43(19)	C(66)-C(61)-B(1)	122.5(2)	C(14)-C(13)-C(12)	121.7(2)
F(632)-C(631)-F(631)	105.36(19)	C(222)-C(221)-C(22)	113.4(2)	F(651)-C(651)-F(653)	108.4(2)
F(633)-C(631)-C(63)	113.3(2)	C(222)-C(221)-C(223)	108.1(2)	F(651)-C(651)-F(652)	105.7(2)
F(632)-C(631)-C(63)	112.38(19)	C(22)-C(221)-C(223)	111.1(2)	F(653)-C(651)-F(652)	104.2(2)
F(631)-C(631)-C(63)	112.1(2)	C(262)-C(261)-C(263)	110.7(2)	F(651)-C(651)-C(65)	113.0(2)
C(54)-C(53)-C(52)	121.4(2)	C(262)-C(261)-C(26)	113.3(2)	F(653)-C(651)-C(65)	113.5(2)
C(65)-C(66)-C(61)	122.1(2)	C(263)-C(261)-C(26)	110.9(2)	F(652)-C(651)-C(65)	111.5(2)
C(16)-C(11)-C(12)	123.2(2)	C(94)-C(95)-C(96)	120.6(2)	C(52)-C(521)-C(522)	111.3(2)
C(16)-C(11)-N(1)	117.5(2)	C(94)-C(95)-C(951)	120.4(2)	C(52)-C(521)-C(523)	112.4(2)
C(12)-C(11)-N(1)	118.8(2)	C(96)-C(95)-C(951)	119.0(2)	C(522)-C(521)-C(523)	109.2(2)
C(56)-C(51)-C(52)	120.8(2)	C(74)-C(73)-C(72)	120.7(2)	C(76)-C(75)-C(74)	120.7(2)
C(56)-C(51)-C(32)	117.8(2)	C(74)-C(73)-C(731)	120.0(2)	C(76)-C(75)-C(751)	119.7(2)
C(52)-C(51)-C(32)	121.2(2)	C(72)-C(73)-C(731)	119.3(2)	C(74)-C(75)-C(751)	119.5(2)
C(63)-C(62)-C(61)	122.7(2)	C(3)-C(2)-N(1)	107.4(2)	C(15)-C(16)-C(11)	117.3(2)
C(76)-C(71)-C(72)	115.4(2)	C(81)-B(1)-C(61)	111.91(18)	C(15)-C(16)-C(161)	119.7(2)
C(76)-C(71)-B(1)	124.07(19)	C(81)-B(1)-C(91)	113.15(18)	C(11)-C(16)-C(161)	123.0(2)
C(72)-C(71)-B(1)	120.49(19)	C(61)-B(1)-C(91)	105.26(18)	C(53)-C(54)-C(55)	120.2(2)
C(94)-C(93)-C(92)	120.9(2)	C(81)-B(1)-C(71)	105.60(18)	C(75)-C(76)-C(71)	122.7(2)
C(94)-C(93)-C(931)	120.8(2)	C(61)-B(1)-C(71)	111.60(18)	C(42)-C(421)-C(422)	114.0(2)
C(92)-C(93)-C(931)	118.2(2)	C(91)-B(1)-C(71)	109.43(18)	C(42)-C(421)-C(423)	108.6(2)
C(91)-C(92)-C(93)	122.3(2)	F(933)-C(931)-F(931)	106.1(2)	C(422)-C(421)-C(423)	110.8(2)
C(85)-C(86)-C(81)	122.7(2)	F(933)-C(931)-F(932)	106.2(2)	C(82)-C(83)-C(84)	120.7(2)
C(23)-C(22)-C(21)	116.7(2)	F(931)-C(931)-F(932)	105.9(2)	C(82)-C(83)-C(831)	121.3(2)
C(23)-C(22)-C(221)	121.8(2)	F(933)-C(931)-C(93)	113.6(2)	C(84)-C(83)-C(831)	118.0(2)

C(55)-C(56)-C(51)	118.7(2)	F(752)-C(751)-F(753)	107.8(2)	C(14)-C(15)-C(16)	120.9(2)
C(55)-C(56)-C(561)	119.0(2)	F(752)-C(751)-F(751)	105.1(2)	C(16)-C(161)-C(162)	111.9(2)
C(51)-C(56)-C(561)	122.3(2)	F(753)-C(751)-F(751)	105.0(2)	C(16)-C(161)-C(163)	109.9(2)
C(24)-C(25)-C(26)	120.9(2)	F(752)-C(751)-C(75)	112.3(2)	C(162)-C(161)-C(163)	110.3(2)
C(23)-C(24)-C(25)	120.8(2)	F(753)-C(751)-C(75)	113.4(2)	F(831)-C(831)-F(833)	107.1(2)
C(463)-C(461)-C(46)	113.23(19)	F(751)-C(751)-C(75)	112.6(2)	F(831)-C(831)-F(832)	105.5(2)
C(463)-C(461)-C(462)	110.8(2)	C(563)-C(561)-C(56)	111.3(2)	F(833)-C(831)-F(832)	106.2(2)
C(46)-C(461)-C(462)	109.83(18)	C(563)-C(561)-C(562)	111.4(2)	F(831)-C(831)-C(83)	111.8(2)
C(12)-C(121)-C(123)	111.4(2)	C(56)-C(561)-C(562)	111.4(2)	F(833)-C(831)-C(83)	113.3(2)
C(12)-C(121)-C(122)	112.7(2)	C(24)-C(23)-C(22)	120.9(2)	F(832)-C(831)-C(83)	112.5(2)
C(123)-C(121)-C(122)	108.34(19)	C(13)-C(14)-C(15)	120.5(2)	C(54)-C(55)-C(56)	120.7(2)

(IV) Computational Methods

All simulations employed the Gaussian 09 suite of programs.[7] DFT geometry optimizations were initiated from the experimental X-ray coordinates of **4**, **5**, **7** and **9**. The initial guess geometry of complexes $\mathbf{4}^+$ and $\mathbf{5}^+$ were generated from the DFT-optimized geometries of **4** and **5**, respectively, by removal of an electron followed by reoptimization of the geometry at the same level of theory. Singlet and triplet states were evaluated for **7** and **9**, doublets for **4** and **5**, and singlets for $\mathbf{4}^+$ and $\mathbf{5}^+$. Cartesian coordinates are given in Table S-2.

For these full complex models (disregarding the counterion for cationic species for $\mathbf{4}^+$, **7** and **9**), the level of theory employed was B3LYP/6-31G(d). Given the potential non-innocence of the ligands vis-à-vis C-H activation we chose to model all atoms quantum mechanically. All complexes were verified as minima at this level of theory via the calculation of the vibrational frequencies and the absence of any imaginary frequencies. Free energy data was calculated using unscaled vibrational frequencies and determined at 1 atm and 298.15 K.

Table S-1. B3LYP/6-31G(d) calculated free energies (in Hartrees).

Complex	Calculated Free Energy (G)
4	-3652.339401
7S	-3652.161479
$\mathbf{4}^+$	-3652.147721
7T	-3652.160772
5	-3888.021902
9T	-3887.859367
$\mathbf{5}^+$	-3887.835503
9S	-3887.839829

Table S-2. Cartesian coordinates (Å) of B3LYP/6-31G(d) optimized complexes discussed in the text. The first column denotes the atomic number of the atomic center. Spin state is denoted.

4 (S = ½)

28	-0.438471000	-0.107995000	0.738042000
7	-1.965284000	-0.613759000	-1.813161000
6	-2.235378000	1.364450000	-2.741643000
1	-2.447257000	2.222093000	-3.359616000
6	-1.205221000	2.768927000	-0.981712000
6	-0.076499000	-0.516263000	2.734922000
7	1.472050000	-0.104020000	0.574777000
6	3.588779000	-0.718329000	1.762005000
7	-1.623461000	1.485771000	-1.498474000
6	-0.649715000	0.641169000	3.368836000
6	1.399347000	-0.761115000	2.841711000
6	-1.433362000	0.262932000	-0.894793000
6	4.142819000	-1.164588000	2.967998000
1	5.221020000	-1.307883000	3.015056000
6	1.984627000	-1.208378000	4.021791000
1	1.353524000	-1.390985000	4.890019000
6	-2.446880000	0.044218000	-2.941712000
1	-2.889470000	-0.489314000	-3.767542000
6	2.177456000	-0.518773000	1.675509000
6	-1.639214000	4.722951000	0.345591000
1	-2.265946000	5.285661000	1.029556000
6	-0.975965000	-2.869444000	-1.893570000
6	-2.011253000	0.677258000	3.638023000
1	-2.418697000	1.541190000	4.160314000
6	-2.062061000	3.466645000	-0.103243000
6	0.389190000	-2.279523000	-2.241144000
1	0.501589000	-1.369290000	-1.643493000
6	-3.380927000	-2.570280000	-1.395335000
6	3.365120000	-1.417021000	4.099210000
1	3.824928000	-1.759351000	5.021815000
6	0.887791000	2.602842000	-2.472836000
1	0.526295000	1.575515000	-2.576432000
6	-2.101162000	-2.045625000	-1.669240000
6	0.470890000	-1.905028000	-3.736639000
1	-0.296930000	-1.181048000	-4.025980000
1	0.349592000	-2.795606000	-4.365763000
1	1.449193000	-1.464790000	-3.963035000
6	0.378267000	4.575587000	-0.968303000
1	1.311734000	5.018827000	-1.301814000
6	0.009090000	3.311587000	-1.446002000

6	1.566908000	-3.193093000	-1.871843000
1	1.506089000	-3.530399000	-0.832644000
1	2.505977000	-2.643221000	-1.990062000
1	1.623522000	-4.078008000	-2.517827000
6	2.357756000	2.520110000	-2.030935000
1	2.442195000	2.047939000	-1.049715000
1	2.825558000	3.510063000	-1.975275000
1	2.936093000	1.926068000	-2.747347000
6	-2.338642000	-1.480216000	2.643039000
1	-2.973253000	-2.332306000	2.406388000
6	-3.510733000	-3.964283000	-1.330565000
1	-4.483669000	-4.399629000	-1.121218000
6	-0.963383000	-1.553648000	2.286611000
6	-1.166131000	-4.253526000	-1.814718000
1	-0.323589000	-4.917516000	-1.973484000
6	-0.429862000	5.270470000	-0.075760000
1	-0.122324000	6.247483000	0.287736000
6	-3.434039000	2.921108000	0.286981000
1	-3.378403000	1.828091000	0.252824000
6	-2.873960000	-0.395875000	3.315788000
6	-4.619618000	-1.694600000	-1.212567000
1	-4.297114000	-0.650303000	-1.168318000
6	0.245387000	1.773060000	3.818218000
1	0.866405000	1.476401000	4.671672000
1	-0.347105000	2.644822000	4.115114000
1	0.931115000	2.075325000	3.019886000
6	-2.417662000	-4.798051000	-1.535335000
1	-2.539127000	-5.876729000	-1.480525000
6	-5.362571000	-1.990835000	0.102555000
1	-4.704153000	-1.853117000	0.964170000
1	-5.753788000	-3.014294000	0.130883000
1	-6.215548000	-1.310844000	0.212476000
6	0.768968000	3.280621000	-3.853843000
1	-0.265953000	3.294500000	-4.214203000
1	1.377258000	2.747691000	-4.594028000
1	1.120336000	4.318483000	-3.814757000
6	-0.415715000	-2.905474000	1.869028000
1	-0.222012000	-3.526882000	2.754067000
1	0.527148000	-2.811650000	1.327094000
1	-1.131005000	-3.438055000	1.234333000
6	-5.576575000	-1.836031000	-2.414479000
1	-5.082921000	-1.584868000	-3.359699000
1	-6.439835000	-1.170616000	-2.296396000
1	-5.953355000	-2.861909000	-2.501464000
6	-4.332089000	-0.342086000	3.706333000

1	-4.875724000	0.426694000	3.140426000
1	-4.452740000	-0.097606000	4.769171000
1	-4.830762000	-1.299788000	3.525167000
6	-4.504856000	3.372910000	-0.730261000
1	-5.485723000	2.962819000	-0.461125000
1	-4.269806000	3.040462000	-1.746310000
1	-4.588626000	4.466339000	-0.744565000
6	-3.867472000	3.310611000	1.709150000
1	-3.103182000	3.048609000	2.445716000
1	-4.789389000	2.779572000	1.972378000
1	-4.079848000	4.382651000	1.795750000
1	2.050743000	-0.034363000	-0.256595000
6	4.484847000	-0.444251000	0.593983000
6	4.848662000	0.884419000	0.278208000
6	5.008947000	-1.503778000	-0.178097000
6	5.691948000	1.128910000	-0.810576000
6	5.846356000	-1.217244000	-1.263532000
6	6.199968000	0.091699000	-1.598798000
1	5.965619000	2.156987000	-1.043566000
1	6.236875000	-2.041809000	-1.858273000
6	4.707271000	-2.945809000	0.166845000
1	4.980879000	-3.612157000	-0.658362000
1	5.268218000	-3.268341000	1.053061000
1	3.649406000	-3.095568000	0.400220000
6	4.362707000	2.036170000	1.129777000
1	4.735526000	1.949421000	2.157445000
1	4.702766000	2.995017000	0.724426000
1	3.269237000	2.056713000	1.193666000
6	7.132680000	0.376672000	-2.753958000
1	6.884830000	1.323231000	-3.247513000
1	8.175971000	0.452396000	-2.417947000
1	7.092643000	-0.417852000	-3.507149000

7S (S = 0)

28	0.052495000	0.025066000	0.035150000
6	2.672699000	-2.326698000	1.980184000
6	-2.118230000	1.814267000	-1.077820000
7	2.415798000	-1.848944000	-0.164572000
7	1.652149000	-1.402901000	1.802972000
6	-3.352685000	1.379640000	-1.588193000
6	-0.133115000	3.373449000	-1.049306000
7	-1.557551000	1.175878000	0.109600000
6	-1.898320000	3.426350000	-2.848300000
6	-4.174572000	0.331213000	-0.899564000
6	0.817392000	-0.870513000	2.858180000

6	-1.390491000	2.859938000	-1.671809000
6	3.152612000	-2.603994000	0.743433000
6	2.627824000	-1.965660000	-1.595853000
6	-3.102957000	2.990431000	-3.395808000
6	1.473255000	-1.099950000	0.480272000
6	1.296596000	0.203910000	3.636852000
6	3.671273000	-1.225676000	-2.193060000
6	3.877235000	-1.402048000	-3.566512000
6	3.092524000	-2.279760000	-4.308735000
6	0.970769000	2.501820000	-0.876232000
6	2.090536000	-3.016738000	-3.686697000
6	-0.802784000	0.132410000	4.867648000
6	0.804791000	-3.788860000	-1.647943000
6	2.156559000	3.011931000	-0.322021000
6	3.584271000	4.893401000	0.599403000
6	4.596907000	-0.307280000	-1.396736000
6	1.839522000	-2.886790000	-2.314961000
6	-4.888272000	0.651970000	0.279301000
6	0.452573000	0.690525000	4.643249000
6	2.284959000	4.348254000	0.055694000
6	-0.545109000	-3.789449000	-2.385762000
6	3.648794000	0.265969000	4.542231000
6	-1.236615000	-0.948978000	4.104729000
6	2.690612000	0.795758000	3.453561000
6	-5.664444000	-0.337391000	0.895003000
6	-5.775801000	-1.627259000	0.368142000
6	-3.828255000	1.986375000	-2.760423000
6	-0.429668000	-1.490076000	3.096710000
6	-0.034649000	4.723476000	-0.640283000
6	1.170769000	5.180602000	-0.097267000
6	5.919240000	-1.028228000	-1.055625000
6	-3.588406000	-1.328782000	-2.748014000
6	-4.283450000	-0.963580000	-1.454760000
6	-6.658712000	-2.663430000	1.022489000
6	-1.188486000	5.698379000	-0.755565000
6	-5.076431000	-1.916631000	-0.807977000
6	-0.903467000	-2.694741000	2.286414000
6	2.689477000	2.334697000	3.439938000
6	-4.874167000	2.051099000	0.861528000
6	4.896214000	1.020778000	-2.117773000
6	1.351755000	-5.225268000	-1.507597000
6	-1.811543000	-2.246696000	1.128325000
6	-1.604809000	-3.762625000	3.144817000
1	-2.310023000	0.647493000	0.560478000
6	0.912349000	1.072212000	-1.278283000

1	2.950551000	-2.695275000	2.954838000
1	-1.275283000	1.910276000	0.766525000
1	-1.334737000	4.216908000	-3.333836000
1	3.936030000	-3.269808000	0.419068000
1	-3.482002000	3.443311000	-4.307059000
1	4.667334000	-0.847835000	-4.062192000
1	3.272191000	-2.398768000	-5.373408000
1	1.502554000	-3.716764000	-4.271893000
1	-1.439062000	0.530249000	5.653188000
1	0.620284000	-3.408836000	-0.638197000
1	3.005754000	2.343234000	-0.204830000
1	4.295508000	4.091922000	0.821612000
1	4.060898000	5.567260000	-0.123539000
1	3.425298000	5.470278000	1.517649000
1	4.099125000	-0.062890000	-0.450661000
1	0.785725000	1.515704000	5.264330000
1	-1.279102000	-4.379961000	-1.825357000
1	-0.466838000	-4.234836000	-3.383490000
1	-0.937782000	-2.774388000	-2.501559000
1	3.706951000	-0.827978000	4.539318000
1	4.659516000	0.658074000	4.384018000
1	3.319375000	0.577117000	5.540079000
1	-2.205761000	-1.391573000	4.310794000
1	3.074181000	0.463494000	2.482885000
1	-6.216566000	-0.083230000	1.797393000
1	-4.785771000	1.667029000	-3.161347000
1	1.240796000	6.220811000	0.214141000
1	5.751565000	-1.943799000	-0.479184000
1	6.570798000	-0.373807000	-0.465578000
1	6.457295000	-1.304841000	-1.969205000
1	-3.573563000	-2.413266000	-2.889717000
1	-2.556910000	-0.962503000	-2.781311000
1	-4.100943000	-0.893437000	-3.614675000
1	-6.259162000	-3.674381000	0.890185000
1	-6.771505000	-2.477782000	2.095446000
1	-7.664964000	-2.654025000	0.583941000
1	-2.153922000	5.224574000	-0.554930000
1	-1.060272000	6.524565000	-0.049781000
1	-1.252959000	6.139356000	-1.757773000
1	-5.157619000	-2.911365000	-1.241789000
1	-0.020663000	-3.171366000	1.846099000
1	3.699218000	2.702995000	3.228264000
1	2.017924000	2.730830000	2.671855000
1	2.390771000	2.753811000	4.407092000
1	-5.603380000	2.138783000	1.671663000

1	-3.897312000	2.333850000	1.275936000
1	-5.120710000	2.801609000	0.102754000
1	3.981602000	1.537848000	-2.424257000
1	5.512861000	0.869053000	-3.010112000
1	5.456875000	1.686320000	-1.451971000
1	2.281997000	-5.247991000	-0.929390000
1	1.559737000	-5.665341000	-2.489309000
1	0.621681000	-5.865972000	-0.999810000
1	-2.134504000	-3.096625000	0.518538000
1	-1.277569000	-1.561081000	0.447456000
1	-2.708760000	-1.733494000	1.492308000
1	-1.805492000	-4.652680000	2.538898000
1	-0.983969000	-4.064144000	3.994607000
1	-2.566688000	-3.413558000	3.535525000
1	1.906915000	0.681759000	-1.480168000
1	0.273463000	0.904480000	-2.156098000

4^{+} (S = 0)

28	-0.808867000	-0.202510000	1.068234000
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6	0.180428000	2.718270000	-0.566995000
6	-0.445848000	-1.380147000	2.750251000
7	1.015720000	-0.346965000	0.851578000
6	2.969162000	-1.855999000	1.296184000
7	-0.955495000	1.922399000	-1.006878000
6	-0.501307000	-0.148457000	3.503528000
6	0.888491000	-2.013607000	2.560696000
6	-1.316323000	0.675796000	-0.570259000
6	3.453068000	-2.899755000	2.099878000
1	4.476165000	-3.228246000	1.937780000
6	1.399307000	-3.048481000	3.336284000
1	0.790532000	-3.484905000	4.124390000
6	-2.491723000	1.245382000	-2.434004000
1	-3.189005000	1.099266000	-3.241985000
6	1.634952000	-1.408956000	1.512268000
6	1.169488000	4.330251000	0.907339000
1	1.110957000	5.002944000	1.755735000
6	-2.064121000	-2.104646000	-2.083638000
6	-1.643914000	0.640508000	3.428989000
1	-1.696629000	1.569440000	3.986430000
6	0.044096000	3.585513000	0.536619000
6	-0.637809000	-1.902101000	-2.587693000
1	-0.279002000	-0.931506000	-2.236030000

6	-4.251493000	-1.212978000	-1.341833000
6	2.694288000	-3.508998000	3.098755000
1	3.112950000	-4.315296000	3.692328000
6	1.454102000	1.872731000	-2.659225000
1	0.576023000	1.226061000	-2.748683000
6	-2.868838000	-1.051665000	-1.594384000
6	-0.629989000	-1.866764000	-4.131583000
1	-1.295459000	-1.088881000	-4.521835000
1	-0.956031000	-2.825289000	-4.550848000
1	0.381807000	-1.665359000	-4.501299000
6	2.448607000	3.420997000	-0.924033000
1	3.373047000	3.385211000	-1.491239000
6	1.356943000	2.650295000	-1.345040000
6	0.349865000	-2.956088000	-2.062988000
1	0.380155000	-2.967524000	-0.968877000
1	1.356992000	-2.726659000	-2.424236000
1	0.102645000	-3.965395000	-2.409829000
6	2.691805000	0.965897000	-2.754225000
1	2.738565000	0.235212000	-1.941847000
1	3.623758000	1.538155000	-2.730324000
1	2.671931000	0.416477000	-3.702310000
6	-2.695401000	-0.995874000	1.966400000
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6	-4.788229000	-2.497879000	-1.496427000
1	-5.844140000	-2.659011000	-1.305773000
6	-1.615541000	-1.892209000	2.118745000
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1	-2.067153000	-4.196297000	-2.585627000
6	2.364004000	4.237850000	0.197325000
1	3.223437000	4.825604000	0.507074000
6	-1.292856000	3.797185000	1.242923000
1	-1.842951000	2.850470000	1.211744000
6	-2.710570000	0.277463000	2.583336000
6	-5.192643000	-0.055610000	-1.006558000
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6	0.689974000	0.315407000	4.289864000
1	1.119966000	-0.500132000	4.878267000
1	0.418445000	1.137080000	4.958378000
1	1.475627000	0.669382000	3.611643000
6	-4.001553000	-3.568603000	-1.910522000
1	-4.442775000	-4.554749000	-2.023775000
6	-6.189619000	-0.383192000	0.122586000
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1	-6.743300000	0.518980000	0.404455000

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1	1.431526000	2.298335000	-4.799736000
1	2.305385000	3.505969000	-3.843639000
6	-1.688799000	-3.295236000	1.580347000
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1	-0.718763000	-3.633113000	1.208829000
1	-2.428933000	-3.379718000	0.781262000
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1	-6.627894000	1.235474000	-2.026764000
1	-6.623891000	-0.435893000	-2.615440000
6	-3.909535000	1.180675000	2.456040000
1	-4.165359000	1.370846000	1.410044000
1	-3.735186000	2.141815000	2.945480000
1	-4.785864000	0.718178000	2.925361000
6	-2.138911000	4.851093000	0.493859000
1	-3.101922000	4.997618000	0.996664000
1	-2.342684000	4.554448000	-0.539927000
1	-1.621216000	5.816550000	0.470276000
6	-1.148594000	4.202935000	2.719355000
1	-0.473834000	3.534173000	3.263709000
1	-2.128300000	4.183098000	3.210384000
1	-0.766217000	5.223649000	2.826122000
1	1.479174000	-0.082698000	-0.011708000
6	3.914588000	-1.231774000	0.315063000
6	4.437398000	0.061188000	0.561885000
6	4.405125000	-1.978602000	-0.781975000
6	5.413851000	0.580034000	-0.293806000
6	5.372086000	-1.410967000	-1.619602000
6	5.899473000	-0.138210000	-1.390066000
1	5.821311000	1.567216000	-0.083732000
1	5.736292000	-1.990900000	-2.465677000
6	3.952769000	-3.396471000	-1.061266000
1	4.033621000	-3.627057000	-2.128820000
1	4.579835000	-4.124635000	-0.530450000
1	2.923592000	-3.576320000	-0.743274000
6	4.000525000	0.875764000	1.758933000
1	4.079939000	0.293775000	2.684567000
1	4.623291000	1.768542000	1.867628000
1	2.957234000	1.200102000	1.666857000
6	6.987679000	0.424596000	-2.274271000
1	6.991104000	1.519608000	-2.263738000
1	7.979103000	0.094855000	-1.937045000
1	6.874410000	0.093837000	-3.312208000

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28	0.731662000	0.555716000	-0.258923000
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7	2.279471000	-2.011671000	-0.019280000
7	0.715167000	-1.965590000	1.456097000
6	-3.109254000	1.986080000	-1.215674000
6	0.420294000	3.245199000	-0.384942000
7	-1.252639000	0.919077000	0.063897000
6	-1.495573000	4.248179000	-1.619474000
6	-4.036772000	0.821260000	-1.026717000
6	-0.457943000	-1.595121000	2.214070000
6	-0.985709000	3.165657000	-0.889670000
6	2.410099000	-3.167801000	0.735340000
6	3.180267000	-1.664741000	-1.099552000
6	-2.782929000	4.213549000	-2.147266000
6	1.228481000	-1.252576000	0.409754000
6	-0.339779000	-0.614051000	3.221492000
6	4.447424000	-1.141596000	-0.766963000
6	5.300447000	-0.809140000	-1.827147000
6	4.914936000	-1.004096000	-3.150345000
6	1.452603000	2.503591000	-1.049622000
6	3.672947000	-1.561157000	-3.443745000
6	-2.728462000	-0.868035000	3.621996000
6	1.466904000	-2.617105000	-2.775601000
6	2.805075000	2.773505000	-0.687746000
6	4.578914000	4.066990000	0.573864000
6	4.938275000	-1.002726000	0.673476000
6	2.777076000	-1.915141000	-2.427343000
6	-4.805657000	0.711719000	0.152975000
6	-1.508929000	-0.258426000	3.908369000
6	3.140570000	3.729278000	0.260815000
6	0.675601000	-1.904060000	-3.886458000
6	1.431022000	-0.538776000	5.013676000
6	-2.803709000	-1.863310000	2.651007000
6	0.997046000	-0.001517000	3.633512000
6	-5.766288000	-0.301410000	0.246453000
6	-5.998191000	-1.201823000	-0.797126000
6	-3.577387000	3.088823000	-1.946676000
6	-1.670826000	-2.258344000	1.927740000
6	0.757029000	4.188187000	0.613956000
6	2.100058000	4.405843000	0.924662000
6	6.006933000	-2.072407000	0.983907000
6	-3.450988000	0.005476000	-3.375182000

6	-4.242870000	-0.089581000	-2.088463000
6	-7.082614000	-2.248862000	-0.698412000
6	-0.305333000	4.988023000	1.338021000
6	-5.216402000	-1.083830000	-1.950886000
6	-1.771570000	-3.404295000	0.922382000
6	0.972765000	1.537726000	3.629241000
6	-4.636703000	1.686750000	1.297614000
6	5.471196000	0.404193000	0.994853000
6	1.737157000	-4.089186000	-3.153649000
6	-2.866021000	-3.178301000	-0.133388000
6	-1.990160000	-4.745560000	1.654291000
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6	1.136280000	1.433281000	-1.991259000
1	1.170769000	-3.827657000	2.457848000
1	-1.352149000	1.097284000	1.068145000
1	-0.859275000	5.112101000	-1.786785000
1	3.183872000	-3.892718000	0.538525000
1	-3.162700000	5.056662000	-2.716689000
1	6.285091000	-0.405277000	-1.612370000
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1	3.399536000	-1.736104000	-4.479511000
1	-3.619539000	-0.579993000	4.172409000
1	0.833069000	-2.620278000	-1.883206000
1	3.589749000	2.242018000	-1.220958000
1	5.272141000	3.518537000	-0.069702000
1	4.766564000	5.137939000	0.433418000
1	4.827961000	3.833258000	1.616358000
1	4.092476000	-1.180884000	1.345448000
1	-1.458111000	0.489353000	4.694130000
1	-0.282184000	-2.412260000	-4.045165000
1	1.208734000	-1.914319000	-4.843343000
1	0.471461000	-0.861373000	-3.623905000
1	1.493150000	-1.632322000	5.017089000
1	2.415860000	-0.141289000	5.282830000
1	0.724286000	-0.242128000	5.796745000
1	-3.755981000	-2.344870000	2.453424000
1	1.755759000	-0.315896000	2.910153000
1	-6.367916000	-0.371024000	1.150442000
1	-4.585561000	3.053331000	-2.349302000
1	2.349797000	5.140298000	1.687284000
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1	6.896914000	-1.933892000	0.359949000
1	-3.636387000	-0.866293000	-4.009309000
1	-2.371615000	0.068106000	-3.192787000

1	-3.721293000	0.897901000	-3.952103000
1	-6.783527000	-3.186030000	-1.179963000
1	-7.339225000	-2.466522000	0.343245000
1	-8.000775000	-1.910292000	-1.195629000
1	-1.187961000	4.383891000	1.571249000
1	0.089148000	5.394427000	2.273969000
1	-0.655304000	5.835114000	0.736001000
1	-5.375995000	-1.777763000	-2.773644000
1	-0.820946000	-3.476930000	0.385686000
1	1.963525000	1.929963000	3.882540000
1	0.700412000	1.939996000	2.646454000
1	0.265374000	1.937652000	4.364208000
1	-5.442653000	1.572309000	2.028390000
1	-3.691520000	1.530906000	1.835052000
1	-4.641913000	2.725130000	0.950186000
1	4.704014000	1.165653000	0.827345000
1	6.345175000	0.661735000	0.386313000
1	5.779814000	0.455569000	2.045055000
1	2.252113000	-4.624635000	-2.348208000
1	2.362069000	-4.158138000	-4.051213000
1	0.795119000	-4.610023000	-3.359515000
1	-2.867924000	-4.006705000	-0.850515000
1	-2.708119000	-2.251379000	-0.694070000
1	-3.864317000	-3.125470000	0.311570000
1	-2.007942000	-5.571716000	0.935004000
1	-1.196542000	-4.947025000	2.382384000
1	-2.943079000	-4.751535000	2.195240000
1	1.986576000	1.048665000	-2.551759000
1	0.248336000	1.568321000	-2.607300000

5 (S = ½)

28	-0.726221000	-0.471151000	-0.232651000
7	-3.134087000	1.150129000	0.688186000
6	-2.339075000	3.104225000	1.313479000
1	-2.147007000	4.099465000	1.680765000
6	0.048139000	2.746540000	0.872562000
6	-0.289434000	-2.337744000	-1.071261000
7	1.183755000	-0.346038000	0.005124000
6	3.373227000	-1.377708000	-0.666933000
7	-1.322558000	2.299101000	0.813479000
6	-1.028754000	-3.260418000	-0.242632000
6	1.208724000	-2.400640000	-1.158135000
6	-1.780127000	1.060097000	0.419020000
6	3.973265000	-2.450106000	-1.341637000
1	5.059095000	-2.467294000	-1.406124000

6	1.846126000	-3.434397000	-1.837118000
1	1.243569000	-4.215022000	-2.296111000
6	-3.477074000	2.382047000	1.237537000
1	-4.489845000	2.615819000	1.522297000
6	1.944240000	-1.323188000	-0.577129000
6	2.102534000	2.934857000	2.101704000
1	2.714734000	2.702146000	2.967602000
6	-5.030153000	0.270387000	-0.602927000
6	-2.390648000	-3.443599000	-0.485724000
1	-2.941023000	-4.151653000	0.129955000
6	0.792223000	2.446832000	2.031088000
6	-4.918313000	1.402071000	-1.624343000
1	-3.923733000	1.849138000	-1.527515000
6	-4.330578000	-0.840721000	1.493250000
6	3.239310000	-3.477188000	-1.934080000
1	3.738918000	-4.287157000	-2.457042000
6	-0.310261000	3.979992000	-1.354367000
1	-1.175744000	3.310418000	-1.394492000
6	-4.155557000	0.145054000	0.498065000
6	-5.962303000	2.503737000	-1.339272000
1	-5.852675000	2.926662000	-0.335817000
1	-6.980564000	2.105949000	-1.423115000
1	-5.859882000	3.322231000	-2.061490000
6	1.853851000	4.045259000	-0.026384000
1	2.270405000	4.681892000	-0.800874000
6	0.546089000	3.563187000	-0.161265000
6	-5.062934000	0.922095000	-3.079800000
1	-4.360288000	0.117236000	-3.307346000
1	-4.864021000	1.752719000	-3.766455000
1	-6.075028000	0.560065000	-3.293845000
6	0.424437000	3.852460000	-2.699624000
1	0.824570000	2.845237000	-2.841843000
1	1.255644000	4.562032000	-2.781710000
1	-0.267126000	4.064599000	-3.523228000
6	-2.378419000	-1.864116000	-2.295775000
1	-2.886284000	-1.381223000	-3.124472000
6	-5.390865000	-1.740752000	1.333412000
1	-5.552807000	-2.513929000	2.077627000
6	-1.011425000	-1.560289000	-2.061186000
6	-6.078120000	-0.653170000	-0.705863000
1	-6.770006000	-0.584698000	-1.539919000
6	2.631676000	3.720653000	1.081923000
1	3.653839000	4.080155000	1.151834000
6	0.190337000	1.683560000	3.207525000
1	-0.763585000	1.261284000	2.881304000

6	-3.059292000	-2.784802000	-1.526665000
6	-3.469462000	-0.882986000	2.754128000
1	-2.511230000	-0.410103000	2.519857000
6	-0.426421000	-4.143841000	0.860188000
1	-1.285637000	-4.425000000	1.485467000
6	-6.254684000	-1.652326000	0.245734000
1	-7.075542000	-2.357849000	0.146180000
6	-3.158419000	-2.307962000	3.239666000
1	-2.732638000	-2.916821000	2.437610000
1	-4.049691000	-2.818077000	3.623410000
1	-2.432212000	-2.268628000	4.059228000
6	-0.839330000	5.418383000	-1.170651000
1	-1.426961000	5.522837000	-0.252205000
1	-1.479718000	5.702244000	-2.014297000
1	-0.011790000	6.135962000	-1.119708000
6	-0.261992000	-0.797062000	-3.162534000
1	0.713663000	-0.511745000	-2.760637000
6	-4.132660000	-0.067690000	3.885410000
1	-4.290248000	0.976438000	3.596121000
1	-3.502166000	-0.076592000	4.782488000
1	-5.106783000	-0.494547000	4.152946000
6	-0.102478000	2.641302000	4.380828000
1	-0.568854000	2.097201000	5.210849000
1	-0.779698000	3.450018000	4.083412000
1	0.820358000	3.099276000	4.756154000
6	1.068047000	0.508598000	3.664005000
1	1.293070000	-0.156284000	2.824712000
1	0.550365000	-0.069185000	4.439164000
1	2.012408000	0.856788000	4.096193000
1	1.734192000	0.437969000	0.342913000
6	4.274578000	-0.315974000	-0.094058000
6	4.769120000	-0.431251000	1.232245000
6	4.716573000	0.750460000	-0.917399000
6	5.659518000	0.536749000	1.714174000
6	5.613585000	1.692639000	-0.395596000
6	6.077548000	1.594887000	0.911655000
1	6.045606000	0.457019000	2.726098000
1	5.963935000	2.506953000	-1.024186000
6	4.296529000	0.852383000	-2.383781000
1	3.395706000	0.243587000	-2.510046000
6	4.413022000	-1.632740000	2.109330000
1	3.417920000	-1.975241000	1.806009000
1	6.776566000	2.332032000	1.300799000
1	-4.108311000	-2.992296000	-1.715830000
6	5.397637000	-2.798566000	1.874150000

1	5.134913000	-3.655458000	2.507298000
1	5.386615000	-3.132401000	0.833842000
1	6.421382000	-2.494077000	2.125499000
6	4.359566000	-1.315942000	3.613821000
1	5.359445000	-1.147296000	4.032095000
1	3.753388000	-0.430715000	3.823516000
1	3.924252000	-2.162528000	4.157430000
6	3.953041000	2.285639000	-2.822753000
1	3.225737000	2.743274000	-2.146604000
1	4.839179000	2.931458000	-2.854718000
1	3.525838000	2.277793000	-3.832922000
6	5.382211000	0.263862000	-3.308539000
1	5.574371000	-0.788470000	-3.080023000
1	5.071851000	0.330746000	-4.358931000
1	6.326430000	0.812003000	-3.199956000
6	0.580175000	-3.462063000	1.799368000
1	0.190854000	-2.515053000	2.186270000
1	0.788193000	-4.121117000	2.651541000
1	1.525836000	-3.254039000	1.295418000
6	0.143695000	-5.473285000	0.319646000
1	-0.574769000	-5.974311000	-0.339187000
1	1.069272000	-5.313011000	-0.238566000
1	0.366439000	-6.149586000	1.154548000
6	-0.976184000	0.493562000	-3.596953000
1	-1.918230000	0.289587000	-4.120159000
1	-1.198787000	1.131037000	-2.735268000
1	-0.342506000	1.059095000	-4.289721000
6	-0.020758000	-1.702259000	-4.386939000
1	0.554947000	-2.591337000	-4.116423000
1	-0.971182000	-2.029950000	-4.826173000
1	0.537658000	-1.160160000	-5.160358000

9T (S = 1)

28	0.563767000	-0.049895000	-0.658297000
7	2.788078000	0.145588000	1.465084000
7	-1.172171000	-0.390668000	-0.132654000
7	1.751169000	2.017644000	1.222387000
6	0.967259000	-2.264442000	-2.352117000
6	1.799847000	0.742624000	0.725377000
6	0.908404000	3.111141000	0.777413000
6	-2.289287000	-2.452557000	-2.968230000
6	-1.503614000	-1.673406000	-2.123565000
6	-0.088806000	-1.313434000	-2.447857000
6	-3.628831000	-2.692544000	-2.660163000
6	-5.063063000	-0.630062000	2.733439000

6	3.312448000	-1.207303000	1.382518000
6	-4.146856000	-0.630600000	0.487770000
6	-0.302952000	3.344339000	1.461126000
6	0.179268000	0.030965000	-2.881988000
6	-3.427386000	-1.317210000	-0.642986000
6	-2.044879000	-1.120587000	-0.925374000
6	-4.179296000	-2.112041000	-1.517677000
6	-4.296228000	-1.264207000	1.747635000
6	2.658345000	2.196304000	2.255727000
6	4.470969000	-1.443697000	0.605180000
6	1.403012000	3.973575000	-0.226205000
6	-0.742160000	2.512709000	2.664314000
6	2.793596000	3.808385000	-0.839135000
6	3.306665000	1.019549000	2.411005000
6	1.520148000	0.405998000	-3.099848000
6	2.277565000	-1.840641000	-2.625096000
6	2.555984000	-0.521540000	-2.974613000
6	5.022392000	-2.729390000	0.656887000
6	3.827888000	4.658752000	-0.067965000
6	-3.703805000	-2.645781000	2.026607000
6	2.745691000	-2.188999000	2.219306000
6	-5.680587000	0.593834000	2.492175000
6	-0.958174000	0.948351000	-3.333999000
6	-4.780598000	0.613380000	0.233759000
6	0.598243000	5.061580000	-0.585780000
6	-0.626128000	5.289827000	0.036756000
6	0.696146000	-3.733095000	-2.044150000
6	5.838152000	-0.873303000	-1.488887000
6	5.169211000	-0.349648000	-0.203678000
6	6.235316000	0.379971000	0.645368000
6	-4.721783000	1.302848000	-1.130493000
6	-0.694451000	2.448262000	-3.149069000
6	-1.064779000	4.447328000	1.053728000
6	4.470859000	-3.724809000	1.460000000
6	0.803344000	-4.569300000	-3.338377000
6	3.348686000	-3.454205000	2.233633000
6	1.566582000	-1.911495000	3.145612000
6	-1.275613000	0.638113000	-4.813677000
6	1.611299000	-4.309347000	-0.952189000
6	-6.076800000	1.189897000	-1.858742000
6	-5.540383000	1.204880000	1.251468000
6	-2.244072000	2.185964000	2.664879000
6	-0.362983000	3.230582000	3.978878000
6	2.855220000	4.161049000	-2.335934000
6	-4.705872000	-3.762187000	1.662125000

6	-4.275655000	2.774191000	-1.041803000
6	-3.240964000	-2.826326000	3.483064000
6	0.419950000	-2.916405000	2.942357000
6	2.023509000	-1.891926000	4.619409000
1	-1.623827000	-0.034724000	0.706675000
1	-1.857008000	-2.860167000	-3.877731000
1	-4.243499000	-3.300125000	-3.316850000
1	-5.193310000	-1.103998000	3.700882000
1	-5.234122000	-2.254955000	-1.301437000
1	2.751659000	3.135986000	2.774910000
1	-0.198425000	1.561580000	2.638384000
1	3.086290000	2.756997000	-0.738550000
1	4.077720000	0.716025000	3.100217000
1	1.745232000	1.412823000	-3.432948000
1	3.089777000	-2.557161000	-2.559978000
1	3.577615000	-0.215250000	-3.174196000
1	5.909881000	-2.952017000	0.074547000
1	4.827274000	4.525247000	-0.497477000
1	3.574678000	5.723235000	-0.127608000
1	3.878637000	4.385485000	0.990288000
1	-2.824832000	-2.768840000	1.381458000
1	-6.279626000	1.063543000	3.267822000
1	-1.844562000	0.697178000	-2.747547000
1	0.937174000	5.747728000	-1.354890000
1	-1.232178000	6.141431000	-0.259107000
1	-0.333917000	-3.810666000	-1.685004000
1	6.142387000	-0.030202000	-2.118802000
1	6.745389000	-1.446508000	-1.269266000
1	5.174047000	-1.517227000	-2.072650000
1	4.411809000	0.386304000	-0.498643000
1	6.737718000	1.146452000	0.044342000
1	6.997213000	-0.325708000	0.995180000
1	5.805836000	0.873892000	1.520667000
1	-3.982822000	0.778680000	-1.744456000
1	-0.417957000	2.698208000	-2.120476000
1	0.091861000	2.815989000	-3.818453000
1	-1.603256000	3.008295000	-3.392392000
1	-2.005452000	4.659322000	1.551158000
1	4.927780000	-4.709885000	1.491310000
1	0.125995000	-4.205288000	-4.117799000
1	1.821878000	-4.544062000	-3.743354000
1	0.550508000	-5.614843000	-3.131598000
1	2.939909000	-4.231071000	2.872272000
1	1.170219000	-0.918381000	2.911470000
1	-1.550772000	-0.411011000	-4.956870000

1	-0.412619000	0.855798000	-5.453815000
1	-2.113520000	1.255848000	-5.154857000
1	1.541744000	-3.736782000	-0.023137000
1	2.663646000	-4.326398000	-1.256341000
1	1.319251000	-5.342787000	-0.735744000
1	-6.020301000	1.650062000	-2.852360000
1	-6.870902000	1.697264000	-1.298834000
1	-6.375487000	0.144005000	-1.985781000
1	-6.040646000	2.150881000	1.064628000
1	-2.572291000	1.733281000	1.725196000
1	-2.476091000	1.486926000	3.474933000
1	-2.856459000	3.079112000	2.829016000
1	0.712372000	3.423311000	4.049809000
1	-0.653536000	2.621342000	4.842066000
1	-0.879469000	4.193885000	4.056977000
1	3.834821000	3.885252000	-2.741324000
1	2.730437000	5.235389000	-2.508170000
1	2.085063000	3.640400000	-2.912399000
1	-4.272270000	-4.748567000	1.865572000
1	-4.984538000	-3.728746000	0.605232000
1	-5.622431000	-3.666983000	2.255862000
1	-4.203374000	3.205857000	-2.047257000
1	-3.296704000	2.871819000	-0.560006000
1	-4.989566000	3.385973000	-0.478740000
1	-2.673417000	-3.757807000	3.582913000
1	-2.604975000	-1.997915000	3.814208000
1	-4.087517000	-2.894055000	4.175240000
1	0.035351000	-2.883506000	1.917140000
1	0.733333000	-3.944326000	3.155282000
1	-0.404941000	-2.680498000	3.620166000
1	2.806830000	-1.145226000	4.790555000
1	1.179416000	-1.653372000	5.275987000
1	2.420913000	-2.866090000	4.925575000

9S (S = 0)

28	-0.764071000	-0.103297000	0.852665000
7	-2.576411000	0.298731000	-1.477156000
7	0.865194000	-0.574079000	0.061025000
7	-1.350557000	2.050299000	-1.174566000
6	-1.281186000	-2.128383000	2.180553000
6	-1.593956000	0.803367000	-0.662507000
6	-0.429139000	3.070359000	-0.703146000
6	1.995294000	-2.796647000	2.778161000
6	1.258323000	-1.886077000	2.024393000
6	-0.082183000	-1.349999000	2.393443000

6	3.290317000	-3.128029000	2.388571000
6	4.943567000	-0.753869000	-2.759665000
6	-3.329699000	-0.941252000	-1.381093000
6	3.929721000	-0.829060000	-0.555355000
6	0.766569000	3.268592000	-1.424523000
6	-0.147441000	-0.003070000	2.914105000
6	3.135424000	-1.550109000	0.504444000
6	1.769184000	-1.297679000	0.830203000
6	3.839176000	-2.482955000	1.280127000
6	4.042702000	-1.350649000	-1.868407000
6	-2.145905000	2.299662000	-2.287155000
6	-4.636584000	-0.884232000	-0.840933000
6	-0.833785000	3.919979000	0.352143000
6	1.111032000	2.492965000	-2.694993000
6	-2.227405000	3.848639000	0.976403000
6	-2.905377000	1.201207000	-2.481641000
6	-1.383800000	0.657581000	2.826426000
6	-2.456017000	-1.402344000	2.011490000
6	-2.474392000	-0.001255000	2.235952000
6	-5.405194000	-2.054113000	-0.889880000
6	-3.235775000	4.673276000	0.143751000
6	3.269147000	-2.592601000	-2.308130000
6	-2.807933000	-2.103537000	-1.983481000
6	5.721162000	0.335647000	-2.379992000
6	1.069907000	0.648357000	3.553182000
6	4.721054000	0.283945000	-0.164639000
6	0.059179000	4.925202000	0.741587000
6	1.277699000	5.102400000	0.090349000
6	-1.241655000	-3.645207000	2.144017000
6	-6.008684000	0.168561000	1.049576000
6	-5.264367000	0.393928000	-0.282421000
6	-6.236999000	1.024516000	-1.303653000
6	4.693081000	0.857975000	1.252324000
6	1.068101000	2.181582000	3.514074000
6	1.616587000	4.294768000	-0.989129000
6	-4.914082000	-3.217055000	-1.475339000
6	-1.302431000	-4.162466000	3.603213000
6	-3.633575000	-3.236017000	-2.017454000
6	-1.435201000	-2.148014000	-2.646937000
6	1.184806000	0.137939000	5.007640000
6	-2.354592000	-4.300446000	1.316891000
6	5.992565000	0.522150000	2.011390000
6	5.604027000	0.849485000	-1.093602000
6	2.574000000	2.027669000	-2.744064000
6	0.802406000	3.344449000	-3.947248000

6	-2.280226000	4.321626000	2.440441000
6	4.135053000	-3.861488000	-2.161568000
6	4.429090000	2.375287000	1.271527000
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