Supporting Information

Catalytic Azoarene Synthesis from Aryl Azides Enabled by a Dinuclear Ni Complex

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1. General Information

General Considerations. All manipulations were carried out using standard Schlenk or glovebox techniques under an atmosphere of N_2. Solvents were dried and degassed by passing through a column of activated alumina and sparging with Ar gas. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc., degassed, and stored over activated 3 Å molecular sieves prior to use. All other reagents and starting materials were purchased from commercial vendors and used without further purification unless otherwise noted. Liquid reagents were degassed and stored over activated 3 Å molecular sieves prior to use. Elemental analyses were performed by Midwest Microlab (Indianapolis, IN). The [$^{i\text{-Pr}}$NDI]$Ni_2(C_6H_6)$ complex (**1**), was prepared according to previously reported procedures.[1]

Physical Methods. ^{1}H NMR spectra were collected at room temperature on Varian INOVA 600 or 300 MHz or Bruker DRX 500 MHz spectrometers. ^{1}H and ^{13}C NMR spectra are reported in parts per million relative to tetramethylsilane, using the residual solvent resonances as an internal standard. GC/MS data was collected on a Shimadzu GC-2010/MS-QP2010 spectrometer containing a mini-bore capillary GC column and single quad EI detector. UV–vis measurements were acquired on a Perkin Elmer Lambda 950 UV–VIS–NIR spectrophotometer using a 1-cm two-window quartz cuvette. High-resolution mass data were obtained using a 6320 Ion Trap MS system.

X-Ray Crystallography. Single-crystal X-ray diffraction studies were carried out at the Purdue X-ray crystallography facility using a Rigaku Rapid II diffractometer or a Bruker AXS D8 Quest CMOS diffractometer.

Procedure for XRD data collected using the Rigaku Rapid II instrument. Single crystal X-ray measurements were conducted on a Rigaku Rapid II curved image plate diffractometer with a Cu-Kα X-ray microsource (λ = 1.54178 Å) with a laterally graded multilayer (Goebel) mirror for monochromatization. Single crystals were mounted on Mitegen microloop mounts using a trace of mineral oil and cooled in-situ to 150(2) K for data collection. Data were collected using the dtrek option of CrystalClear-SM Expert 2.1 b32.[2] Data were processed using HKL3000 and data were corrected for absorption and scaled using Scalepack.[3]

Procedure for XRD data collected using the Bruker Quest instrument. Single crystals were coated with mineral oil or fomblin and quickly transferred to the goniometer head of a Bruker Quest diffractometer with kappa geometry, an I-μ-S microsource X-ray tube, laterally graded multilayer (Goebel) mirror single crystal for monochromatization, a Photon2 CMOS area detector and an Oxford Cryosystems low temperature device. Examination and data collection were performed with Cu Kα radiation (λ = 1.54178 Å) at 100 K. Data were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX3.[4]

Structure Solution and Refinement. The space groups were assigned and the structures were solved by direct methods using XPREP within the SHELXTL suite of programs[5] and refined by full matrix least squares against F^2 with all reflections using Shelxl2016[6] using the graphical interface Shelxle.[7] If not specified otherwise H atoms attached to carbon and nitrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with carbon hydrogen bond distances of 0.95 Å for and aromatic C-H, 1.00, 0.99 and 0.98 Å for aliphatic C-H, CH_2 and CH_3 moieties, respectively.

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Methyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. U_{iso}(H) values were set to a multiple of U_{eq}(C) with 1.5 for CH_3, and 1.2 for C-H units, respectively. Additional data collection and refinement details, including description of disorder and/or twinning (where present) can be found in Section 9.

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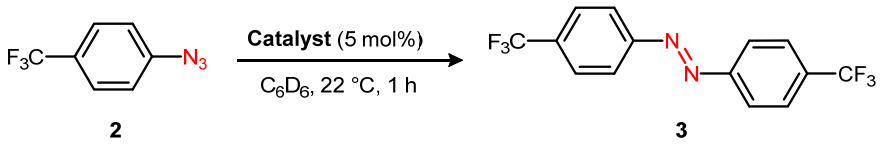
2. N=N Coupling Catalyst Comparison Studies



2 **3**

General procedure. In an N_2 filled glovebox, an NMR tube equipped with a J. Young valve was charged with catalyst (0.0015 mmol, 5 mol %) and C_6H_6 (550 µL). A solution of 4-trifluoromethylphenylazide **2** (50 µL of a 0.60 M stock solution in C_6D_6 containing 0.41 M 1,3,5-trimethoxybenzene, 0.3 mmol, 1.0 equiv) was added. The reaction components were allowed to react for 1 h, and the yield of the azoarene product was determined by ^{1}H NMR integration against 1,3,5-trimethoxybenzne as an internal standard. In all cases, no additional conversion or yield of azoarene was observed after 2 h or after heating for an additional hour at 80 °C. For entries 3 and 4, the catalyst was formed by mixing the corresponding ligand (28% and 14% for PPh_3 and $^{i\text{-Pr}}$IPr respectively) with $Ni(COD)_2$ (5 mol%). For entry 9, 0.5 mol% **1** was used.

entry	catalyst	conversion	yield
1	none	<2%	<2%
2	$Ni(COD)_2$	24%	<2%
3	$Ni(COD)_2$ + PPh_3	35%	<2%
4	$Ni(COD)_2$ + IPr	32%	<2%
5	[$^{i\text{-Pr}}$IP]Ni(COD) (**4**)	24%	13%
6	[BPY]Ni(COD) (**5**)	23%	13%
7	[$^{i\text{-Pr}}$DAD]Ni(COD) (**6**)	<2%	<2%
8	[$^{i\text{-Pr}}$NDI]$Ni_2(C_6H_6)$ (**1**)	>98%	90%
9	[$^{i\text{-Pr}}$NDI]$Ni_2(C_6H_6)$ (**1**)	>98%	96%

Identification of reaction products in entries 3 and 4. To determine the identity of the products formed in entries 3 and 4, **2** was reacted with the PPh_3 and IPr ligands respectively. Both reactions immediately evolved N_2 gas, leading to the formation of the respective nitrene transfer products, [$^{i\text{-Pr}}$IPr]=NAr and Ph_3P=NAr.[8] ^{1}H, ^{19}F, and ^{31}P (for entry 3) NMR spectra confirmed that the group transfer products formed in these stoichiometric reactions were the same as those formed in the catalytic reactions of entries 3 and 4.

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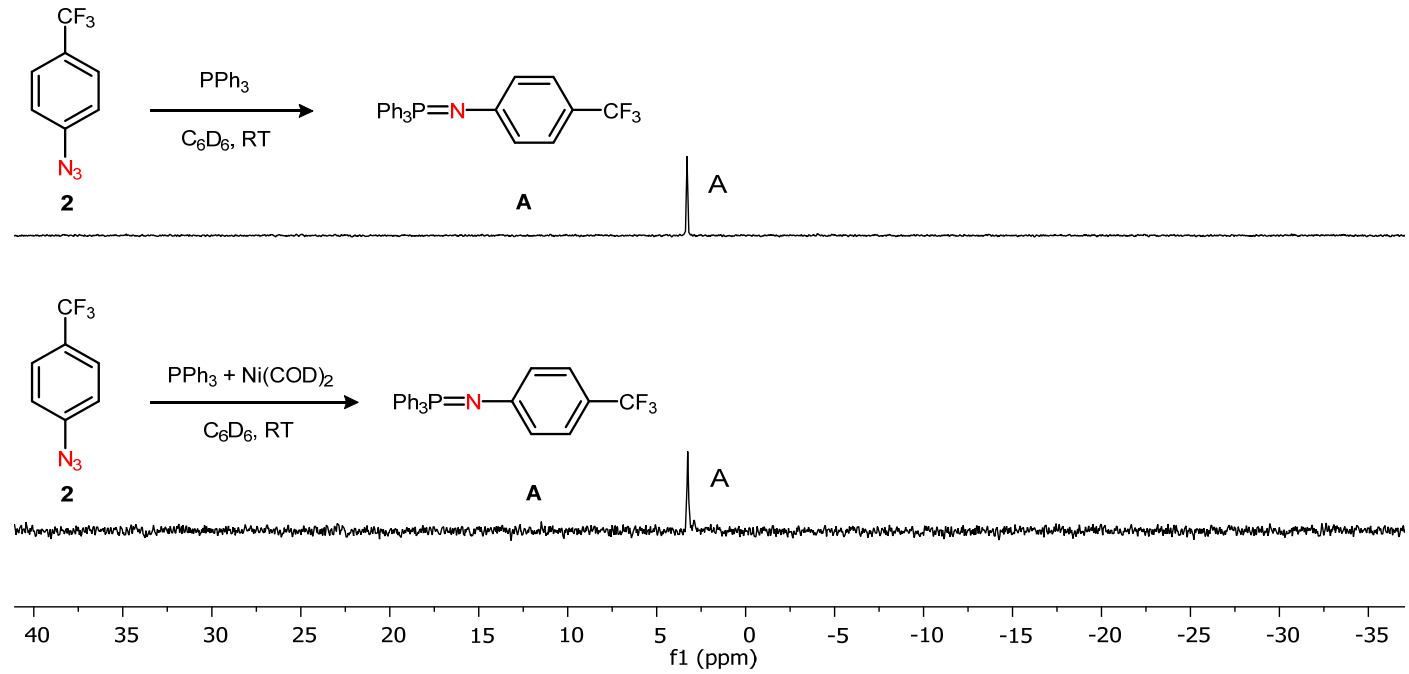

Figure S1. ^{31}P NMR comparison of the stoichiometric reaction between $^{i\text{-Pr}}$IPr and **2** (top) and the catalytic reaction mixture from entry 3 (bottom).

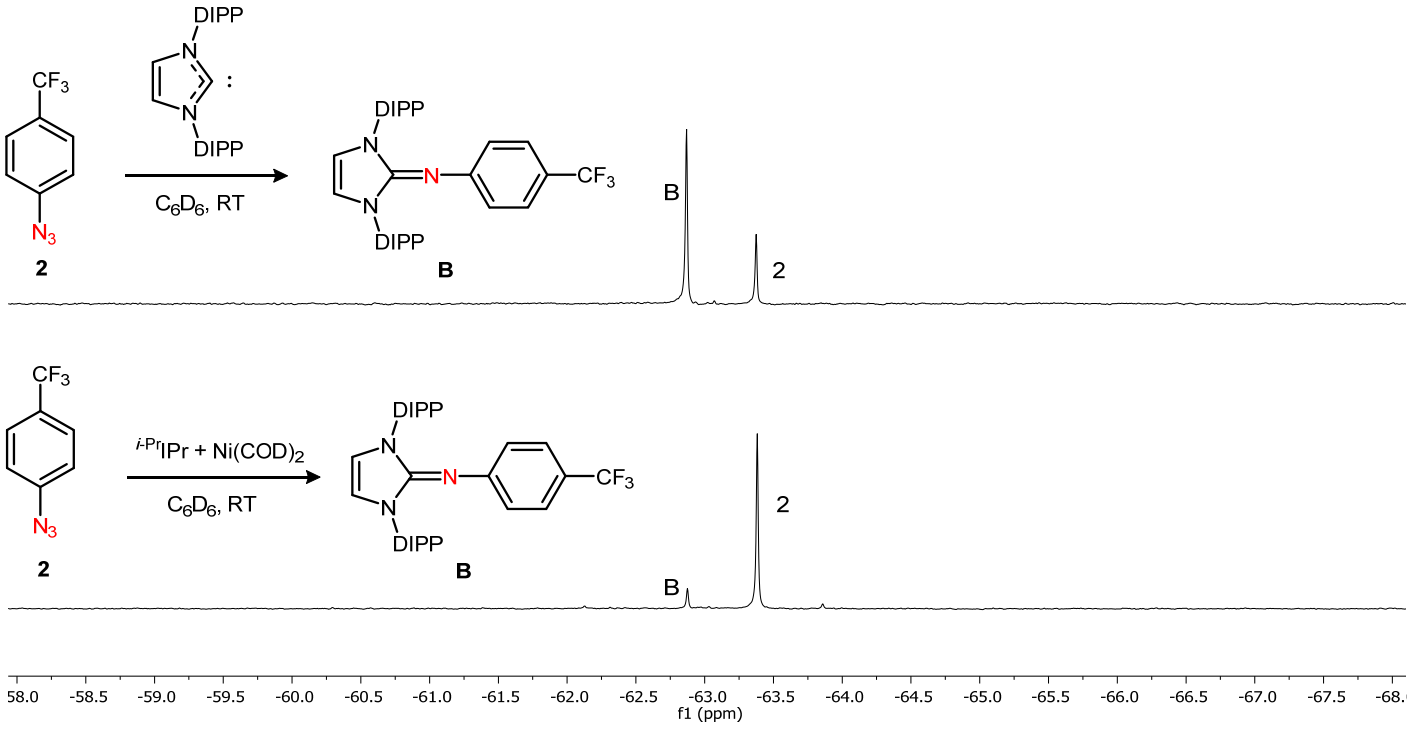

Figure S2. ^{19}F NMR comparison of the stoichiometric reaction between $^{i\text{-Pr}}$IPr and **2** (top) and the catalytic reaction mixture from entry 4 (bottom).

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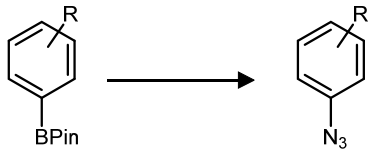
3. Synthesis of Azides and Characterization of Novel Azide Compounds



General Procedure for azidification of pinacolborane.[9] Pinacol boranes were synthesized from the corresponding aryl triflates according to a previously reported procedure.[10] To the aryl pinacol boronate (1.0 equiv) in MeOH (5 mL/mmol) was added NaN_3 (1.5 equiv) and $Cu(OAc)_2$ (0.1 equiv). The solution was vigorously stirred at 55 °C under air for 24 hours. The mixture was filtered through celite and concentrated. The residue was purified by silica gel column chromatography.

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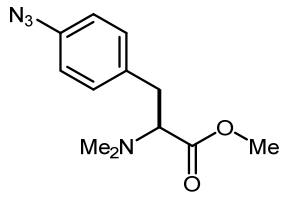

S1

Compound S1. Synthesized according to the general procedure using crude (*S*)-methyl 2-(dimethylamino)-3-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)phenyl)propanoate (1.21 g, 3.63 mmol). Isolated yields were determined following column chromatography (SiO_2, 15% EtOAc/hexanes). The product was isolated as an orange solid. (0.187 g, 0.753 mmol 21% yield). ^1H NMR (800 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H), 3.61 (s, 3H), 3.38 (dd, *J* = 9.4, 5.8 Hz, 1H), 3.08 – 2.86 (m, 2H), 2.38 (s, 6H). $^{13}C\{^1H\}$ NMR (201 MHz, $CDCl_3$) δ 171.70, 138.18, 134.91, 130.42, 119.00, 69.50, 51.10, 41.84, 35.09. HRMS(ESI): calcd for $C_{12}H_{17}N_4O_2^+$: 249.1346; found: 249.1344.

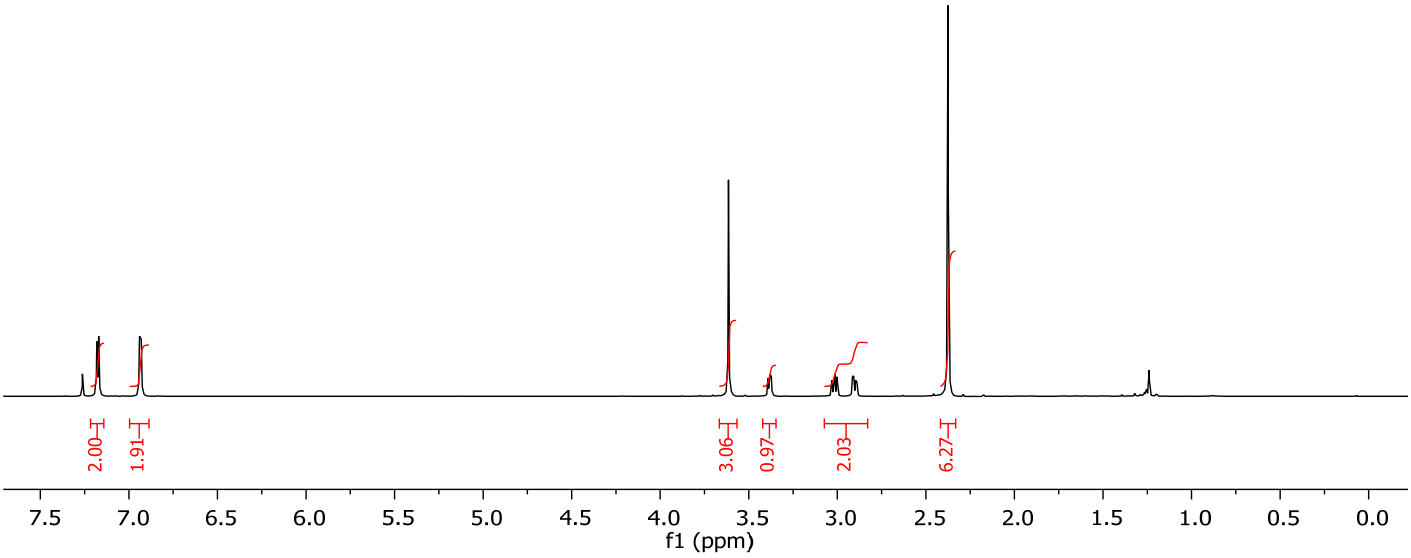

Figure S3. ^1H NMR spectrum of **S1** in $CDCl_3$.

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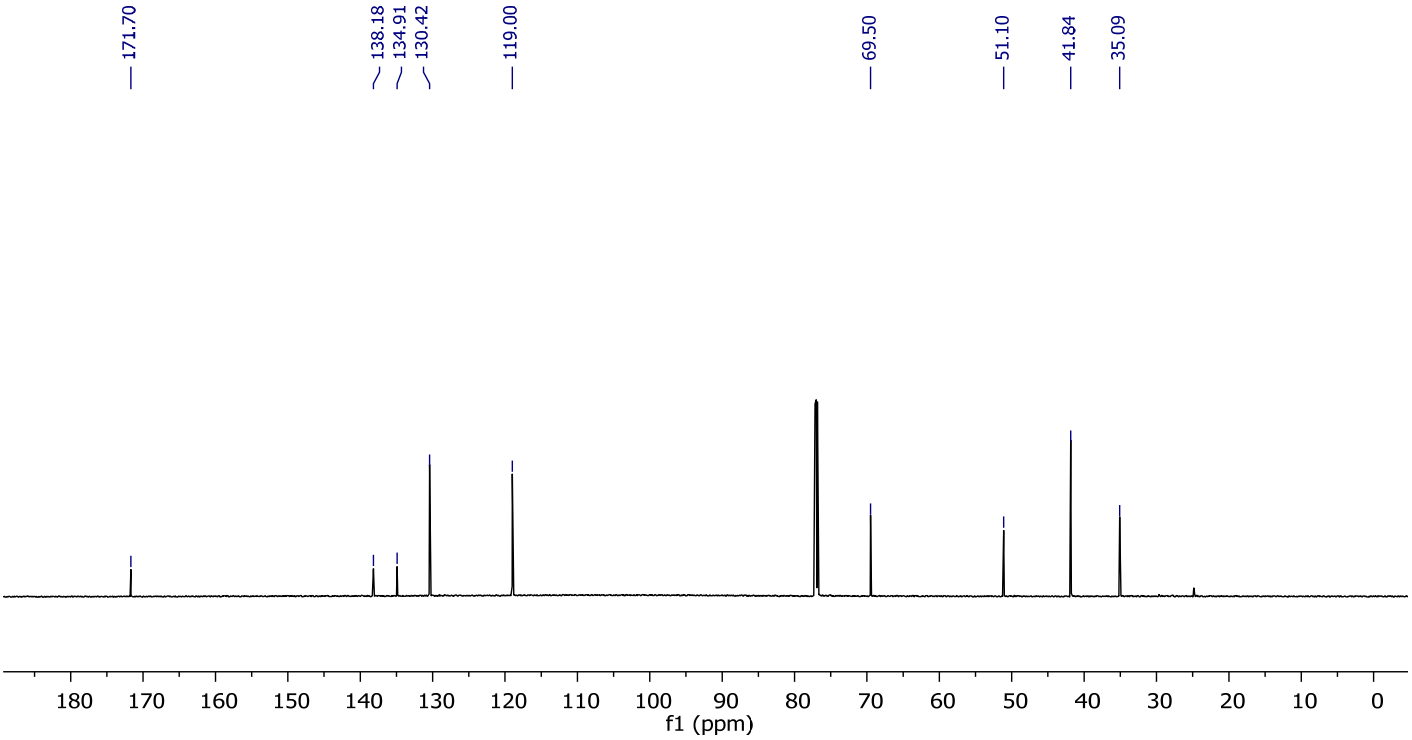

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **S1** in $CDCl_3$.

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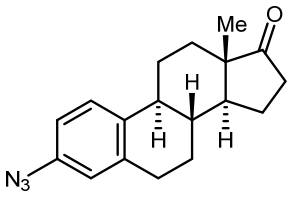

Compound S2. Synthesized according to the general procedure using 3-deoxyestrone-3-boronic acid pinacol ester (0.5267 g, 1.38 mmol). The isolated yield was determined following column chromatography (SiO_2, 10% EtOAc/hexanes) to yield a light-yellow oil (0.511g, >99% yield). ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.1 Hz, 1H), 6.82 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.76 (dd, *J* = 2.5, 1.2 Hz, 1H), 2.90 (dd, *J* = 9.2, 4.2 Hz, 2H), 2.51 (dd, *J* = 9.3, 8.7 Hz, 1H), 2.43 – 2.38 (m, 1H), 2.31 – 2.24 (m, 1H), 2.19 – 2.11 (m, 1H), 2.10 – 2.00 (m, 2H), 2.00 – 1.94 (m, 1H), 1.67 – 1.56 (m, 2H), 1.56 – 1.48 (m, 3H), 1.48 – 1.41 (m, 1H), 0.97 – 0.87 (m, 3H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 220.62, 138.31, 137.41, 136.67, 126.77, 119.11, 116.48, 50.40, 47.93, 44.12, 38.10, 35.82, 31.52, 29.37, 26.31, 25.79, 21.57, 13.83. HRMS(ESI): calcd for $C_{18}H_{22}N_3O^+$: 296.1757; found: 296.1760.

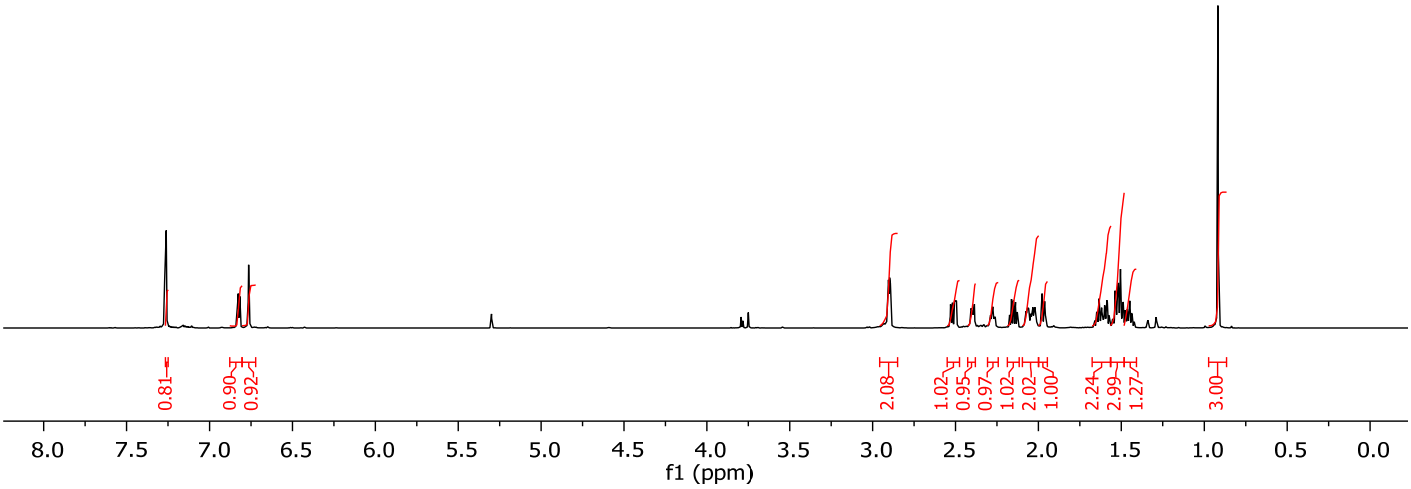

Figure S5. ^{1}H NMR spectrum of **S2** in $CDCl_3$.

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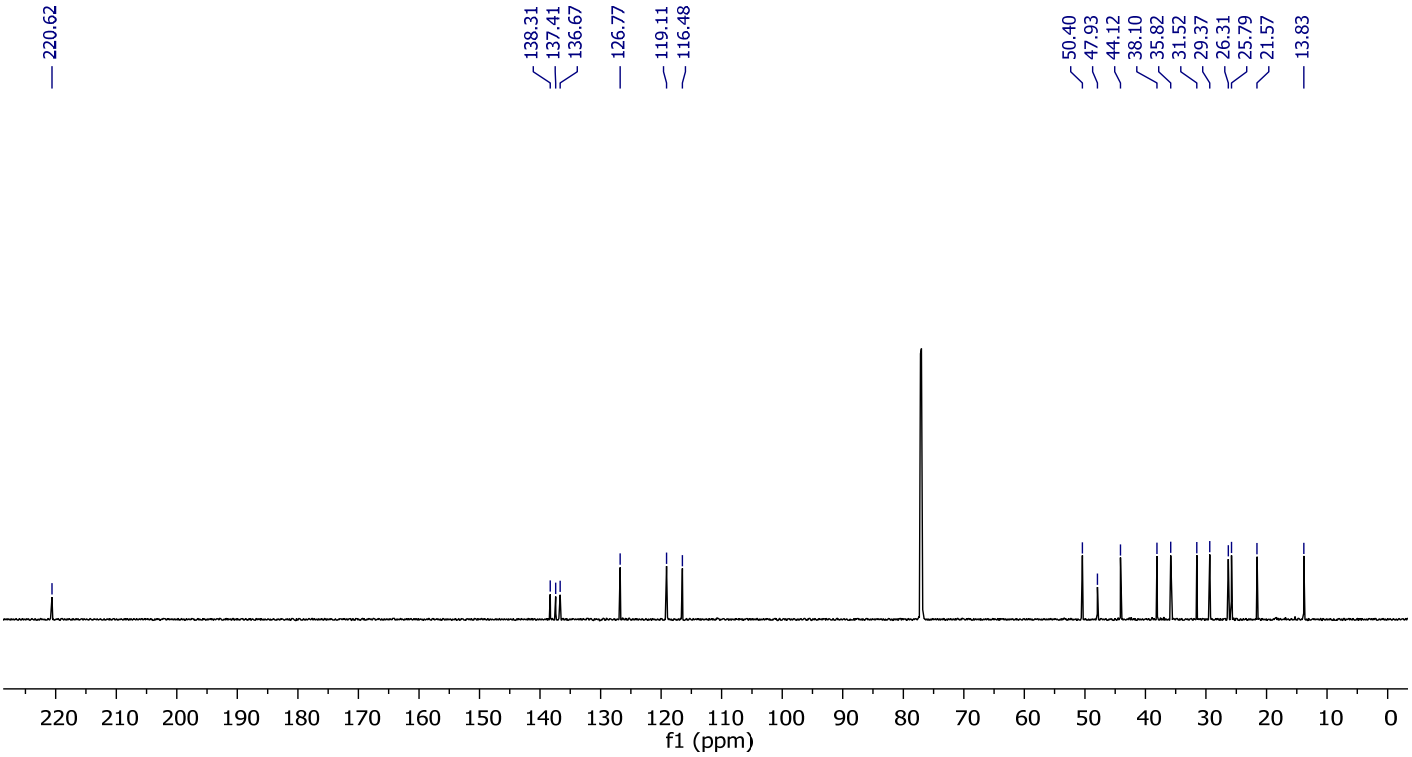

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **S2** in $CDCl_3$.

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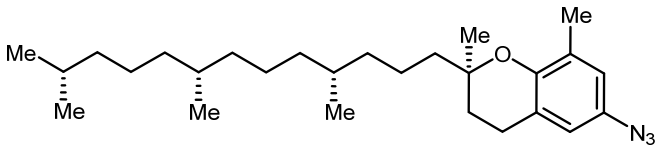

Compound S3. Synthesized according to the general procedure using crude 4,4,5,5-Tetramethyl-1,3,2-dioxaborolane δ-tocopherol (1.2 g, 2.34 mmol). Isolated yields were determined following column chromatography (SiO_2, 10% CH_2Cl_2/hexanes). The product was isolated as a colorless oil (0.624 g, 62% yield). ^1H NMR (800 MHz, C_6D_6) δ 6.61 (s, 1H), 6.50 (s, 1H), 2.32 (t, *J* = 6.9 Hz, 2H), 2.12 (s, 3H), 1.55 – 1.09 (m, 23H), 1.07 (s, 3H), 0.94 – 0.85 (m, 12H). $^{13}C\{^1H\}$ NMR (201 MHz, C_6D_6) δ 149.51, 130.47, 127.93, 121.50, 119.28, 117.14, 75.78, 39.94, 39.39, 37.54, 37.47, 37.43, 37.36, 32.88, 32.67, 30.82, 27.98, 24.92, 24.58, 23.70, 22.55, 22.46, 22.07, 20.92, 19.63, 19.51, 15.88. HRMS(ESI): calcd for $[C_{27}H_{45}N_3O^+]$ - N_2 + H: 400.3574; found: 400.3572. The temperature required to vaporize the sample resulted in the loss of N_2 from the azide.

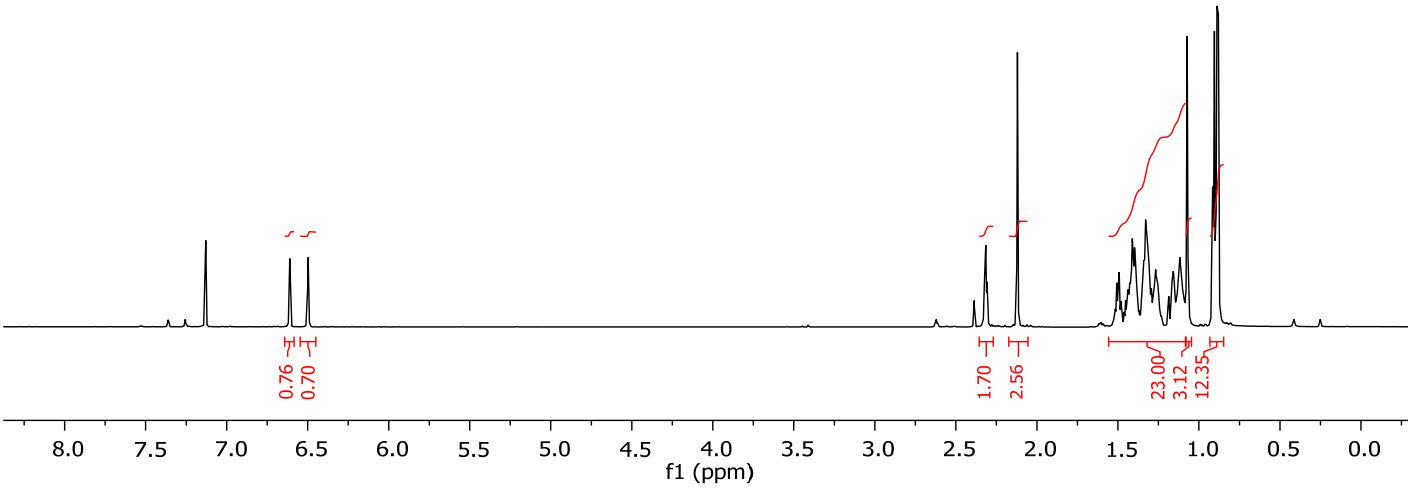

Figure S7. ^1H NMR spectrum for **S3** in $CDCl_3$.

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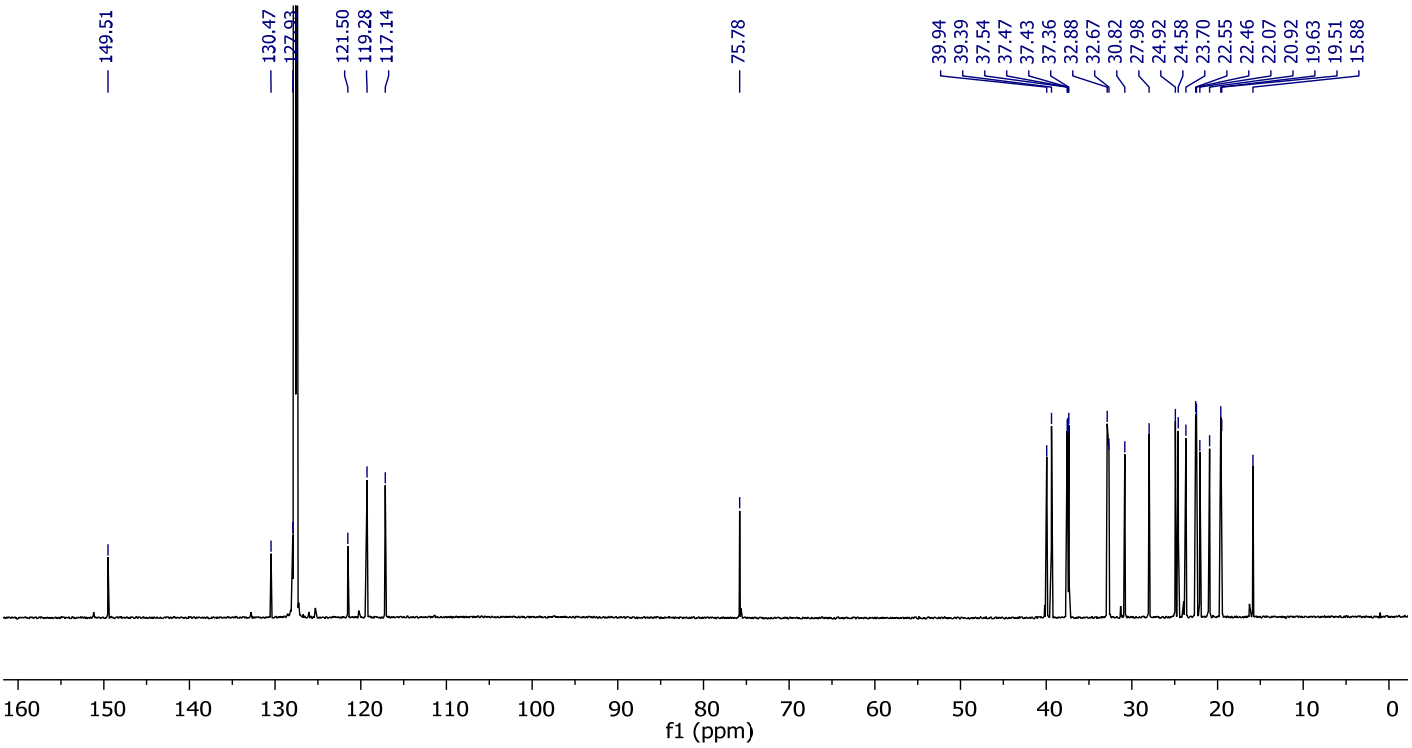

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum for **S3** in $CDCl_3$.

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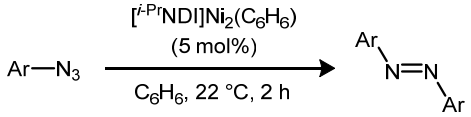
4. Catalytic N=N Coupling Reactions and Azoarene Characterization Data



General procedure for the synthesis of azoarenes from aryl azides. In an N_2 filled glovebox, a 20-mL vial was charged with **1** (11.0 mg, 0.015 mmol, 5 mol%), C_6H_6 (3.0 mL), and a magnetic stir bar. A solution of the aryl azide (0.3 mmol, 1.0 equiv) dissolved in C_6H_6 (3.0 mL) was added. The vial was sealed, and the reaction mixture was stirred at room temperature. After 2 h, the reaction vial was opened to air and stirred for 30 min in order to quench the catalyst. The solution volume was reduced by half under reduced pressure, and the crude mixture was directly loaded onto a SiO_2 column. Isolated yields were determined following purification.

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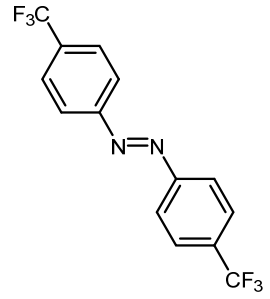

Azoarene 3.[11] The reaction was conducted according to the general procedure using 4-trifluoromethylphenyl azide (56.1 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 1% EtOAc/hexanes). The product was isolated as an orange solid. Run 1: 45.5 mg, 96% yield; Run 2: 43.6 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.2 Hz, 4H), 7.81 (d, *J* = 8.3 Hz, 4H). ^{19}F NMR (300 MHz, $CDCl_3$) δ -63.85. ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 154.07, 132.97 (q, *J* = 32.6 Hz), 126.41 (q, *J* = 3.8 Hz), 123.79 (q, *J* = 272.4 Hz), 123.32.

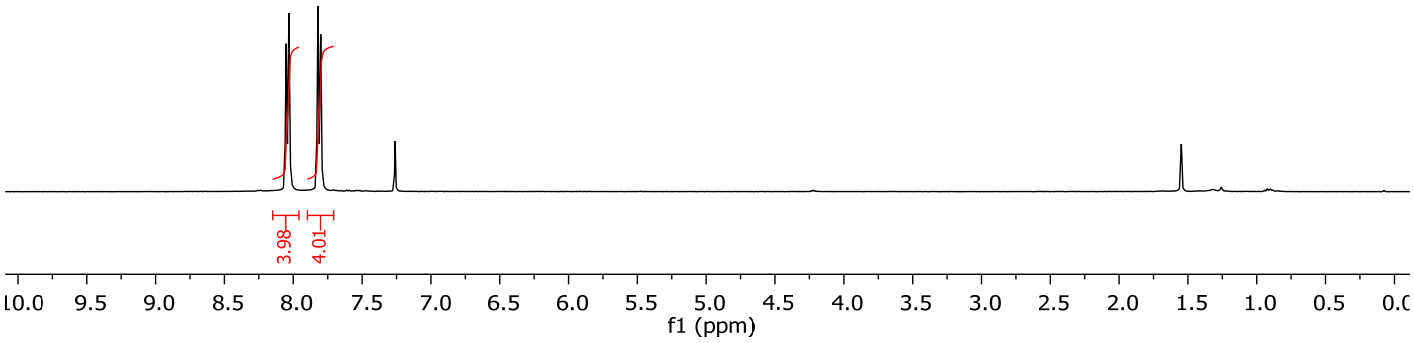

Figure S9. ^{1}H NMR spectrum for **3** in $CDCl_3$.

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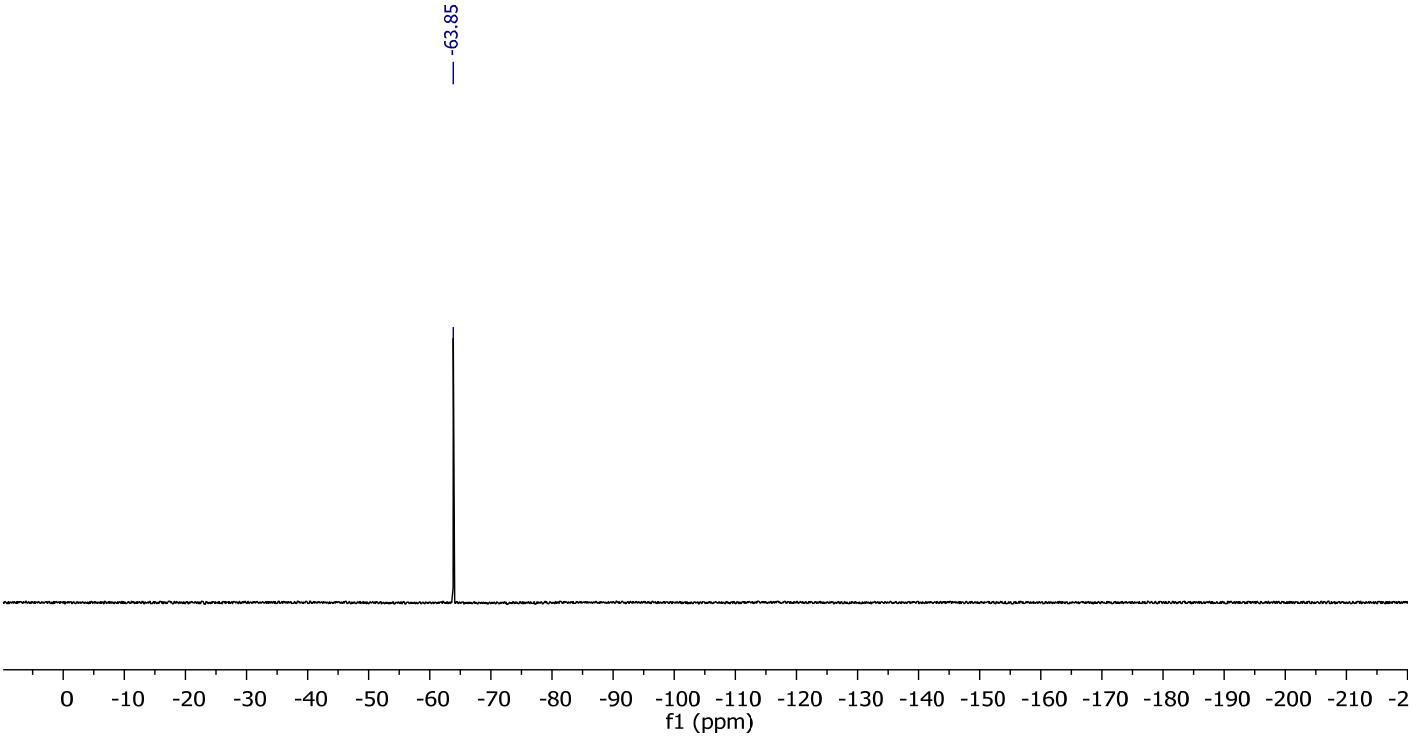

Figure S10. ^{19}F NMR spectrum for **3** in $CDCl_3$.

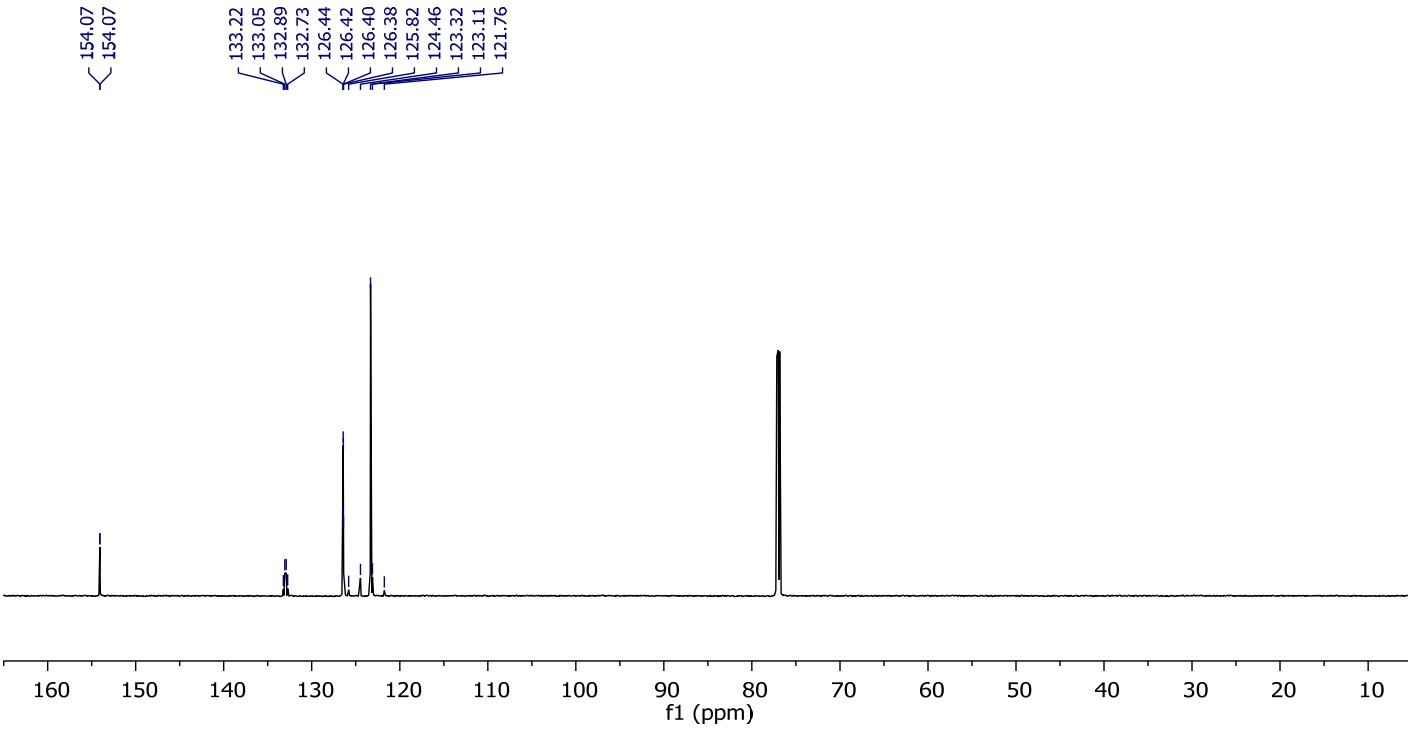

Figure S11. $^{13}C\{^1H\}$ NMR spectrum for **3** in $CDCl_3$.

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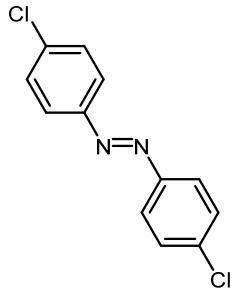

Azoarene 8.[11] The reaction was conducted according to the general procedure using 4-chlorophenyl azide (46.1 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 0-3% EtOAc/hexanes). The product was isolated as an orange solid. Run 1: 34.7 mg, 92% yield; Run 2: 32.4 mg, 86% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.8 Hz, 4H), 7.49 (d, *J* = 8.8 Hz, 4H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 150.68, 137.12, 129.29, 124.08.

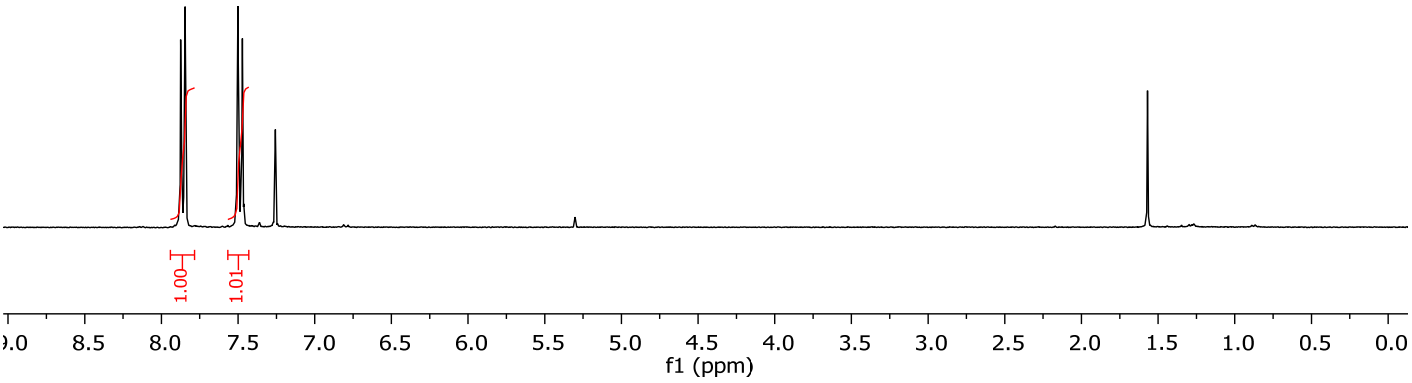

Figure S12. ^{1}H NMR spectrum for **8** in $CDCl_3$.

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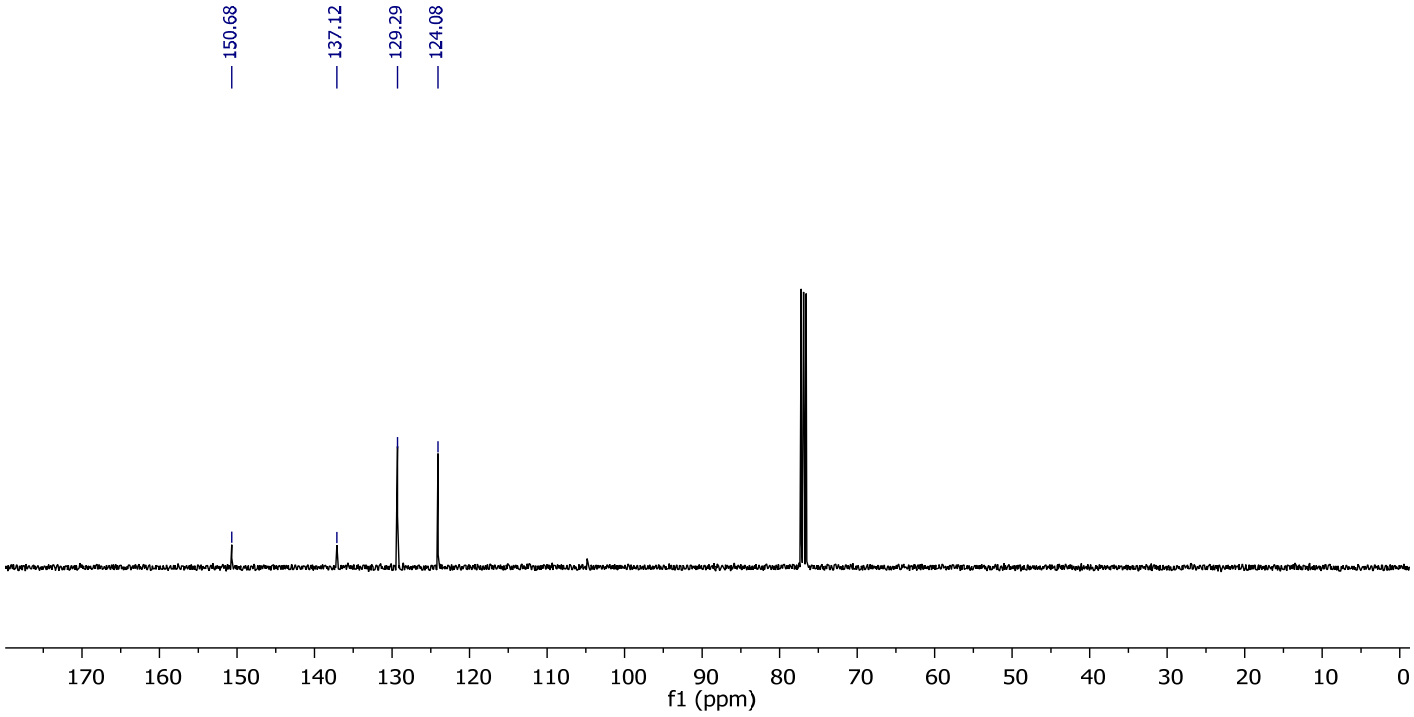

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum for **8** in $CDCl_3$.

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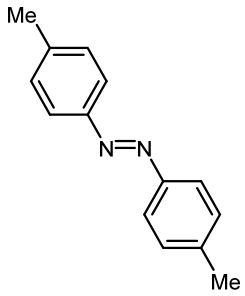

Azoarene 9.[11] The reaction was conducted according to the general procedure using 4-methylphenyl azide (39.9 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (hexanes). The product was isolated as an orange solid. Run 1: 29.3mg, 93% yield; Run 2: 28.7 mg, 91% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 4H), 7.31 (d, *J* = 7.8 Hz, 4H), 2.43 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 150.72, 141.08, 129.59, 122.60, 21.37.

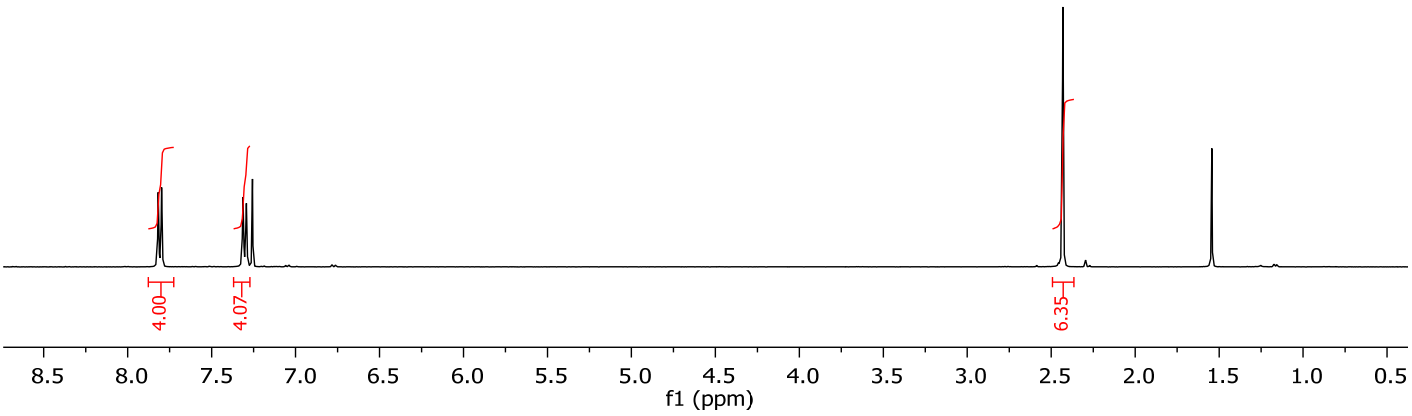

Figure S14. ^{1}H NMR spectrum for **9** in $CDCl_3$.

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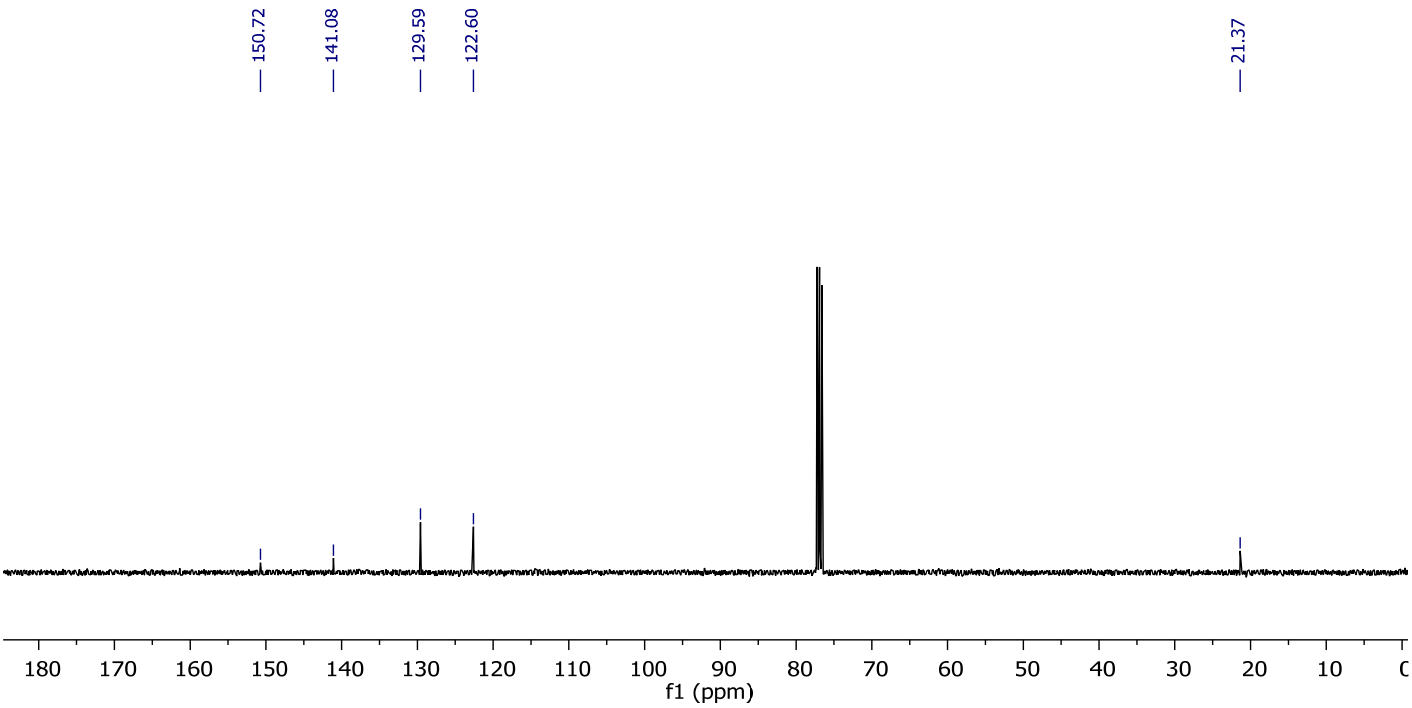

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum for **9** in $CDCl_3$.

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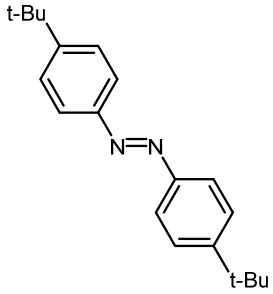

Azoarene 10.[12] The reaction was conducted according to the general procedure using 4-*tert*-butylphenyl azide (52.6 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 1% EtOAc/hexanes). The product was isolated as an orange solid. Run 1: 42.5mg, 96% yield; Run 2: 41.1 mg, 94% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.9 Hz, 4H), 7.53 (d, *J* = 8.9 Hz, 4H), 1.38 (s, 18H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 154.11, 150.65, 125.85, 122.32, 34.88, 31.18.

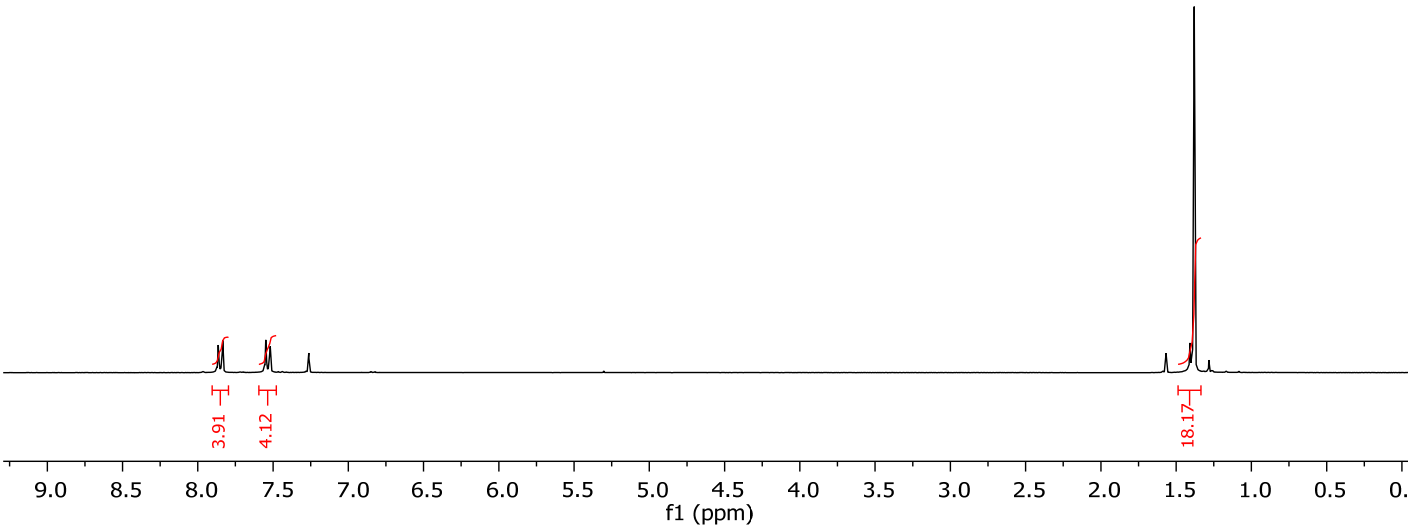

Figure S16. ^{1}H NMR spectrum for **10** in $CDCl_3$

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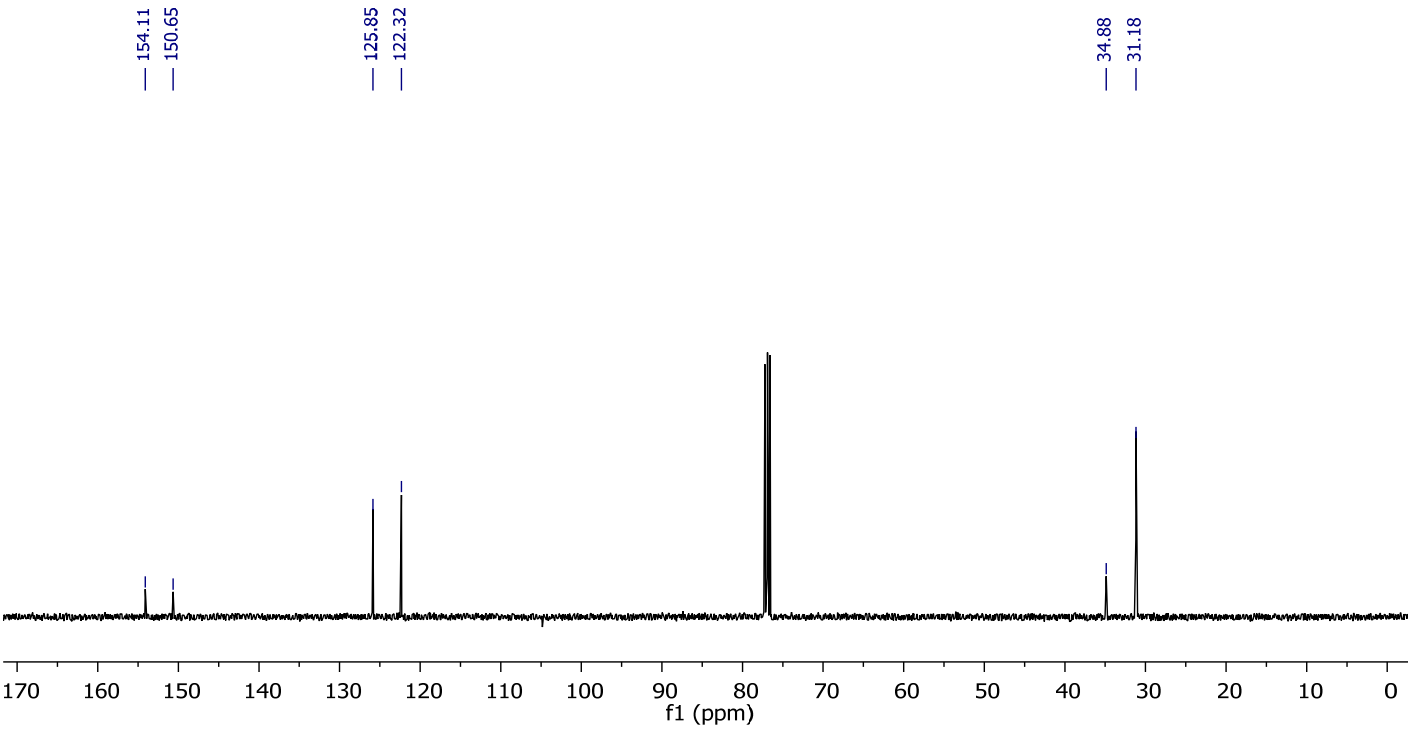

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum for **10** in $CDCl_3$.

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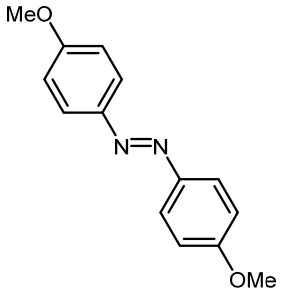

Azoarene 11.[13] The reaction was conducted according to the general procedure using 4-(methoxy)phenyl azide (44.7 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 0-3% EtOAc/hexanes). Run 1: 25 mg, 75% yield; Run 2: 28mg, 77% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (d, *J* = 9.0 Hz, 4H), 7.01 (d, *J* = 8.9 Hz, 4H), 3.89 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.47, 147.00, 124.25, 114.08, 55.47.

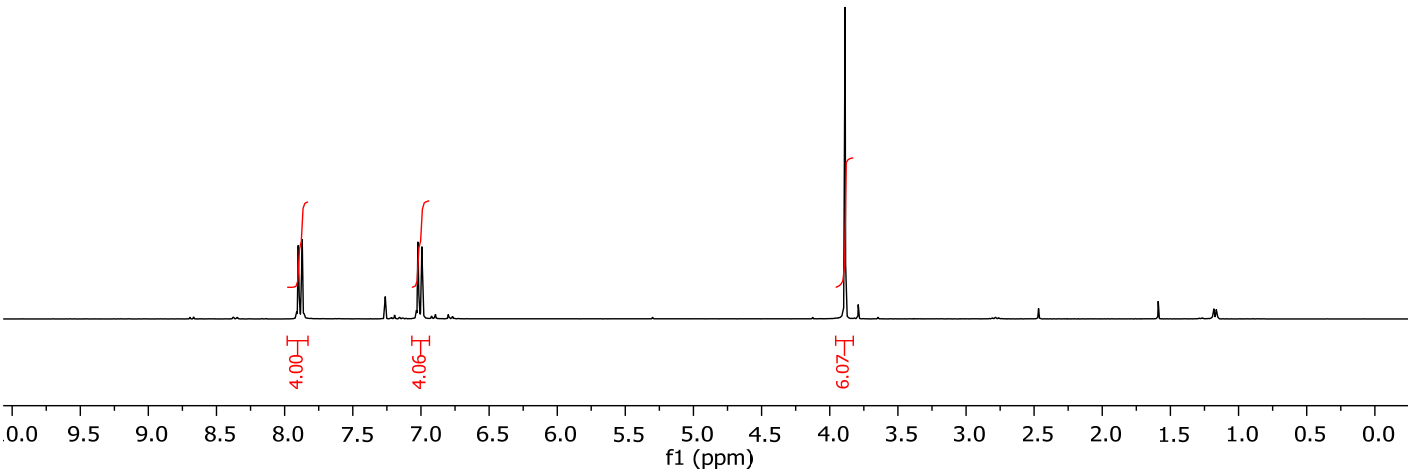

Figure S18. ^{1}H NMR spectrum for **11** in $CDCl_3$.

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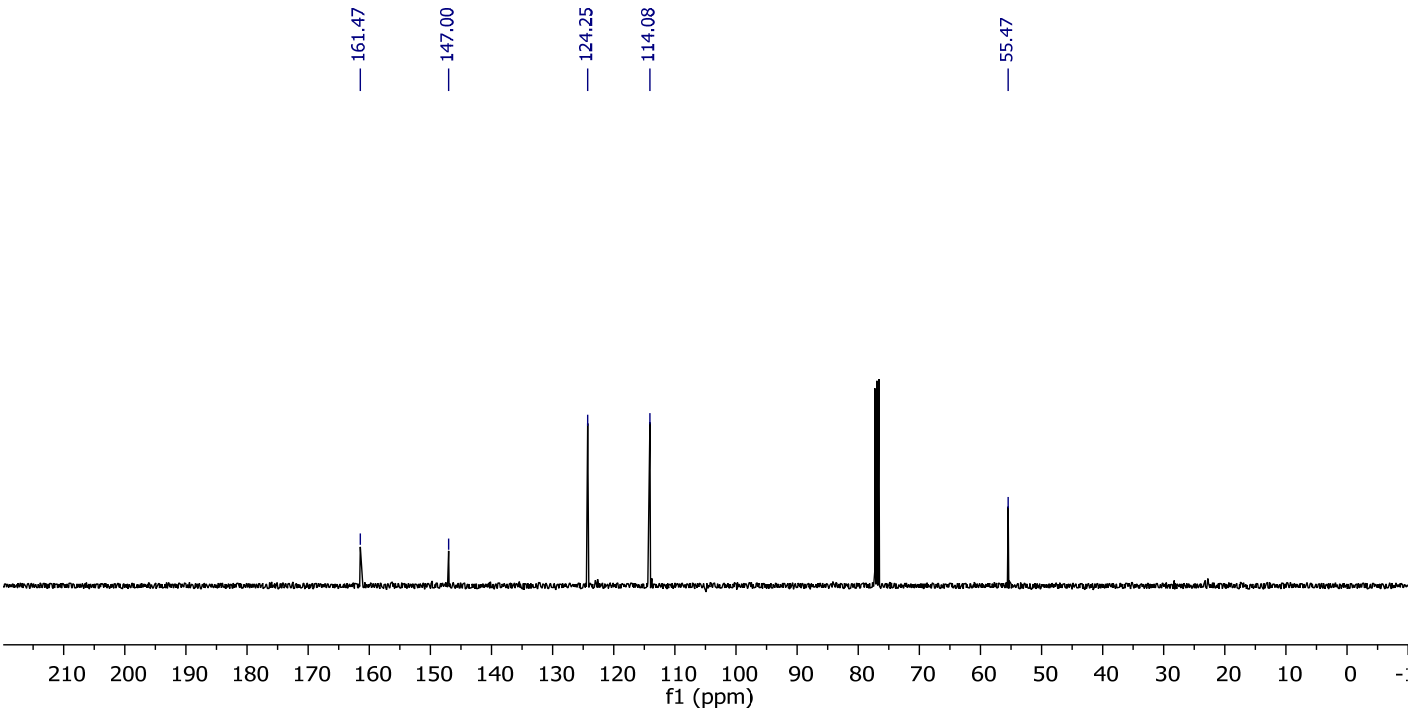

Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum for **11** in $CDCl_3$.

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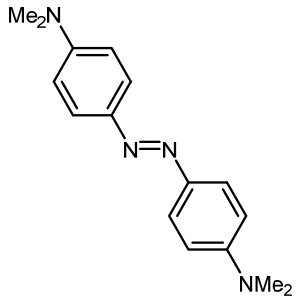

Azoarene 12.[14] The reaction was conducted according to the general procedure using 4-(N,N′-dimethyl)penyl azide (48.7 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 10% EtOAc/hexanes). Run 1: 20 mg, 50% yield; Run 2: 19 mg 48% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (d, *J* = 9.1 Hz, 4H), 6.76 (d, *J* = 9.2 Hz, 4H), 3.06 (d, *J* = 0.6 Hz, 12H). $^{13}C\{^1H\}$ NMR (201 MHz, $CDCl_3$) δ 151.50, 144.12, 123.97, 111.76, 40.43.

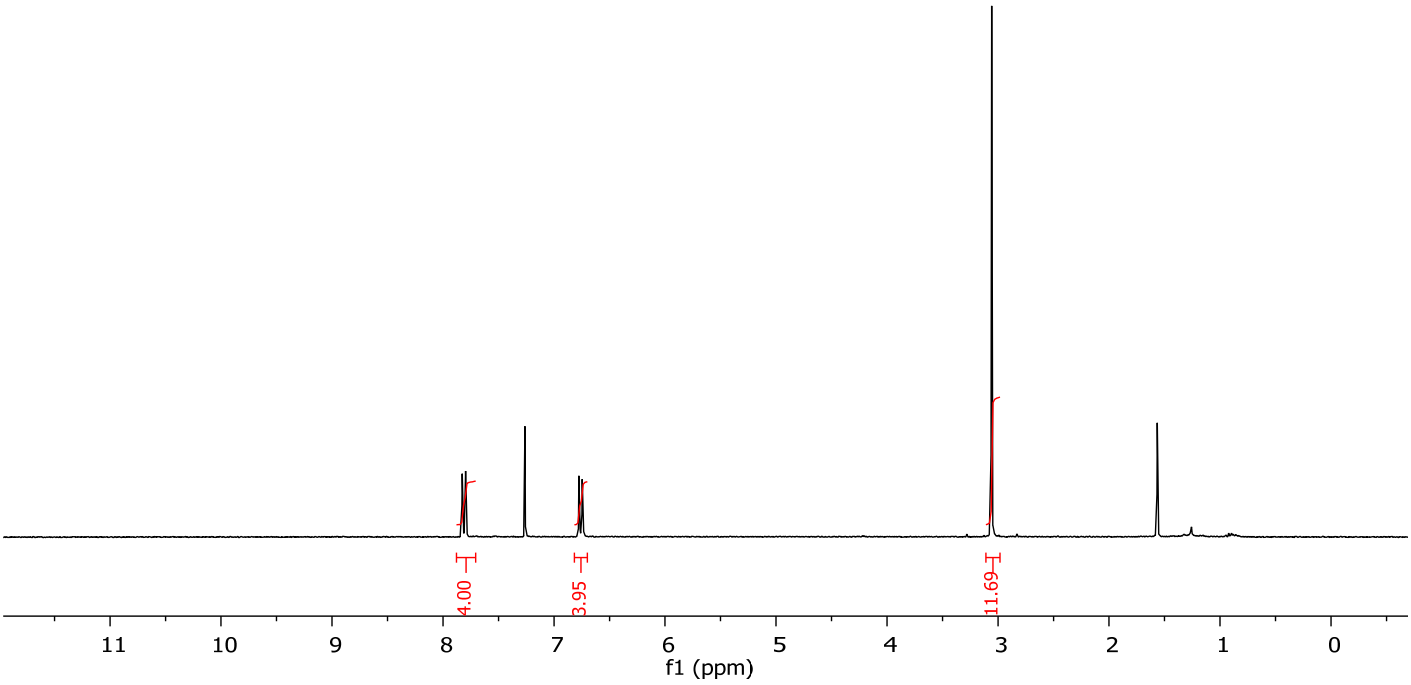

Figure S20. ^{1}H NMR spectrum for **12** in $CDCl_3$.

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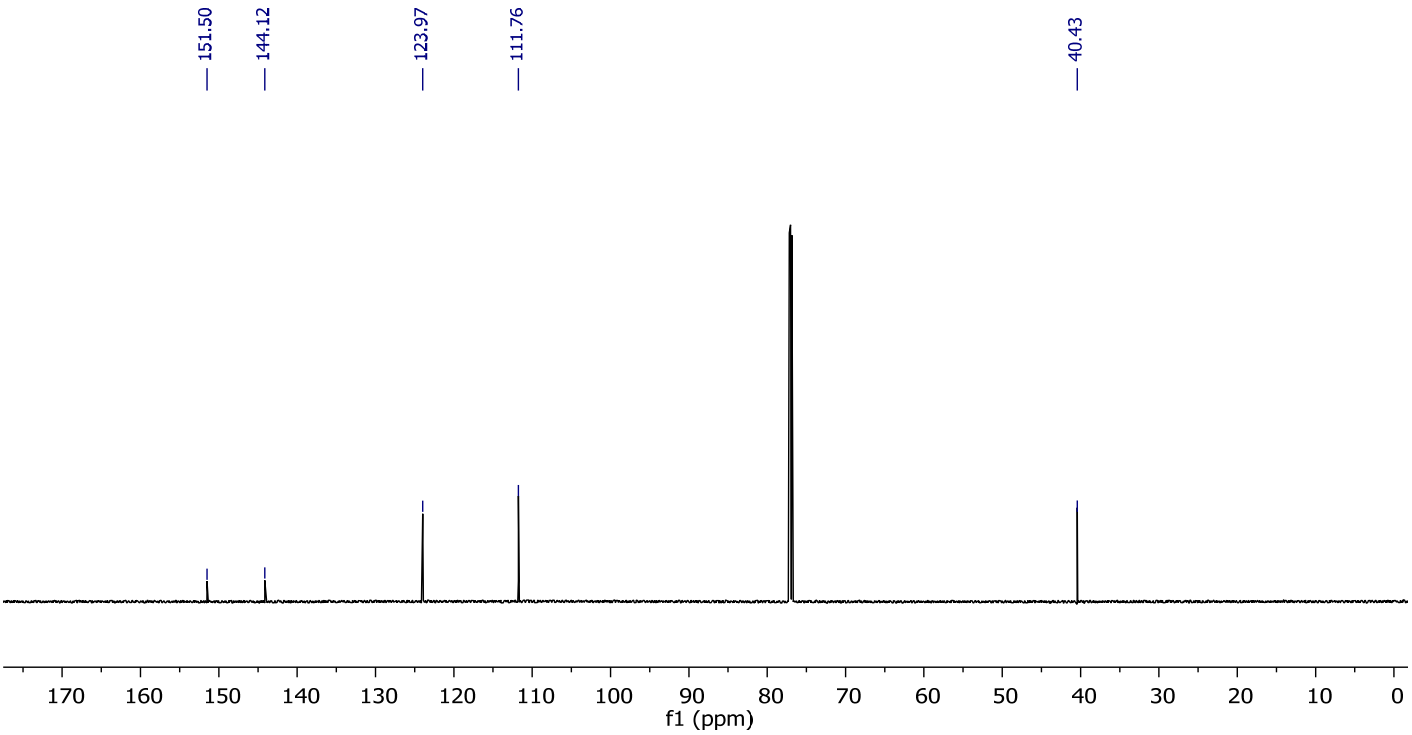

Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum for **12** in $CDCl_3$.

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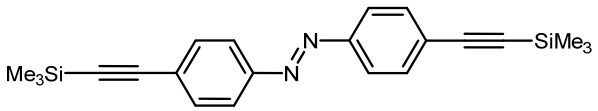

Azoarene 13.[15] The reaction was conducted according to the general procedure using 4-(trimethylsilylethynyl)phenyl azide (65 mg, 0.3 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, 1% EtOAc/hexanes). Run 1: 46 mg, 82% yield; Run 2: 51 mg 91% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 4H), 7.60 (d, *J* = 8.5 Hz, 4H), 0.29 (s, 18H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 151.75, 132.71, 125.92, 122.76, 104.47, 97.22, -0.20.

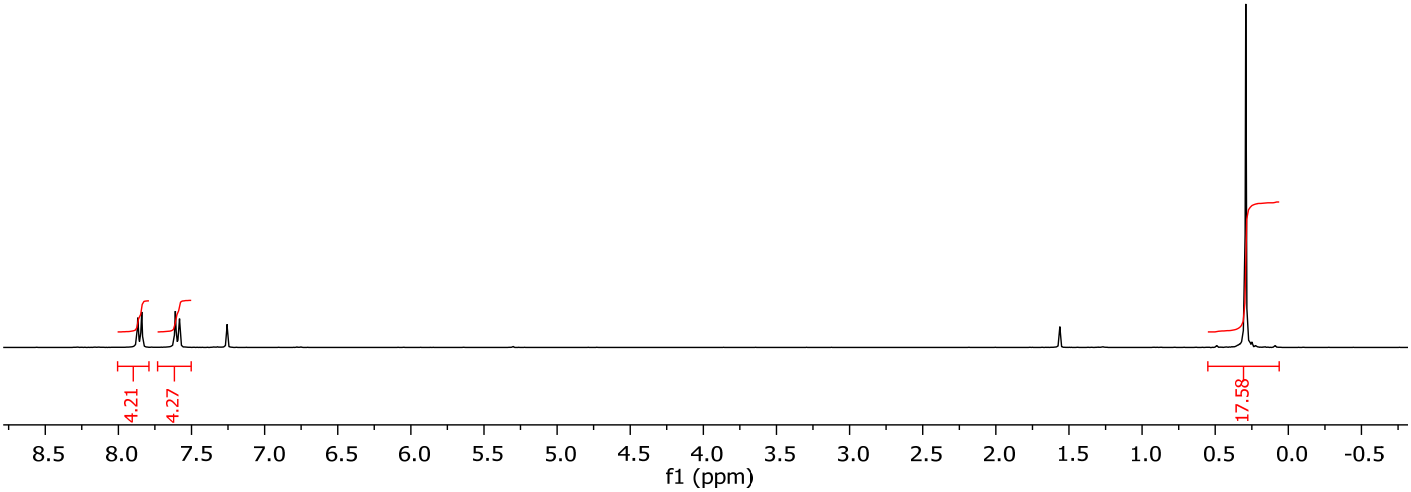

Figure S22. ^{1}H NMR spectrum for **13** in $CDCl_3$

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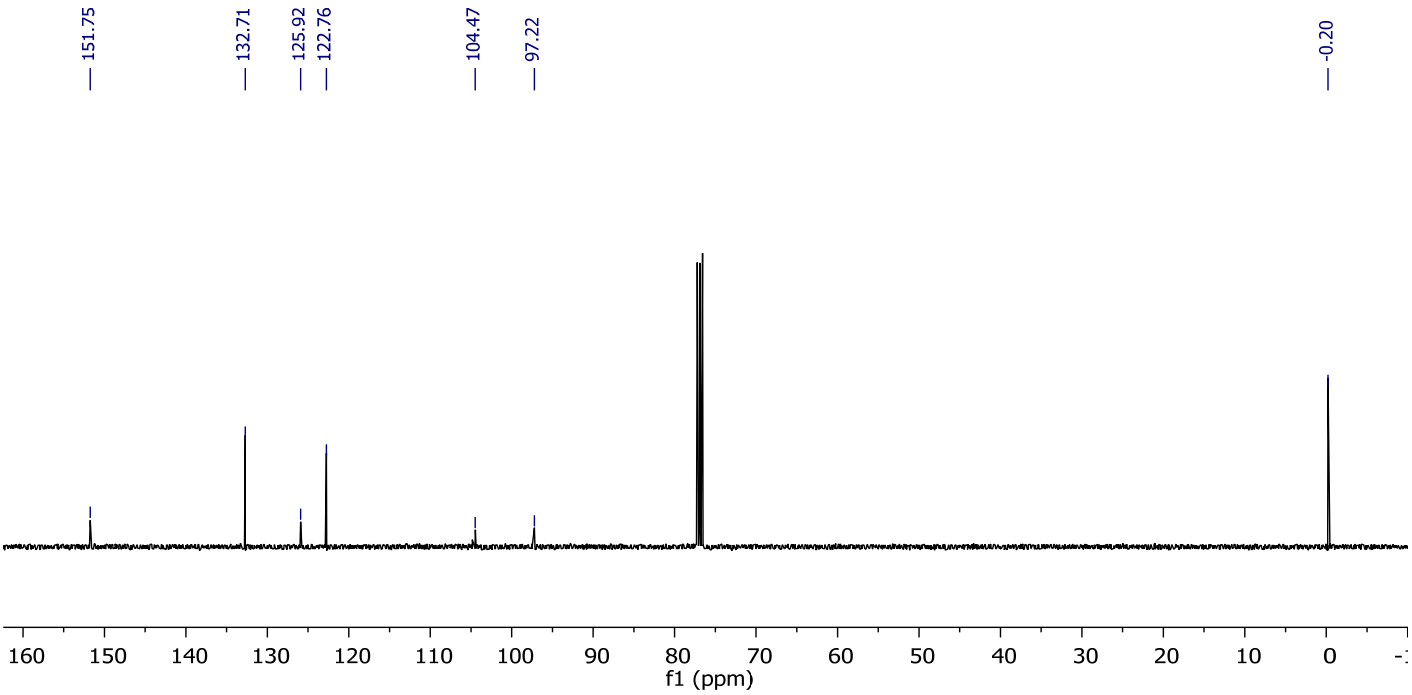

Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum for **13** in $CDCl_3$.

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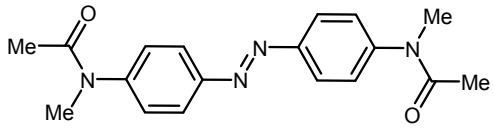

Azoarene 14. The reaction was conducted according to the general procedure using *N*-(4-azidophenyl)-*N*-methylacetamide (44.3 mg, 0.22 mmol, 1.0 equiv). The product was isolated without chromatography by the following workup procedure: after opening the vial to air and stirring, the solution was filtered through a glass fiber pad and the solvent was removed. The solid residue was then washed with 5 mL hexane and dried to yield a brown-orange solid. Run 1: 39.3 mg, >99% yield; Run 2: 41.0 mg, >99% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 4H), 7.36 (d, *J* = 8.7 Hz, 4H), 3.34 (s, 6H), 1.98 (s, 6H). $^{13}C\{^{1}H\}$ NMR (201 MHz, $CDCl_3$) δ 170.26, 151.23, 146.96, 127.75, 124.19, 37.14, 22.58. HRMS(ESI): calcd for $C_{26}H_{28}N_4O_4^+$: 325.1665; found: 325.1675.

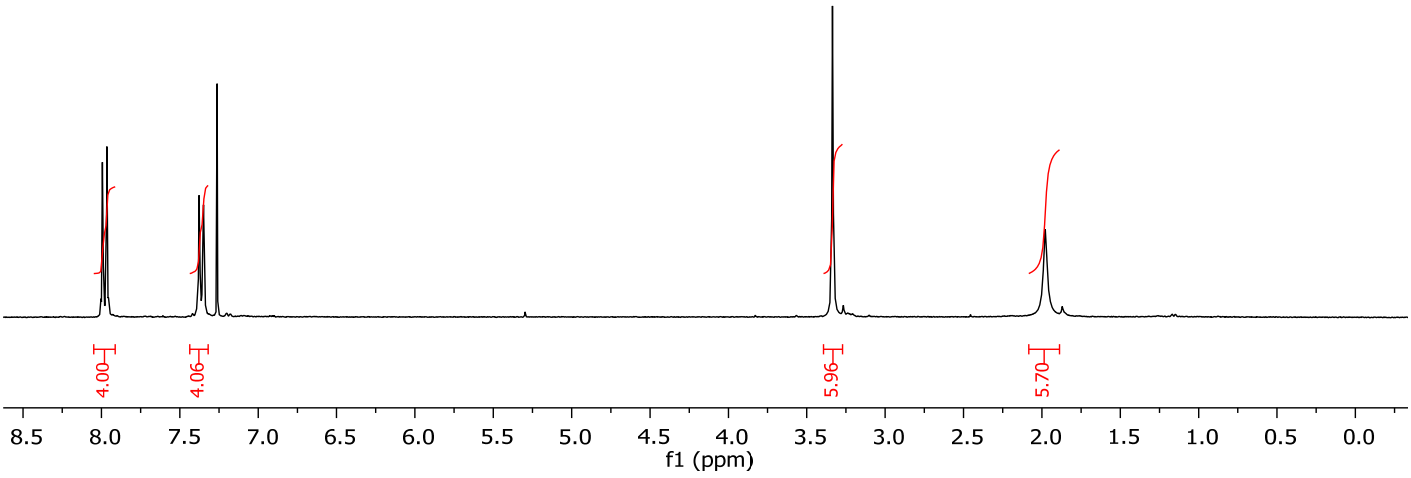

Figure S24. ^{1}H NMR spectrum for **14** in $CDCl_3$.

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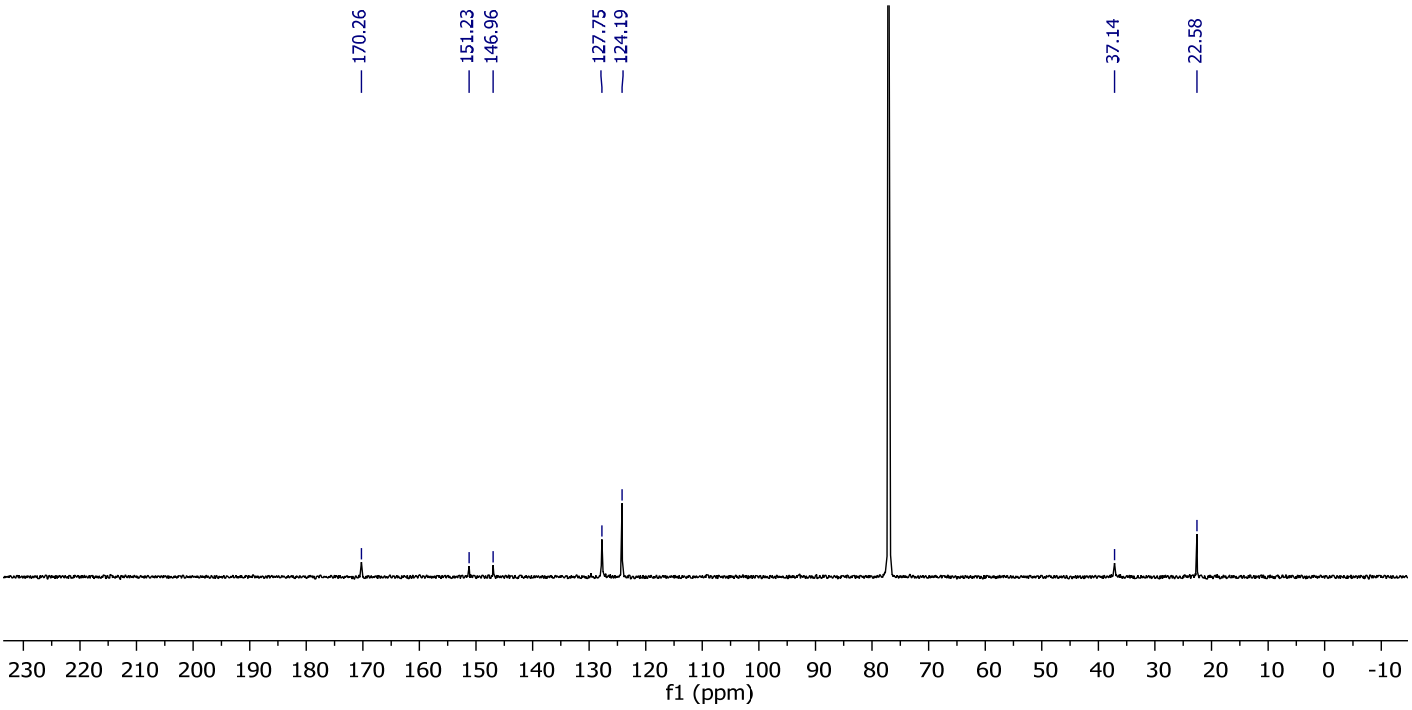

Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum for **14** in $CDCl_3$.

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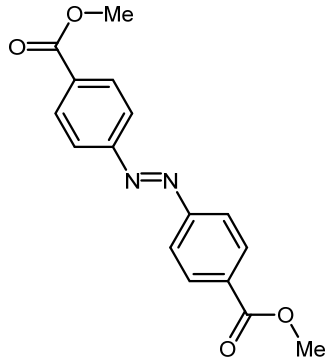

Azoarene 15.[14] The reaction was conducted according to the general procedure using methyl 4-azidobenzoate (46.1 mg, 0.3 mmol, 1.0 equiv). The product was isolated without chromatography by the following workup procedure: after opening the vial to air and stirring, the solution was filtered through a glass fiber pad and the solvent was removed. The solid residue was then washed with 5 mL hexane and dried to yield a brown-orange solid. Run 1: 46.2 mg, >99% yield; Run 2: 45.4 mg, >99% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.6 Hz, 4H), 7.99 (d, *J* = 8.3 Hz, 4H), 3.97 (s, 6H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 166.29, 154.81, 132.31, 130.57, 122.80, 52.30.

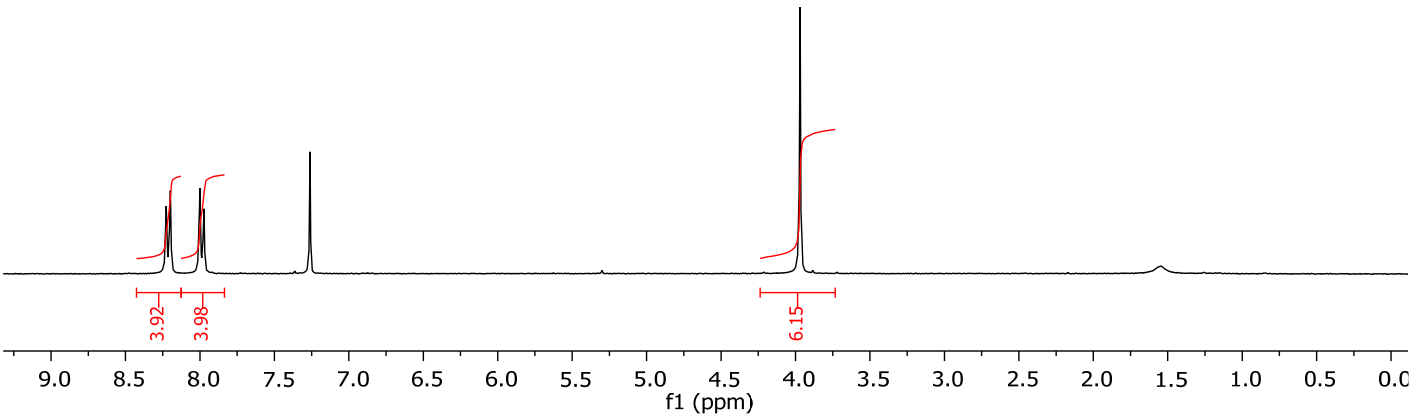

Figure S26. ^{1}H NMR spectrum for **15** in $CDCl_3$.

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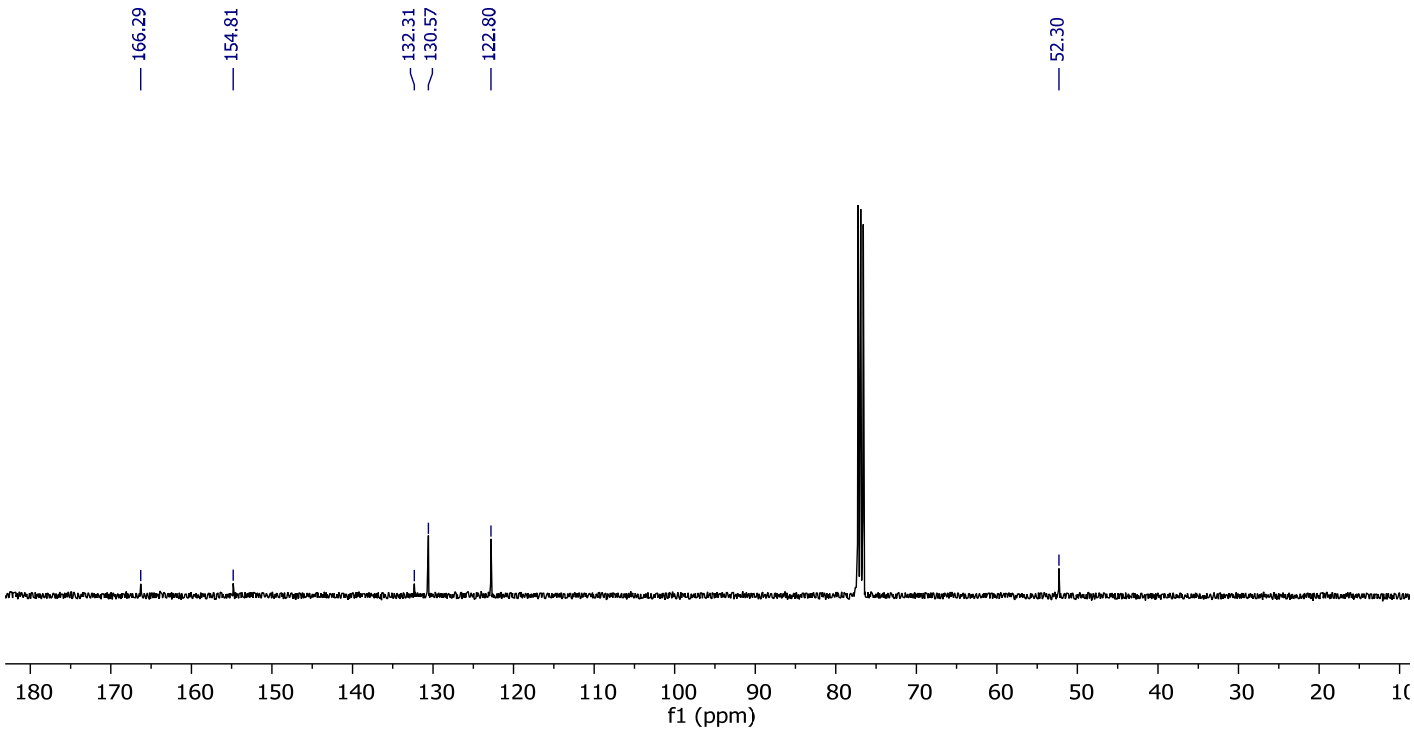

Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum for **15** in $CDCl_3$.

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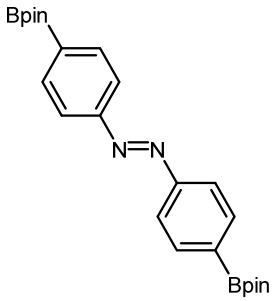

Azoarene 16.[16] The reaction was conducted according to the general procedure using 4-(pinacolboronato)phenyl azide (73.5 mg, 0.3 mmol, 1.0 equiv) and toluene as the solvent. The product was isolated without chromatography by the following workup procedure: after opening the vial to air and stirring, the solution was filtered through a glass fiber pad and the solvent was removed. The solid residue was then washed with 5 mL hexane and dried to yield a brown-orange solid. Run 1: 65.1 mg, >99% yield; Run 2: 65.0 mg, 99% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.3 Hz, 4H), 7.90 (d, *J* = 8.2 Hz, 4H), 1.37 (s, 24H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 154.27, 135.52, 121.94, 83.97, 24.80.

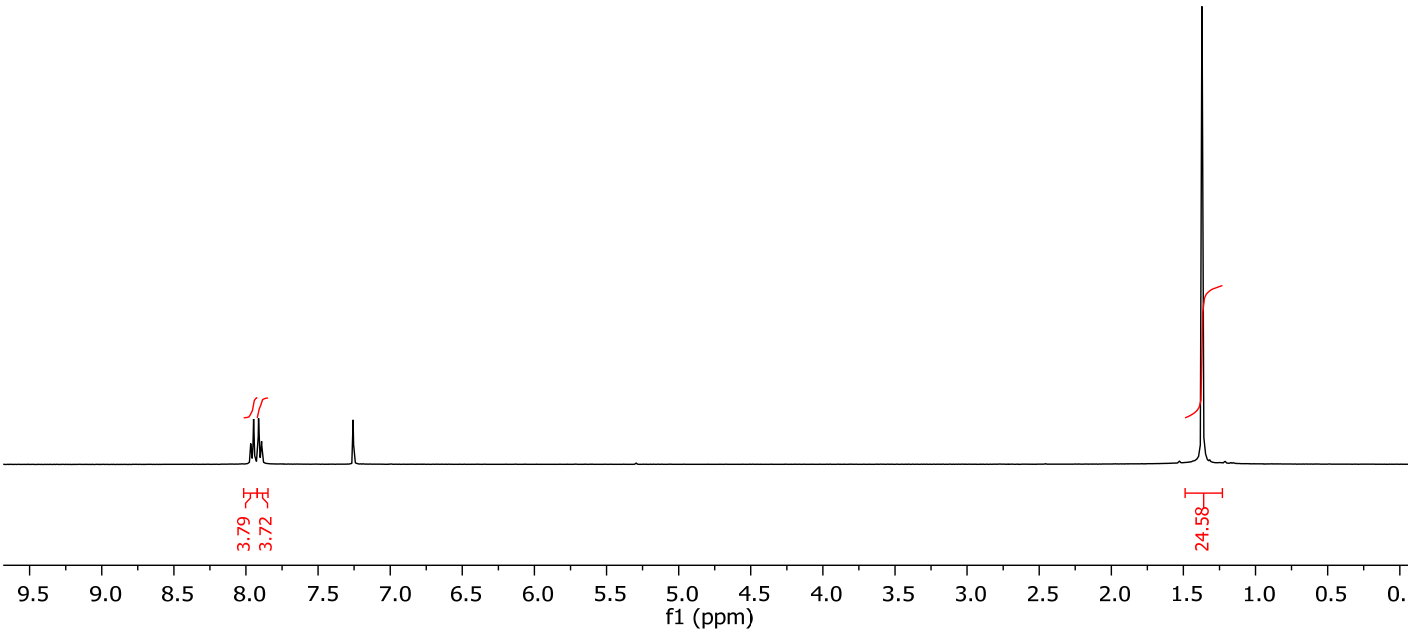

Figure S28. ^{1}H NMR spectrum for **16** in $CDCl_3$.

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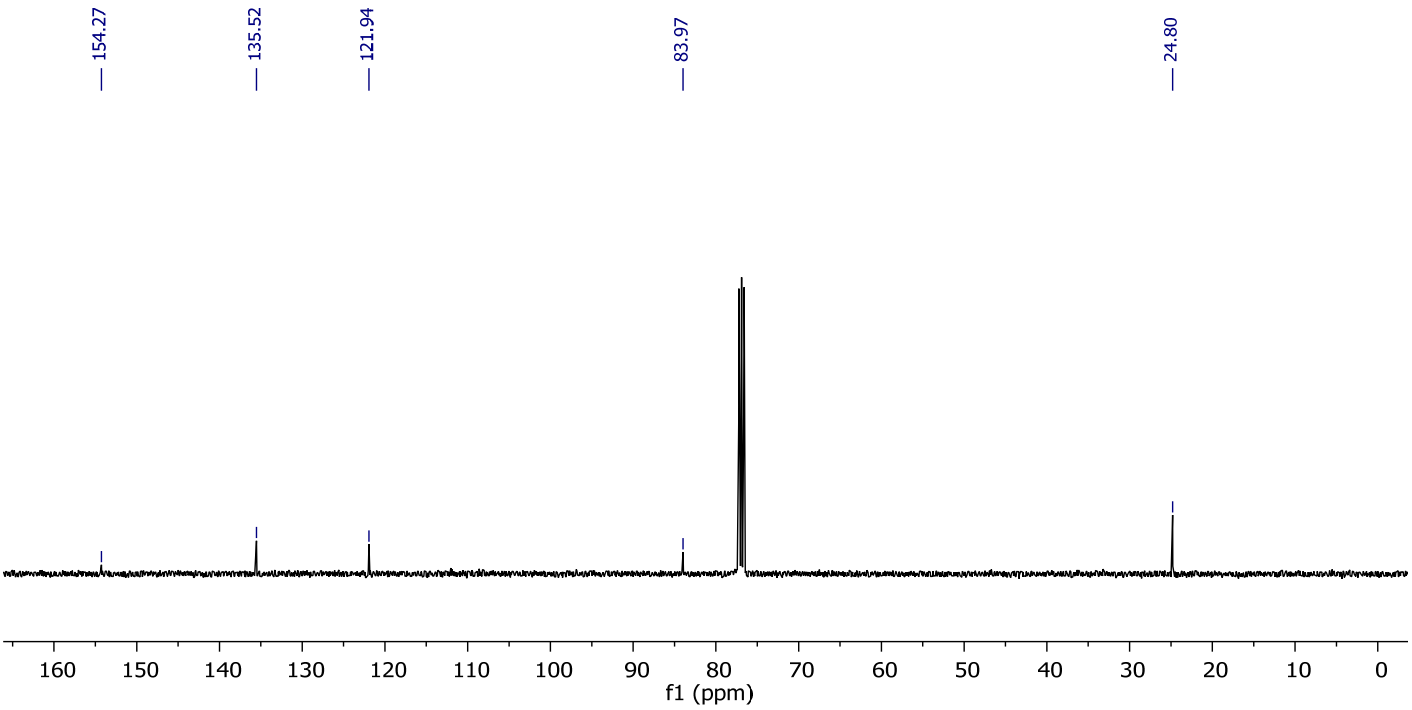

Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum for **16** in $CDCl_3$.

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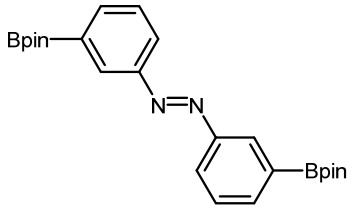

Azoarene 17.[16] The reaction was conducted according to the general procedure using 3-(pinacolboronato)phenylazide (73.5 mg, 0.3 mmol, 1.0 equiv.) and toluene as the solvent. The product was isolated without chromatography by the following workup procedure: after opening the vial to air and stirring, the solution was filtered through a glass fiber pad and the solvent was removed. The solid residue was then washed with 5 mL hexane and dried to yield a brown-orange solid. Run 1: 53.0 mg, 81% yield; Run 2: 54.0 mg, 83% yield. ^{1}H (400 MHz, $CDCl_3$) δ 8.36 (s, 2H), 8.00 (d, *J* = 1.3 Hz, 2H), 7.90 (d, *J* = 1.3 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 1.37 (s, 24H). ^{13}C{H} NMR (101 MHz, CDCl3) δ 152.01, 137.05, 129.22, 128.42, 125.22, 83.94, 77.11, 24.81.

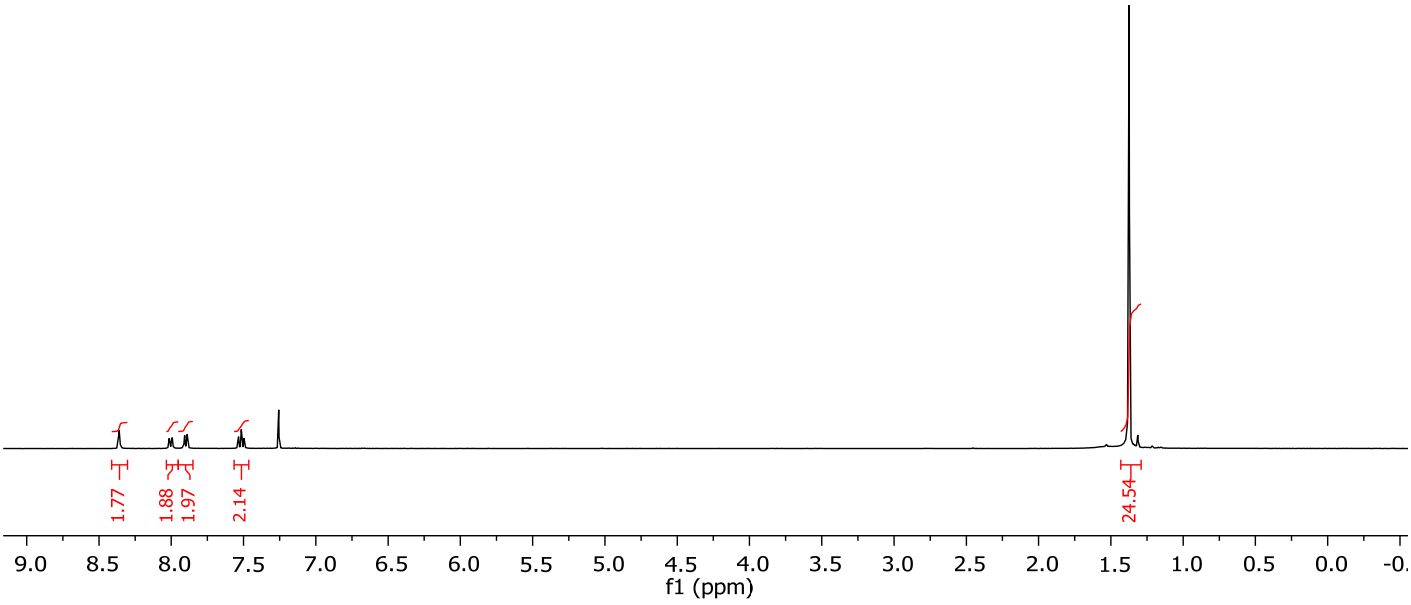

Figure S30. ^{1}H NMR spectrum for **17** in $CDCl_3$.

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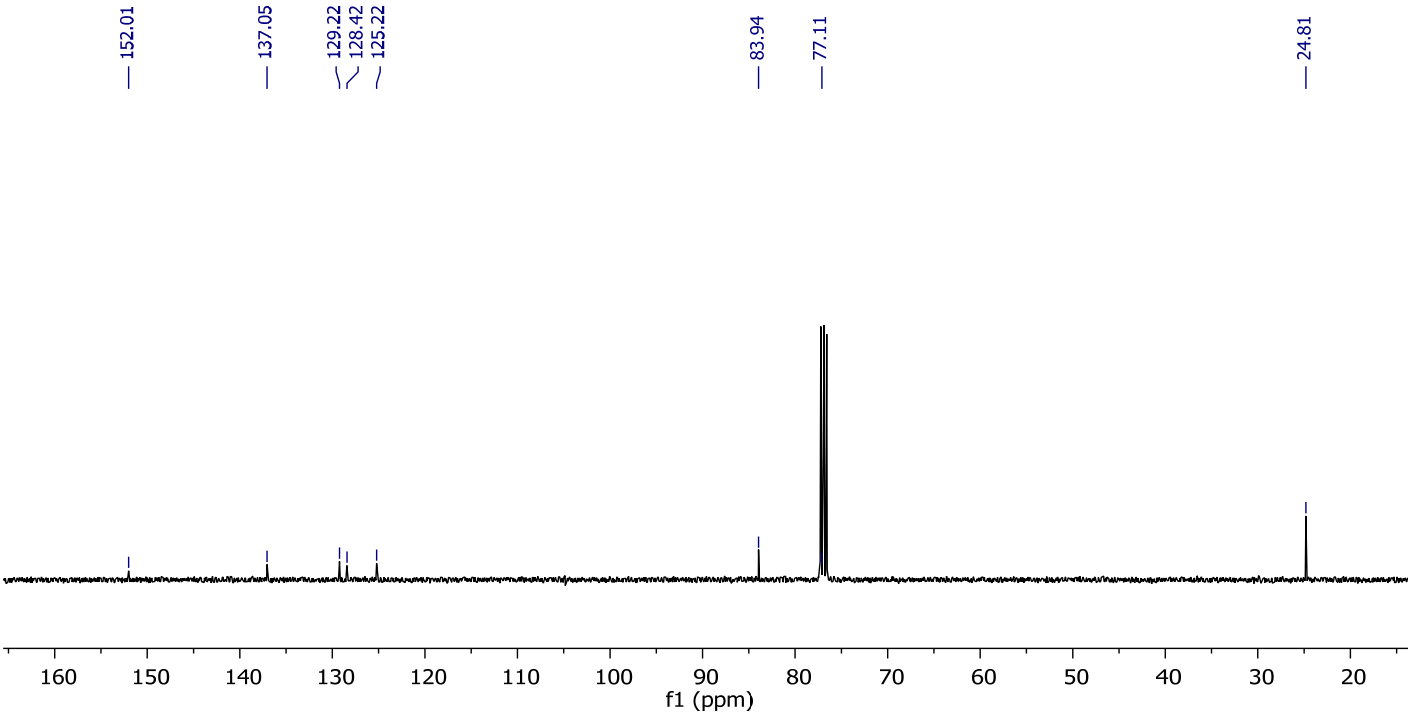

Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum for **17** in $CDCl_3$.

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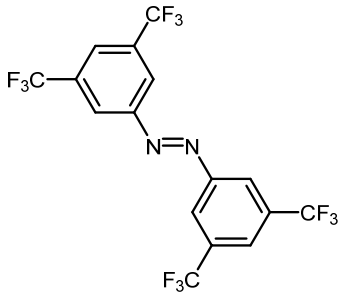

Azoarene 18.[17] The reaction was conducted according to the general procedure using 3,5-bis-trifluoromethylphenyl azide (68.1 mg, 0.27 mmol, 1.0 equiv). Isolated yields were determined following column chromatography (SiO_2, hexanes). The product was isolated as an orange solid. Run 1: 55 mg, 90% yield; Run 2: 58 mg, 97% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.45 (d, *J* = 1.6 Hz, 4H), 8.06 (s, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.50. ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 152.12 , 133.13 (q, *J* = 34.2 Hz), 125.20 (hept, *J* = 4.1 Hz), 123.53 – 123.27 (m), 122.86 (q, *J* = 273.0 Hz).

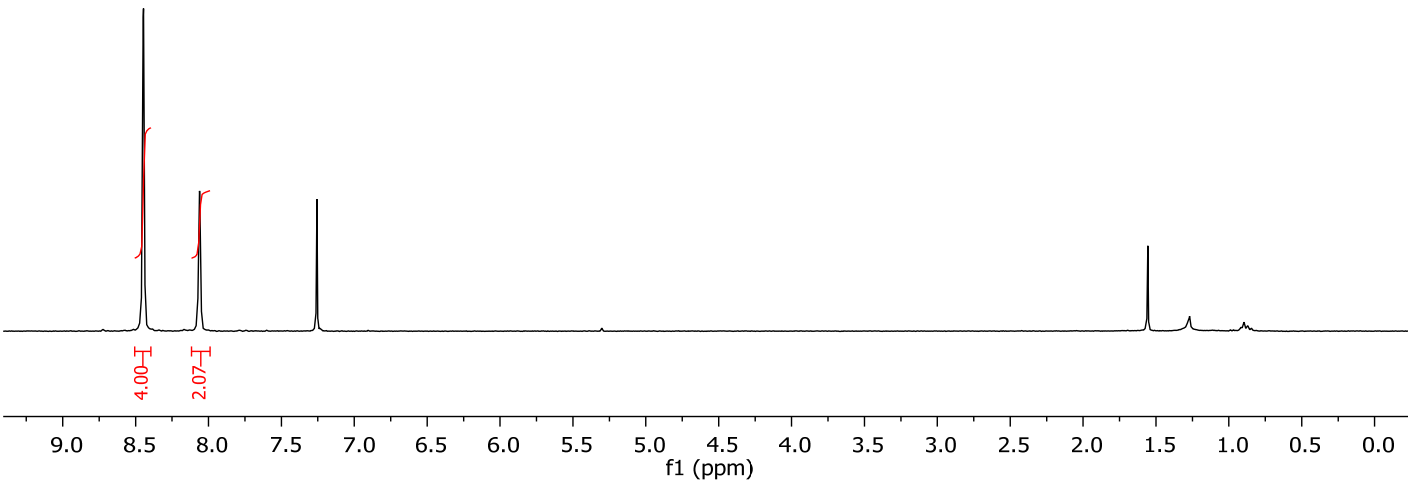

Figure S32. ^{1}H NMR spectrum for **18** in $CDCl_3$.

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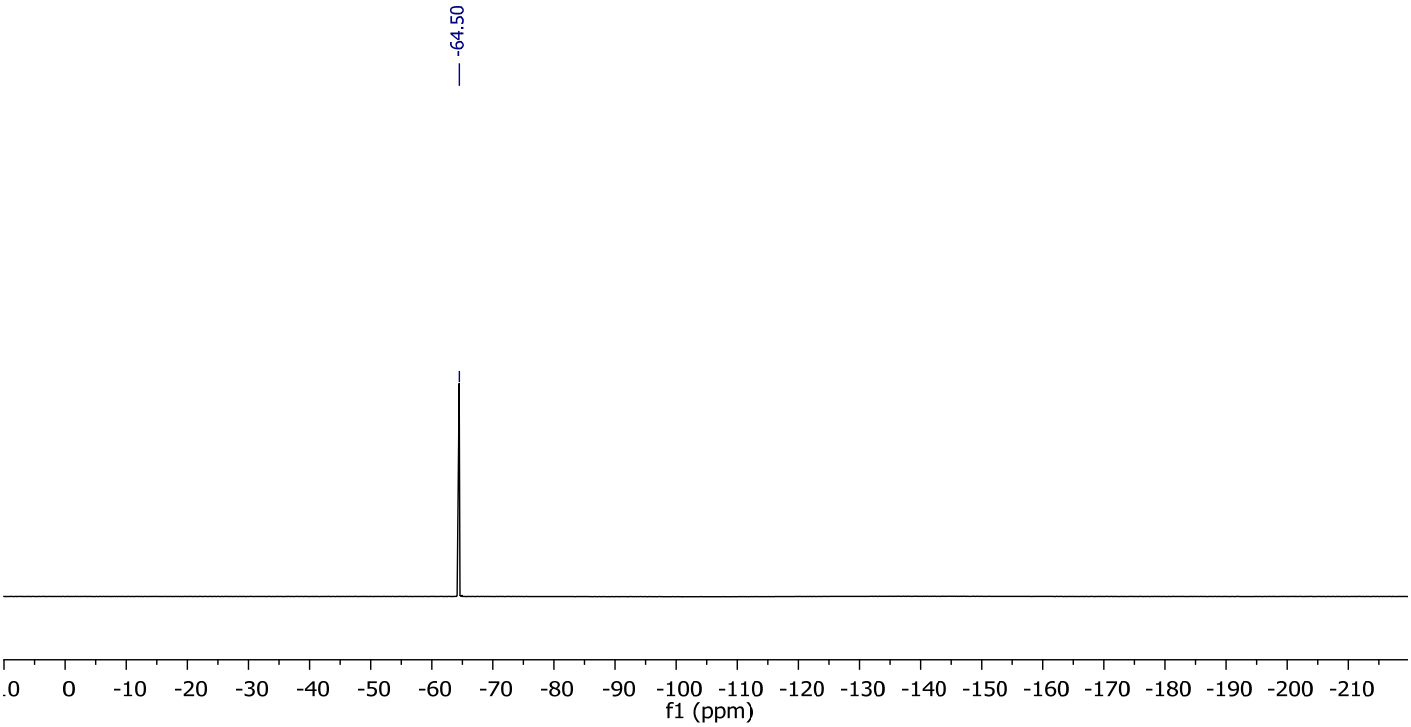

Figure S33. ^{19}F NMR spectrum for **18** in $CDCl_3$.

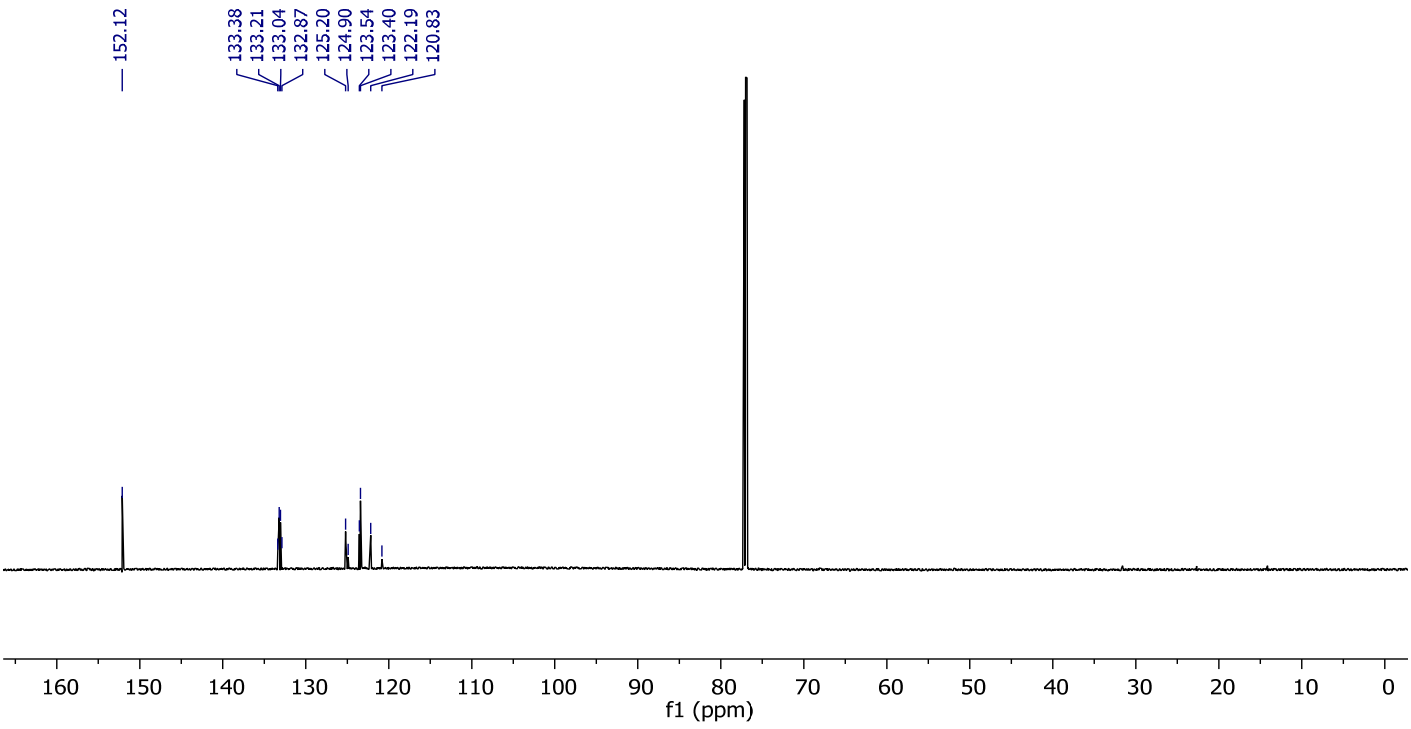

Figure S34. $^{13}C\{^1H\}$ NMR spectrum for **18** in $CDCl_3$.

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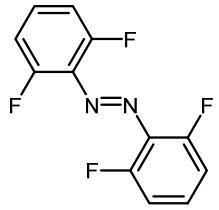

Azoarene 19.[18] The reaction was conducted according to the following modified general procedure using 2,6-difluorophenyl azide (46.5 mg, 0.3 mmol, 1.0 equiv): the reagents were mixed in a microwave vial, which was then sealed and heated to 80 °C for 2 h. Isolated yields were determined following column chromatography (SiO_2, 1% EtOAc/hexanes). The product was isolated as an orange solid in a 15:85 mixture of *Z* and *E* isomers. Run 1: 32.1 mg, 84% yield; Run 2: 34.2 mg, 90% yield. ^{1}H NMR (300 MHz, $CDCl_3$) *E* isomer: δ 7.47 – 7.31 (m, 2H), 7.12 – 7.00 (m, 4H); *Z* isomer: δ 7.24 – 7.14 (m, 2H), 6.95 – 6.75 (m, 4H). ^{19}F NMR (282 MHz, $CDCl_3$) *E* isomer: δ -122.81; Z isomer: δ -121.03. ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) *E* isomer: δ 155.49 (d, J = 260.8 Hz), 131.70 (t, J = 9.3 Hz), 131.37 (t, J = 9.7 Hz), 112.54 (d, J = 24.1 Hz).

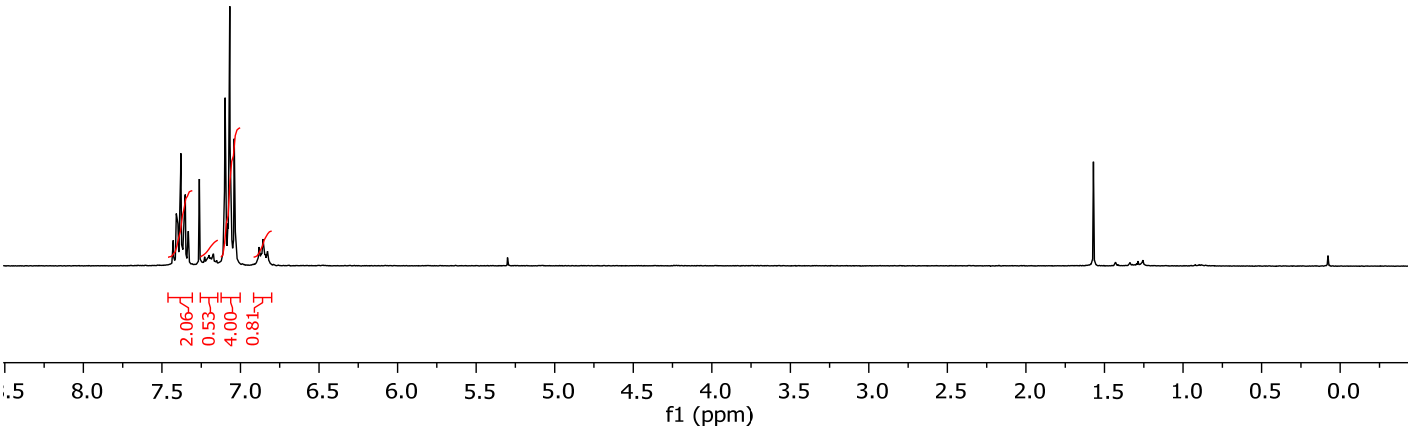

Figure S35. ^{1}H NMR spectrum for **19** in $CDCl_3$.

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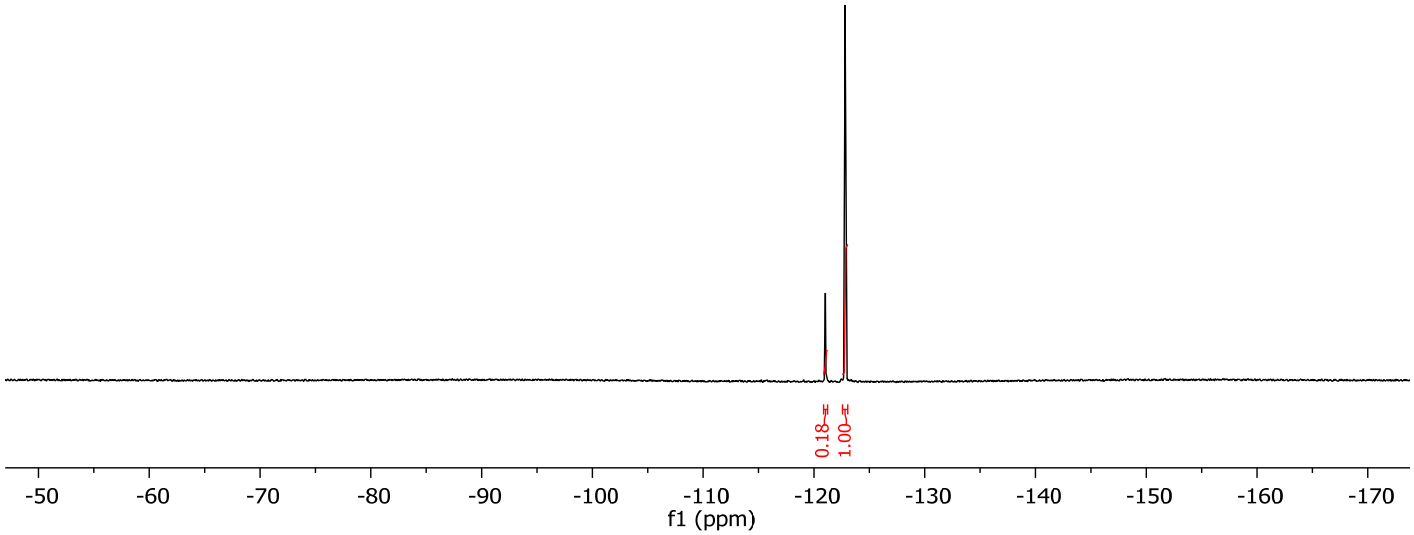

Figure S36. ^{19}F NMR spectrum for **19** in $CDCl_3$.

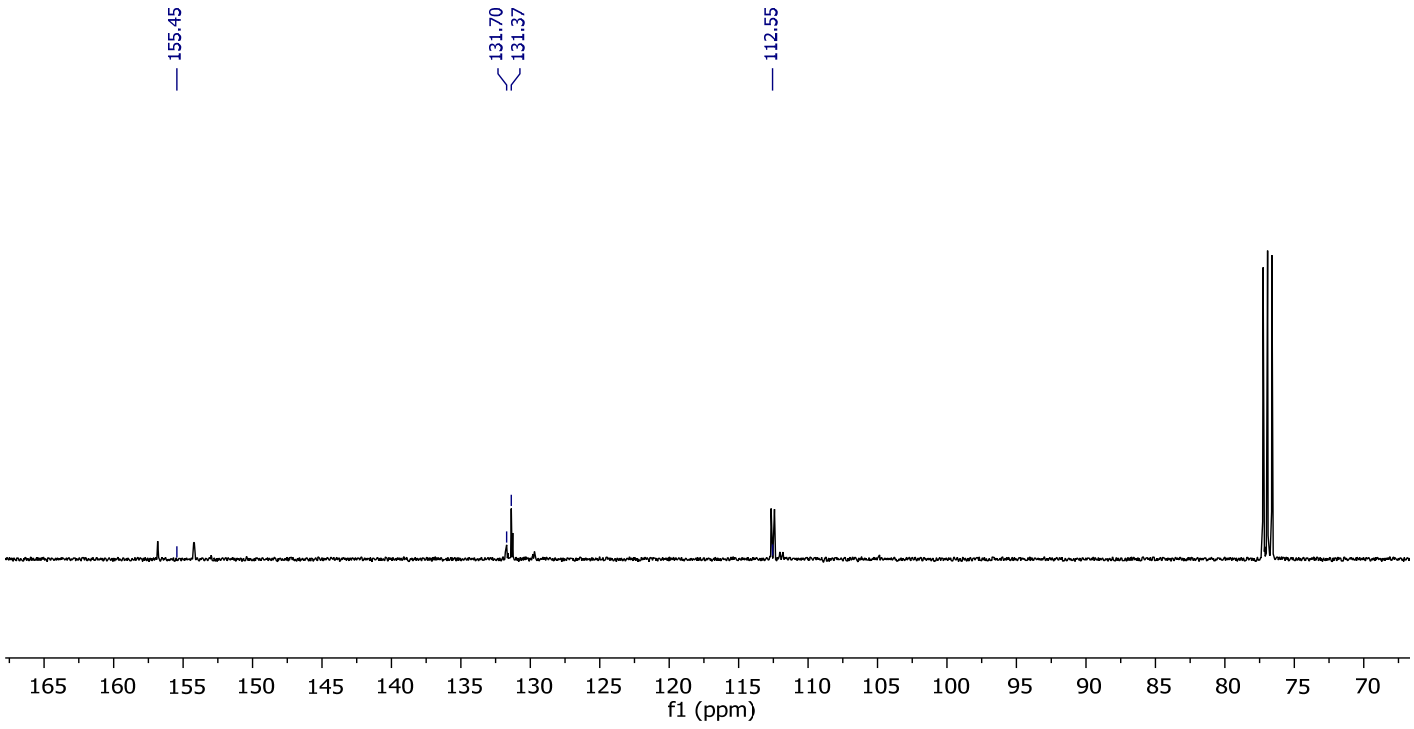

Figure S37. $^{13}C\{^1H\}$ NMR spectrum for **19** in $CDCl_3$.

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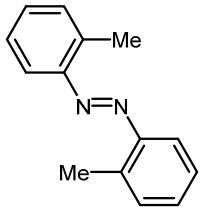

Azoarene 20.[14] The reaction was conducted according to the following modified general procedure using 2-tolyl azide (39.9 mg, 0.3 mmol, 1.0 equiv): the reagents were mixed in a microwave vial, which was then sealed and heated to 100 °C for 4 h. Isolated yields were determined following column chromatography (hexanes). The product was isolated as an orange oil. Run 1: 26.1 mg, 83% yield; Run 2: 24.3 mg, 77% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.44 – 7.32 (m, 4H), 7.31 – 7.22 (m, 2H), 2.76 (s, 6H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 151.01, 137.91, 131.17, 130.59, 126.27, 115.76, 17.54.

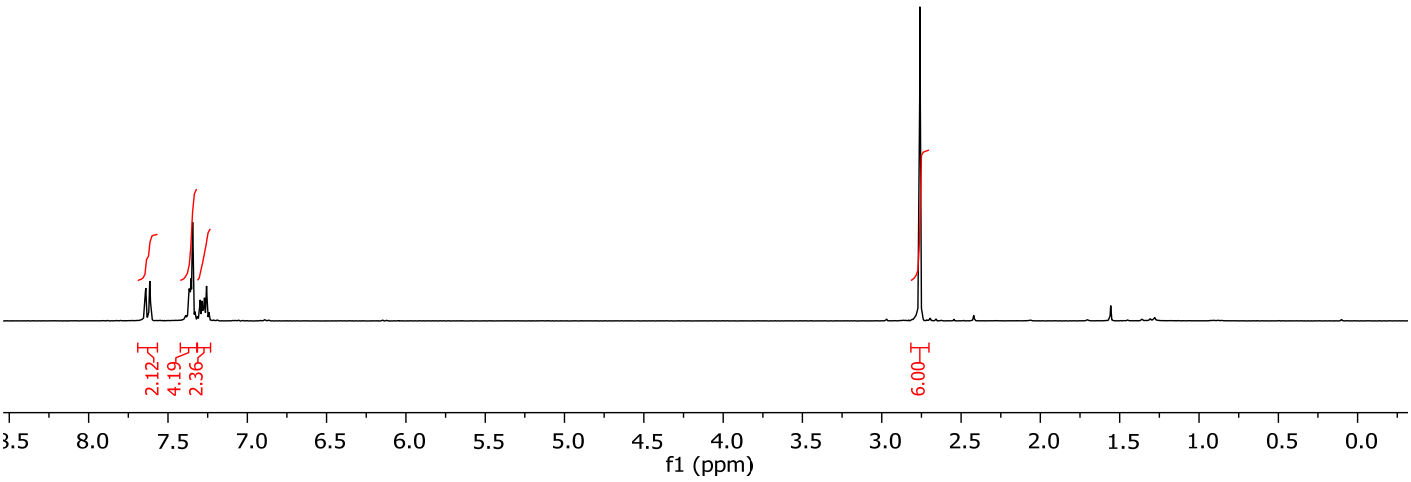

Figure S38. ^{1}H NMR spectrum for **20** in $CDCl_3$.

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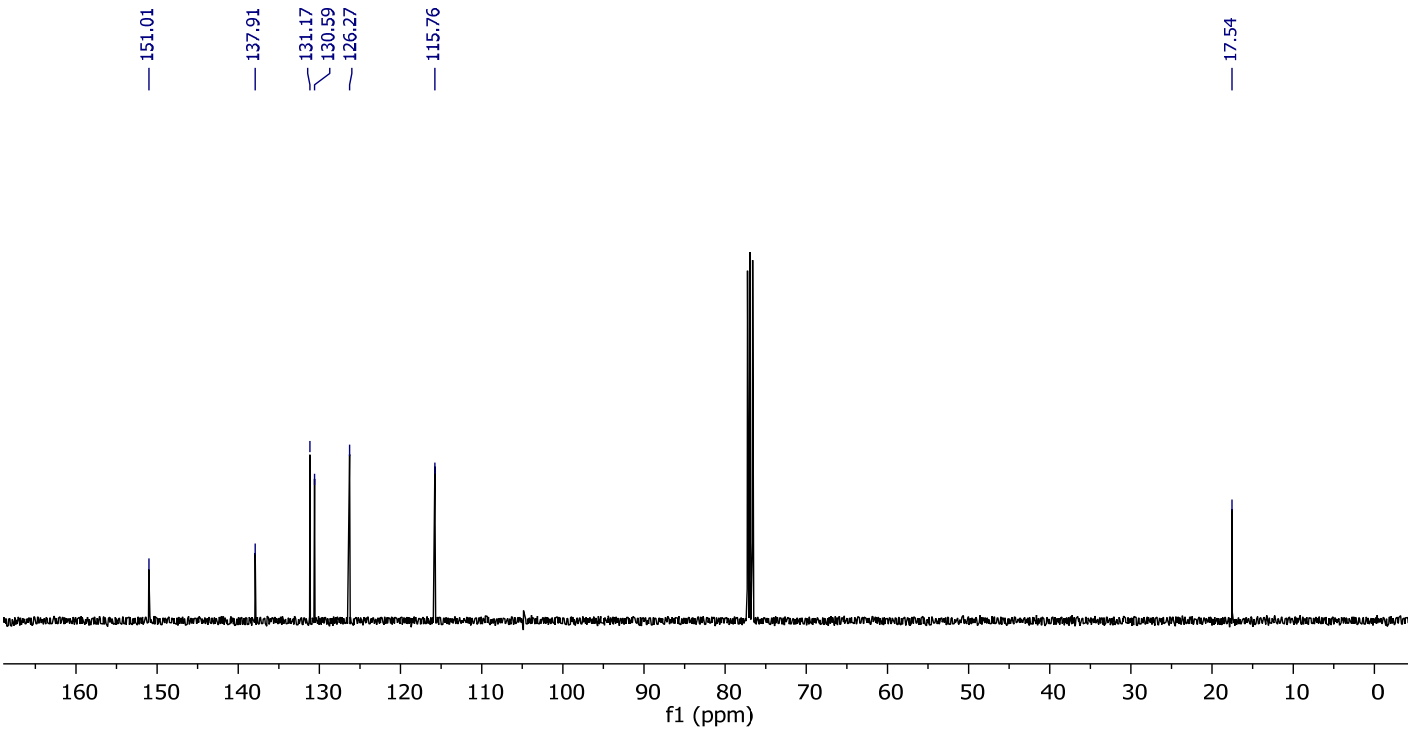

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum for **20** in $CDCl_3$.

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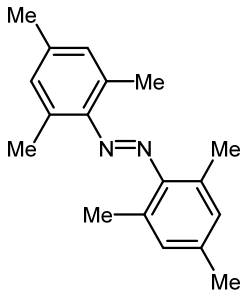

Azoarene 21.[19] The reaction was conducted according to the following modified general procedure using 2,4,6-trimethylphenyl azide (48.4 mg, 0.3 mmol, 1.0 equiv): the reagents were mixed in a microwave vial, which was then sealed and heated to 100 °C for 4 h. Isolated yields were determined following column chromatography (hexanes). The product was isolated as an orange solid. Run 1: 33 mg, 83% yield; Run 2: 37 mg, 93% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.97 (s, 4H), 2.43 (s, 12H), 2.35 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 149.03, 138.23, 131.54, 129.97, 20.94, 19.92.

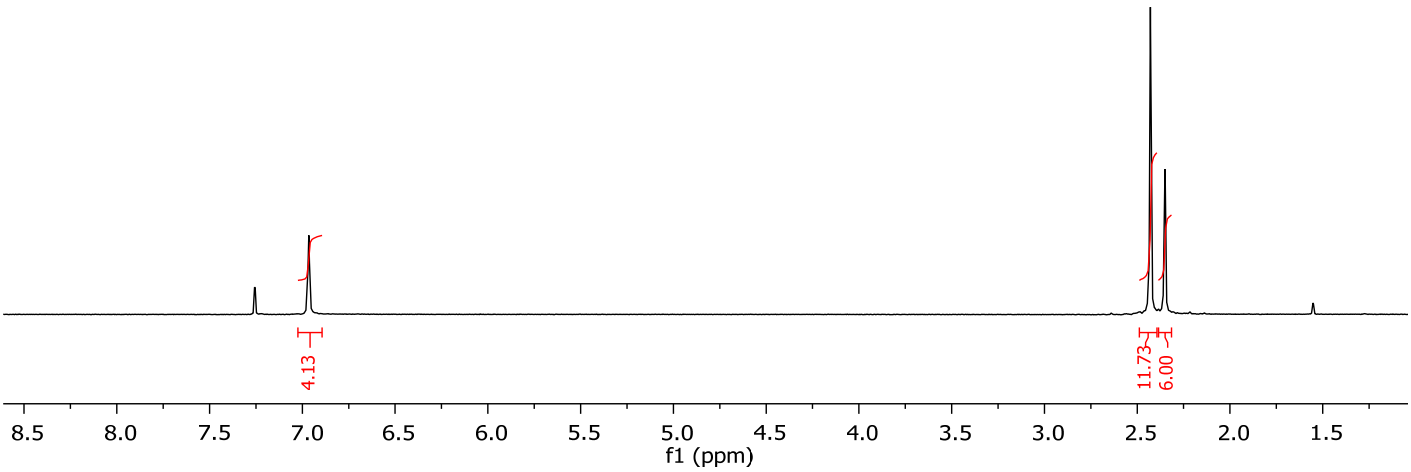

Figure S40. ^{1}H NMR spectrum for **21** in $CDCl_3$.

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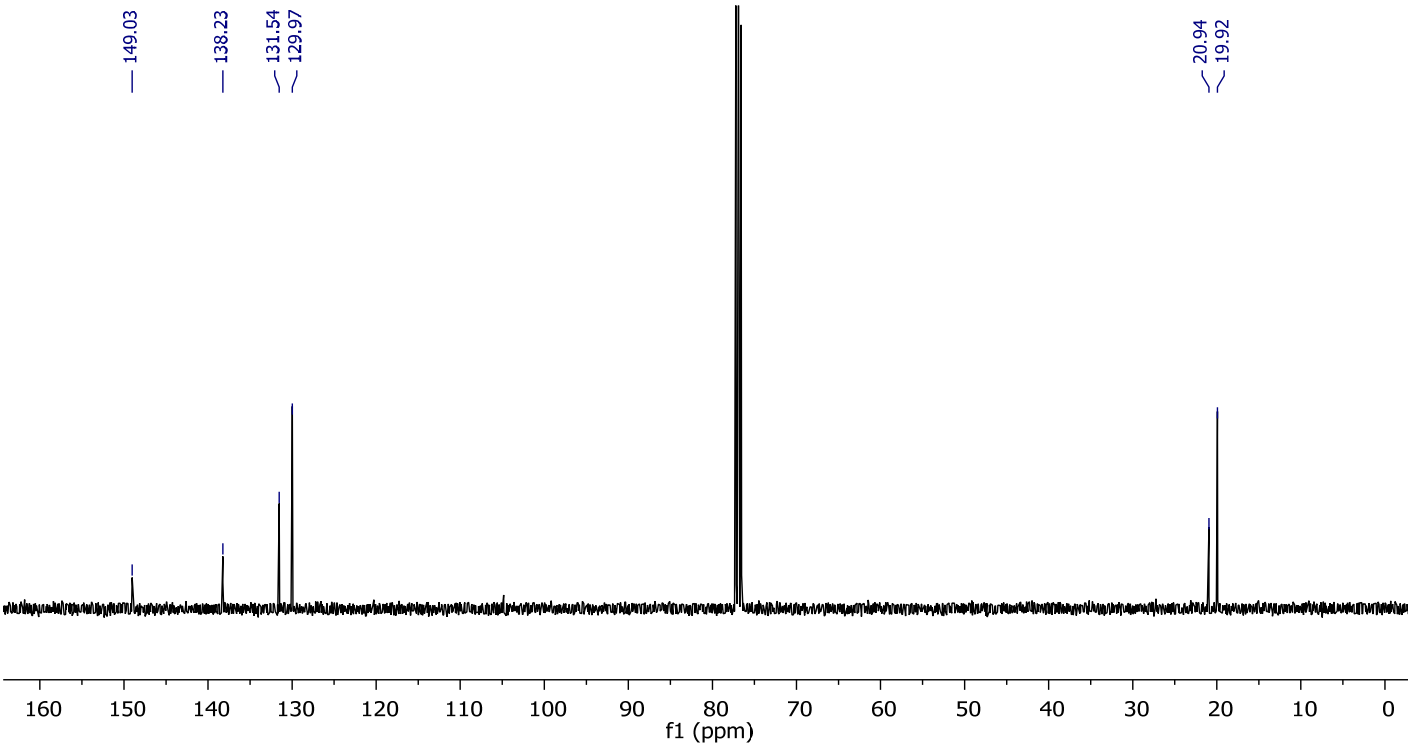

Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum for **21** in $CDCl_3$.

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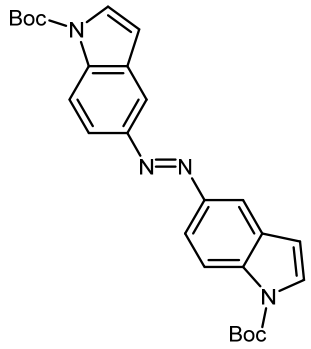

Azoarene 22. The reaction was conducted according to a modified general procedure using *tert*-butyl 5-azido-1*H*-indole-1-carboxylate (77.5 mg, 0.3 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). Isolated yields were determined following column chromatography (SiO_2, 0 – 3% EtOAc/Hexanes). The product was isolated as a yellow solid. Run 1: 30.9 mg, 45% yield; Run 2: 31.3 mg, 48% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.9 Hz, 2H), 8.17 (d, *J* = 1.9 Hz, 2H), 7.98 (dd, *J* = 8.9, 2.0 Hz, 2H), 7.66 (d, *J* = 3.7 Hz, 2H), 6.70 (dd, *J* = 3.7, 0.7 Hz, 2H), 1.70 (s, 18H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 149.42, 148.71, 136.45, 130.92, 127.07, 118.74, 116.34, 115.35, 108.07, 84.04, 28.10. HRMS(ESI): calcd for $C_{26}H_{28}N_4O_4^{+\cdot}$: 461.2183; found: 461.2181.

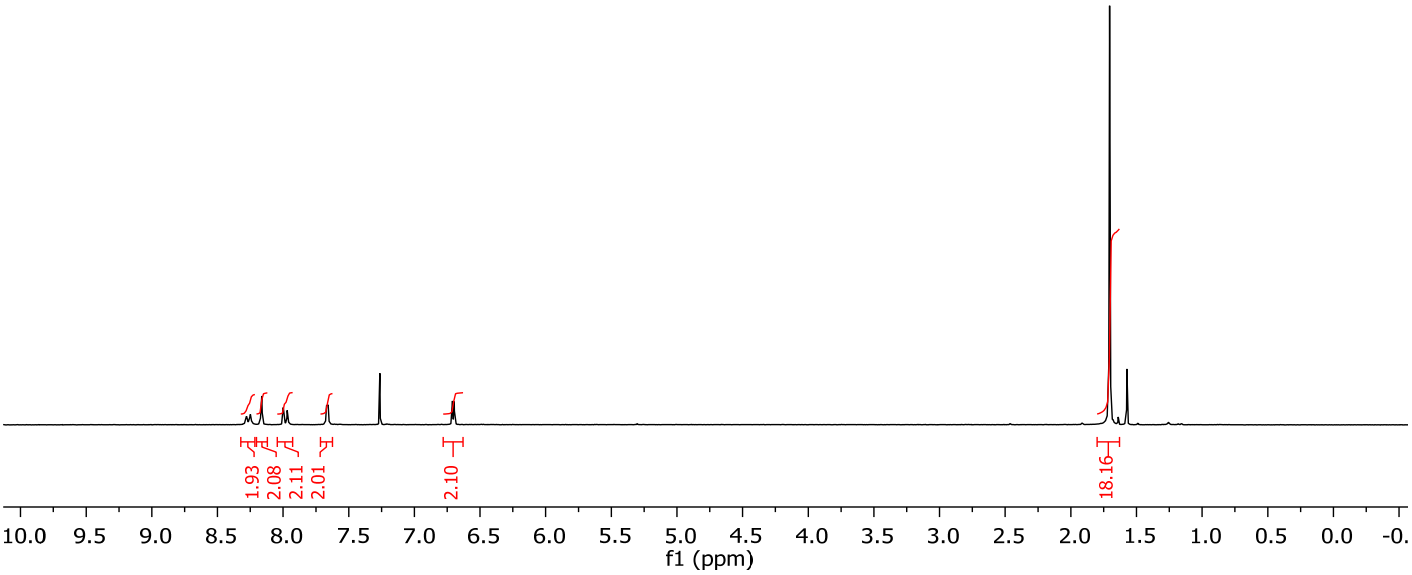

Figure S42. ^{1}H NMR spectrum for **22** in $CDCl_3$.

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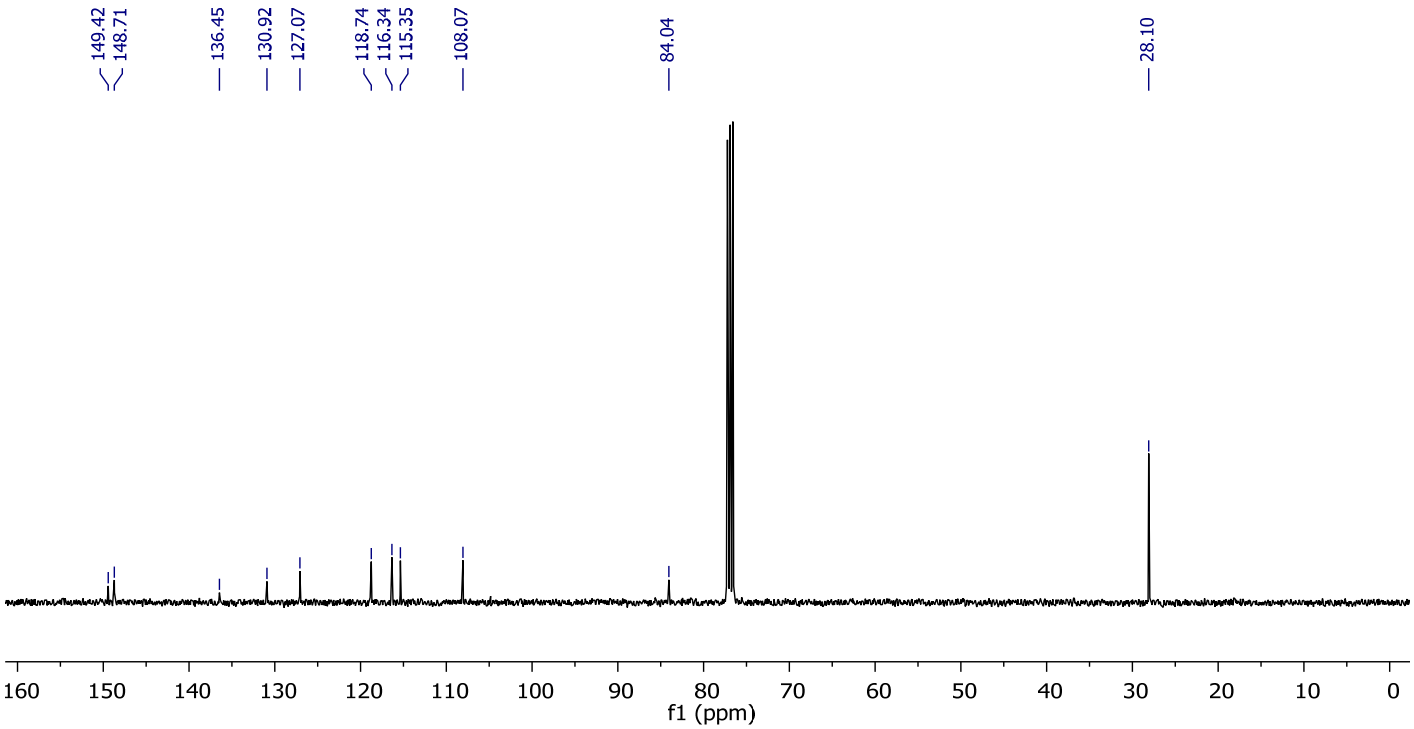

Figure S43. $^{13}C\{^{1}H\}$ NMR spectrum for **22** in $CDCl_3$.

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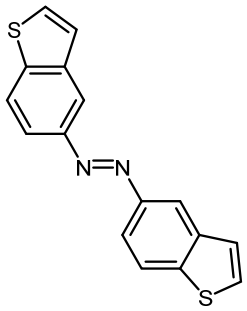

Azoarene 23.[20] The reaction was conducted according to a modified general procedure using 5-azidobenzo[*b*]thiophene (52.6 mg, 0.3 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol), with an additional 5 mol% **1** added after one hour. Isolated yields were determined following column chromatography (SiO_2, 0 – 3% EtOAc/Hexanes). The product was isolated as a yellow solid. Run 1: 30 mg, 68% yield; Run 2: 34 mg, 77% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 1.7, 0.8 Hz, 2H), 8.06 – 7.93 (m, 4H), 7.55 (dd, *J* = 5.5, 0.4 Hz, 2H), 7.50 (dd, *J* = 5.5, 0.6 Hz, 2H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 150.16, 142.09, 140.12, 127.85, 124.80, 122.89, 120.29, 117.35.

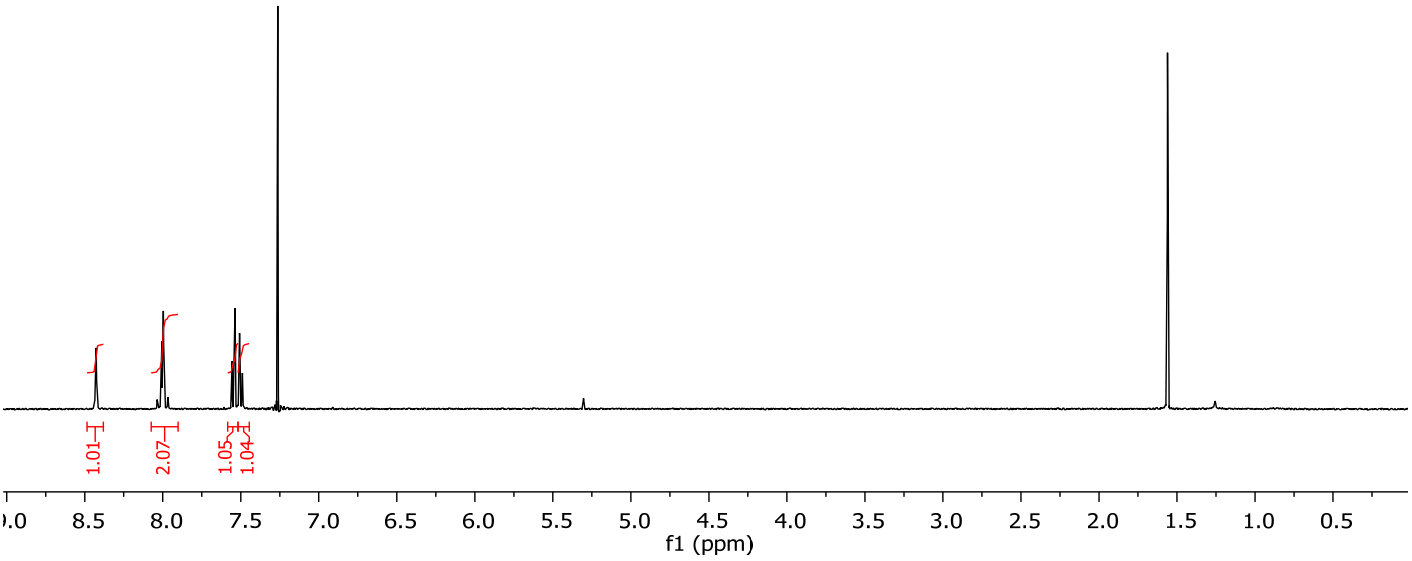

Figure S44. ^{1}H NMR spectrum for **23** in $CDCl_3$.

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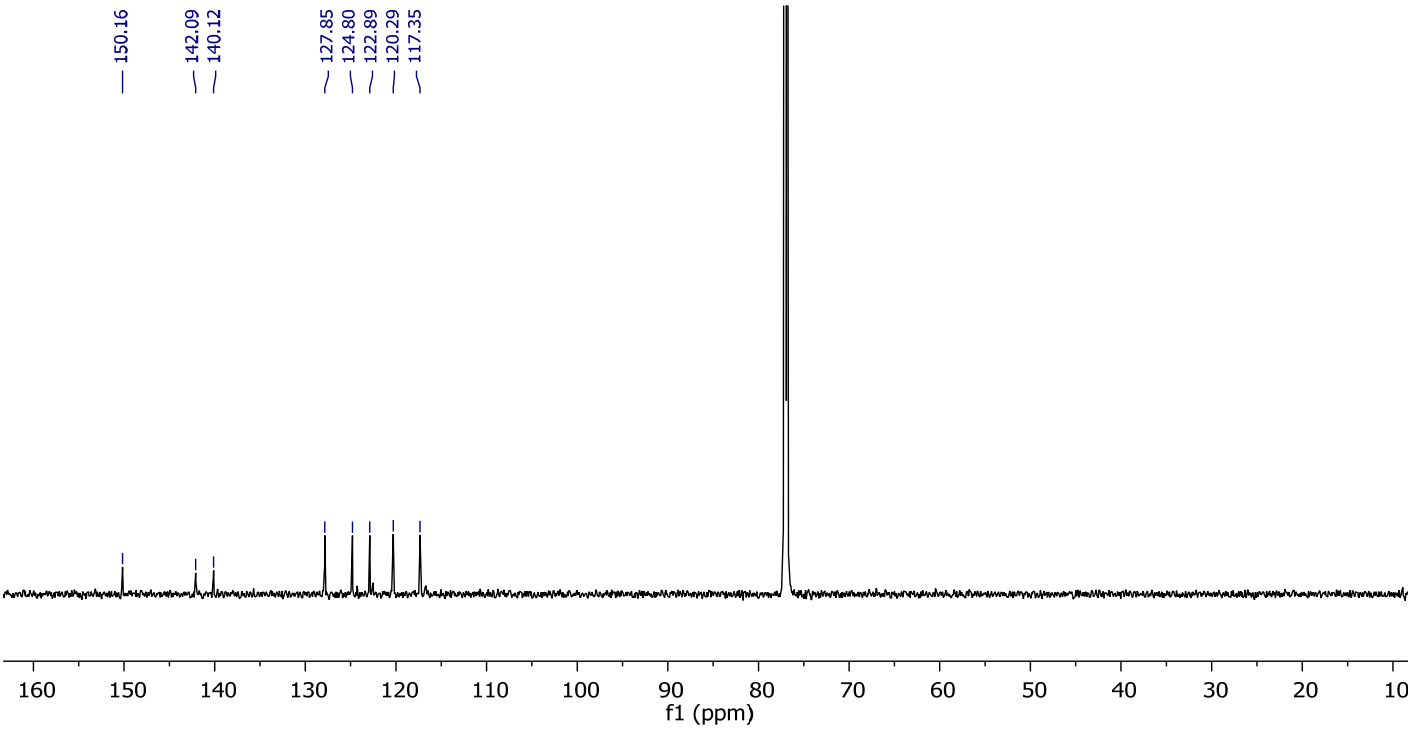

Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum for **23** in $CDCl_3$.

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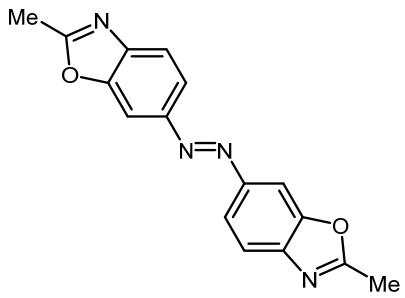

Azoarene 24. The reaction was conducted according to a modified general procedure using 6-azido-2-methylbenzo[*d*]oxazole (52.2 mg, 0.3 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). Isolated yields were determined following column chromatography (SiO_2, 0 – 1% CH_2Cl_2/MeOH). The product was isolated as a yellow solid. Run 1: 35.4 mg, 81% yield; Run 2: 33.8 mg, 77% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (d, *J* = 1.9 Hz, 2H), 7.99 (dd, *J* = 8.7, 1.9 Hz, 2H), 7.58 (dd, *J* = 8.6, 0.5 Hz, 2H), 2.68 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 165.24, 152.55, 149.80, 142.18, 120.09, 114.14, 110.24, 14.57. HRMS(ESI): calcd for $C_{16}H_{12}N_4O_2^+$: 293.1033; found: 293.1034.

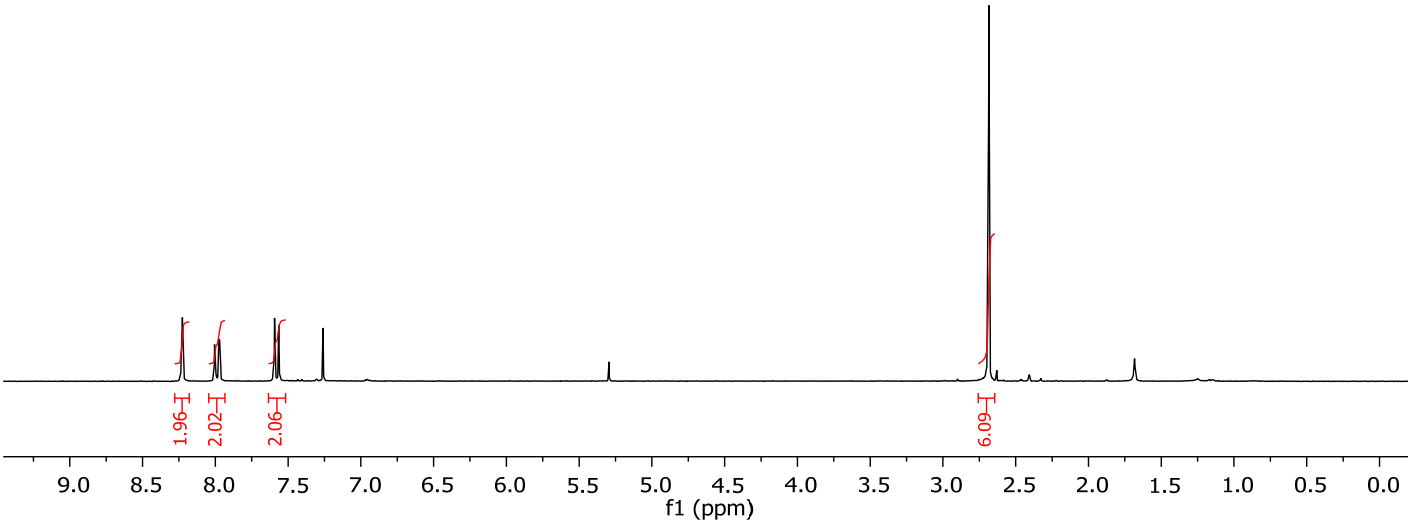

Figure S46. ^{1}H NMR spectrum for **24** in $CDCl_3$.

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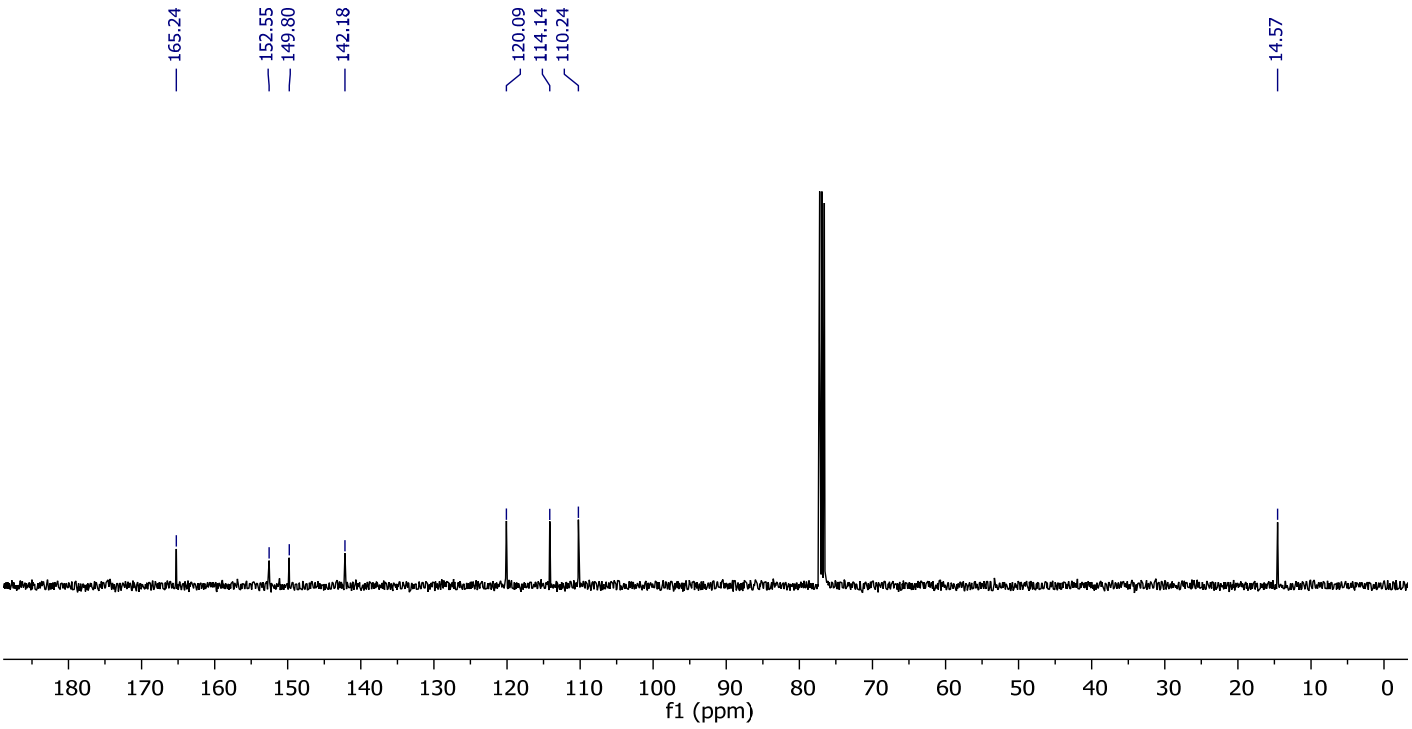

Figure S47. $^{13}C\{^{1}H\}$ NMR spectrum for **24** in $CDCl_3$.

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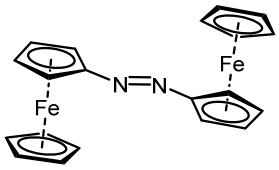

Azoarene 25.[21] The reaction was conducted according to a modified general procedure using 1-azidoferrocene (68.1 mg, 0.3 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). The product was isolated without chromatography by the following workup procedure: After opening the vial to air and stirring, the solution was filtered through a glass fiber pad, and residual solid product was washed through the filter with chloroform. The solvent was then removed, and the solid residue was washed with 2 x 5 mL hexane and dried to yield a purple solid. Run 1: 59.8 mg, >99% yield; Run 2: 59.7 mg, >99% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 4.94 (t, *J* = 2.0 Hz, 2H), 4.49 (t, *J* = 2.0 Hz, 2H), 4.25 (s, 5H). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 107.93, 69.64, 69.44, 64.01.

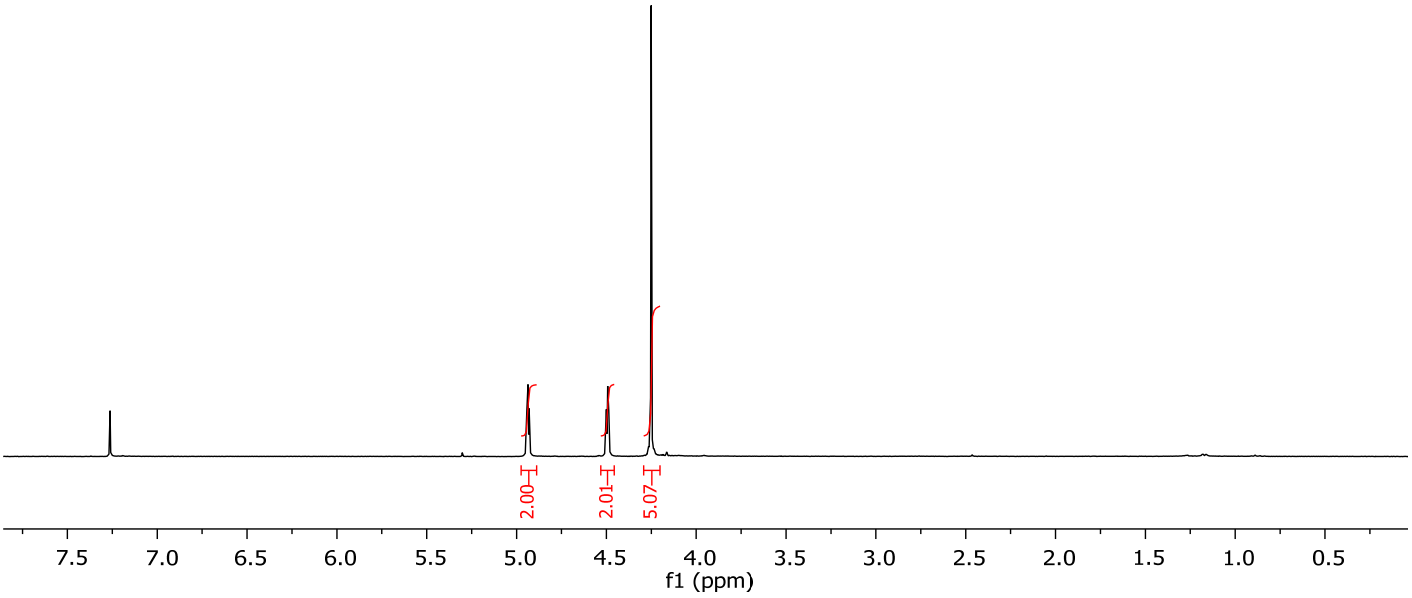

Figure S48. ^{1}H NMR spectrum for **25** in $CDCl_3$.

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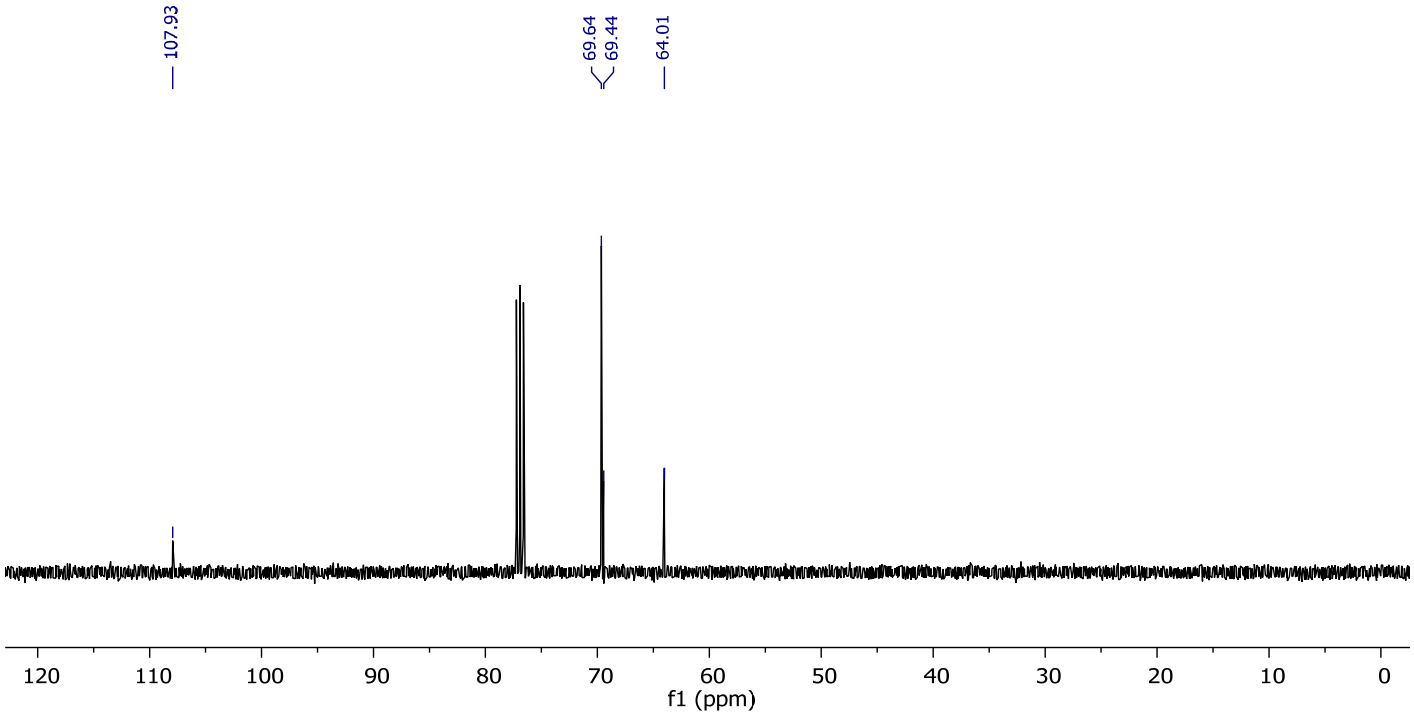

Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum for **25** in $CDCl_3$.

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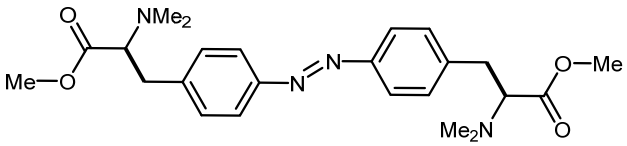

Azoarene 26. The reaction was conducted according to a modified general procedure using **S1** (57.1 mg, 0.3 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). The product was isolated without chromatography by the following workup procedure: After opening the vial to air and stirring, the solution was filtered through a glass fiber pad, and residual solid product was washed through the filter with chloroform. The solvent was then removed, and the solid residue was washed with 2 x 5 mL hexane and dried to yield a dark brown solid. Run 1: 31 mg, 67% yield; Run 2: 33 mg, 69% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 4H), 7.34 (d, *J* = 8.1 Hz, 4H), 3.62 (s, 6H), 3.46 – 3.39 (m, 2H), 3.22 – 2.90 (m, 4H), 2.40 (s, 12H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 171.68, 151.38, 141.49, 129.80, 122.83, 69.35, 51.15, 41.87, 35.56. HRMS(ESI): calcd for $C_{24}H_{33}N_4O_4^+$: 441.2496; found: 441.2494.

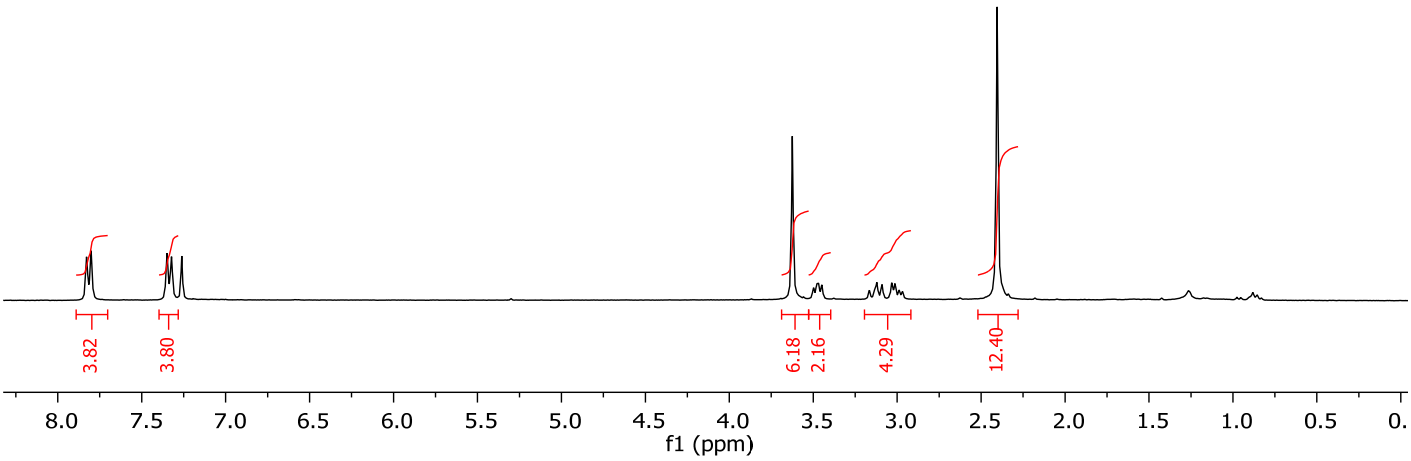

Figure S50. ^{1}H NMR spectrum for **26** in $CDCl_3$.

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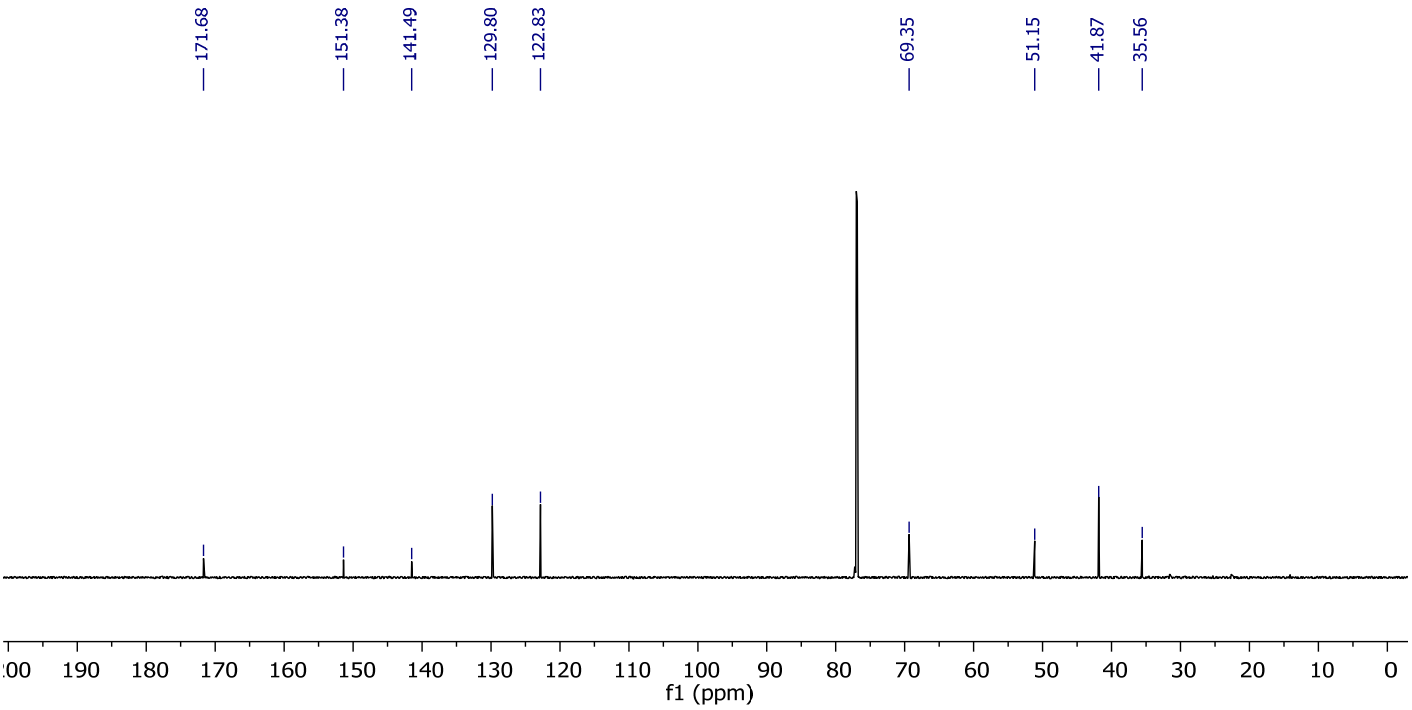

Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum for **26** in $CDCl_3$.

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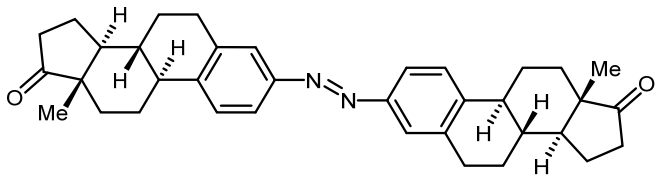

Azoarene 27. The reaction was conducted according to a modified general procedure using **S2** (88.6 mg, 0.30 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). The product was isolated without chromatography by the following workup procedure: after opening the vial to air and stirring, the solution was filtered through a glass fiber pad, and residual solid product was washed through the filter with dichloromethane. The solvent was then removed, and the solid residue was washed with 2 x 5 mL hexane and dried to yield a yellow solid. Run 1: 84 mg, >99% yield; Run 2: 83 mg, >99% yield. ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.65 (s, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 3.13 – 2.92 (m, 4H), 2.61 – 2.46 (m, 4H), 2.38 (td, *J* = 11.3, 4.2 Hz, 2H), 2.22 – 2.12 (m, 2H), 2.12 – 2.04 (m, 4H), 2.01 (dt, *J* = 13.4 Hz, 2H), 1.74 – 1.59 (m, 6H), 1.57 – 1.44 (m, 6H), 0.94 (s, 6H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 220.42, 150.92, 142.96, 137.43, 126.02, 122.87, 120.36, 50.63, 47.93, 44.74, 38.08, 35.82, 31.65, 29.44, 26.42, 25.77, 21.63, 13.86. HRMS(ESI): calcd for $C_{36}H_{42}N_2O_2^{+}$: 535.3319; found: 535.3323.

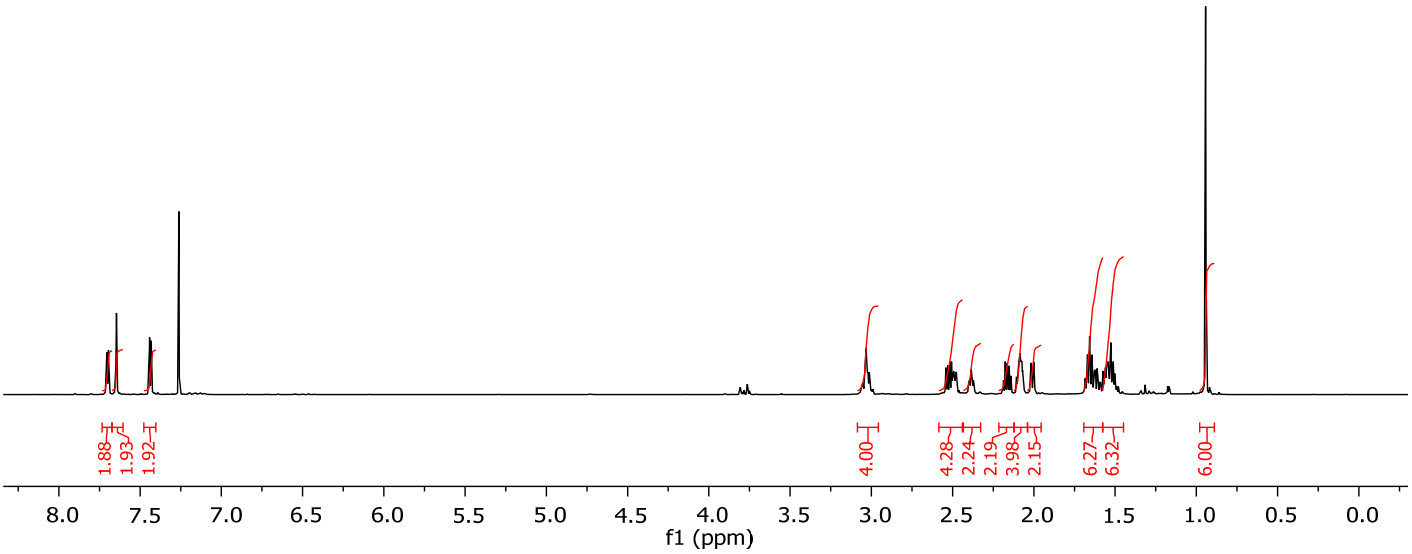

Figure S52. ^{1}H NMR spectrum for **27** in $CDCl_3$.

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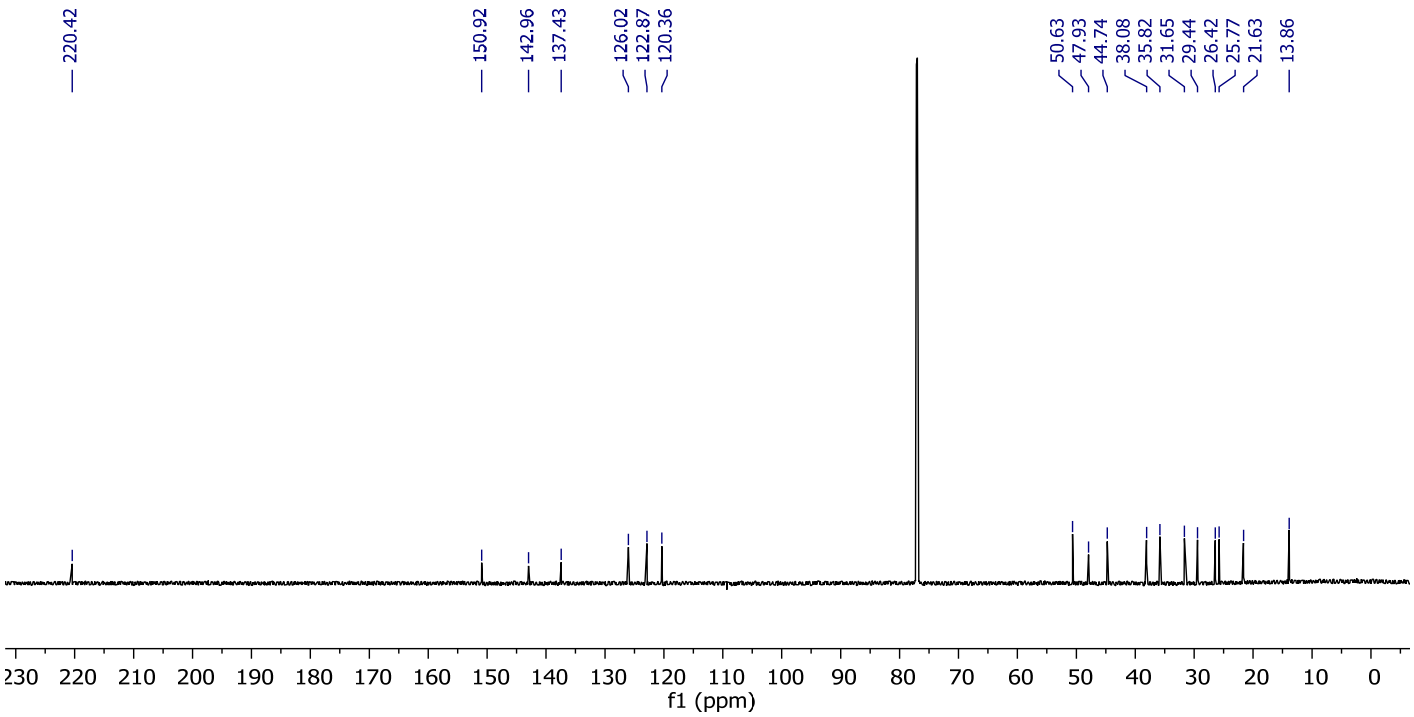

Figure S53. $^{13}C\{^{1}H\}$ NMR spectrum for **27** in $CDCl_3$.

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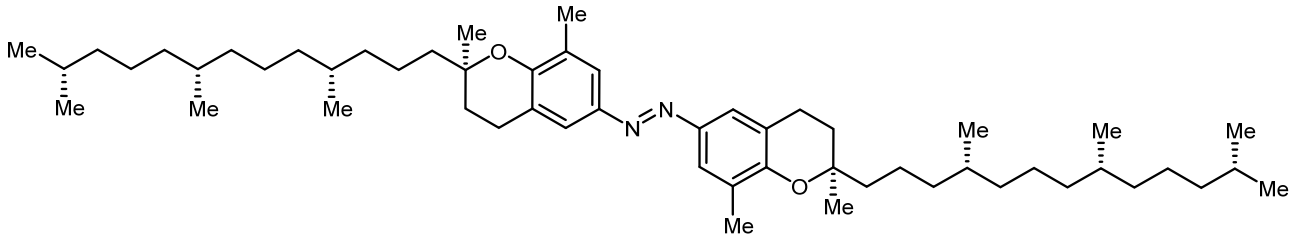

Azoarene 28. The reaction was conducted according to a modified general procedure using **S3** (128 mg, 0.30 mmol, 1.0 equiv) and 5 mol% **1** (11.0 mg, 0.015 mmol). Isolated yields were determined following column chromatography (SiO_2, 0 – 1% EtOAc/Hexanes). The product was isolated as a yellow oil. Run 1: 116 mg, 97% yield; Run 2: 117 mg, 98% yield. ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.55 (d, *J* = 2.4 Hz, 2H), 7.48 (d, *J* = 2.4 Hz, 2H), 2.89 – 2.80 (m, 4H), 2.24 (s, 6H), 1.92 – 1.83 (m, 2H), 1.83 – 1.77 (m, 2H), 1.66 – 1.56 (m, 4H), 1.56 – 1.50 (m, 3H), 1.50 – 1.44 (m, 2H), 1.44 – 1.35 (m, 6H), 1.35 – 1.30 (m, 9H), 1.30 – 1.16 (m, 12H), 1.16 – 1.10 (m, 6H), 1.10 – 1.02 (m, 6H), 0.87 (d, *J* = 7.0 Hz, 18H), 0.85 (d, *J* = 6.7 Hz, 6H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 154.46, 145.69, 126.92, 122.44, 122.00, 120.65, 76.97, 40.17, 39.39, 37.46, 37.43, 37.30, 32.81, 32.69, 31.15, 28.00, 24.82, 24.47, 24.35, 22.74, 22.65, 22.40, 20.99, 19.77, 19.67, 16.21. HRMS(ESI): calcd for $C_{54}H_{90}N_2O_2^+$: 799.7075; found: 799.7068.

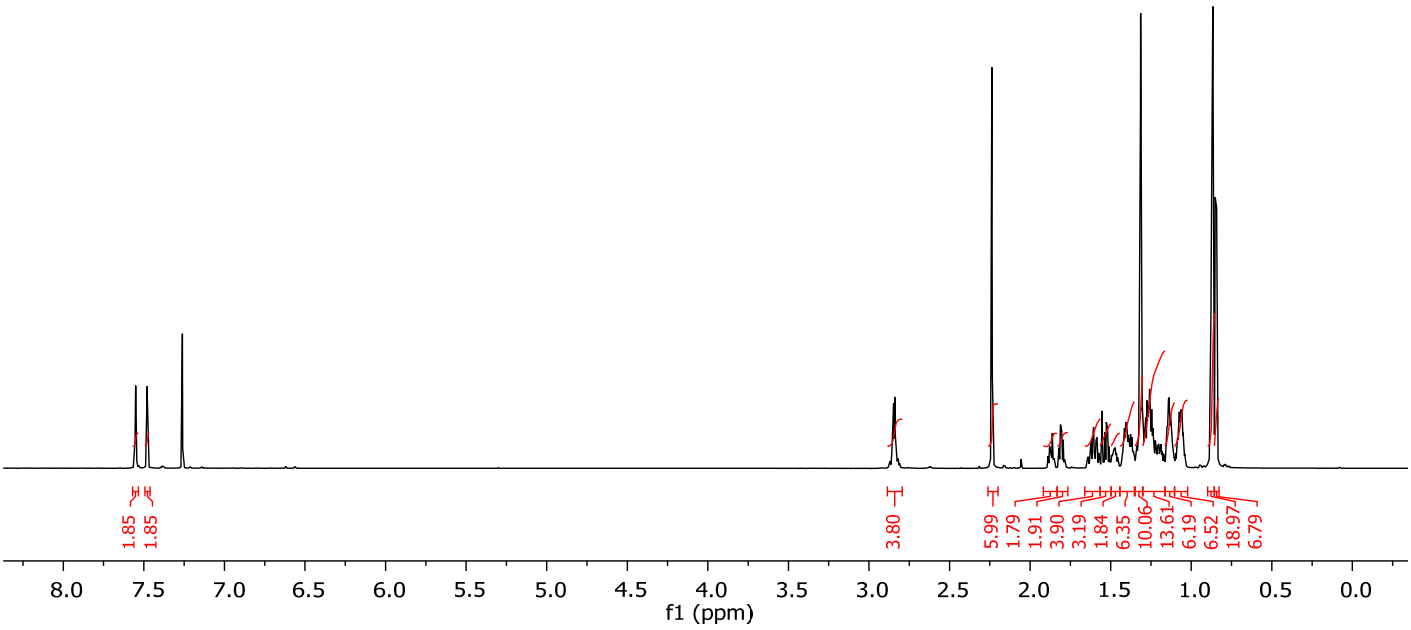

Figure S54. ^{1}H NMR spectrum for **28** in $CDCl_3$.

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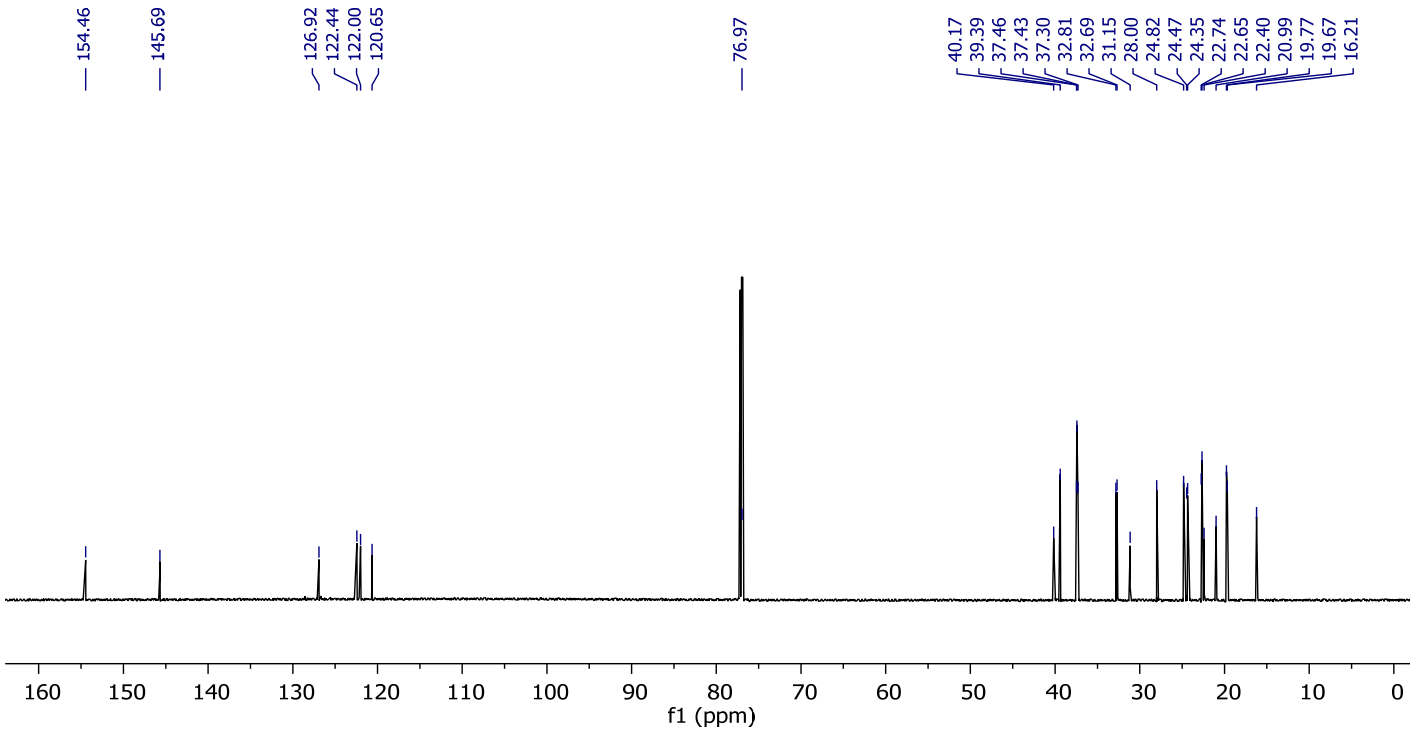

Figure S55. $^{13}C\{^{1}H\}$ NMR spectrum for **28** in $CDCl_3$.

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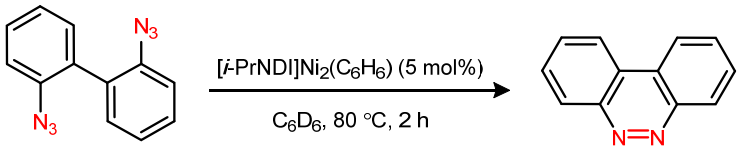

Intramolecular N=N Coupling. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with 2,2'-diazido-1,1'-biphenyl **29** (7.1 mg, 0.03 mmol, 1.0 equiv), **1** (2.2 mg, 0.003 mmol, 10 mol%) and C_6D_6 (600 µL), along with 1,3,5-trimethoxybenzene (2.0 mg, 0.012 mmol) as an internal standard. The mixture was then heated to 80 °C for 2 h, leading to the formation of **30** in 80% yield. The ^{1}H NMR spectrum of **30** was consistent with previous reports.[14]

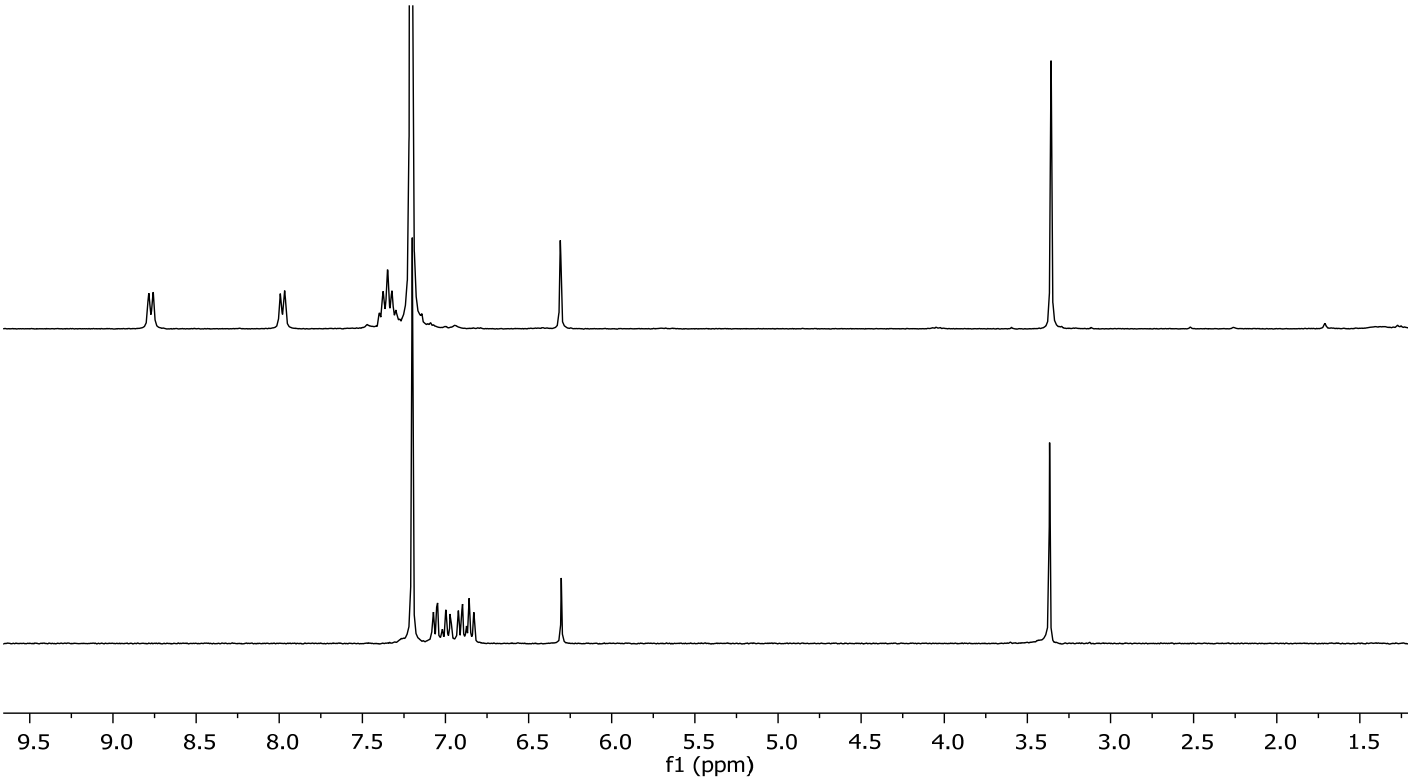

Figure S56. ^{1}H NMR spectrum for the intramolecular N=N coupling of **29** (bottom) to form **30** (top).

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5. Polymerization Experiments

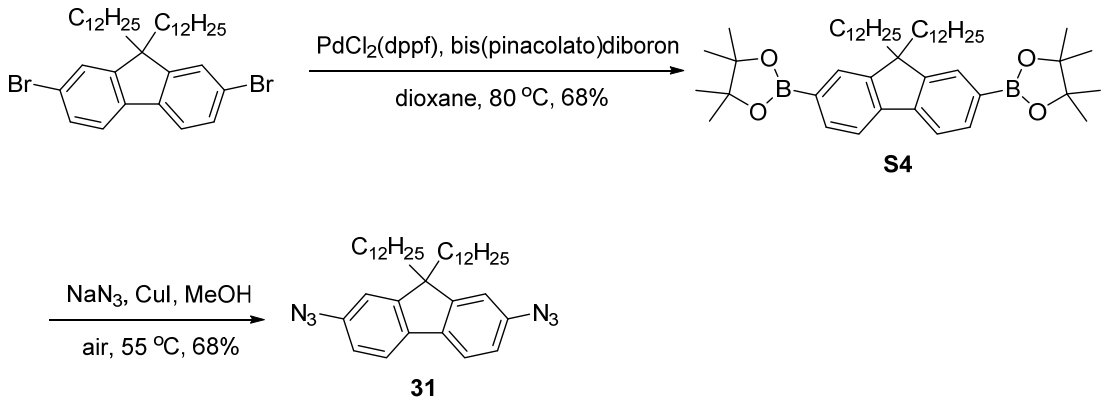
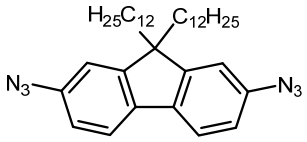


Figure S57. Synthetic route to the diazofluorene monomer **31**.

2,2'-(9,9-didodecyl-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) **S4** was synthesized according to previously reported methods.[22]



Synthesis of Compound 31. NaN_3 (139.6 mg, 2.147 mmol) and CuI (27.3 mg, 0.143 mmol) were added to a mixture of 2,2'-(9,9-didodecyl-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) **S4** (542.0 mg 0.718 mmol) and MeOH (40 mL). The resulting mixture was kept from light and bubbled with air at 50 °C for 8 h before being allowed to cool to room temperature. After removal of the solvent under reduced pressure, the residue was purified by silica gel chromatography (hexanes) to give the product **31** as a light yellow solid (285.0 mg, 68%). ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.0, 1.0 Hz, 2H), 7.00 (dd, *J* = 8.0, 2.2 Hz, 2H), 6.94 (d, *J* = 2.1 Hz, 2H), 1.93 – 1.89 (m, 4H), 1.27 (dt, *J* = 9.6, 4.8 Hz, 4H), 1.25 – 1.21 (m, 8H), 1.21 – 1.11 (m, 12H), 1.11 – 1.06 (m, 4H), 1.06 – 1.00 (m, 8H), 0.87 (d, *J* = 7.3 Hz, 6H), 0.60 – 0.54 (m, 4H). ^{13}C{^{1}H} NMR (201 MHz, $CDCl_3$) δ 152.55, 138.69, 137.57, 120.51, 117.84, 113.56, 109.31, 55.43, 40.35, 31.88, 29.88, 29.59, 29.54, 29.52, 29.31, 29.23, 23.64, 22.67, 14.10. HRMS(ESI): calcd for [$C_{37}H_{56}N_6^+$] - N_2 + H : 557.4578; found: 557.4571. The temperature required to vaporize the sample resulted in the loss of N_2 from the azide.

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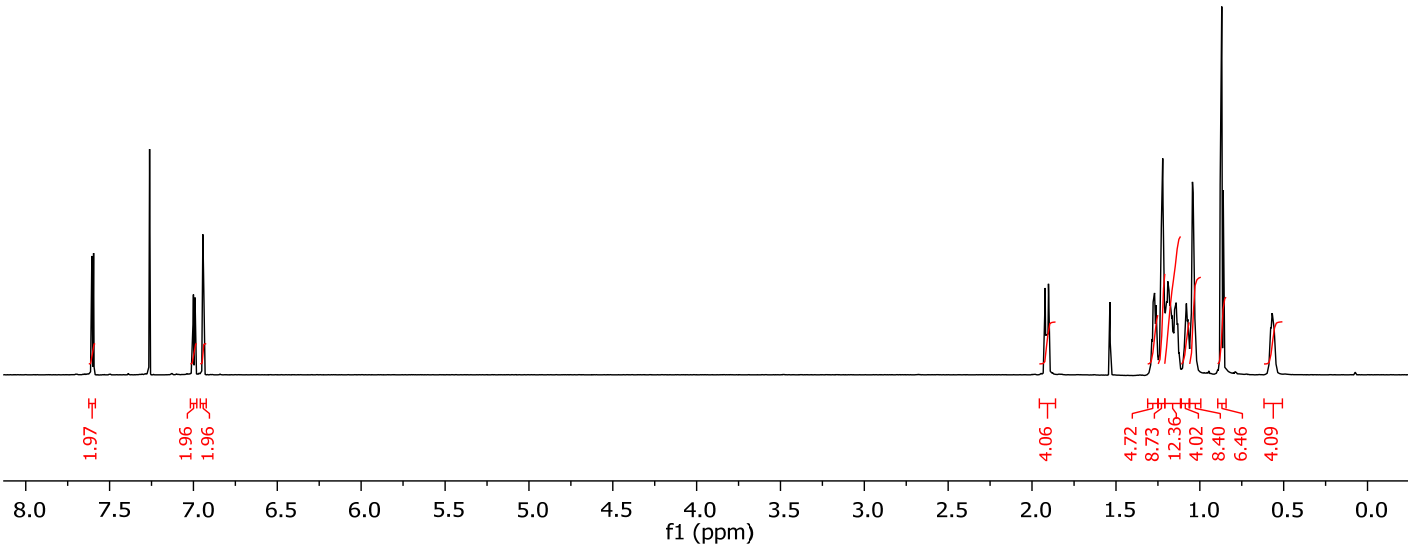

Figure S58. ^{1}H NMR spectrum for **31** in $CDCl_3$.

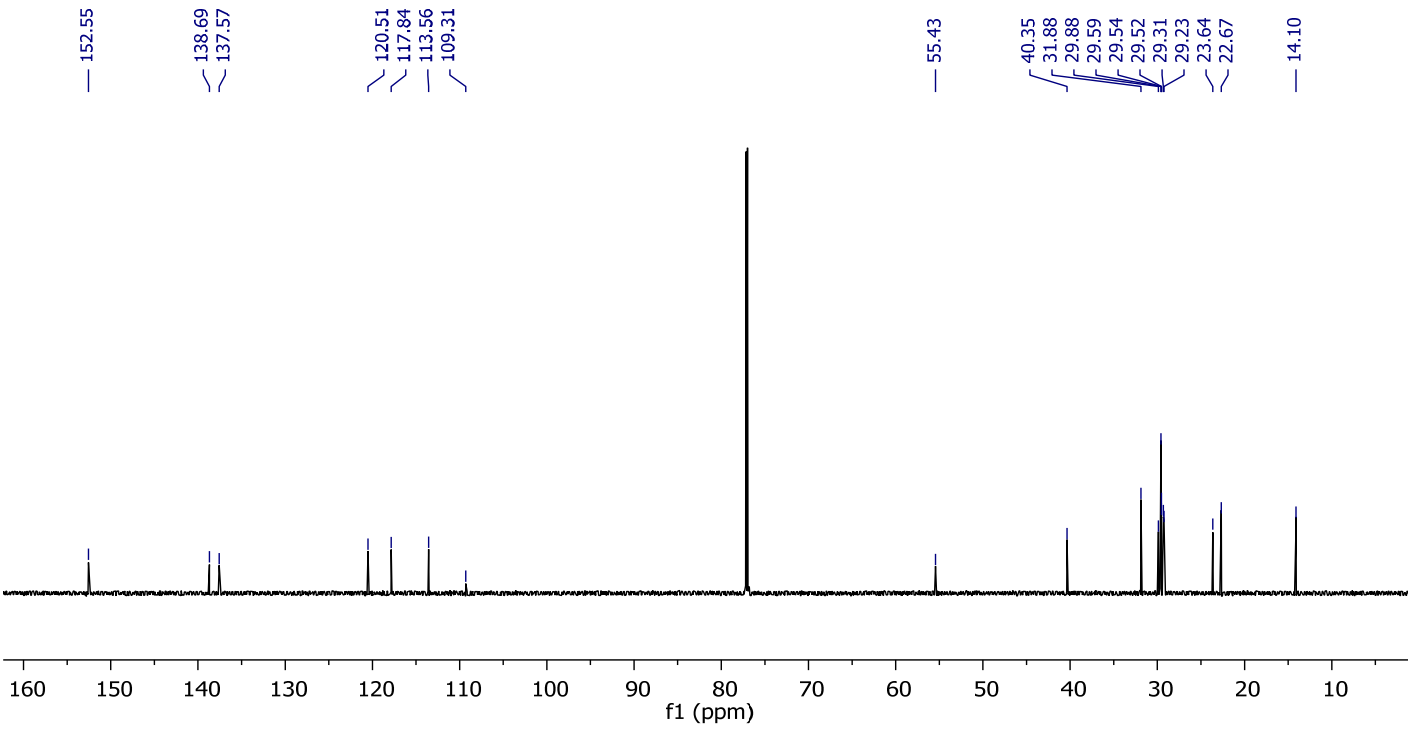

Figure S59. $^{13}C\{^{1}H\}$ NMR spectrum of **31** in $CDCl_3$.

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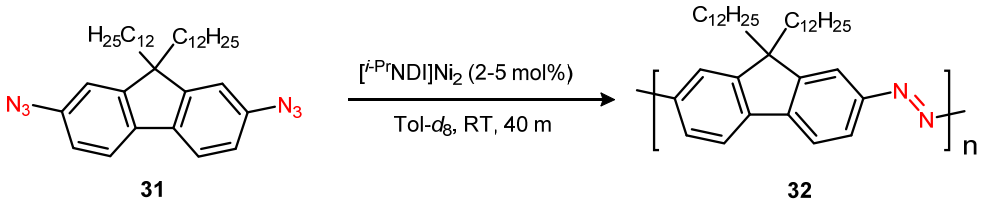

31 **32**

Catalytic Polymerization Procedure. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with **31** (29.0 mg, 0.050 mmol, 1.0 equiv), **1** (1.8 mg, 0.0025 mmol, 5 mol% or 0.7 mg, 0.001 mmol, 2 mol%), and toluene-d_8 (600 µL). Immediate gas evolution was observed, and the solution color turned from pale yellow to a deep red-orange. Over the course of 40 min at room temperature, complete consumption of the monomer was observed by ^{1}H NMR spectroscopy, and the solution darkened and became more viscous. The reaction was then quenched by opening the NMR tube to air. The polymeric material was removed from the tube using CH_2Cl_2 and added to methanol to precipitate the product. The precipitated solids were purified by Soxhlet extraction successively with acetone, hexane, and chloroform. The fraction extracted from chloroform was precipitated into methanol, filtered and dried at 60 °C under vacuum to afford the polymer.

32(2% loading). The first precipitation provided 17.1 mg (76% yield) of a dark orange solid. 12.2 mg of polymer was collected after Soxhlet extraction. ^{1}H NMR (300 MHz, toluene-*8d*, ppm) δ: 8.36 (s, 2H), 8.21 (d, *J* = 7.7 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 1.23-0.89 (m, *J* = 50H). 2% loading gives M_n of 18.1 kDa with a PDI of 2.48.

32(5% loading). The first precipitation provided 16.3 mg (72% yield) of a dark orange solid. 11.6 mg of polmer was collected after Soxhlet extraction. ^{1}H NMR (300 MHz, toluene-*8d*, ppm) δ: 8.36 (s, 2H), 8.21 (m, 2H), 7.65 (m, 2H), 1.23-0.89 (m, *J* = 50H). 5% loading gives M_n of 41.4 kDa with a PDI of 3.23.

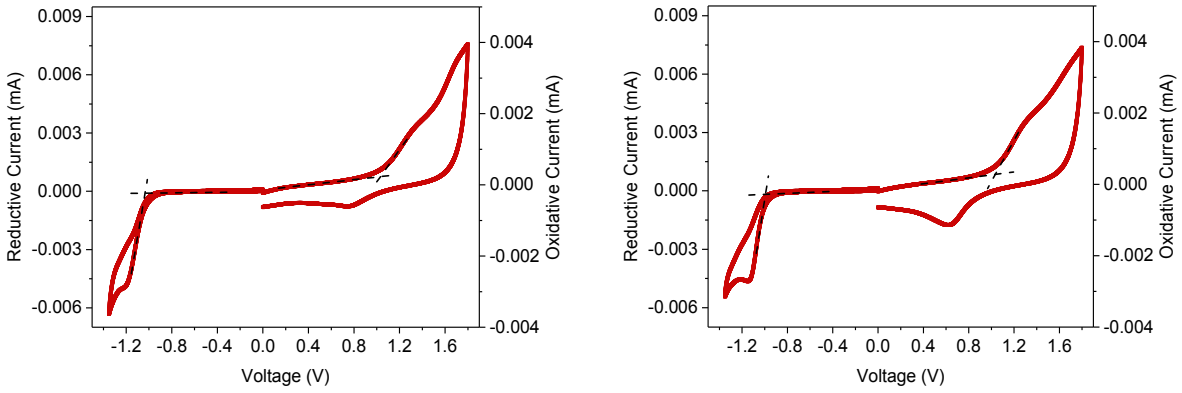

Figure S60. Cyclic voltammograms of **32(2% loading)** (left) and **32(5% loading)** (right) films in Propylene Carbonate with 0.2 M n-Bu_4NPF_6 as supporting electrolyte (scan rate: 20 mV s^{-1}).

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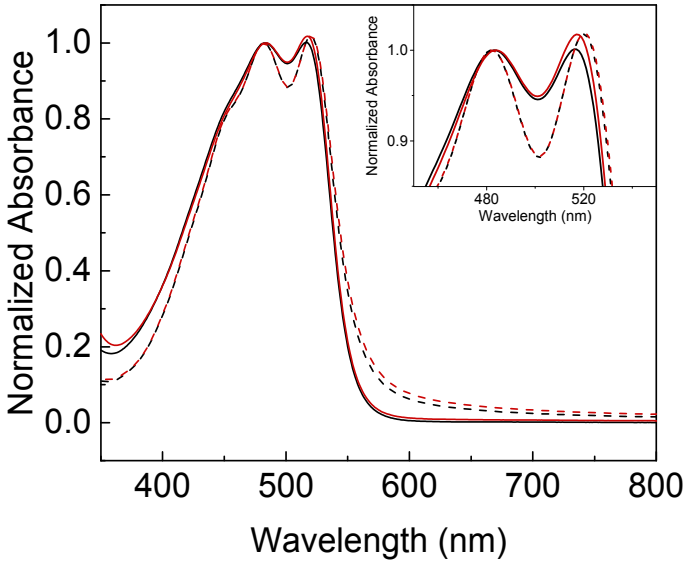

Figure S61. Absorption spectra of **32(2% loading)** (black) and **32(5% loading)** (red) in $CHCl_3$ solutions (solid lines) and as film (dashed lines).

The electrochemical properties of the azo-fluorene polymer were evaluated by cyclic voltammetry, shown in **Figure 1**. Azo polymer **32** exhibited an irreversible redox behavior. HOMO/LUMO levels were estimated around -5.52/-3.47 eV for the low M_n polymer and -5.53/-3.49 eV for the high M_n polymer. UV-Vis absorption spectra for the azo-fluorene polymers are shown in **Figure S60**. The peaks around 480 nm and 520 nm are attributed to intramolecular charge transfer peaks and aggregation peaks, respectively. The 520nm peak of **32(5% loading)** is relatively more intense, indicative of a stronger aggregation in $CHCl_3$ solution owing to a higher molecular weight. Both thin films show slightly red-shifted absorption spectra, which is evidence of a stronger intermolecular interaction in films. Small CV and UV-Vis spectra difference two azo-fluorenes suggests that the molecular weight of azo-fluorenes has a negligible impact on their energy levels between this range.

Table 1. Molecular, Optical, and Electrochemical Properties

	Cat. Loading	Mn[a] (KDa)	PDI	HOMO[b] (eV)	LUMO[b] (eV)	E_g^{CV}[c] (eV)	E_g^{Opt}[d] (eV)
L	2%	18.1	2.48	-5.52	-3.47	2.05	2.20
H	5%	41.4	3.23	-5.53	-3.49	2.04	2.20

[a]Determined by GPC using polystyrene standards in THF. [b]The HOMO and LUMO energy levels are estimated from HOMO = − (4.80 + E_{ox} − E_{Fc/Fc^+}) and LUMO = − (4.80 + E_{red} − E_{Fc/Fc^+}), where E_{ox} and E_{red} are onsets of redox potentials. [c]Calculated from E_g = LUMO-HOMO. [d]Calculated from absorption band edge of the polymer films, $E_g = 1240/\lambda_{edge}$.

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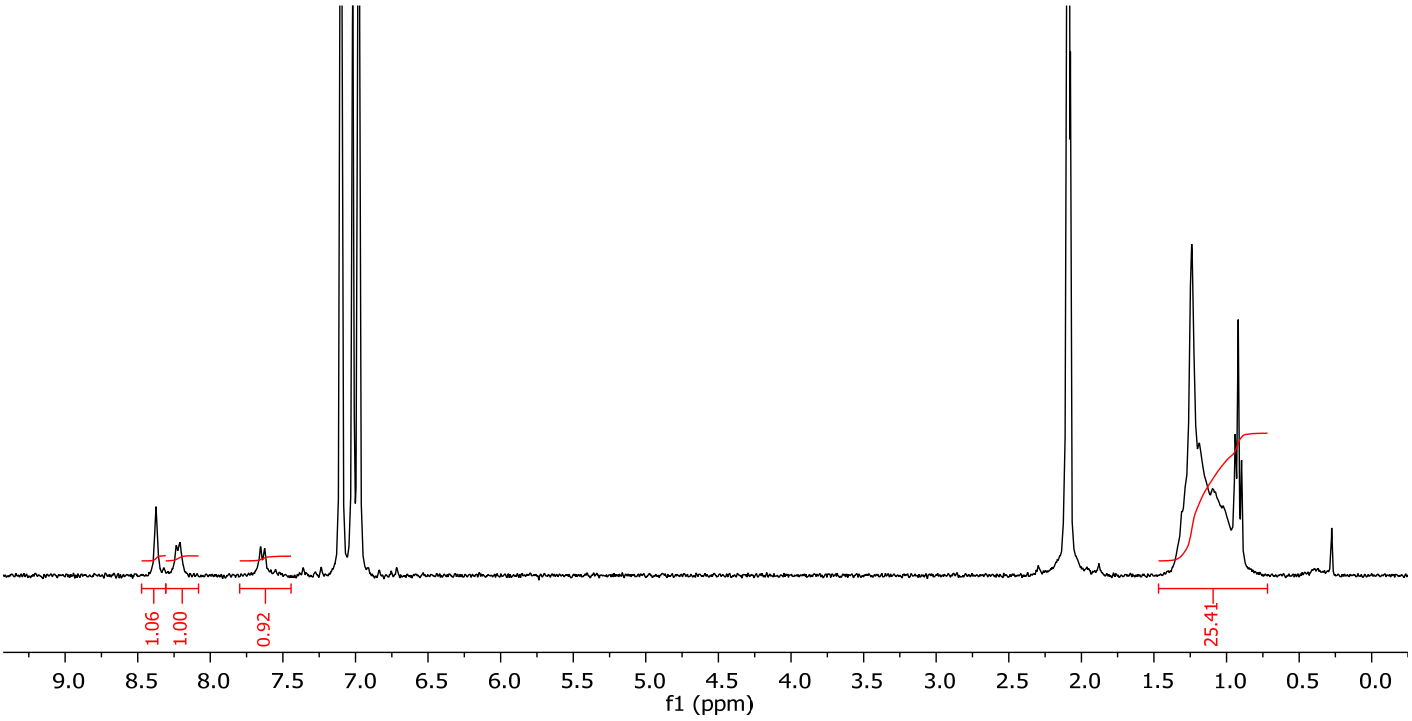

Figure S62. ^{1}H NMR spectrum for the polymerization of **31** using 2 mol% **1** (toluene-d_8).

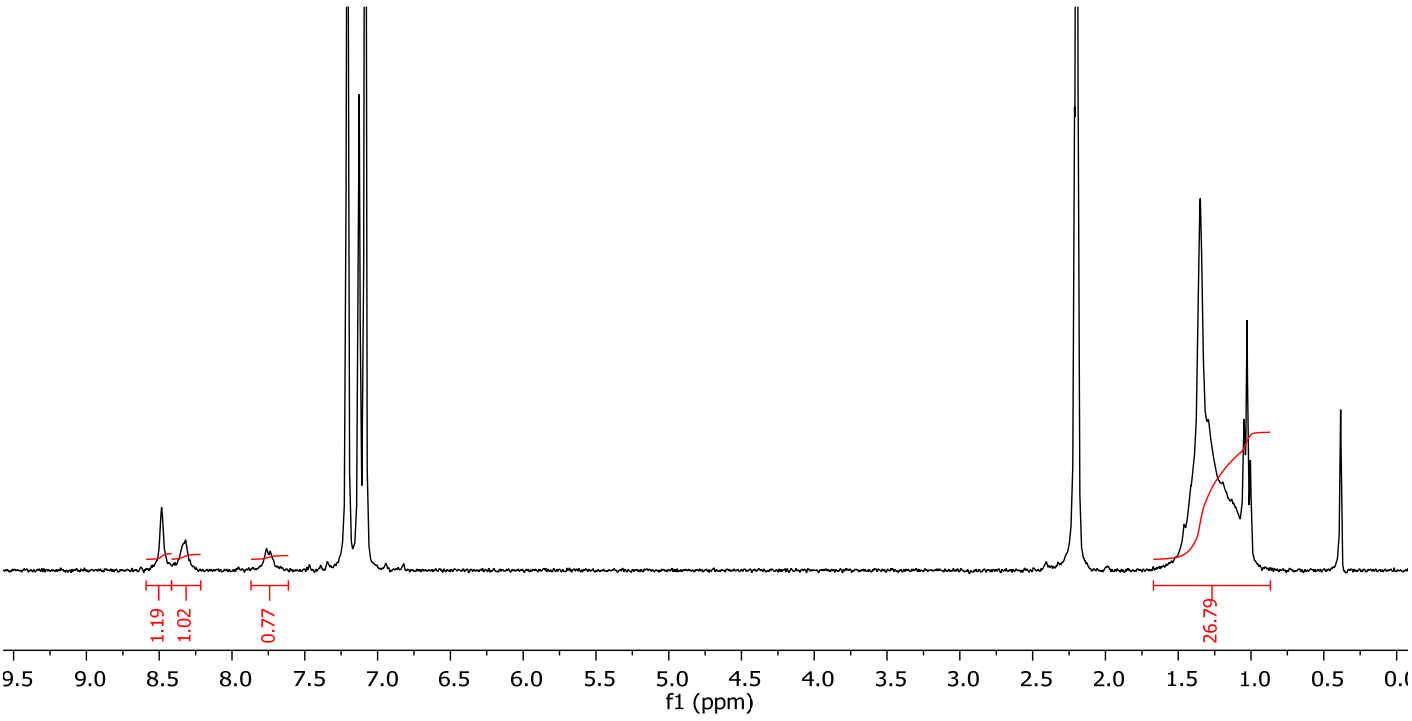

Figure S63. ^{1}H NMR spectrum for the polymerization of **31** using 5 mol% **1** (toluene-d_8).

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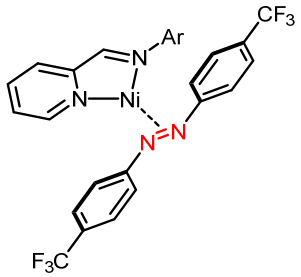
6. Synthesis and Characterization of Nickel Complexes



[*i*-PrIP]Ni(4,4′-bis-trifluoromethylazobenzene) (7). In an N_2 filled glovebox, a 20-mL vial was charged with **4** (50.0 mg, 0.115 mmol, 1.0 eq), C_6H_6 (2.0 mL), and a magnetic stir bar. A solution of 4-trifluoromethylphenyl azide (36 mg, 0.192 mmol, 1.7 equiv) in 2.0 mL C_6H_6 was added. Immediate gas evolution was observed, and the reaction solution turned from dark purple to dark blue-green. The reaction mixture was stirred at room temperature. After 5 min, the solvent was removed under reduced pressure. The solid residue was purified by recrystallization from a saturated pentane/toluene solution at –30 °C. Brown cube-like single crystals of **7** obtained by this procedure were suitable for X-ray diffraction studies (22 mg 44% yield). ^{1}H NMR (300 MHz, C_6D_6) δ 8.75 (d, *J* = 5.0 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.43 (m, 3H), 7.33 – 7.20 (m, 4H), 7.06 – 6.92 (m, 3H), 6.67 (t, *J* = 7.5 Hz, 1H), 6.45 (t, *J* = 6.4 Hz, 1H), 6.17 (d, *J* = 7.6 Hz, 1H), 4.32 (s, 1H), 2.28 (s, 1H), 1.77 (d, *J* = 6.6 Hz, 3H), 1.00 (d, *J* = 6.8 Hz, 3H), 0.78 (d, *J* = 6.6 Hz, 3H), 0.69 (d, *J* = 5.3 Hz, 3H). ^{13}C{^{1}H} NMR (201 MHz, C_6D_6) δ 162.09 , 161.32 , 159.83 , 152.58 , 150.46 , 144.91 , 140.54 , 139.29 , 135.39 , 127.94 , 127.73 (q, *J* = 39.2 Hz), 127.39 , 126.90 , 126.77 , 126.61 (q, *J* = 3.8 Hz), 126.42 (q, *J* = 3.8 Hz), 125.56 , 125.42 , 125.28 , 123.65 , 123.45 , 121.23 (q, *J* = 32.9 Hz), 120.74 (q, *J* = 31.9 Hz), 119.71 , 119.31 , 28.76 , 27.63 , 24.72 , 24.20 , 22.57 , 21.55. UV–Vis–NIR (C_6H_6, nm {M^{-1} cm^{-1}}): 326 {sh}, 386 {5200}, 549 {3700}, 656 {5700}. Anal. Calcd for $C_{32}H_{30}F_6N_4Ni$: C 59.75 H 4.70, N, 8.71; found: C 59.49 H 4.71 N 8.56.

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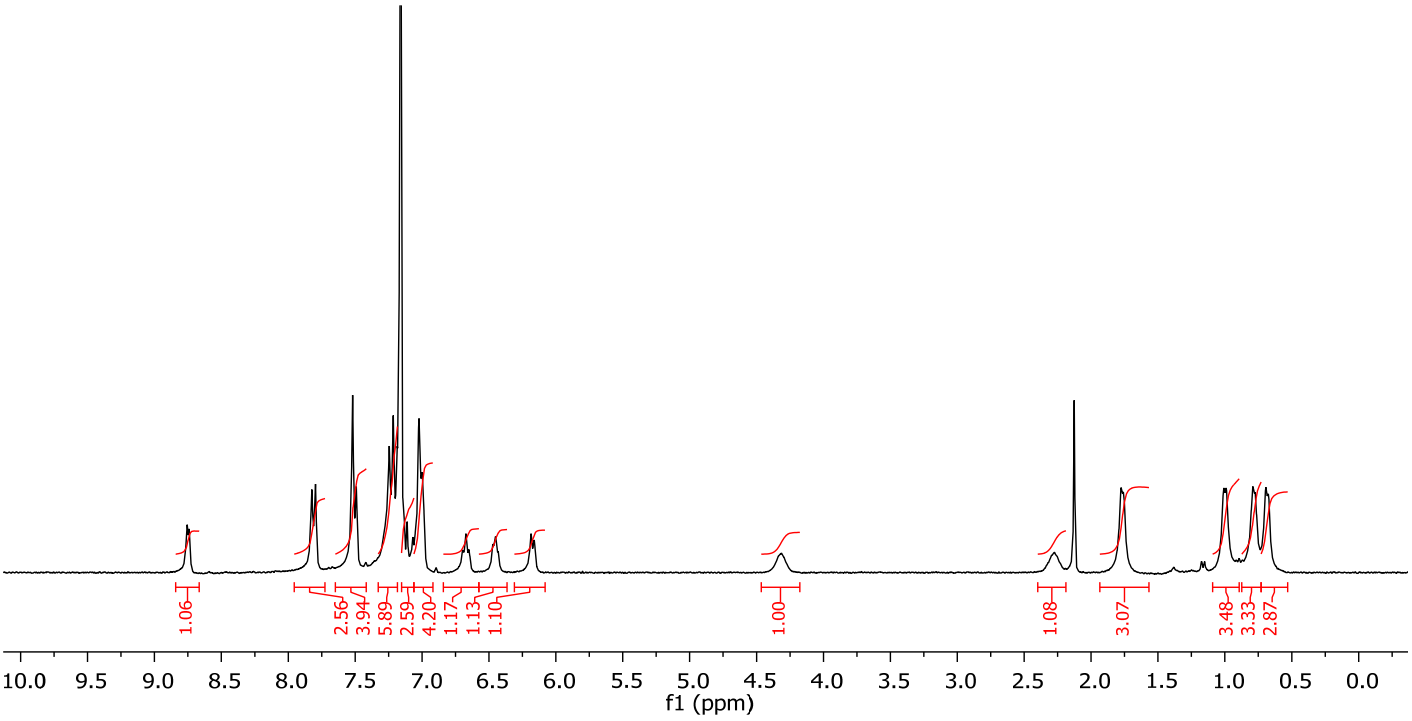

Figure S64. ^{1}H NMR spectrum of **7**.

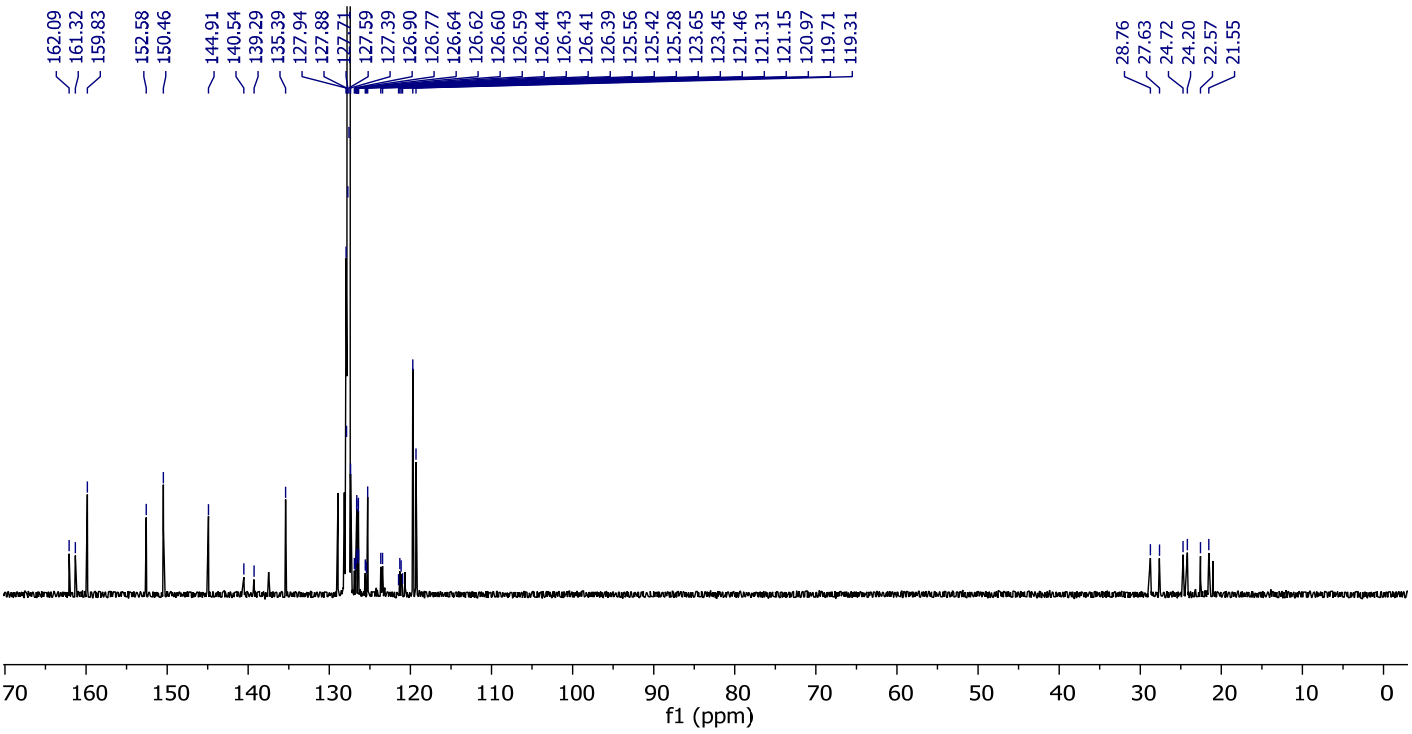

Figure S65. $^{13}C\{H\}$ NMR spectrum of **7** in C_6D_6.

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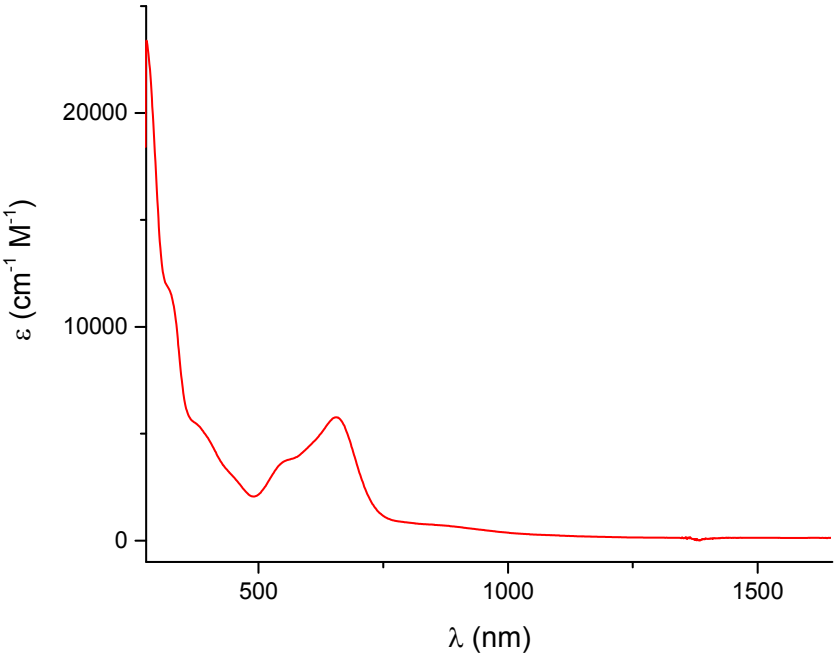

Figure S66. UV-Vis-NIR spectrum of **7** in C_6H_6 (0.012 mM).

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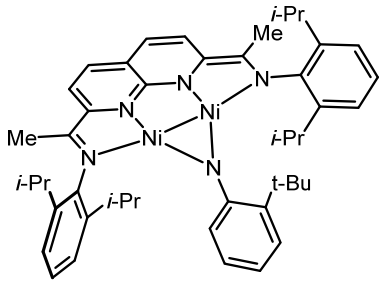

[*i*-^{Pr}NDI]Ni_2((2-$C(CH_3)_3C_6H_5$) (33). Under an atmosphere of N_2, a 20-mL vial was charged with [*i*-^{Pr}NDI]$Ni_2(C_6H_6)$ (**1**) (15 mg, 0.021 mmol, 1.0 equiv.), 1-*tert*-butyl-phenyl azide (3.6 mg, 0.021 mmol, 1.0 equiv), and C_6D_6 (900 µL). Immediate gas evolution was observed, and the reaction mixture turned brown-purple. After 2 min, the solvent was then removed under reduced pressure. The solid residue was purified by recrystallization from a saturated 3:1 pentane/toluene solution at –30 °C. Brown plate-like single crystals of **33** obtained by this procedure were suitable for X-ray diffraction studies (8.7 mg 53% yield). ^{1}H NMR (800 MHz, C_6D_6) δ 45.54 (s, 6H), 29.19 (s, 1H), 26.39 (s, 1H), 19.22 (s, 2H), 13.74 (m, 4H), 10.87 (s, 1H), 7.11 – 6.81 (m, 4H), 4.13 (s, 9H), 3.38 (s, 2H), 2.33 (s, 12H), 1.90 (s, 12H), -3.63 (s, 1H), -102.45 (s, 2H). UV–Vis–NIR (C_6H_6, nm {M^{-1} cm^{-1}}): 288 {sh}, 342 {2300}, 516 {7500}, 707 {5900}, 812 {5600}, 979 {5700}. Anal. Calcd for $C_{46}H_{57}N_5Ni_2$: C 69.29 H 7.21, N, 8.78; found: C 68.86 H 7.28 N 8.47.

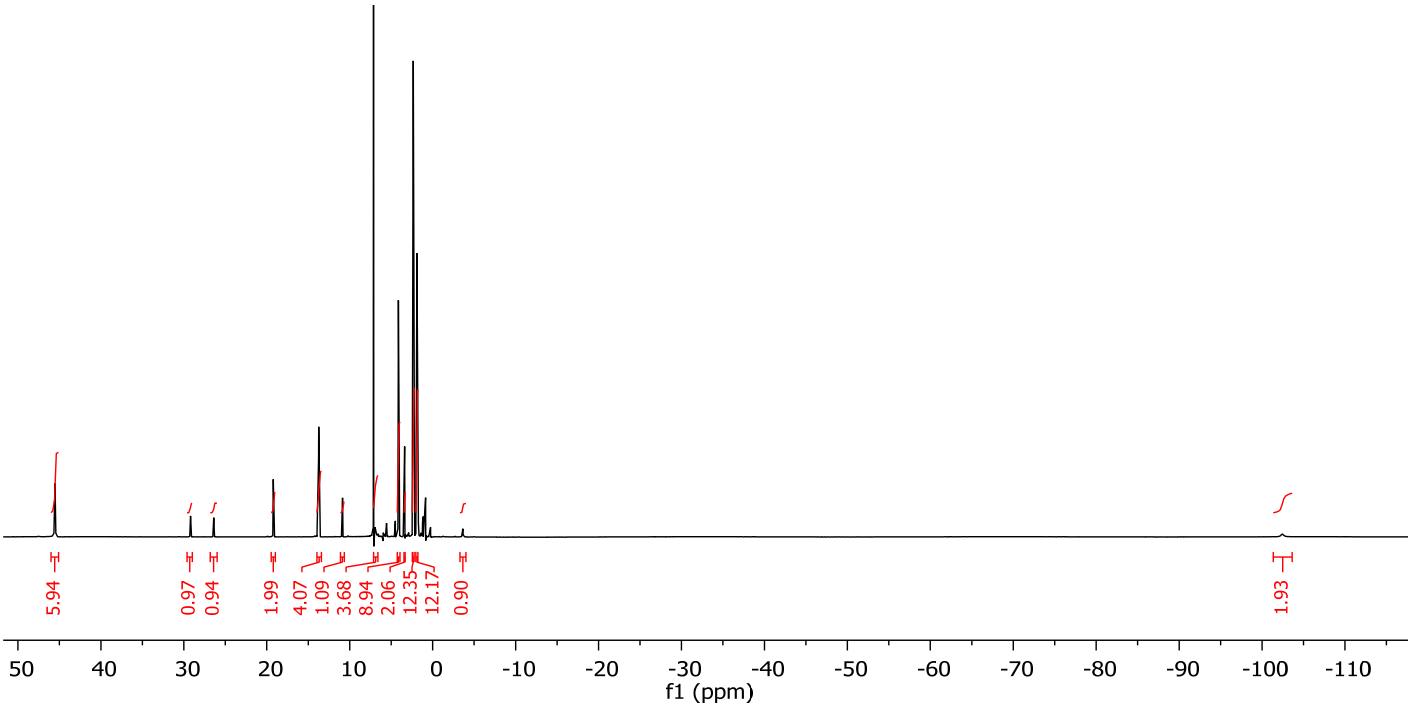

Figure S67. ^{1}H NMR spectrum of **33** in C_6D_6.

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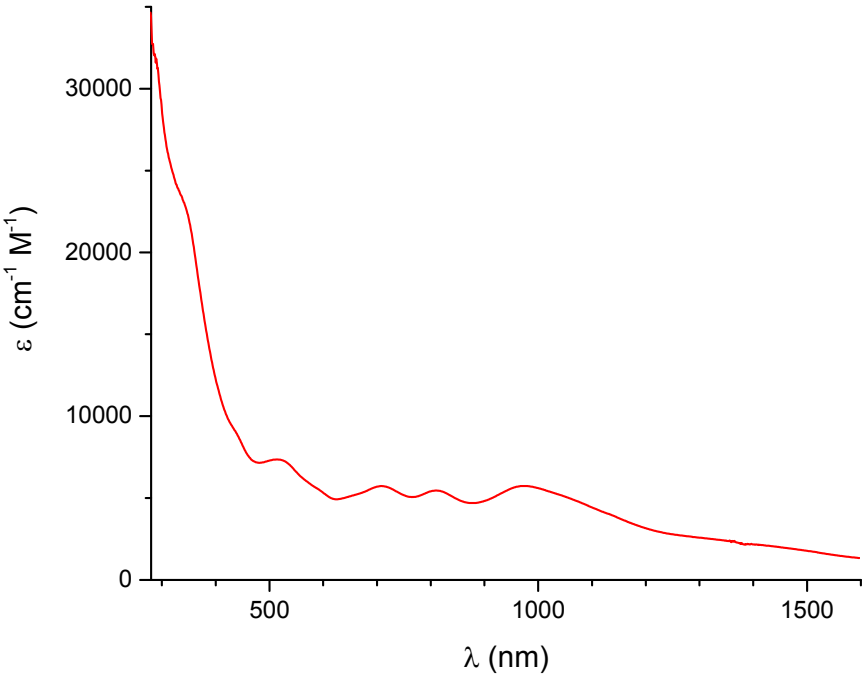

Figure S68. UV–Vis–NIR spectrum of **33** in C_6H_6 (0.13 mM).

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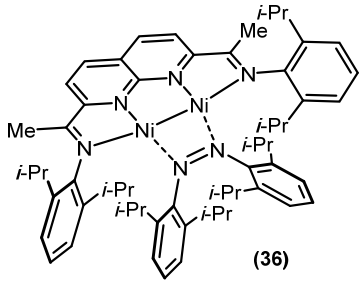

(36)

[*i*-PrNDI]Ni$_2$(N$_2$Ar$_2$) (36). Under an atmosphere of N_2, a 20-mL vial was charged with [*i*-PrNDI]Ni$_2$(C_6H_6) (**1**) (40 mg, 0.055 mmol, 1.0 equiv.), 2,6-diisopropylphenyl azide (23 mg, 0.11 mmol, 2.0 equiv.), and C_6H_6 (8.0 mL). Immediate gas evolution was observed, and the solution turned dark green-brown. After allowing the reactants to mix for 2 min, the mixture was filtered through a glass fiber pad, and the filtrate was evaporated under reduced pressure. The crude solid was washed with pentane (approx. 3 mL) and dried under vacuum. The solid residue was redissolved in C_6H_6 and lyophilized to yield **2** as a dark brown solid (43 mg, 78% yield). Single crystals suitable for XRD analysis were obtained from concentrated C_6H_6 solutions. ^{1}H NMR (500 MHz, C_6D_6) δ 7.15–7.12 (m, 2H), 7.07 (t, *J* = 7.7 Hz, 2H), 6.99 (d, *J* = 7.7 Hz, 1H), 6.87–6.82 (m, 4H), 6.48 (dd, *J* = 6.1, 3.2 Hz, 2H), 6.43 (d, *J* = 8.2 Hz, 2H), 5.94 (d, *J* = 8.2 Hz, 2H), 3.70 (hept, *J* = 6.2, 2H), 3.10 (hept, *J* = 6.6 Hz, 2H), 2.84 (hept, *J* = 6.6 Hz, 2H), 2.36 (hept, *J* = 6.3 Hz, 2H), 2.19 (d, *J* = 6.7 Hz, 6H), 1.75 (d, *J* = 6.8 Hz, 6H), 1.59 (s, 6H), 1.29 (d, *J* = 6.8 Hz, 6H), 1.16 (d, *J* = 6.8 Hz, 6H), 0.94 (d, *J* = 6.7 Hz, 6H), 0.69 (d, *J* = 6.8 Hz, 6H), 0.07 (d, *J* = 6.7 Hz, 6H), –0.19 (d, *J* = 6.6 Hz, 6H). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6) δ 161.9, 150.0, 147.0, 142.1, 142.3, 141.7, 141.1, 137.3, 125.8, 125.7, 124.2, 123.9, 123.5, 123.4, 114.8, 29.6, 28.4, 28.4, 28.4, 28.0, 26.5, 24.5, 24.3, 24.2, 24.0, 23.9, 23.7, 23.2, 16.9. UV–Vis–NIR (C_6H_6, nm {M^{-1} cm^{-1}}): 284 {sh}, 338 {29300}, 446 {10500}, 506 {8000}, 704 {8700}, 969 {sh}, 1080 {10600}, 1329 {8200}. Anal. calcd for $C_{60}H_{78}N_6Ni_2$: C 73.48, H 7.85, N 7.79; found: C 73.27, H 7.76, N 7.76.

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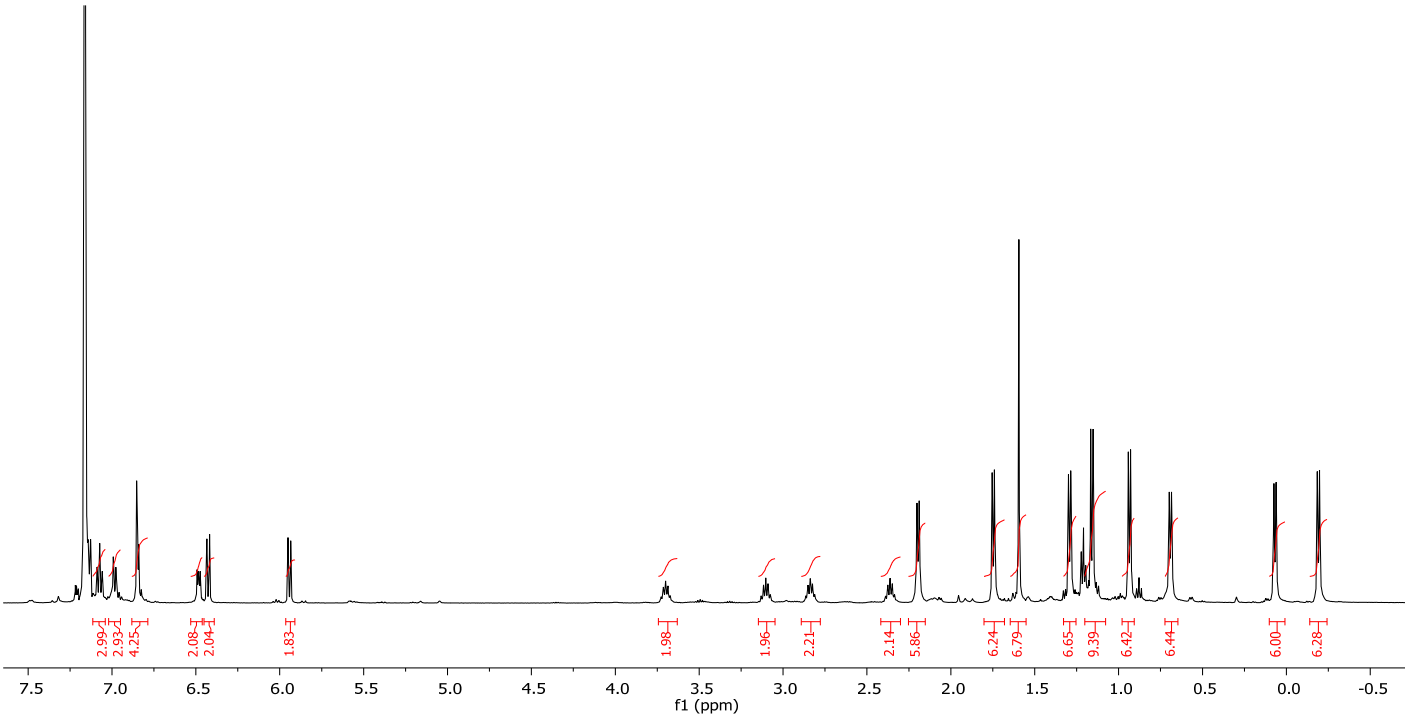

Figure S69. ^{1}H NMR spectrum of **36** in C_6D_6.

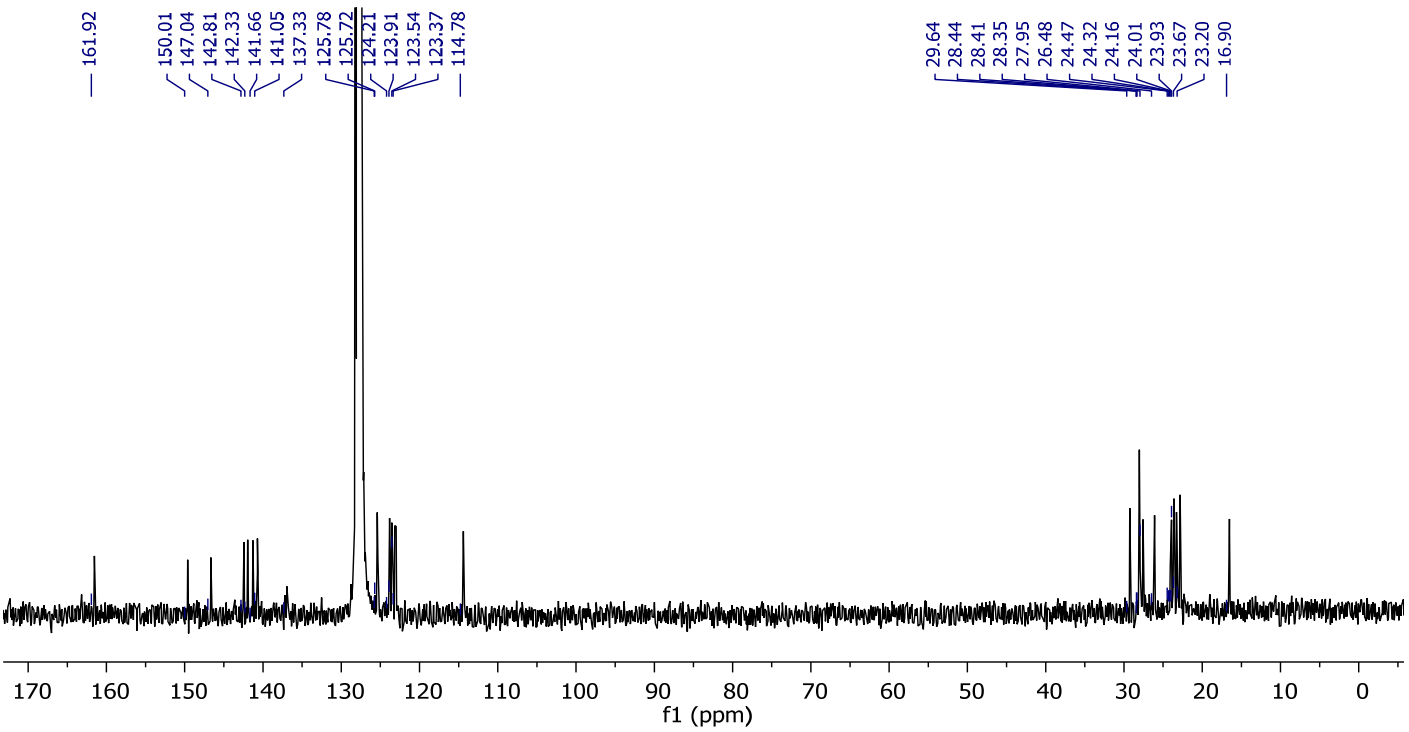

Figure S70. $^{13}C\{^{1}H\}$ NMR spectrum of **36** in C_6D_6.

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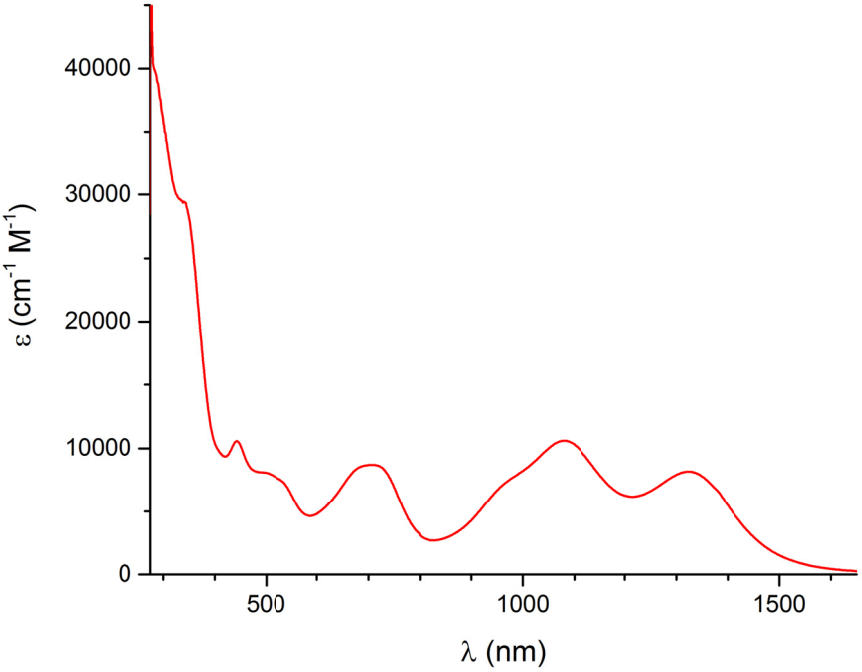

Figure S71. UV–Vis–NIR spectrum of **36** in C_6H_6 (0.10 mM).

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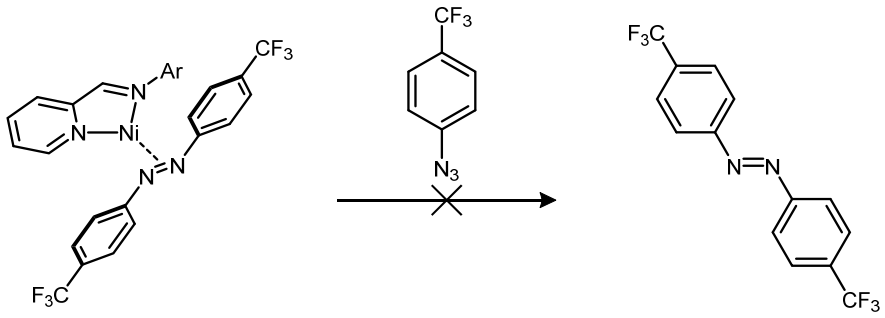
7. Mechanistic Experiments



Reaction of 7 with 4-trifluoromethylphenyl azide. In an N_2 filled glovebox, an NMR tube equipped with a J. Young valve was charged with 4-trifluoromethylphenyl azide (**2**) (5.8 mg, 0.031 mmol, 1.0 equiv), C_6D_6 (500 µL), **7** (1.0 mg, 0.0015 mmol, 5 mol %), and 1,3,5-trimethoxybenzene (5.2 mg, 0.031mmol) as an internal standard. The reaction components were allowed to react for 1 h. No conversion of **2** was observed by ^{1}H NMR integration against 1,3,5-trimethoxybenzene as an internal standard. No additional conversion or yield of azoarene was observed after an additional 2 h at room temperature or after heating for 1 h at 80 °C.

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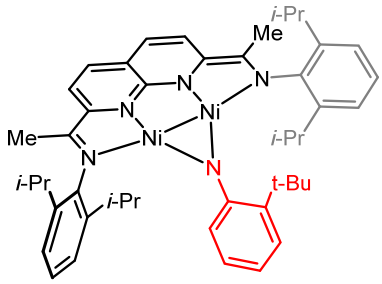

Variable temperature ^{1}H NMR data for 33.

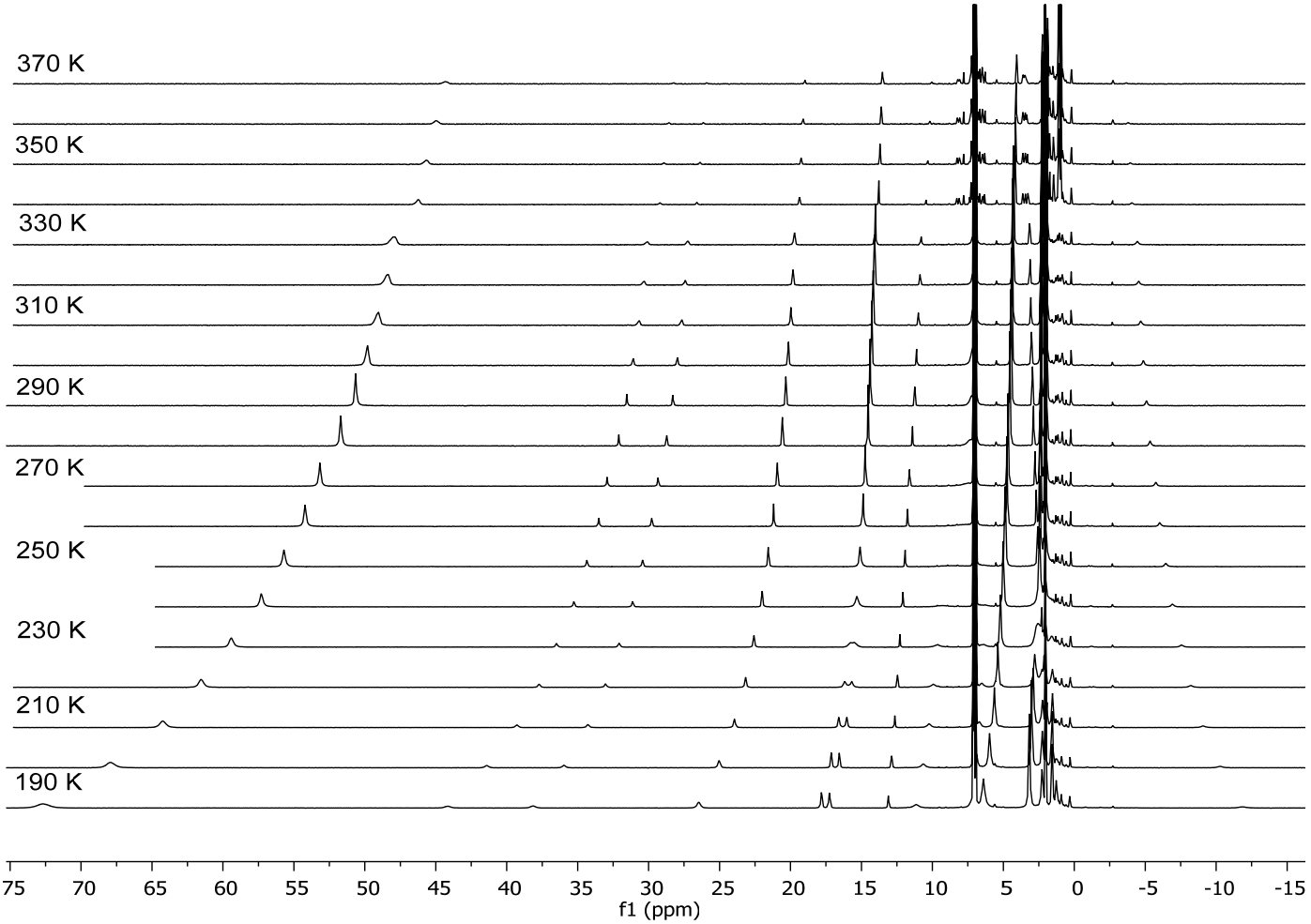

Figure S72. Variable temperature ^{1}H NMR spectrum overlay (toluene-d_8) showing selected peaks of **33** as a function of temperature.

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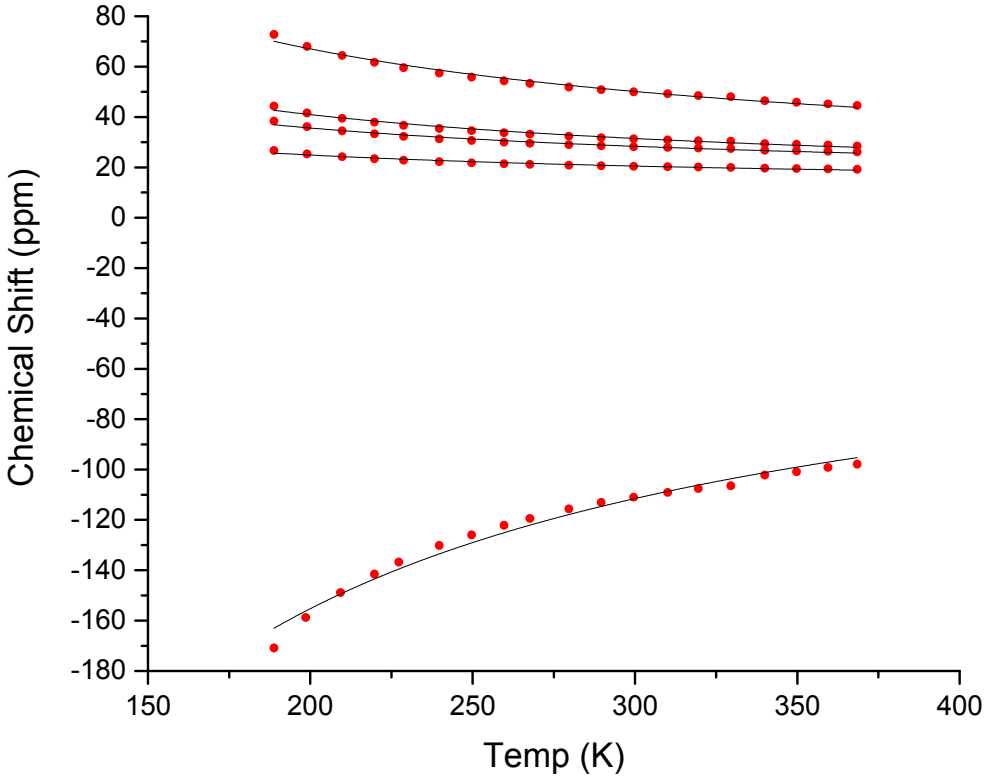

Figure S73. Selected ^{1}H NMR peaks for **33** are plotted as a function of temperature (red points), and each set of points was fit (black lines) to simple Curie behavior according to the equation below.

$$chemical\ shift = a + b * \frac{1}{T}$$

Curve	Adj. R^2	a	b
1	0.984	16 ± 1	10200 ± 300
2	0.979	12.2 ± 0.7	5700 ± 200
3	0.974	13.6 ± 0.6	4400 ± 200
4	0.965	11.5 ± 0.5	2600 ± 100
5	0.980	-24 ± 3	-26300 ± 900

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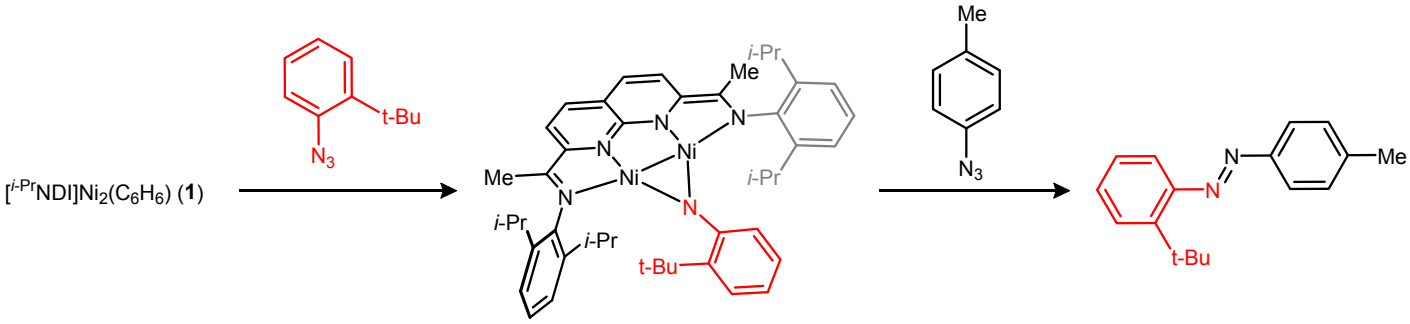

Reaction of 1 with 2-tert-butylphenyl azide and cross-azoarene formation with 4-tolyl azide. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with 2-*tert*-butylphenyl azide (50 µL of a 0.28 M solution in C_6D_6, 0.0137 mmol, 1.0 equiv), **1** (10.0 mg, 0.0137 mmol, 1.0 equiv), and C_6D_6 (600 µL). Immediate gas evolution was observed, and the clean formation of **33** was confirmed by ^{1}H NMR. 4-Tolyl azide was then added to the reaction mixture (250 µL of a 0.28 M solution in C_6D_6, 0.067 mmol, 5.0 equiv) along with 1,3,5-trimethoxybenzene (2.6 mg, 0.017 mmol) as an internal standard. Full consumption of the **33** was observed by ^{1}H NMR, and the solution was then filtered through a short plug of silica. The yield of the cross-azoarene product was determined by ^{1}H NMR integration (89% yield). The yield of the homocoupled 4-azotoluene product was 81%. The material was run through a silical column (hexanes) to remove the free NDI ligand and most of the 1,3,5-trimethoxybenzene. This material was then analyzed by ^{1}H NMR, COSY, and GC-MS, confirming the identity of the cross-coupled product.

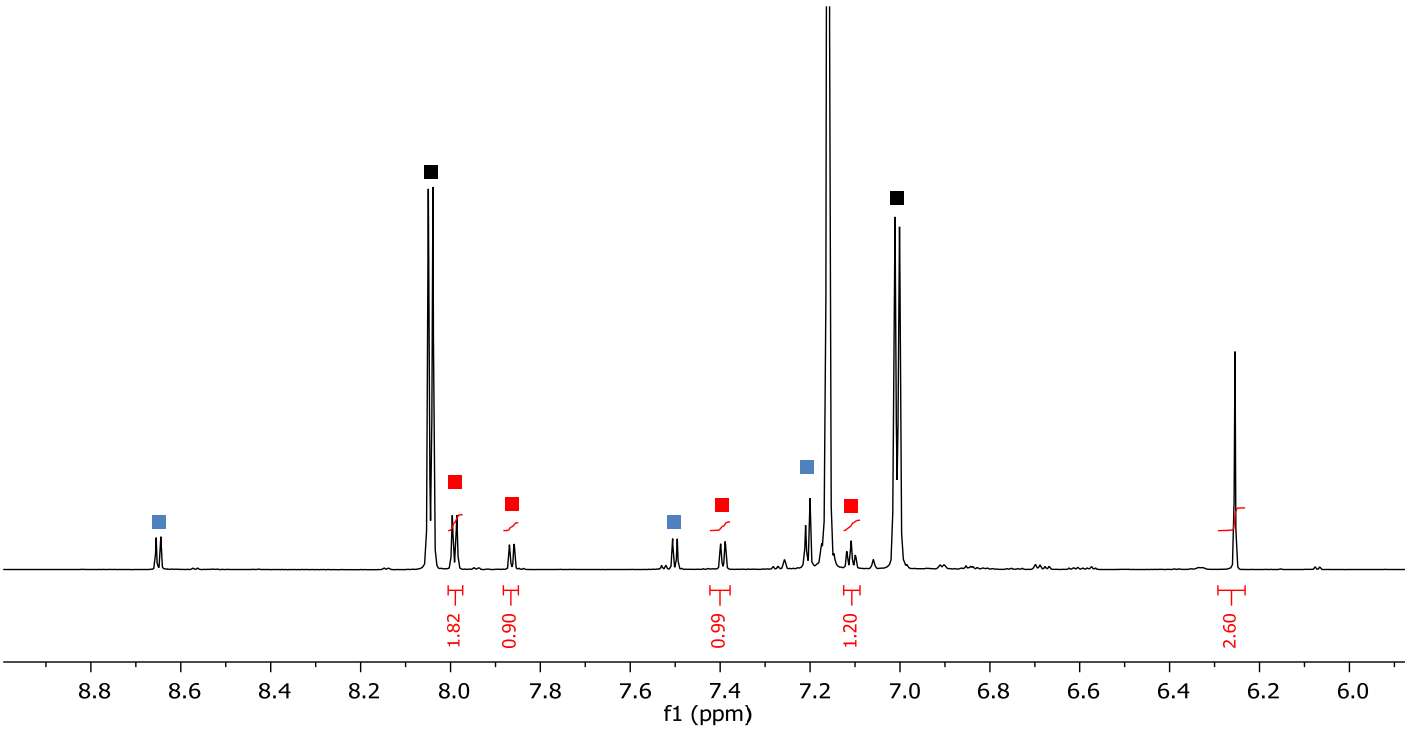

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Figure S74. ^{1}H NMR spectrum (C_6H_6) of the product mixture after reaction of the imido intermediate with 4-tolylazide and running through a silica plug. Black, red, and blue squares correspond to 4-azotoluene (**9**), the cross-coupled product (**34**), and free NDI ligand respectively.

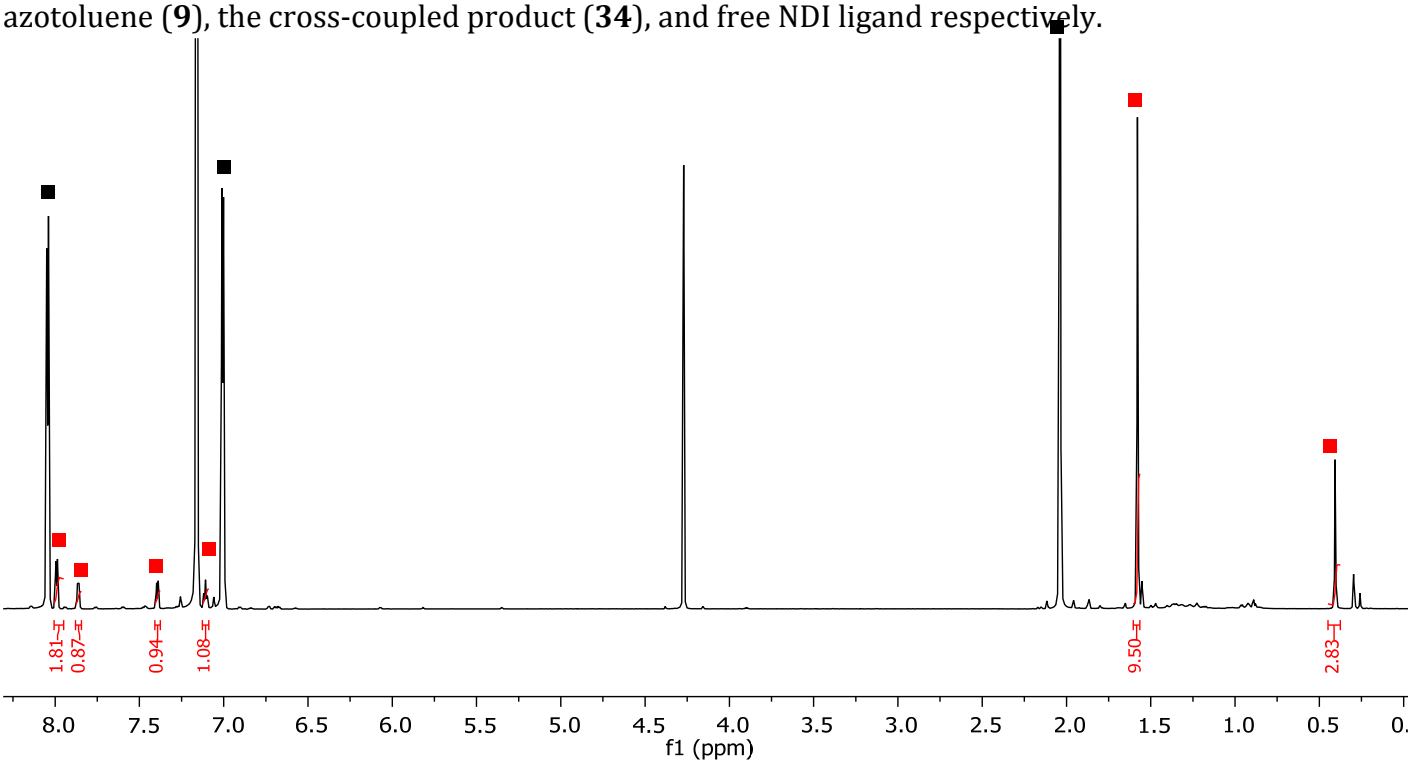

Figure S75. ^{1}H NMR spectrum (C_6H_6) of the product mixture after running through a column to remove the $^{i\text{-Pr}}$NDI ligand and 1,3,5-trimethoxybenzene. Black and red squares correspond to 4-azotoluene (**9**) and the cross-coupled product (**34**) respectively.

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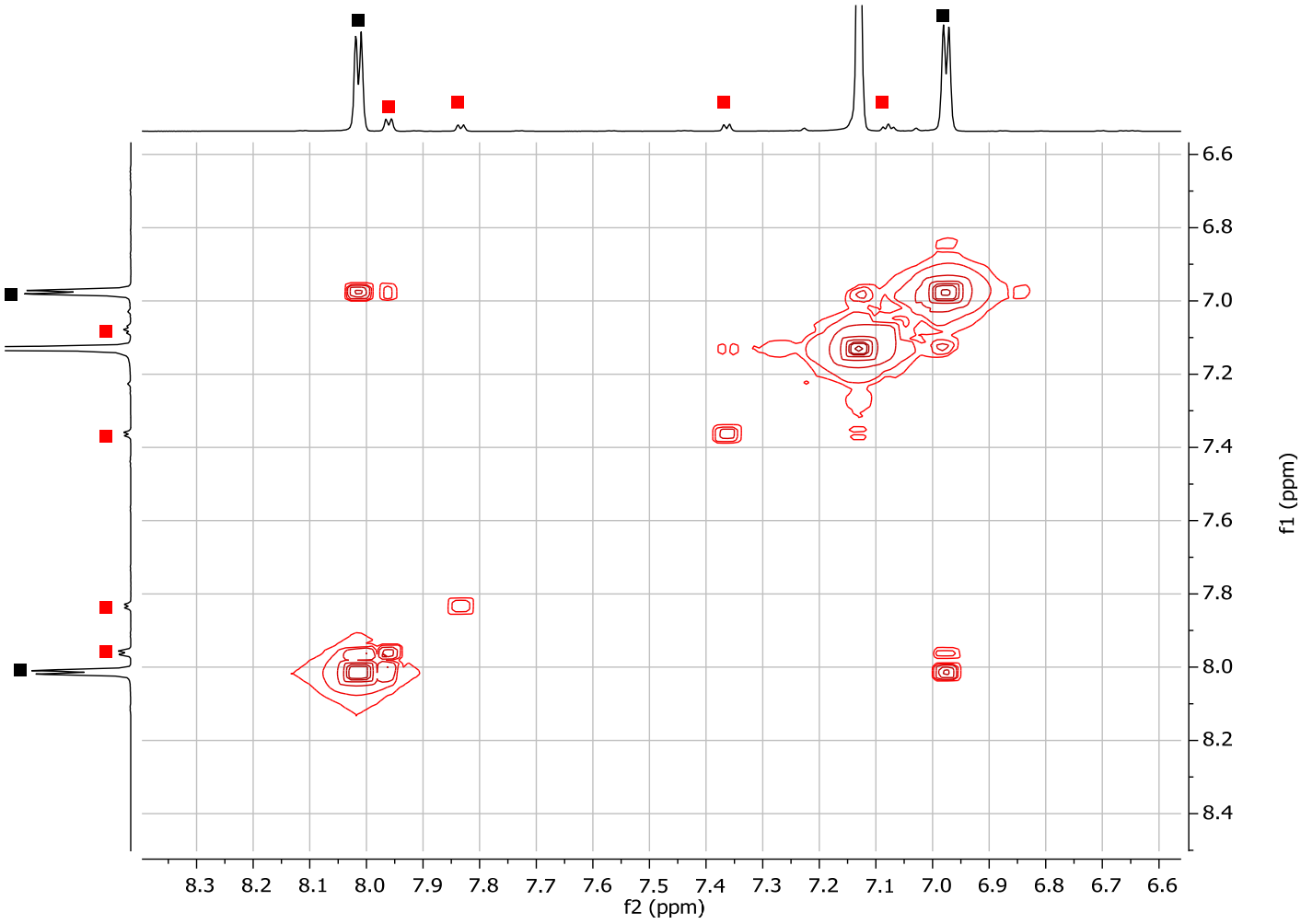

Figure S76. COSY spectrum of product mixture after column. Black and red squares correspond to 4-azotoluene (**9**) and the cross-coupled product (**34**) respectively.

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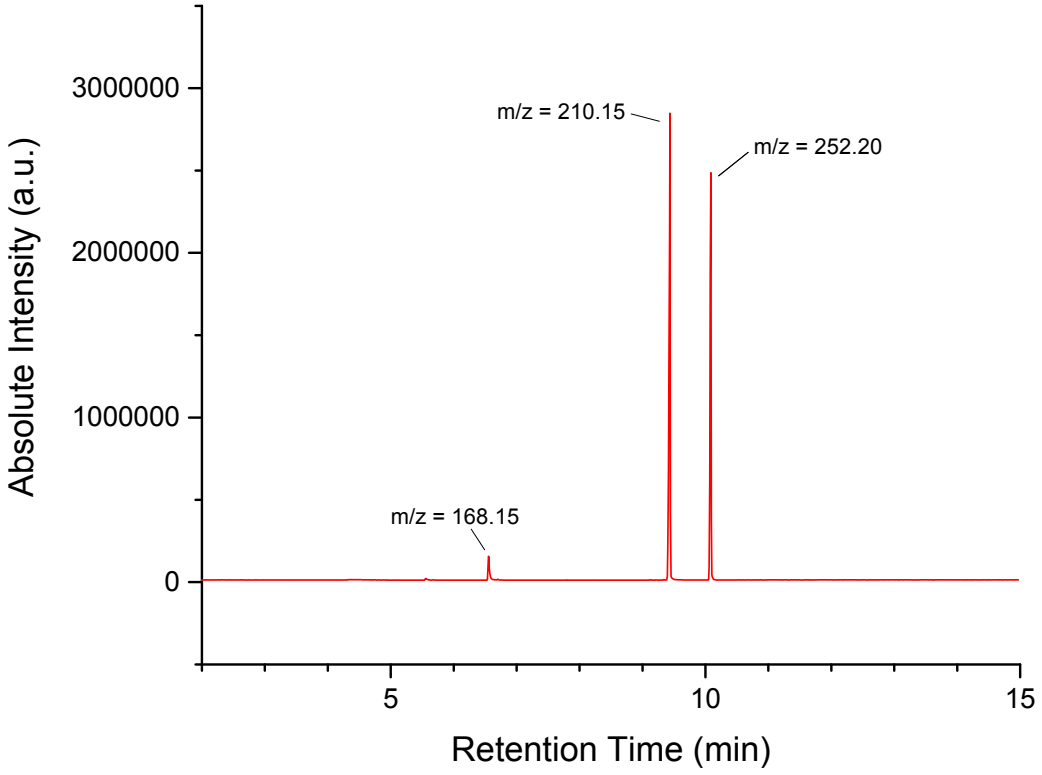

Figure S77. GCMS trace of the cross-coupling reaction following a silica plug. The masses at m/z = 168.15, 210.15, and 252.20 correspond to the masses of 1,3,5-trimethoxybenzene, 4-azotoluene (**9**), and the cross-coupled product (**34**) respectively.

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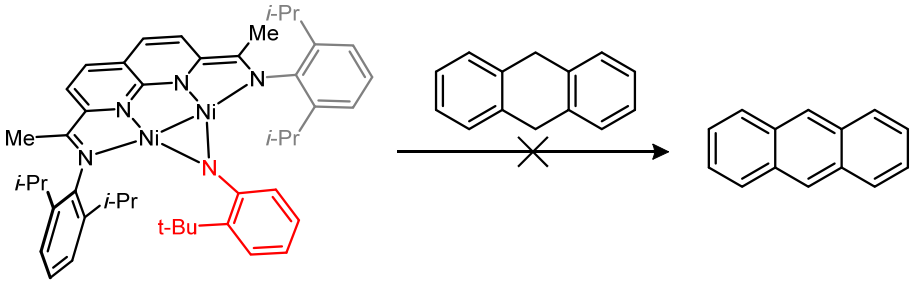

Comparison of the decomposition of 33 in the presence and absence of 9,10-dihydroanthracene. Under an atmosphere of N_2, a 20-mL vial was charged with 2-*tert*-butylphenyl azide (2.5 mg, 0.014 mmol, 1.0 equiv), **1** (10.0 mg, 0.014 mmol, 1.0 equiv), 1,3,5-trimethoxybenzene (2.5 mg, 0.015 mmol) as an internal standard, and C_6D_6 (1200 µL). This solution was then divided equally between two J. Young NMR tubes. To the first tube was added a solution of 9,10-dihydroanthracene (0.0068 mmol, 1.0 equiv) in C_6D_6 (150 µL). To the second was added C_6D_6 (150 µL). The decomposition of **33** in each solution was the monitored over several hours: over the time period of the catalytic N–N coupling reaction (2 h), a 13% decomposition of **33** in the solution without 9,10-dihydroanthracene was observed; the solution containing dihydroanthracene showed 14% decomposition of **33**. Measurement of the decomposition over a longer period showed minimal difference in the rate of decomposition between the two solutions. For the solution containing dihydroanthracene, no measurable amount of anthracene was formed by ^{1}H NMR.

Time	% Remaining **33**	% Remaining **33** (DHA)	% Remaining DHA
1 h	88%	89%	>95%
2 h	87%	86%	>95%
3 h	75%	74%	>95%
4 h	64%	72%	>95%
6 h	48%	51%	>95%
20 h	<5%	<5%	>95%

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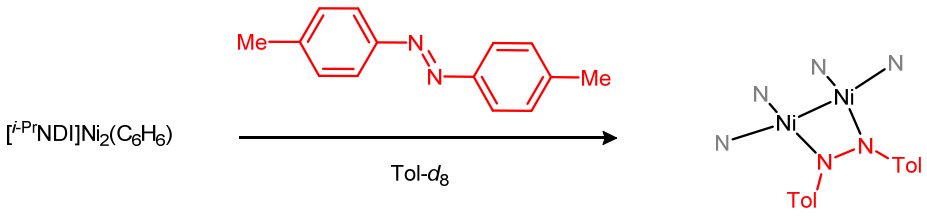

Variable-temperature NMR data for 1 + 4-tolylazobenzene. Under an atmosphere of N_2, a J-Young NMR tube was charged with 4-tolyl azide (2.8 mg, 0.014 mmol, 1.0 equiv), **1** (10.0 mg, 0.014 mmol, 1.0 equiv), and toluene-d_8 (600 µL). This lead to the formation of a new set up broad peaks observed by ^{1}H NMR. The spectrum was then taken over a range of temperatures from 200 to 350K, leading to a sharp set of diamagnetic peaks at low temperature, which broadened at high temperature.

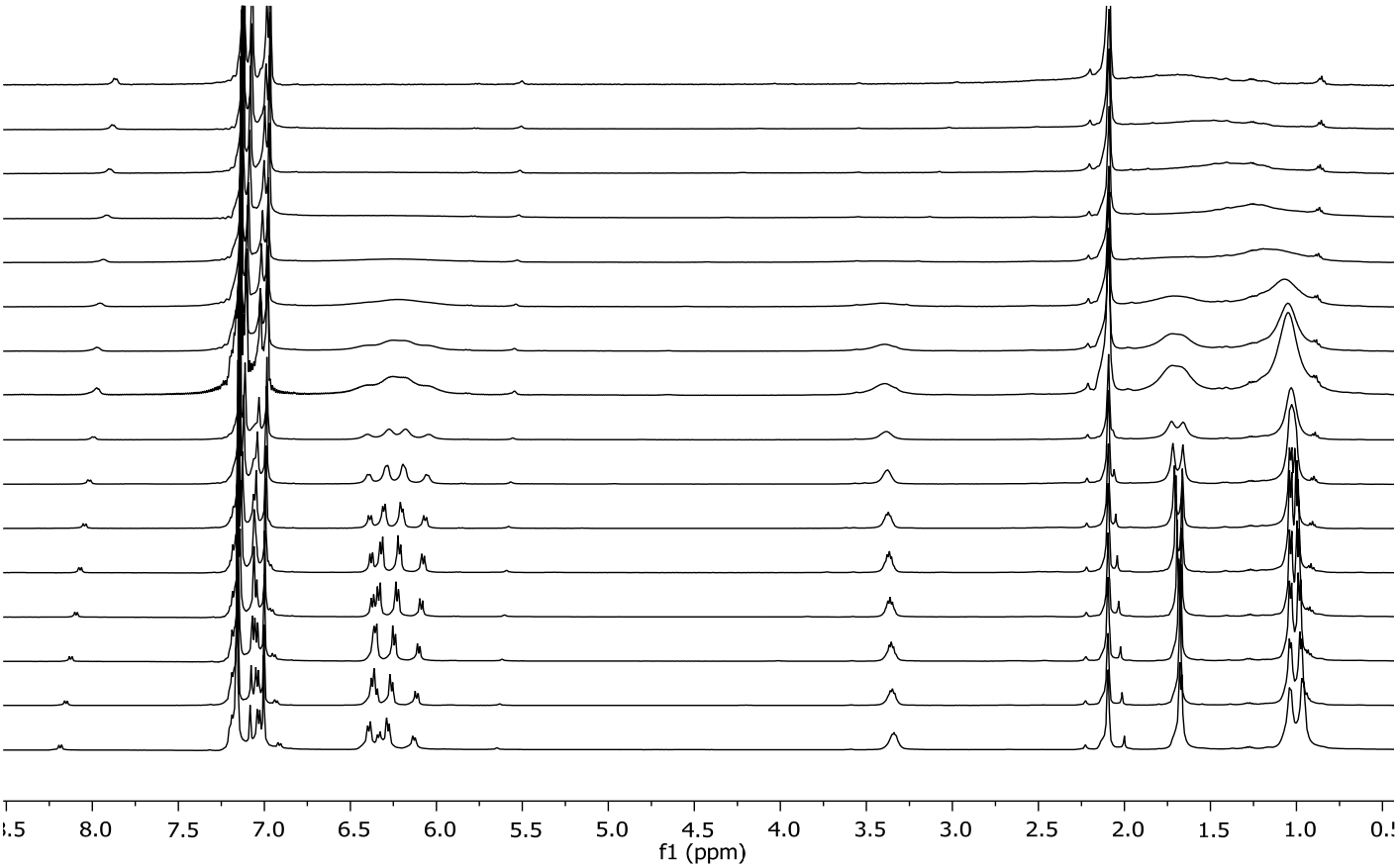

Figure S78. Variable-temperature ^{1}H NMR spectrum of the azoarene adduct formed on reaction of 4-azotoluene with **1** (200 to 350 K).

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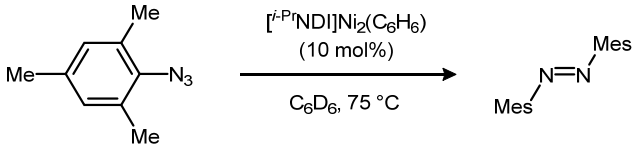

NMR kinetics studies for mesitylazide homocoupling. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with mesityl azide (103 µL of a 0.29 M solution in C_6D_6, 0.30 mmol, 1.0 equiv), **1** (400 µL of a 7.5 mM solution in C_6D_6, 0.03 mmol, 10 mol%) and C_6D_6 (97 µL). The reaction was then placed in an NMR spectrometer and heated at 75 °C. Data points were collected in 3-min intervals over 8 h.

The reaction rate was found to be zero order in [mesityl azide] (k = 7.86 ± 0.08 mM/min).

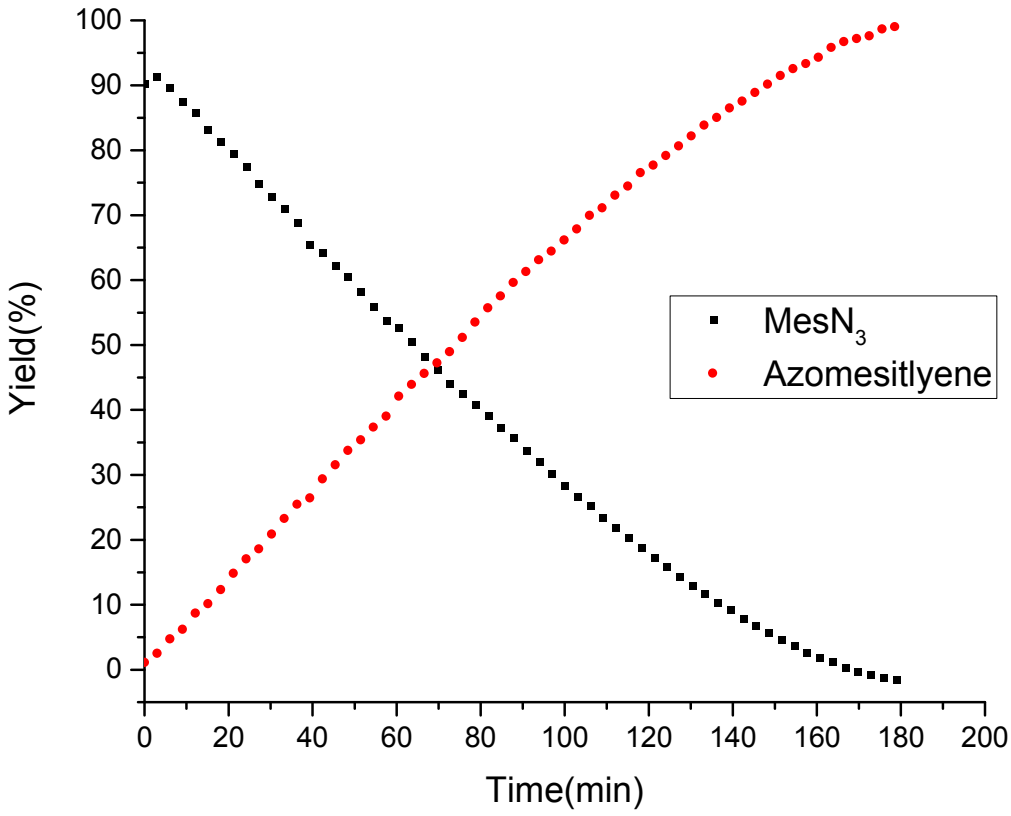

Figure S79. NMR kinetics plot of the formation of azomesitlyene catalyzed by **1**.

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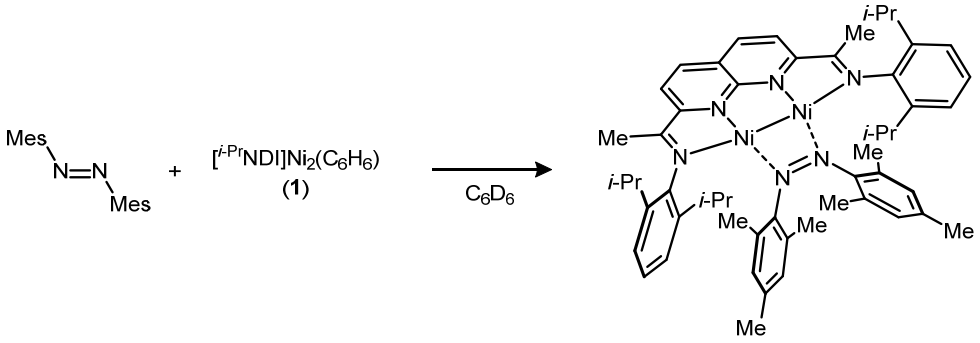

Azomesitylene binding under thermal conditions. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with **1** (3.9 mg, 0.005 mmol, 1.0 equiv), azomesitylene (10.6 mg, 0.040 mmol, 8.0 equiv), and C_6D_6 (600 µL). The NMR tube was placed in an oil bath and heated at 80 °C. Full conversion of **1** to the azomesitylene complex was observed after 30 days.

Azomesitylene binding under photolytic conditions. Under an atmosphere of N_2, an NMR tube equipped with a J. Young valve was charged with **1** (5.0 mg, 0.0069 mmol, 1.0 equiv), azomesitylene (1.8 mg, 0.0069 mmol, 1 equiv), and C_6D_6 (600 µL). The NMR tube was placed in a photobox and irradiated with 254 nm UV light[23] for 1.5 h. Full conversion to the azoarene complex was observed after 1.5 h.

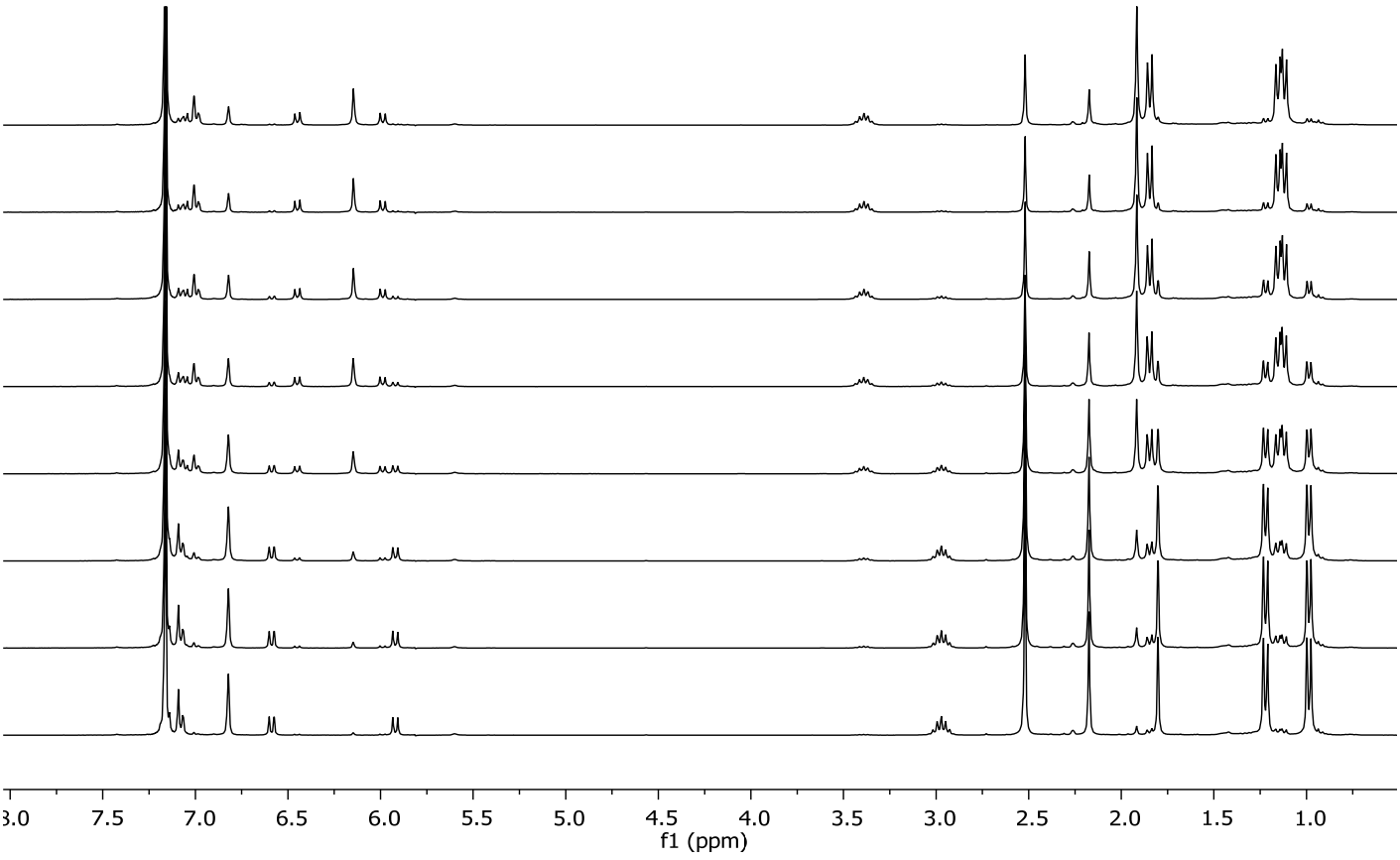

Figure S80. ^{1}H NMR spectrum of the azomesitylene binding experiment under thermal conditions.

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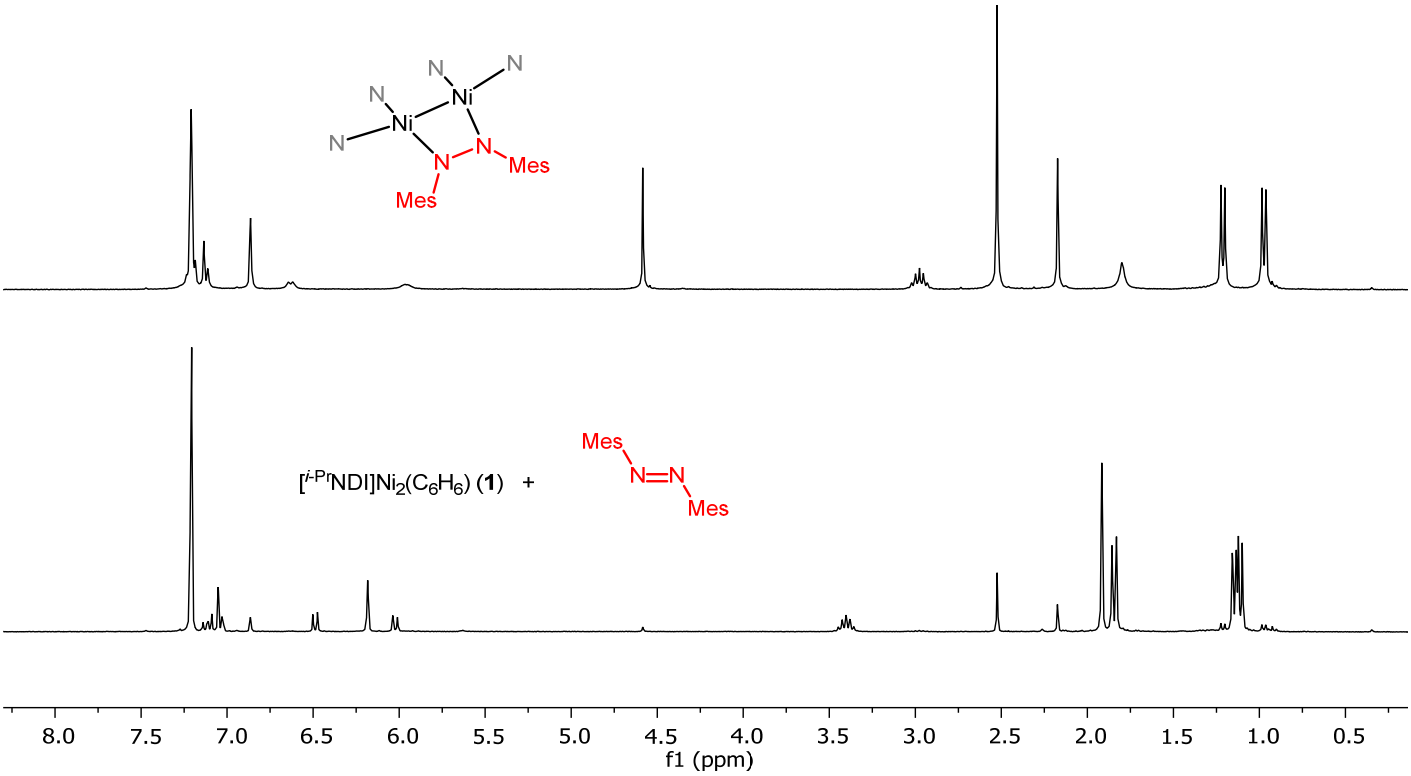

Figure S81. ^{1}H NMR spectrum of the asomesitylene binding experiment under photolytic conditions just after mixing (top) and after irradiation with UV light for 1.5 h (bottom).

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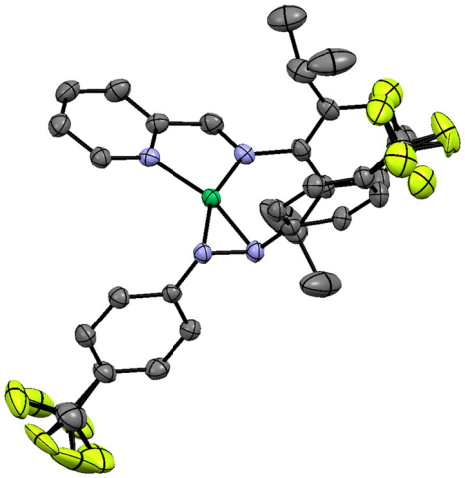
8. X-Ray Diffraction Data



Compound 7

Crystal data	
Chemical formula	$C_{32}H_{30}F_6N_4Ni \cdot 0.146(C_7H_8) \cdot 0.104(C_5H_{12})$
M_r	664.24
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	150
a, *b*, *c* (Å)	16.3481 (3), 22.1973 (4), 35.0360 (7)
V (Å^3)	12714.0 (4)
Z	16
Radiation type	Cu *K*α
μ (mm^{-1})	1.44
Crystal size (mm)	0.12 × 0.08 × 0.06
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.650, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	40453, 11767, 9216
R_{int}	0.040
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.118, 1.01
No. of reflections	11767
No. of parameters	1052
No. of restraints	1070
H-atom treatment	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.54, -0.37

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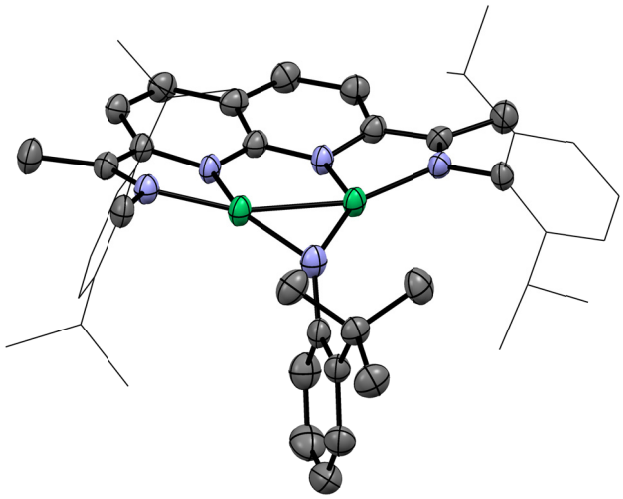

Compound 33

Crystal data	
Chemical formula	$2(C_{46}H_{57}N_5Ni_2)\cdot C_7H_8$
M_r	1686.90
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	8.6475 (7), 22.8313 (17), 22.7875 (16)
β (°)	98.535 (3)
V (Å^3)	4449.2 (6)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.34
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan TWINABS 2012/1: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.300, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	73107, 8851, 7121
R_{int}	0.150
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.177, 1.03
No. of reflections	8851
No. of parameters	544
No. of restraints	46
H-atom treatment	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.75, -0.68

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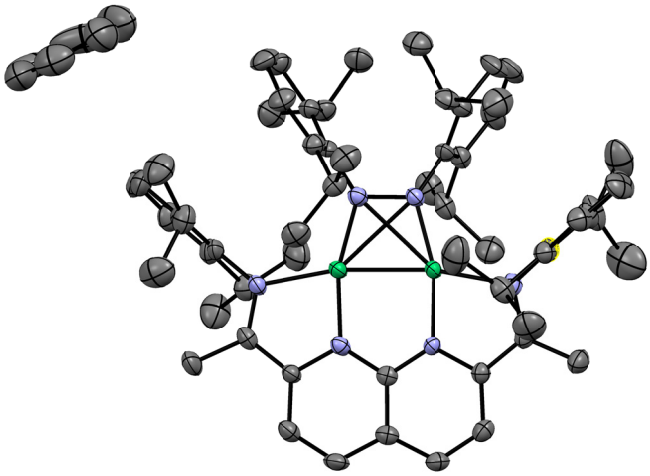

Compound 36

Crystal data	
Chemical formula	$C_{66}H_{84}N_6Ni_2$
M_r	1078.81
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	123
a, b, c (Å)	12.0220 (5), 26.4576 (8), 18.2600 (6)
β (°)	97.465 (3)
V (Å^3)	5758.8 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.15
Crystal size (mm)	0.30 × 0.20 × 0.16
Data collection	
Diffractometer	Rigaku Rapid II curved image plate diffractometer
Absorption correction	Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.816, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	40091, 10681, 9279
R_{int}	0.063
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.166, 1.08
No. of reflections	10681
No. of parameters	717
No. of restraints	186
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, -0.47

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9. DFT Calculations and Optimized Structures

Calculations addressing the thermodynamics of free nitrene release and comparison to imido formation. We were interested in the potential for free triplet nitrene release from a dinickel azide complex as an alternative mechanism to imido formation. We located a stable coordination mode for an $S = 1$ azide complex and found the formation of free triplet nitrene and a singlet N_2 complex to be endergonic by 16.3 kcal/mol (Figure S82). The subsequent substitution of N_2 for C_6H_6 is exergonic by 4.2 kcal/mol relative to the azide complex. By contrast, the formation of an imido species is much more energetically favorable, and the process is exergonic by 52.1 kcal/mol

From the imido intermediate we considered the possibility of the formation of tetrazene intermediates upon addition of a second equivalent of azide. The formation of a 1,4-tetrazene complex is nearly energetically neutral from the imido complex. From this intermediate, the bis(imido) species is energetically accessible.

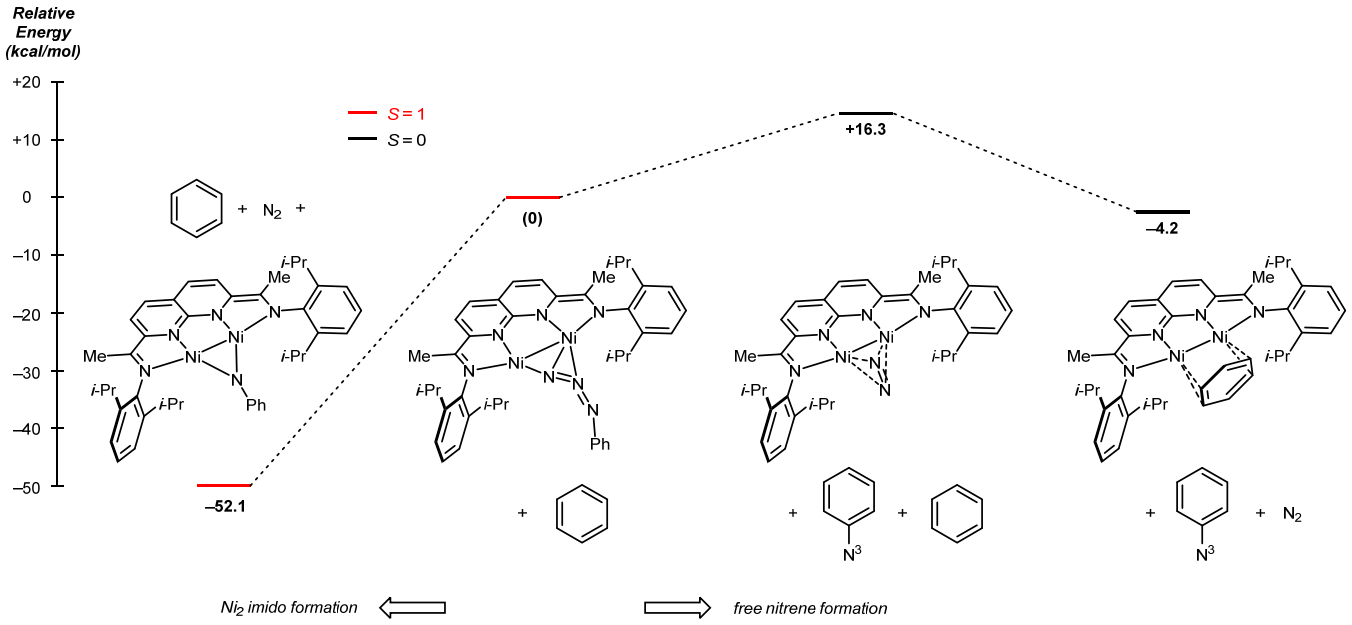

Figure S82. Thermodynamics of Ni_2(imido) formation (left pathway) vs. free triplet nitrene formation (right pathway) from an initial $Ni_2(N_3Ph)$ adduct. Energies are relative to: $Ni_2(N_3Ph)$ ($S = 1$) + C_6H_6. All structures are fully optimized and verified by frequency analysis.

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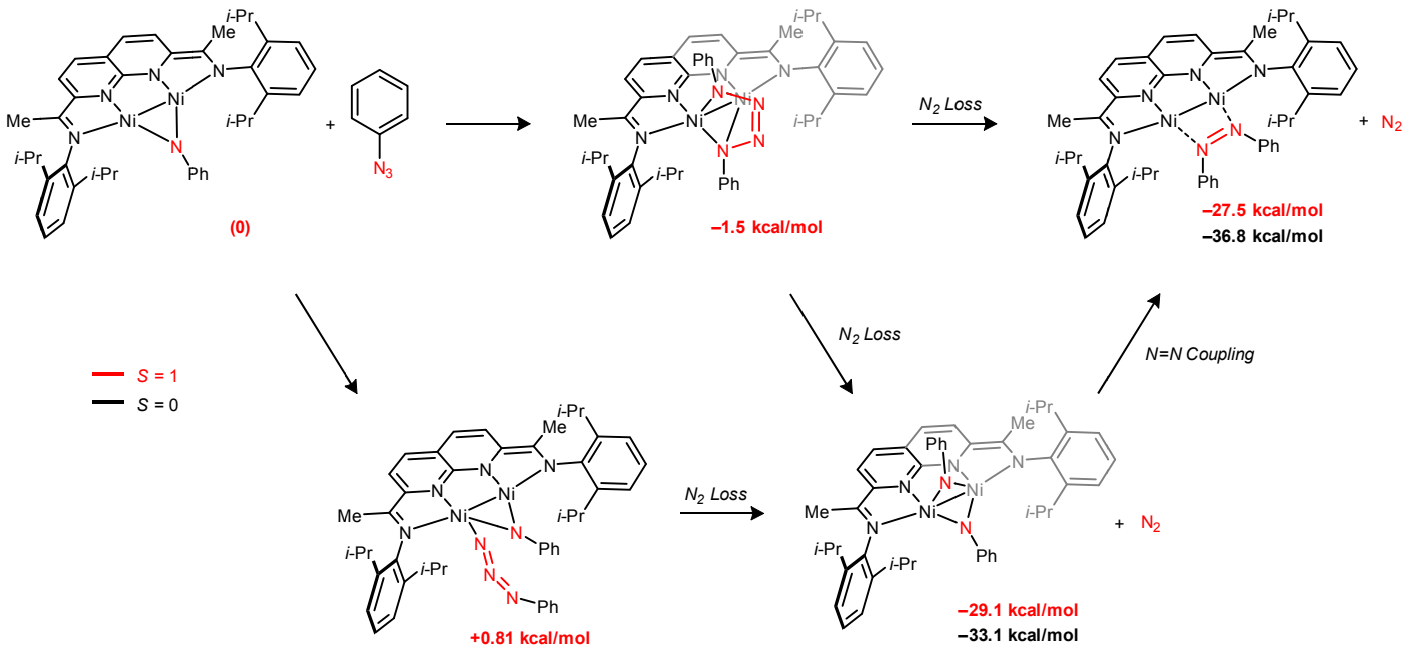

Figure S83. Calculated energies for possible intermediates leading from the Ni_2(imido) complex to the Ni_2(azoarene) product. Energies are relative to: Ni_2(imido) (S = 1) + PhN_3. All structures are fully optimized and verified by frequency analysis.

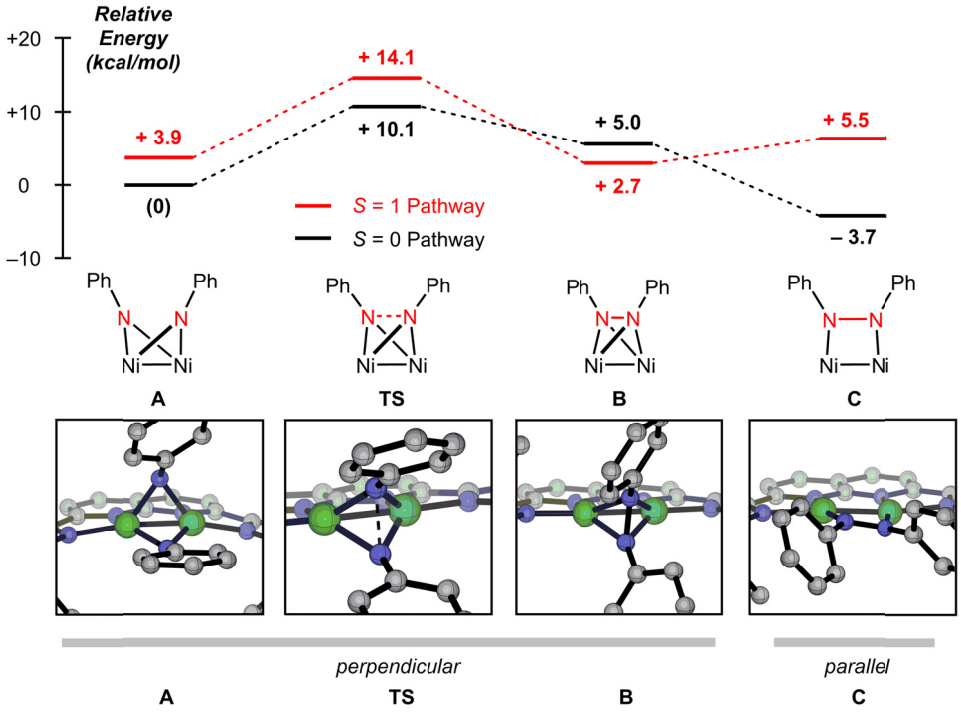

Figure S84. Energy profile for azoarene formation from a Ni_2 bis(imido) complex.

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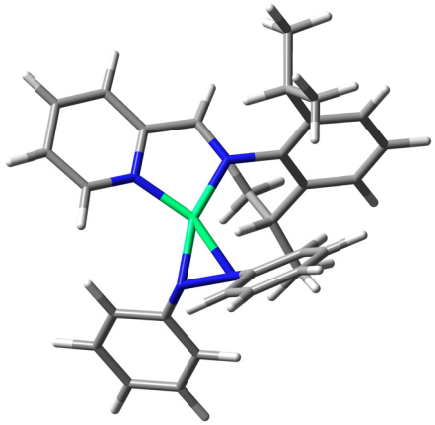
Computational Methods.[24] Geometry optimizations were performed using the Gaussian09 software package.[25] All geometries were fully optimized at the BP86/6-31G(d,p) level of DFT. Stationary points were verified by frequency analysis.



Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -2889.91086561 Hartrees
Gibbs Free Energy (298.15 K): –2889.439275 Hartrees

Ni	0.5926660	0.3886680	-0.4362580
N	1.9741340	-0.6907440	-0.9781270
N	0.8922860	-1.4721310	-0.5512590
N	0.8712950	2.2301130	-0.7464130
N	-0.9190210	0.9401770	0.5010680
C	-1.4341860	-3.2060950	-3.6599600
C	-1.9206730	-3.1166050	-2.3424230
H	-2.9031310	-3.5315820	-2.0915230
C	-1.1511190	-2.5173610	-1.3385460
H	-1.5138420	-2.4643820	-0.3071160
C	0.1233180	-1.9792610	-1.6401180
C	0.6170250	-2.0862120	-2.9616890
H	1.6155610	-1.6971820	-3.1786960
C	-0.1618330	-2.6910020	-3.9575180
H	0.2350830	-2.7694660	-4.9760090
C	3.1207560	-0.8023280	-0.1536800
C	3.4143040	-1.9934300	0.5534050
H	2.6955800	-2.8152380	0.5067480
C	4.6059010	-2.1061290	1.2822000
H	4.8186350	-3.0369250	1.8199460
C	5.5299460	-1.0489580	1.3188320
C	5.2458620	0.1325540	0.6104230
H	5.9566010	0.9661320	0.6271120
C	4.0604790	0.2557100	-0.1220190
H	3.8459900	1.1770130	-0.6721320
C	-0.0455680	3.0321250	-0.0873050

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C	-0.0421880	4.4314800	-0.2208540
H	-0.7749830	5.0271840	0.3316630
C	0.8866780	5.0325020	-1.0775320
H	0.9086010	6.1193600	-1.1982310
C	1.7800840	4.2122920	-1.7916610
H	2.5151710	4.6381430	-2.4795250
C	1.7362860	2.8265560	-1.6031830
H	2.4158210	2.1507080	-2.1293890
C	-0.9955270	2.2539760	0.6733400
H	-1.7394640	2.7135880	1.3346130
C	-1.8775250	0.1146860	1.1873700
C	-3.2313290	0.0960450	0.7579170
C	-4.1258200	-0.7348580	1.4622470
H	-5.1761020	-0.7653050	1.1526940
C	-3.7000900	-1.5260330	2.5340670
H	-4.4154800	-2.1631510	3.0643790
C	-2.3528140	-1.5087150	2.9212830
H	-2.0210180	-2.1367630	3.7537690
C	-1.4156870	-0.6971480	2.2598190
C	0.0466000	-0.6367370	2.6926480
H	0.6143180	-0.3618180	1.7822290
C	0.2669130	0.4717880	3.7472680
H	-0.0613220	1.4585890	3.3782270
H	1.3360220	0.5462420	4.0113670
H	-0.2994810	0.2539880	4.6703320
C	0.5961090	-1.9862930	3.1851890
H	1.6850340	-1.9113340	3.3398190
H	0.4133460	-2.7801690	2.4436080
H	0.1455620	-2.2919960	4.1467560
C	-3.7382730	0.9068090	-0.4378740
H	-2.8692120	1.3902060	-0.9163570
C	-4.7106380	2.0224400	0.0079570
H	-5.6052940	1.5984930	0.4966800
H	-5.0505130	2.6128770	-0.8607150
H	-4.2387340	2.7128450	0.7281450
C	-4.3931000	0.0022290	-1.5057250
H	-5.3039850	-0.4888500	-1.1205890
H	-3.6969330	-0.7830890	-1.8418870
H	-4.6876750	0.6019620	-2.3845350
H	6.4622810	-1.1452300	1.8840890
H	-2.0353050	-3.6836180	-4.4404070

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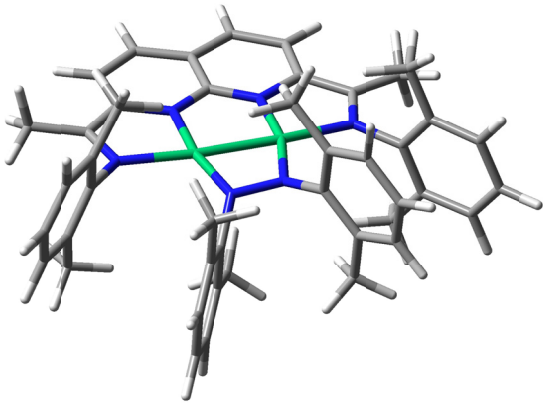

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –5049.84544543 Hartrees
Gibbs Free Energy (298.15 K): –5049.155070 Hartrees

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Ni	-1.16945400	0.77999500	0.11863400
N	3.05013000	1.12072700	-0.02882400
N	-3.13432500	0.96492800	0.12889400
N	1.05414200	2.64968100	0.03410400
N	-1.22699600	2.60063800	0.12394800
N	0.68510900	-0.90195100	0.15432500
N	-0.69103000	-0.93954100	0.04376900
C	3.38716000	2.42012500	-0.06033400
C	-3.54330200	2.24275400	0.16129700
C	2.27230600	3.32586800	-0.01349400
C	2.29964800	4.73244700	-0.05514200
H	3.26206200	5.25100700	-0.09182800
C	1.11219100	5.46931400	-0.06552900
H	1.13605400	6.56246300	-0.10682800
C	-0.14162900	4.79722100	-0.02582100
C	-0.10499500	3.36034300	0.03616300
C	-1.42890800	5.40389300	-0.04467700
H	-1.50846700	6.49377400	-0.10138600
C	-2.57888600	4.61045300	0.00230700
H	-3.56561200	5.08176900	-0.02136000
C	-2.47941300	3.20872300	0.07821900
C	4.08281300	0.14164800	-0.16587600
C	4.63470400	-0.44570200	1.00114400
C	5.62280300	-1.43519800	0.85300100
H	6.05045000	-1.89454000	1.75123500
C	6.05702800	-1.83780600	-0.41720400
H	6.82430000	-2.61265700	-0.51593800
C	5.50352500	-1.24641400	-1.56112400
H	5.84126700	-1.55665500	-2.55694000
C	4.51301500	-0.25198500	-1.45961200

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C	-4.09929300	-0.07173900	0.32999400
C	-4.25666200	-0.61124800	1.63246200
C	-5.19315400	-1.64261400	1.82539900
H	-5.32015600	-2.06205300	2.83018200
C	-5.95345300	-2.13608400	0.75618400
H	-6.67786500	-2.94030300	0.92124700
C	-5.77295700	-1.60456100	-0.52796400
H	-6.35327500	-1.99759500	-1.37049600
C	-4.84545000	-0.57378900	-0.76737600
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C	2.72605800	-4.05858400	0.25847100
H	3.24334500	-4.73608500	-0.43022900
C	2.76173000	-4.30080800	1.63585400
C	2.11320800	-3.42024500	2.51231100
H	2.14924100	-3.59489700	3.59395500
C	1.41491400	-2.29876200	2.02865600
C	0.72087500	-1.36091500	2.98931300
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C	2.00633100	-2.73656700	-1.76826200
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H	5.09328200	3.09326900	-1.22370400
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H	-5.20616900	2.79570900	1.42831400
C	4.18087900	0.01844000	2.36475800
H	3.08192300	0.09926800	2.40127700
C	3.92543400	0.38888600	-2.69721200
H	4.29386500	1.42134900	-2.84212900
C	-3.41016800	-0.08436500	2.76818500
H	-3.72414300	0.92622900	3.08878100
C	-4.64905500	-0.01052600	-2.15598800
H	-3.58172500	-0.01543700	-2.43304200
H	1.15020700	-3.26413900	-2.22495900
H	2.92991100	-3.11561200	-2.23431800
H	-0.35722800	-1.58650600	3.06523900
H	1.15378800	-1.43711800	3.99985400

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H	-2.58935300	-4.14936000	1.54551600
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H	0.17986400	-0.79731900	-3.48792500
H	-1.40221100	0.00608200	-3.43744600
H	-5.20393200	-0.60250700	-2.90092600
H	-4.99264300	1.03722800	-2.23465200
H	-3.45993600	-0.74671400	3.64738200
H	-2.35967400	0.00591400	2.43483800
H	3.30494700	-5.16688900	2.02848000
H	-2.88532200	-4.65845700	-3.11783200
H	4.18874800	-0.18413800	-3.60075000
H	2.82564300	0.45776200	-2.63051600
H	4.51485400	-0.67454000	3.15288300
H	4.57829700	1.02213000	2.60587400

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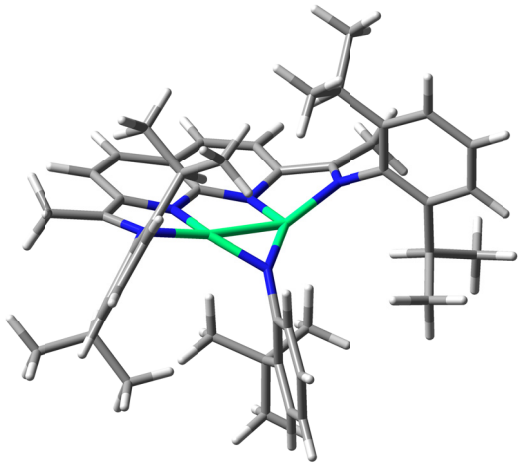

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Multiplicity: 1
Imaginary Frequencies: 0
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Gibbs Free Energy (298.15 K): –5077.109486 Hartrees

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N	-2.9920050	0.8765940	0.2111620
N	-1.1542260	2.3146450	-0.6991760
N	1.1548260	2.3145270	-0.6990770
N	2.9924570	0.8761600	0.2110470
N	0.0001490	-0.7369790	-0.4104430
C	-4.8776300	2.5098170	-0.1420500
H	-5.3886950	2.3406470	-1.1071250
H	-4.9646490	3.5832010	0.0903480
H	-5.4251050	1.9404340	0.6252020
C	-3.4331210	2.0897550	-0.1924890
C	-2.3807370	2.9757910	-0.6022050
C	-2.4412090	4.3676600	-0.7976210
H	-3.4078750	4.8790850	-0.7712650
C	-1.2677160	5.1058490	-0.9810460
H	-1.3114730	6.1917860	-1.1094580
C	0.0004490	4.4634380	-0.9250280
C	0.0003550	3.0301060	-0.7467050
C	1.2687300	5.1056400	-0.9812290
H	1.3126340	6.1915610	-1.1097430
C	2.4421250	4.3672990	-0.7979070
H	3.4088730	4.8785770	-0.7717930
C	2.3814710	2.9754460	-0.6023050
C	3.4337340	2.0892780	-0.1926100
C	4.8783060	2.5091290	-0.1420970
H	5.4254820	1.9401660	0.6256890
H	4.9654450	3.5826470	0.0896110
H	5.3896130	2.3392000	-1.1069030
C	-3.8889510	-0.1547760	0.6222500
C	-3.8243510	-0.5641480	1.9894870

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C	-4.6954910	-1.5748280	2.4285180
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C	-5.5891270	-2.1938680	1.5434880
H	-6.2627850	-2.9787990	1.9031010
C	-5.5993870	-1.8245470	0.1939920
H	-6.2728410	-2.3409560	-0.4986020
C	-4.7546470	-0.8112110	-0.2999930
C	-4.7327100	-0.5185980	-1.8015610
H	-4.1230050	0.3866750	-1.9650870
C	-6.1410820	-0.2528680	-2.3780640
H	-6.0712990	0.0441130	-3.4387810
H	-6.6681000	0.5469380	-1.8307850
H	-6.7741970	-1.1561860	-2.3337230
C	-4.0446570	-1.6744240	-2.5659880
H	-3.0151810	-1.8405100	-2.2095240
H	-3.9986810	-1.4504790	-3.6461030
H	-4.6046270	-2.6177020	-2.4386500
C	-2.8081110	0.0923350	2.9213930
H	-1.9216830	0.2848900	2.2786710
C	-3.3054590	1.4593080	3.4447490
H	-4.2142710	1.3335370	4.0601710
H	-3.5430270	2.1488970	2.6190950
H	-2.5333860	1.9380140	4.0724220
C	-2.3702100	-0.8043080	4.0919480
H	-2.0354310	-1.7948180	3.7429330
H	-3.1835490	-0.9547910	4.8246910
H	-1.5330460	-0.3316020	4.6331350
C	3.8891750	-0.1552960	0.6223300
C	4.7551370	-0.8117270	-0.2996670
C	5.5997760	-1.8250440	0.1945360
H	6.2734480	-2.3414080	-0.4978770
C	5.5890970	-2.1944220	1.5440080
H	6.2626570	-2.9793460	1.9038210
C	4.6951380	-1.5754610	2.4287770
H	4.6673770	-1.8924250	3.4757760
C	3.8241390	-0.5647640	1.9895380
C	2.8076580	0.0917110	2.9211790
H	1.9213740	0.2842530	2.2782140
C	3.3048890	1.4586850	3.4446320
H	4.2137580	1.3329390	4.0599790
H	2.5328080	1.9372390	4.0724120
H	3.5423390	2.1483780	2.6190380
C	2.3694450	-0.8049250	4.0916120
H	2.0347760	-1.7954480	3.7425270
H	1.5321200	-0.3322310	4.6325650
H	3.1825630	-0.9553970	4.8246130
C	4.7333970	-0.5192840	-1.8012650
H	4.1239730	0.3861370	-1.9649880
C	4.0449600	-1.6750510	-2.5654610
H	3.9989110	-1.4512700	-3.6456080
H	3.0154840	-1.8407960	-2.2088320
H	4.6046970	-2.6184520	-2.4380150
C	6.1418430	-0.2540770	-2.3778000

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H	6.7746710	-1.1575920	-2.3334250
H	6.6691190	0.5455970	-1.8305770
H	6.0721440	0.0428620	-3.4385340
C	-0.0002250	-1.6715680	-1.4592790
C	0.0000250	-1.1819610	-2.7953210
H	0.0004900	-0.0963400	-2.9410060
C	-0.0004120	-2.0499400	-3.8891080
H	-0.0002410	-1.6430530	-4.9058990
C	-0.0010440	-3.4349420	-3.6702860
H	-0.0013890	-4.1339980	-4.5126780
C	-0.0012170	-3.9249560	-2.3551940
H	-0.0016730	-5.0081170	-2.2095660
C	-0.0008150	-3.0885710	-1.2205500
C	-0.0009010	-3.6753600	0.2080730
C	1.2698030	-3.2074150	0.9658610
H	1.2625490	-3.6081400	1.9958570
H	1.3214660	-2.1089560	1.0174700
H	2.1841180	-3.5704820	0.4662100
C	-1.2711980	-3.2066630	0.9660420
H	-1.2639410	-3.6072340	1.9960960
H	-2.1858170	-3.5693210	0.4666430
H	-1.3222910	-2.1081730	1.0174720
C	-0.0013540	-5.2214390	0.2074360
H	0.8941040	-5.6380550	-0.2860010
H	-0.8971690	-5.6375190	-0.2858040
H	-0.0013520	-5.5810620	1.2508420

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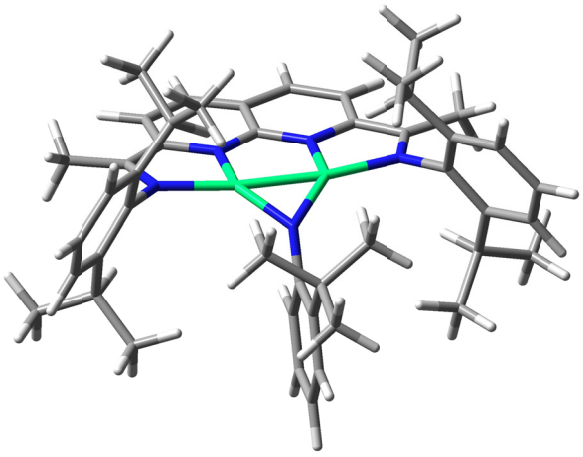

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: –5077.92754475 Hartrees
Gibbs Free Energy (298.15 K): –5077.112786 Hartrees

Ni	1.1093600	0.6003990	0.0561330
Ni	-1.1093620	0.6002530	0.0559660
N	-3.0209030	0.8402980	0.1264300
N	-1.1400370	2.4134160	-0.3228530
N	1.1400740	2.4134870	-0.3224860
N	3.0208800	0.8401300	0.1262050
N	0.0001480	-0.7637350	-0.2663970
C	-4.8894040	2.5125010	-0.1441070
H	-5.3452690	2.4233890	-1.1473680
H	-4.9902860	3.5626460	0.1731640
H	-5.4779080	1.8805180	0.5389010
C	-3.4440940	2.0911590	-0.1509400
C	-2.3761070	3.0225930	-0.4247050
C	-2.4489210	4.3997690	-0.7349620
H	-3.4248780	4.8811740	-0.8457900
C	-1.2802630	5.1492810	-0.9060440
H	-1.3410540	6.2162110	-1.1426120
C	0.0000650	4.5335980	-0.7739180
C	0.0000150	3.1316880	-0.4722700
C	1.2804060	5.1491260	-0.9065040
H	1.3412170	6.2160120	-1.1432720
C	2.4490600	4.3995120	-0.7357600
H	3.4250360	4.8807200	-0.8472450
C	2.3761710	3.0224300	-0.4251120
C	3.4441420	2.0909250	-0.1514140
C	4.8894510	2.5122940	-0.1447410
H	5.4781360	1.8800540	0.5378630
H	4.9903210	3.5623130	0.1729630
H	5.3451010	2.4236480	-1.1481410
C	-3.9458660	-0.1880100	0.4904700
C	-3.9205850	-0.6422900	1.8438210

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C	-4.8108820	-1.6598440	2.2248870
H	-4.8115730	-2.0139850	3.2602820
C	-5.6886060	-2.2381690	1.2971570
H	-6.3778360	-3.0287720	1.6118150
C	-5.6628760	-1.8191800	-0.0374350
H	-6.3253070	-2.3009130	-0.7649240
C	-4.7951430	-0.7989150	-0.4742020
C	-4.7322910	-0.4452620	-1.9611670
H	-4.1105750	0.4603690	-2.0694080
C	-6.1220750	-0.1399340	-2.5621010
H	-6.0217500	0.1965710	-3.6086040
H	-6.6529860	0.6454780	-1.9977890
H	-6.7677000	-1.0357580	-2.5691260
C	-4.0334630	-1.5741440	-2.7551790
H	-3.0164900	-1.7657230	-2.3766660
H	-3.9549410	-1.3047600	-3.8231510
H	-4.6058240	-2.5159460	-2.6846910
C	-2.9209540	-0.0273730	2.8210770
H	-2.0154560	0.1738470	2.2028720
C	-3.4140150	1.3280850	3.3770500
H	-4.3343450	1.1901670	3.9724350
H	-3.6336590	2.0468030	2.5715930
H	-2.6491750	1.7796070	4.0330660
C	-2.5192490	-0.9602960	3.9758590
H	-2.1902760	-1.9459830	3.6097180
H	-3.3516620	-1.1160600	4.6855770
H	-1.6886010	-0.5123470	4.5472210
C	3.9458990	-0.1880460	0.4905170
C	4.7954170	-0.7989210	-0.4739860
C	5.6634130	-1.8188220	-0.0369300
H	6.3260980	-2.3004760	-0.7642340
C	5.6891010	-2.2375680	1.2977530
H	6.3785620	-3.0278850	1.6126240
C	4.8110730	-1.6593800	2.2252600
H	4.8117150	-2.0133370	3.2607200
C	3.9205320	-0.6421230	1.8439100
C	2.9207060	-0.0272570	2.8210010
H	2.0152320	0.1737830	2.2027070
C	3.4135910	1.3283290	3.3768320
H	4.3339650	1.1905740	3.9721790
H	2.6487270	1.7798410	4.0328300
H	3.6331100	2.0469650	2.5712610
C	2.5190090	-0.9601050	3.9758560
H	2.1904920	-1.9459690	3.6097900
H	1.6880470	-0.5123350	4.5468900
H	3.3512820	-1.1154440	4.6858360
C	4.7323910	-0.4456800	-1.9610290
H	4.1106830	0.4599220	-2.0694850
C	4.0334100	-1.5748050	-2.7545810
H	3.9547350	-1.3057640	-3.8226250
H	3.0164880	-1.7662540	-2.3758670
H	4.6057880	-2.5165840	-2.6838570
C	6.1220680	-0.1405310	-2.5623090

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H	6.7675150	-1.0364800	-2.5697200
H	6.6532740	0.6446840	-1.9980020
H	6.0214940	0.1961860	-3.6087200
C	0.0000160	-1.6831940	-1.3220590
C	0.0000210	-1.1767500	-2.6541510
H	0.0001540	-0.0882170	-2.7784080
C	-0.0001140	-2.0203950	-3.7670020
H	-0.0001160	-1.5943550	-4.7760490
C	-0.0002530	-3.4091810	-3.5741250
H	-0.0003640	-4.0924430	-4.4296550
C	-0.0002370	-3.9241380	-2.2685130
H	-0.0003410	-5.0101600	-2.1446500
C	-0.0000900	-3.1078960	-1.1194200
C	-0.0000810	-3.7234960	0.2948440
C	1.2701370	-3.2641470	1.0571290
H	1.2647620	-3.6777540	2.0822410
H	1.3138870	-2.1657710	1.1176760
H	2.1850190	-3.6178190	0.5518340
C	-1.2702270	-3.2640290	1.0571830
H	-1.2648060	-3.6775470	2.0823250
H	-2.1851490	-3.6176840	0.5519550
H	-1.3139140	-2.1656460	1.1176590
C	-0.0001550	-5.2690330	0.2685810
H	0.8953680	-5.6771510	-0.2319210
H	-0.8957250	-5.6770680	-0.2319000
H	-0.0001550	-5.6467780	1.3056810

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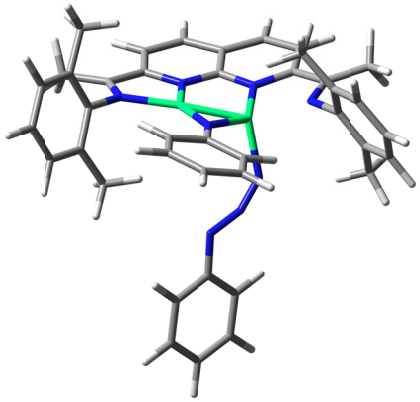

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: –5002.06345819 Hartrees
Gibbs Free Energy (298.15 K): –5001.47561 Hartrees

Ni	-1.1194420	0.8882740	0.1354620
Ni	1.0468870	0.5894860	-0.0543640
N	2.9967560	1.1277200	0.2898650
N	1.1313270	2.2635490	-0.9983360
N	-1.1426180	2.2886380	-1.0620010
N	-3.0085530	1.1342010	0.0754150
N	-0.1425110	-0.2552670	1.0554280
C	4.8013190	2.7591680	-0.3525190
H	4.7900370	3.8230200	-0.0589670
H	5.2757990	2.7021700	-1.3486090
H	5.4283720	2.2062920	0.3613280
C	3.3993060	2.2026370	-0.3860920
C	2.3519320	2.8807930	-1.1325000
C	2.4600940	4.0780720	-1.8755360
H	3.4374950	4.5528130	-2.0004060
C	1.3210990	4.6640190	-2.4416700
H	1.4067770	5.5892000	-3.0202360
C	0.0345210	4.0914610	-2.2160770
C	0.0123110	2.8842890	-1.4447240
C	-1.2345070	4.5996180	-2.6304060
H	-1.2755960	5.5055570	-3.2433290
C	-2.4183710	3.9679940	-2.2299540
H	-3.3873240	4.3814070	-2.5249400
C	-2.3650810	2.8205170	-1.4076640
C	-3.4385500	2.0958040	-0.7672700
C	-4.8857180	2.4054950	-1.0435870
H	-5.0731130	2.4517350	-2.1301930
H	-5.1762730	3.3858910	-0.6227110
H	-5.5447350	1.6410650	-0.6070680
C	3.9060520	0.3650360	1.0801960
C	4.8384250	-0.5165230	0.4679180
C	5.6618290	-1.2968770	1.3019030
H	6.3805450	-1.9817220	0.8374710
C	5.5709060	-1.2173550	2.6977190
H	6.2203970	-1.8341860	3.3272100

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C	4.6341910	-0.3545630	3.2835040
H	4.5483970	-0.2952010	4.3743320
C	3.7837060	0.4397460	2.4946170
C	2.7553900	1.3503080	3.1234610
H	1.7429790	1.1104840	2.7503890
C	4.9388410	-0.6340800	-1.0371730
H	3.9388010	-0.6884760	-1.4978870
C	-3.9425850	0.3562310	0.8279380
C	-4.5603730	0.9054330	1.9827240
C	-5.4329540	0.0849390	2.7222580
H	-5.9131980	0.4970500	3.6170390
C	-5.6834790	-1.2398950	2.3392750
H	-6.3658900	-1.8614880	2.9279870
C	-5.0416720	-1.7723200	1.2120690
H	-5.2155270	-2.8142670	0.9210660
C	-4.1569300	-0.9939040	0.4448730
C	-3.4046510	-1.5693080	-0.7288030
H	-2.3176130	-1.4194610	-0.5883160
C	-4.2630310	2.3196620	2.4278220
H	-4.7249480	3.0738770	1.7652350
C	-0.1180610	-1.2730650	1.9644670
C	-1.2939530	-1.6198550	2.6995480
H	-2.2151310	-1.0621600	2.5075180
C	-1.2613450	-2.6472780	3.6429560
H	-2.1733900	-2.8963070	4.1961660
C	-0.0727640	-3.3631150	3.8863090
H	-0.0558070	-4.1691250	4.6268110
C	1.0927440	-3.0345880	3.1673680
H	2.0214510	-3.5865350	3.3471900
C	1.0801100	-2.0076620	2.2227740
H	5.5013180	-1.5392530	-1.3170340
H	5.4645910	0.2281580	-1.4877880
H	1.9825070	-1.7492400	1.6607210
H	2.7573740	1.2492160	4.2201540
H	2.9388340	2.4111840	2.8757760
H	-4.6466590	2.4970510	3.4451790
H	-3.1769300	2.5172640	2.4259240
H	-3.5997190	-2.6467420	-0.8408680
H	-3.6699960	-1.0702440	-1.6778760
C	-0.0369030	-3.7765440	-2.4559390
C	0.8039980	-3.7942170	-3.5930690
C	-1.0075140	-4.7906600	-2.2978000
C	0.6678640	-4.8097460	-4.5471570
H	1.5578910	-3.0092950	-3.7155480
C	-1.1350710	-5.7984180	-3.2606650
H	-1.6451200	-4.7697000	-1.4090250
C	-0.3004450	-5.8164640	-4.3912160
H	1.3255410	-4.8135600	-5.4233200
H	-1.8913030	-6.5789170	-3.1247330
H	-0.4014790	-6.6065820	-5.1417060
N	1.4521150	-0.9227280	-1.1400970
N	0.9101600	-1.9056760	-1.5229160
N	0.0059090	-2.7985750	-1.4369230

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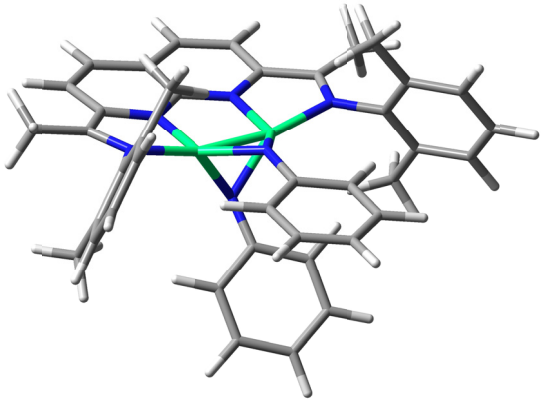

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –4892.57829958 Hartrees
Gibbs Free Energy (298.15 K): – 4891.989757 Hartrees

Ni	1.1058060	0.4884460	-0.0369120
Ni	-1.0675660	0.5093420	-0.0886400
N	3.0086090	0.7351880	-0.3576340
N	-2.9666680	0.8082180	-0.4245080
N	1.1835740	2.3634310	0.1090160
N	-1.0996510	2.3914960	0.0504030
N	0.0223710	-0.8453550	-0.7390280
N	-0.0309020	0.2489280	1.4537760
C	3.4555600	2.0006080	-0.1884610
C	-3.3766650	2.0895800	-0.2868720
C	2.4178340	2.9636610	0.0862670
C	2.5116730	4.3672800	0.2554900
H	3.4919610	4.8523570	0.2722310
C	1.3528580	5.1375820	0.3846370
H	1.4265830	6.2233580	0.5030070
C	0.0642560	4.5261770	0.3197690
C	0.0485850	3.0990570	0.1842690
C	-1.2090050	5.1715920	0.3301110
H	-1.2593960	6.2591120	0.4444550
C	-2.3808730	4.4296990	0.1590000
H	-3.3497420	4.9374240	0.1404360
C	-2.3163010	3.0243160	-0.0058930
C	3.9383040	-0.3148940	-0.6397050
C	4.7869160	-0.8388900	0.3717480
C	5.6407270	-1.9087860	0.0384510
H	6.2910660	-2.3248180	0.8165160
C	5.6674800	-2.4424470	-1.2549880
H	6.3401510	-3.2726560	-1.4934250
C	4.8186280	-1.9176740	-2.2409130
H	4.8259110	-2.3383830	-3.2525320
C	3.9375020	-0.8617340	-1.9538280
C	-3.9275680	-0.2267860	-0.6494140
C	-4.7656660	-0.6810590	0.4053520

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C	-5.6493230	-1.7456070	0.1412960
H	-6.2925270	-2.1084770	0.9511270
C	-5.7153020	-2.3401590	-1.1247950
H	-6.4104930	-3.1655910	-1.3089080
C	-4.8793290	-1.8809610	-2.1529370
H	-4.9208690	-2.3469380	-3.1437820
C	-3.9698680	-0.8310500	-1.9362600
C	0.0183950	-2.2117840	-0.7180640
C	-1.2019980	-2.9518290	-0.7957780
C	-1.1900910	-4.3468120	-0.8676540
H	-2.1411550	-4.8869440	-0.9318470
C	0.0233300	-5.0573170	-0.8483200
C	1.2346010	-4.3457990	-0.7498110
H	2.1868500	-4.8866720	-0.7202190
C	1.2403020	-2.9525480	-0.6786100
C	-0.0813530	-0.9231200	2.1771310
C	1.0412910	-1.3157590	2.9694620
C	0.9567860	-2.3886750	3.8588400
H	1.8340710	-2.6603890	4.4567230
C	-0.2392750	-3.1182120	3.9955170
C	-1.3503850	-2.7598160	3.2138050
H	-2.2845140	-3.3263100	3.2971890
C	-1.2770970	-1.6921840	2.3143640
C	4.9012760	2.4023290	-0.3154790
H	5.4504420	1.7006870	-0.9617070
H	5.4082550	2.4125320	0.6671790
H	4.9887880	3.4143090	-0.7419540
C	-4.8040990	2.5430010	-0.4508050
H	-5.4081570	1.7788670	-0.9617300
H	-4.8477360	3.4744490	-1.0396160
H	-5.2801510	2.7526440	0.5247820
C	4.7923450	-0.2843490	1.7795760
H	3.8410980	0.2108130	2.0296210
C	2.9886250	-0.3299320	-3.0018400
H	3.1597730	0.7416090	-3.2073260
C	-4.7241670	-0.0512740	1.7810410
H	-3.7004900	0.2322200	2.0751910
C	-3.0436780	-0.3598720	-3.0329720
H	-1.9905300	-0.4264900	-2.7048200
H	-5.1201890	-0.7466010	2.5383820
H	-5.3414270	0.8648260	1.8292200
H	-3.1693350	-0.9685550	-3.9422080
H	-3.2249090	0.6970070	-3.2976860
H	3.0958390	-0.8842330	-3.9475110
H	1.9440720	-0.4214460	-2.6526060
H	5.5978660	0.4611300	1.9188810
H	4.9701270	-1.0870810	2.5138220
H	-2.1480090	-2.4033490	-0.8119880
H	0.0261840	-6.1507770	-0.8998490
H	2.1818620	-2.4021240	-0.5996040
H	1.9649660	-0.7365420	2.8795360
H	-0.3004480	-3.9568020	4.6961390
H	-2.1392060	-1.4168860	1.6998050

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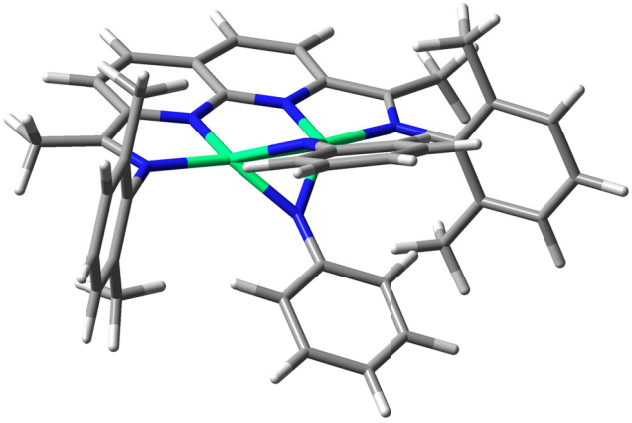

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy: – 4892.56156792 Hartrees
Gibbs Free Energy (298.15 K): – 4891.973713 Hartrees

Ni	-1.1206390	0.6317380	-0.0000320
Ni	1.1206180	0.6317260	-0.0000520
N	-3.0291450	0.8645590	0.0000990
N	3.0291190	0.8645290	0.0000160
N	-1.1426520	2.4807110	-0.0000510
N	1.1426500	2.4807020	-0.0000820
N	-0.0000060	-0.6082030	0.8962560
N	-0.0000250	-0.6080750	-0.8965230
C	-3.4457930	2.1501330	0.0000730
C	3.4457820	2.1501000	-0.0000130
C	-2.3804770	3.1099600	-0.0000220
C	-2.4445370	4.5226590	-0.0000680
H	-3.4180220	5.0215330	-0.0000530
C	-1.2775880	5.2871950	-0.0001330
H	-1.3338830	6.3802150	-0.0001640
C	0.0000080	4.6521550	-0.0001440
C	0.0000020	3.2198760	-0.0001000
C	1.2776100	5.2871850	-0.0001820
H	1.3339130	6.3802040	-0.0002240
C	2.4445510	4.5226400	-0.0001540
H	3.4180400	5.0215070	-0.0001930
C	2.3804820	3.1099410	-0.0000890
C	-4.0073870	-0.1762850	0.0002120
C	-4.4668390	-0.6986020	-1.2381720
C	-5.3960930	-1.7553310	-1.2126180
H	-5.7559570	-2.1663330	-2.1628400
C	-5.8607500	-2.2826450	0.0004640
H	-6.5805940	-3.1074980	0.0005620
C	-5.3957490	-1.7553430	1.2134220
H	-5.7553470	-2.1663520	2.1637420
C	-4.4664860	-0.6986190	1.2387240
C	4.0073930	-0.1762870	0.0001700
C	4.4668060	-0.6986840	-1.2381940

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C	5.3960900	-1.7553850	-1.2126000
H	5.7559220	-2.1664510	-2.1628070
C	5.8608180	-2.2825910	0.0005020
H	6.5806850	-3.1074240	0.0006310
C	5.3958600	-1.7552070	1.2134400
H	5.7555140	-2.1661310	2.1637760
C	4.4665660	-0.6985080	1.2387020
C	-0.0000060	-1.8931270	1.4236000
C	1.2216950	-2.5515420	1.7199340
C	1.2145560	-3.8073840	2.3366500
H	2.1659440	-4.2996410	2.5648940
C	-0.0000030	-4.4396960	2.6542980
C	-1.2145610	-3.8074760	2.3364620
H	-2.1659470	-4.2998070	2.5645590
C	-1.2217030	-2.5516340	1.7197490
C	-0.0000220	-1.8929270	-1.4240390
C	-1.2217200	-2.5513140	-1.7204490
C	-1.2145780	-3.8070820	-2.3373130
H	-2.1659650	-4.2993200	-2.5656070
C	-0.0000180	-4.4393500	-2.6550460
C	1.2145380	-3.8071590	-2.3371440
H	2.1659240	-4.2994570	-2.5653080
C	1.2216760	-2.5513900	-1.7202810
C	-4.9033190	2.5293870	0.0001420
H	-5.4240910	2.1230240	0.8848630
H	-5.4241120	2.1232660	-0.8846700
H	-5.0325670	3.6212930	0.0002730
C	4.9033320	2.5292650	-0.0000210
H	5.0326370	3.6211540	0.0007730
H	5.4239320	2.1236810	-0.8852040
H	5.4242460	2.1223320	0.8843370
C	-3.9672250	-0.1223040	-2.5444240
H	-2.8677240	-0.0246330	-2.5388720
C	-3.9664590	-0.1223520	2.5448290
H	-4.3691960	0.8907180	2.7287760
C	3.9671130	-0.1225010	-2.5444670
H	2.8676010	-0.0249560	-2.5389090
C	3.9665770	-0.1221600	2.5447870
H	2.8670230	-0.0250600	2.5391360
H	4.2615540	-0.7578780	-3.3947640
H	4.3702120	0.8904010	-2.7285620
H	4.2612220	-0.7571860	3.3952740
H	4.3692360	0.8909630	2.7286190
H	-4.2609960	-0.7574810	3.3952770
H	-2.8669130	-0.0251660	2.5391120
H	-4.3704470	0.8905580	-2.7284720
H	-4.2615990	-0.7576780	-3.3947460
H	2.1628800	-2.0580130	1.4620290
H	-0.0000030	-5.4215140	3.1385360
H	-2.1628860	-2.0581720	1.4617110
H	-2.1629050	-2.0578210	-1.4624780
H	-0.0000160	-5.4211090	-3.1394020
H	2.1628560	-2.0579550	-1.4621860

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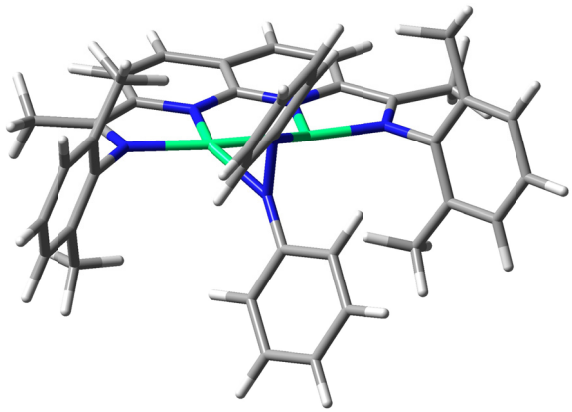

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: – 4892.57068902 Hartrees
Gibbs Free Energy (298.15 K): – 4891.981767 Hartrees

Ni	-1.1248290	0.6441090	0.0214700
Ni	1.1246700	0.6442220	-0.0213740
N	-3.0245890	0.8548120	0.0755050
N	3.0243990	0.8550180	-0.0752170
N	-1.1413850	2.4658590	0.0310270
N	1.1411560	2.4659630	-0.0310120
N	0.0806970	-0.7738870	0.7127240
N	-0.0807540	-0.7738010	-0.7127850
C	-3.4488120	2.1372800	0.0973650
C	3.4485750	2.1375150	-0.0972110
C	-2.3803320	3.0943090	0.0758950
C	-2.4453690	4.5066250	0.0811850
H	-3.4223080	4.9986180	0.1091650
C	-1.2795670	5.2729440	0.0430170
H	-1.3363790	6.3659040	0.0444730
C	-0.0002180	4.6381970	0.0001020
C	-0.0001510	3.2091600	0.0000460
C	1.2790940	5.2730480	-0.0427520
H	1.3358160	6.3660130	-0.0441010
C	2.4449540	4.5068430	-0.0809770
H	3.4218340	4.9989560	-0.1088480
C	2.3800700	3.0945050	-0.0758000
C	-3.9486300	-0.2322780	0.0706070
C	-4.6062790	-0.6161900	-1.1286180
C	-5.4562000	-1.7373910	-1.0938310
H	-5.9651760	-2.0432340	-2.0152290
C	-5.6510510	-2.4648030	0.0882650
H	-6.3140050	-3.3361790	0.0932200
C	-4.9825180	-2.0816600	1.2597640
H	-5.1220340	-2.6527820	2.1845890
C	-4.1210940	-0.9706850	1.2723880
C	3.9486020	-0.2319300	-0.0704480
C	4.1216750	-0.9697670	-1.2724860

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C	4.9833310	-2.0805690	-1.2600160
H	5.1233400	-2.6512490	-2.1850390
C	5.6514660	-2.4641000	-0.0884170
H	6.3146030	-3.3353370	-0.0935010
C	5.4559880	-1.7372660	1.0939340
H	5.9646560	-2.0434180	2.0153990
C	4.6058350	-0.6162510	1.1288710
C	-0.0432180	-1.9283470	1.5203540
C	0.7363880	-1.9728400	2.6980720
C	0.5995500	-3.0387600	3.5948140
H	1.2151380	-3.0644170	4.5001540
C	-0.3188130	-4.0706970	3.3362220
C	-1.1052660	-4.0201930	2.1720670
H	-1.8315230	-4.8137120	1.9666320
C	-0.9785050	-2.9607180	1.2651600
C	0.0434260	-1.9281120	-1.5205870
C	-0.7365170	-1.9728060	-2.6980800
C	-0.5995140	-3.0385700	-3.5949750
H	-1.2153680	-3.0643870	-4.5001310
C	0.3193520	-4.0701600	-3.3367660
C	1.1061230	-4.0194580	-2.1728350
H	1.8327610	-4.8127050	-1.9676940
C	0.9792070	-2.9601300	-1.2657800
C	-4.8980720	2.5443520	0.1507210
H	-5.5334720	1.7025530	0.4641810
H	-5.2616660	2.8923970	-0.8342620
H	-5.0442390	3.3748350	0.8617070
C	4.8978990	2.5443720	-0.1503730
H	5.5326300	1.7036550	-0.4681250
H	5.2628570	2.8878620	0.8357250
H	5.0435910	3.3778540	-0.8578880
C	-4.3909800	0.1517970	-2.4132970
H	-3.3269390	0.4096920	-2.5529700
C	-3.3802650	-0.5539680	2.5202400
H	-3.8192400	0.3546000	2.9723050
C	3.3812110	-0.5526440	-2.5204210
H	2.3364160	-0.3043270	-2.2650760
C	4.3897700	0.1511040	2.4137950
H	3.3255070	0.4081520	2.5533660
H	3.3892110	-1.3509100	-3.2782460
H	3.8199330	0.3564220	-2.9717350
H	4.7281500	-0.4356870	3.2828400
H	4.9478430	1.1054210	2.4247300
H	-3.3875260	-1.3527080	3.2775730
H	-2.3357180	-0.3049870	2.2645450
H	-4.9498170	1.1056760	-2.4238130
H	-4.7290590	-0.4349520	-3.2824890
H	1.4453330	-1.1606680	2.8861890
H	-0.4246030	-4.9046220	4.0372170
H	-1.6079160	-2.9198930	0.3729160
H	-1.4458730	-1.1609100	-2.8858530
H	0.4252830	-4.9039690	-4.0378760
H	1.6088720	-2.9191420	-0.3737190

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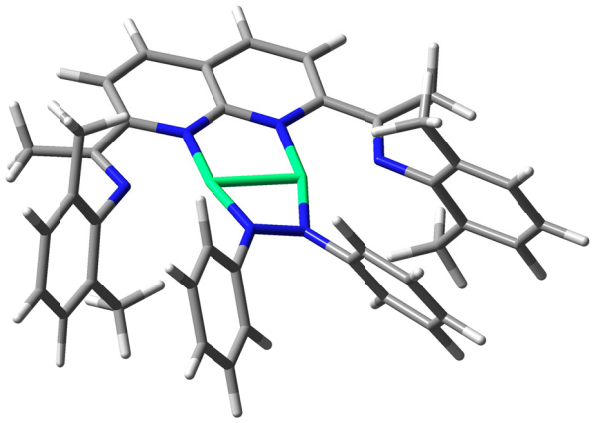

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: – 4892.59061696 Hartrees
Gibbs Free Energy (298.15 K): – 4891.995589 Hartrees

Ni	-1.1315060	0.6856050	0.0652260
Ni	1.1315500	0.6856000	-0.0648270
N	-3.1058010	0.9314550	-0.0331540
N	3.1058650	0.9314700	0.0336190
N	-1.1404980	2.5028810	-0.0000420
N	1.1405310	2.5028800	-0.0000540
N	-0.6731360	-1.0432590	0.1240930
N	0.6731850	-1.0432220	-0.1238750
C	-3.4667910	2.2236310	-0.0962270
C	3.4668340	2.2236750	0.0962820
C	-2.3722350	3.1504580	-0.0464670
C	-2.4375490	4.5550170	-0.0659430
H	-3.4144970	5.0460400	-0.1015290
C	-1.2693700	5.3216100	-0.0332800
H	-1.3194840	6.4146500	-0.0381980
C	0.0000220	4.6797270	-0.0001830
C	0.0000160	3.2396780	-0.0000620
C	1.2694110	5.3216190	0.0328510
H	1.3195220	6.4146590	0.0376140
C	2.4375860	4.5550260	0.0656770
H	3.4145420	5.0460370	0.1012480
C	2.3722620	3.1504660	0.0464230
C	-4.1260940	-0.0655100	-0.0999310
C	-4.2721000	-0.7978890	-1.3058860
C	-5.2709390	-1.7839310	-1.3780440
H	-5.3869950	-2.3533660	-2.3069720
C	-6.1064270	-2.0460200	-0.2834890
H	-6.8816080	-2.8159720	-0.3552580
C	-5.9349110	-1.3307210	0.9098530
H	-6.5744220	-1.5451540	1.7741990
C	-4.9437720	-0.3387840	1.0286930
C	4.1261160	-0.0655230	0.1002640
C	4.9438780	-0.3387090	-1.0283340

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C	5.9349440	-1.3307140	-0.9095180
H	6.5745110	-1.5450960	-1.7738360
C	6.1063310	-2.0461620	0.2837540
H	6.8814780	-2.8161510	0.3554860
C	5.2707550	-1.7841820	1.3782640
H	5.3867060	-2.3537510	2.3071230
C	4.2719560	-0.7980980	1.3061340
C	-1.4236380	-2.2487280	0.0366430
C	-2.3483460	-2.5411800	1.0594910
C	-3.1093530	-3.7158640	1.0081320
H	-3.8220290	-3.9312280	1.8102000
C	-2.9601090	-4.6108150	-0.0634530
C	-2.0469770	-4.3161160	-1.0901060
H	-1.9300130	-5.0034730	-1.9347290
C	-1.2810850	-3.1449740	-1.0474980
C	1.4236510	-2.2487590	-0.0368170
C	2.3482980	-2.5410010	-1.0597670
C	3.1092720	-3.7157260	-1.0086870
H	3.8219070	-3.9309420	-1.8108310
C	2.9600460	-4.6109020	0.0627100
C	2.0469650	-4.3164070	1.0894670
H	1.9300190	-5.0039440	1.9339450
C	1.2811130	-3.1452300	1.0471400
C	-4.8824430	2.7158540	-0.2786730
H	-5.6002380	1.8842650	-0.2876240
H	-4.9800480	3.2669780	-1.2308400
H	-5.1663570	3.4140130	0.5283150
C	4.8825400	2.7159930	0.2781140
H	5.6000520	1.8841850	0.2896600
H	4.9798200	3.2697620	1.2287600
H	5.1671460	3.4118030	-0.5306850
C	-3.3589790	-0.4988720	-2.4707590
H	-2.3416460	-0.2937180	-2.0926270
C	-4.7486330	0.4086000	2.3293540
H	-5.1139190	1.4503880	2.2732480
C	4.7487720	0.4086920	-2.3289790
H	3.6807520	0.4670610	-2.6026990
C	3.3587040	-0.4992180	2.4709360
H	2.3414660	-0.2938290	2.0926850
H	5.2937810	-0.0853830	-3.1495080
H	5.1135240	1.4506480	-2.2727100
H	3.3259330	-1.3384800	3.1830400
H	3.6778580	0.4053080	3.0216710
H	-5.2931970	-0.0857890	3.1499920
H	-3.6805700	0.4674530	2.6027680
H	-3.6780750	0.4058380	-3.0212280
H	-3.3264320	-1.3379690	-3.1830630
H	-2.4445190	-1.8429980	1.8962110
H	-3.5532370	-5.5300320	-0.1011230
H	-0.5722130	-2.9139540	-1.8467320
H	2.4444720	-1.8426410	-1.8963360
H	3.5531570	-5.5301390	0.1001510
H	0.5722850	-2.9143370	1.8464490

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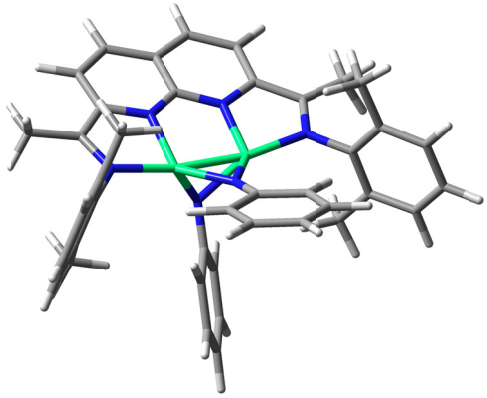

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: – 4892.56655345 Hartrees
Gibbs Free Energy (298.15 K): – 4891.9835 Hartrees

Ni	1.0818440	0.3973800	-0.0577150
Ni	-1.1157420	0.4064160	-0.0022170
N	2.9963280	0.6342870	-0.2954770
N	-3.0085250	0.5863070	-0.2480530
N	1.0993610	2.2633280	-0.4640610
N	-1.1785130	2.2623090	-0.3173740
N	-0.0388850	-1.0015190	-0.5280510
N	0.0823250	0.5301940	1.5071980
C	3.3972990	1.9170240	-0.4710180
C	-3.4579560	1.8614670	-0.3221610
C	2.3307630	2.8823370	-0.4824690
C	2.3941210	4.3006990	-0.5023070
H	3.3650630	4.8041370	-0.5176340
C	1.2248600	5.0611220	-0.4947670
H	1.2802330	6.1540330	-0.5221380
C	-0.0534820	4.4245940	-0.4366910
C	-0.0406210	2.9935370	-0.3892280
C	-1.3393770	5.0437260	-0.4305850
H	-1.4084370	6.1358840	-0.4643700
C	-2.5030560	4.2725170	-0.3910450
H	-3.4803400	4.7632200	-0.3992210
C	-2.4164430	2.8573880	-0.3396420
C	3.9860920	-0.3997140	-0.3310820
C	4.5935800	-0.8292490	0.8779210
C	5.5358040	-1.8727900	0.8153550
H	6.0102990	-2.2105450	1.7437520
C	5.8697550	-2.4786070	-0.4034190
H	6.6031850	-3.2909720	-0.4306190
C	5.2613000	-2.0400870	-1.5875210
H	5.5193740	-2.5092100	-2.5438070
C	4.3149740	-0.9981220	-1.5771750
C	-3.9694460	-0.4756920	-0.2916050
C	-4.4375260	-1.0462720	0.9192960

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C	-5.3630180	-2.1034920	0.8426960
H	-5.7288950	-2.5525260	1.7728740
C	-5.8140130	-2.5842020	-0.3937910
H	-6.5343440	-3.4076690	-0.4332500
C	-5.3316120	-2.0150150	-1.5805860
H	-5.6718950	-2.3959910	-2.5501490
C	-4.4010800	-0.9594990	-1.5555560
C	-0.0627000	-2.2196630	-1.1293450
C	-1.2958450	-2.8703070	-1.4519770
C	-1.3012830	-4.1320840	-2.0476750
H	-2.2600050	-4.6086290	-2.2804990
C	-0.0951060	-4.7953650	-2.3464220
C	1.1280030	-4.1742490	-2.0258510
H	2.0737330	-4.6837430	-2.2415700
C	1.1542080	-2.9153590	-1.4248170
C	0.1226810	-0.3856740	2.5302550
C	0.7992740	-1.6461530	2.4837200
C	0.8041070	-2.4950420	3.5939550
H	1.3225050	-3.4580010	3.5273860
C	0.1549040	-2.1297830	4.7876320
C	-0.5116200	-0.8915150	4.8562100
H	-1.0161620	-0.5915720	5.7815240
C	-0.5330330	-0.0335210	3.7549420
C	4.8452580	2.2923880	-0.6461430
H	5.4637510	1.9131610	0.1855250
H	4.9725250	3.3830790	-0.7051920
H	5.2603730	1.8531790	-1.5708780
C	-4.9231810	2.2031330	-0.3733650
H	-5.4568240	1.8041100	0.5069690
H	-5.4094170	1.7619340	-1.2609590
H	-5.0770480	3.2914640	-0.4054850
C	4.2345460	-0.1837610	2.1967630
H	3.1778800	-0.3692690	2.4602600
C	3.6532150	-0.5360690	-2.8564970
H	3.8432870	0.5323490	-3.0622180
C	-3.9495680	-0.5279110	2.2511550
H	-2.8465590	-0.5249990	2.3011590
C	-3.8439020	-0.3825440	-2.8375930
H	-2.7480050	-0.5167470	-2.8837130
H	-4.3312690	-1.1462670	3.0786170
H	-4.2728240	0.5138980	2.4306480
H	-4.2879950	-0.8787010	-3.7149800
H	-4.0297620	0.7019430	-2.9294270
H	4.0191960	-1.1171070	-3.7177860
H	2.5561270	-0.6537040	-2.8031000
H	4.3617990	0.9125570	2.1702550
H	4.8624080	-0.5811660	3.0100580
H	-2.2320990	-2.3623350	-1.2054680
H	-0.1080020	-5.7848390	-2.8140390
H	2.1037900	-2.4397140	-1.1601270
H	1.2897890	-1.9390380	1.5519190
H	0.1702530	-2.7991670	5.6534270
H	-1.0364240	0.9371730	3.8036600

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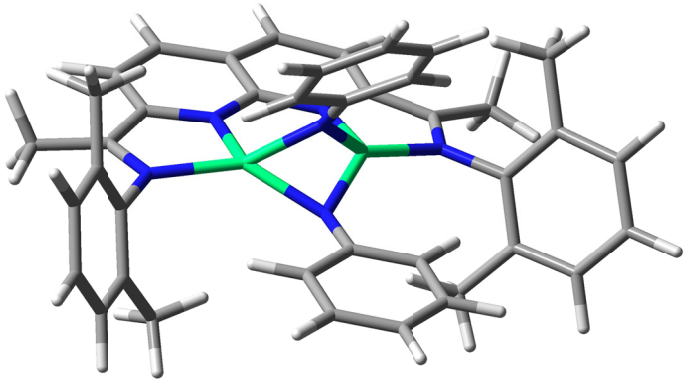

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 1
Electronic Energy: – 4892.55222118 Hartrees
Gibbs Free Energy (298.15 K): – 4891.967319 Hartrees

Ni	1.2874080	0.4595140	-0.0523250
Ni	-1.2627740	0.4808470	-0.0895000
N	3.1481210	0.8127380	-0.3079810
N	-3.1202680	0.8589490	-0.3349080
N	1.1829800	2.3451600	0.0579540
N	-1.1362240	2.3628200	0.0411370
N	0.0032280	-0.8422080	-0.7078030
N	-0.0080590	-0.3245510	0.9961100
C	3.5070030	2.1107870	-0.2048380
C	-3.4628080	2.1605980	-0.2255710
C	2.4067400	3.0010550	0.0331470
C	2.4743510	4.4024920	0.1965580
H	3.4488090	4.8996530	0.1957510
C	1.3065030	5.1442990	0.3470130
H	1.3477870	6.2312860	0.4703980
C	0.0376690	4.4991350	0.2971080
C	0.0280350	3.0639440	0.1511490
C	-1.2220750	5.1623050	0.3392970
H	-1.2486390	6.2495350	0.4645740
C	-2.3995910	4.4372630	0.1820900
H	-3.3670580	4.9479080	0.1788090
C	-2.3507710	3.0356100	0.0147980
C	4.1221950	-0.2096030	-0.5058470
C	4.9581800	-0.6304170	0.5653730
C	5.8527180	-1.6933680	0.3382860
H	6.4956080	-2.0257890	1.1615700
C	5.9285760	-2.3274160	-0.9086900
H	6.6310560	-3.1525180	-1.0644770
C	5.0912050	-1.9076750	-1.9525350
H	5.1394270	-2.4040200	-2.9284510
C	4.1761890	-0.8555690	-1.7730020
C	-4.1059360	-0.1534720	-0.5223200
C	-4.9231630	-0.5746580	0.5634770
C	-5.8284490	-1.6309970	0.3484310

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H	-6.4574220	-1.9635930	1.1823290
C	-5.9326980	-2.2580030	-0.9001870
H	-6.6431910	-3.0779770	-1.0463280
C	-5.1140820	-1.8373700	-1.9584890
H	-5.1856150	-2.3276240	-2.9360810
C	-4.1893440	-0.7914350	-1.7918430
C	-0.0003220	-2.2301990	-0.8595120
C	-1.2203730	-2.9381940	-1.0108050
C	-1.2136680	-4.3162730	-1.2557930
H	-2.1647430	-4.8458190	-1.3765190
C	0.0009730	-5.0184200	-1.3419620
C	1.2149810	-4.3283450	-1.1776710
H	2.1664760	-4.8673080	-1.2381690
C	1.2196370	-2.9506320	-0.9338300
C	-0.0535810	-1.3245790	1.9611020
C	1.1398890	-1.7884650	2.5691210
C	1.0854400	-2.7498460	3.5834380
H	2.0132200	-3.0962080	4.0508720
C	-0.1510110	-3.2760840	3.9982590
C	-1.3376510	-2.8357470	3.3856920
H	-2.3020700	-3.2504230	3.6972930
C	-1.2950100	-1.8723920	2.3725590
C	4.9186100	2.6154950	-0.3671270
H	5.5881730	1.8093370	-0.7013740
H	5.3191570	3.0186860	0.5813760
H	4.9628590	3.4312080	-1.1093650
C	-4.8690290	2.6825140	-0.3796280
H	-5.5527250	1.8817530	-0.6978420
H	-4.9101810	3.4903180	-1.1308520
H	-5.2539260	3.1022000	0.5681150
C	4.8926650	0.0376900	1.9210580
H	3.8550760	0.2837000	2.2039550
C	3.2530940	-0.4171330	-2.8851750
H	3.4930960	0.6010200	-3.2408950
C	-4.8250940	0.0870650	1.9205690
H	-3.7769030	0.2874680	2.2010880
C	-3.2882080	-0.3500490	-2.9209470
H	-2.2375080	-0.3238130	-2.5791670
H	-5.2800690	-0.5472780	2.6982730
H	-5.3505150	1.0593400	1.9435730
H	-3.3686110	-1.0302380	-3.7833990
H	-3.5307390	0.6716980	-3.2643790
H	3.3105640	-1.1038850	-3.7441960
H	2.2109410	-0.3832860	-2.5191690
H	5.4585370	0.9873180	1.9397110
H	5.3241530	-0.6128400	2.6988500
H	-2.1626110	-2.3841740	-0.9491380
H	0.0017050	-6.0964130	-1.5332810
H	2.1610440	-2.4048140	-0.8136690
H	2.0924380	-1.3692050	2.2302620
H	-0.1889230	-4.0298180	4.7911650
H	-2.2075960	-1.5193050	1.8817760

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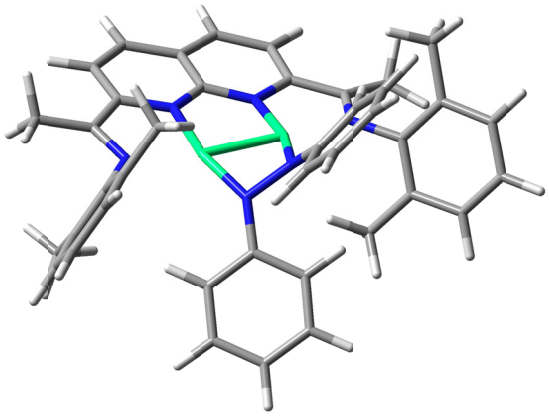

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: – 4892.57464079 Hartrees
Gibbs Free Energy (298.15 K): – 4891.985531 Hartrees

Ni	-1.1329050	0.5903970	0.0338640
Ni	1.1088150	0.6026510	-0.0785620
N	-3.0653220	0.8516890	0.2640960
N	3.0372150	0.8443090	-0.3510620
N	-1.1225880	2.4279470	0.1898410
N	1.1128890	2.4344940	-0.2414300
N	0.6004070	-1.0843260	0.3597430
N	-0.6606950	-1.1554010	-0.2381900
C	-3.4254540	2.1298800	0.4816700
C	3.4085350	2.1207600	-0.5585220
C	-2.3382000	3.0647310	0.3757070
C	-2.4064020	4.4737880	0.4118190
H	-3.3740530	4.9610510	0.5617090
C	-1.2551290	5.2422370	0.2247440
H	-1.3077990	6.3352250	0.2392330
C	-0.0015530	4.6028270	-0.0049120
C	-0.0045520	3.1694320	-0.0179970
C	1.2542670	5.2409150	-0.2253760
H	1.3099250	6.3338750	-0.2187920
C	2.4041360	4.4742930	-0.4334980
H	3.3724500	4.9625190	-0.5759190
C	2.3300010	3.0655490	-0.4255850
C	-4.0508530	-0.1803650	0.3374940
C	-5.0060170	-0.3415390	-0.7036310
C	-5.9175700	-1.4106150	-0.6126630
H	-6.6527510	-1.5459980	-1.4142770
C	-5.8864400	-2.3023940	0.4676360
H	-6.5994590	-3.1316940	0.5157200
C	-4.9282840	-2.1375130	1.4771180
H	-4.8922350	-2.8375170	2.3194280
C	-3.9984680	-1.0842930	1.4314940
C	3.9973360	-0.2080420	-0.4656670
C	3.8743650	-1.1080610	-1.5589260

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C	4.7733850	-2.1843770	-1.6490270
H	4.6824820	-2.8791540	-2.4916450
C	5.7718030	-2.3767530	-0.6838660
H	6.4592630	-3.2248970	-0.7644140
C	5.8768950	-1.4860880	0.3914630
H	6.6465100	-1.6403420	1.1565500
C	4.9999610	-0.3926470	0.5247860
C	0.9291680	-1.9672920	1.3928310
C	2.1032980	-1.7017180	2.1412030
C	2.4934010	-2.5515670	3.1776820
H	3.4057500	-2.3280410	3.7408770
C	1.7170640	-3.6770900	3.5099570
C	0.5348510	-3.9275610	2.7910790
H	-0.0884450	-4.7907580	3.0494950
C	0.1313330	-3.0881080	1.7465200
C	-0.9018810	-2.1559720	-1.1873880
C	-2.1579530	-2.1908510	-1.8439970
C	-2.4384350	-3.1836390	-2.7860470
H	-3.4190780	-3.1928440	-3.2739620
C	-1.4804510	-4.1617380	-3.1093320
C	-0.2278530	-4.1225820	-2.4726220
H	0.5348900	-4.8694590	-2.7195740
C	0.0701600	-3.1355680	-1.5264810
C	-4.8131120	2.5825060	0.8601880
H	-5.4780770	1.7236370	1.0290810
H	-5.2619660	3.2139480	0.0719910
H	-4.7842860	3.1888350	1.7820620
C	4.7940810	2.5640640	-0.9534420
H	5.4349640	1.7008770	-1.1834560
H	5.2786020	3.1446280	-0.1472120
H	4.7523500	3.2171010	-1.8420420
C	-5.0240420	0.5833630	-1.9014270
H	-4.0030900	0.7855060	-2.2688000
C	-2.9650830	-0.8949250	2.5148580
H	-3.2268620	-0.0591070	3.1897330
C	2.8081370	-0.8845400	-2.6042200
H	1.8609760	-0.5922940	-2.1158430
C	5.1321340	0.5433270	1.7072540
H	4.1517020	0.9125530	2.0519970
H	2.6336280	-1.7897170	-3.2055690
H	3.0766720	-0.0609980	-3.2916210
H	5.6291730	0.0366770	2.5502730
H	5.7398320	1.4339270	1.4617880
H	-2.8471770	-1.8030820	3.1257350
H	-1.9935600	-0.6418920	2.0550990
H	-5.4782910	1.5634350	-1.6675240
H	-5.6086310	0.1420360	-2.7244470
H	2.6791550	-0.8078680	1.8917560
H	2.0215630	-4.3409240	4.3249970
H	-0.7943420	-3.2878580	1.2027280
H	-2.9058170	-1.4367440	-1.5920440
H	-1.7041980	-4.9364420	-3.8492580
H	1.0519630	-3.1055450	-1.0485490

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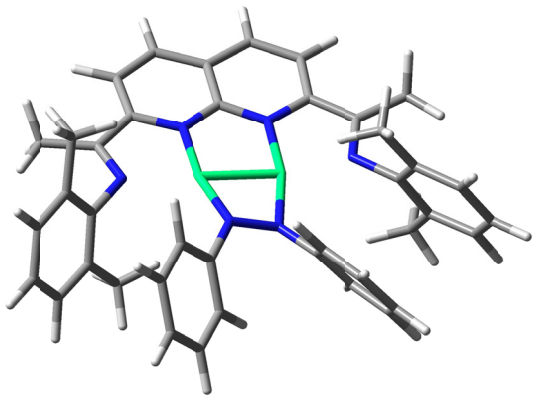

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: – 4892.57170575 Hartrees
Gibbs Free Energy (298.15 K): – 4891.980935 Hartrees

Ni	-1.1061010	0.6811670	0.0893090
Ni	1.1061370	0.6811600	-0.0893820
N	-3.0810590	0.9347910	-0.0150790
N	3.0811300	0.9347980	0.0154680
N	-1.1357260	2.5228790	0.0145460
N	1.1357950	2.5229020	-0.0153230
N	-0.6651760	-1.0859210	0.1966040
N	0.6651500	-1.0859110	-0.1966640
C	-3.4551320	2.2238220	-0.0847700
C	3.4551870	2.2238640	0.0848730
C	-2.3638600	3.1584120	-0.0356490
C	-2.4389190	4.5650440	-0.0596970
H	-3.4175580	5.0517960	-0.0957860
C	-1.2721710	5.3350080	-0.0296500
H	-1.3265110	6.4280010	-0.0364380
C	0.0000200	4.6963980	-0.0002150
C	0.0000290	3.2599240	-0.0002820
C	1.2722110	5.3350250	0.0293700
H	1.3265440	6.4280150	0.0362670
C	2.4389520	4.5650600	0.0595110
H	3.4175750	5.0518280	0.0958440
C	2.3639270	3.1584300	0.0353640
C	-4.1013870	-0.0634100	-0.1020910
C	-4.2257390	-0.7896810	-1.3133010
C	-5.2309440	-1.7669740	-1.4094090
H	-5.3306130	-2.3336770	-2.3416980
C	-6.0907050	-2.0259960	-0.3334050
H	-6.8695140	-2.7901880	-0.4238330
C	-5.9383400	-1.3170270	0.8661060
H	-6.5958380	-1.5310560	1.7168270
C	-4.9423680	-0.3335030	1.0093580
C	4.1013770	-0.0634430	0.1025730
C	4.9426670	-0.3334170	-1.0086910

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C	5.9385600	-1.3170000	-0.8652990
H	6.5962850	-1.5309290	-1.7158690
C	6.0905720	-2.0261590	0.3341440
H	6.8693280	-2.7903930	0.4246660
C	5.2305050	-1.7672850	1.4099360
H	5.3298860	-2.3341350	2.3421660
C	4.2253590	-0.7899450	1.3136870
C	-1.4386220	-2.2606690	0.0635660
C	-2.3938670	-2.5511280	1.0641680
C	-3.1667540	-3.7155160	0.9934820
H	-3.8983060	-3.9235620	1.7807630
C	-3.0024590	-4.6151070	-0.0732410
C	-2.0574980	-4.3299400	-1.0740200
H	-1.9235330	-5.0203800	-1.9140280
C	-1.2791220	-3.1684520	-1.0132450
C	1.4385950	-2.2606800	-0.0638750
C	2.3939250	-2.5508590	-1.0644790
C	3.1668380	-3.7152430	-0.9940370
H	3.8984490	-3.9230680	-1.7813200
C	3.0024990	-4.6151080	0.0724500
C	2.0574630	-4.3302170	1.0732360
H	1.9234650	-5.0208690	1.9130650
C	1.2790530	-3.1687390	1.0126990
C	-4.8719270	2.7086560	-0.2764340
H	-5.5827960	1.8720310	-0.3105600
H	-4.9621250	3.2781390	-1.2183770
H	-5.1725470	3.3876040	0.5411200
C	4.8719300	2.7087390	0.2768540
H	5.5827860	1.8721130	0.3112930
H	4.9618580	3.2783170	1.2187670
H	5.1728180	3.3875900	-0.5406820
C	-3.2869300	-0.4947720	-2.4586440
H	-2.2721660	-0.3117350	-2.0625320
C	-4.7668830	0.4059160	2.3174650
H	-5.1196250	1.4519270	2.2594770
C	4.7674990	0.4060340	-2.3168200
H	3.7055440	0.4493070	-2.6154620
C	3.2862460	-0.4951880	2.4588170
H	2.2716080	-0.3120110	2.0624430
H	5.3359360	-0.0861070	-3.1223480
H	5.1194910	1.4522730	-2.2585630
H	3.2527610	-1.3299400	3.1758540
H	3.5807670	0.4185000	3.0082440
H	-5.3345290	-0.0866540	3.1232890
H	-3.7047800	0.4498660	2.6154560
H	-3.5815610	0.4190250	-3.0078300
H	-3.2537050	-1.3293950	-3.1758420
H	-2.4964710	-1.8595970	1.9059230
H	-3.6021400	-5.5294450	-0.1236550
H	-0.5441260	-2.9516390	-1.7924470
H	2.4965750	-1.8591160	-1.9060560
H	3.6022070	-5.5294380	0.1226760
H	0.5440130	-2.9521470	1.7919210

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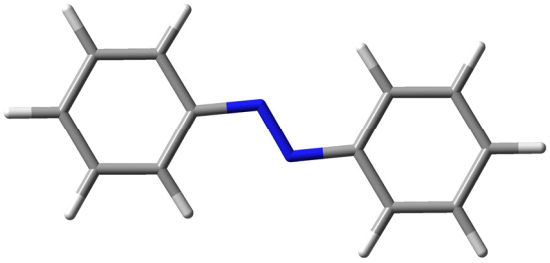

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –572.77189910 Hartrees
Gibbs Free Energy (298.15 K): –572.6256841 Hartrees

C	-3.6828550	-1.3128000	-0.0002940
C	-2.2988110	-1.1252990	-0.0002840
C	-1.7709460	0.1878230	-0.0000160
C	-2.6448630	1.2956590	0.0001430
C	-4.0319220	1.0995480	0.0002620
C	-4.5534580	-0.2042880	0.0000180
H	-4.0944880	-2.3277710	-0.0005940
H	-1.6009030	-1.9667500	-0.0004710
H	-2.2047460	2.2976630	0.0002290
H	-4.7064050	1.9617390	0.0004790
H	-5.6371160	-0.3610700	-0.0000230
C	1.7710750	-0.1882340	0.0003110
C	2.6453270	-1.2957740	0.0003240
C	2.2983300	1.1251090	0.0000080
C	4.0322790	-1.0991350	0.0001270
H	2.2053720	-2.2978600	0.0005990
C	3.6823260	1.3131100	-0.0002790
H	1.6001570	1.9663300	-0.0000830
C	4.5533190	0.2049110	-0.0002140
H	4.7070520	-1.9610980	0.0000690
H	4.0937050	2.3281920	-0.0005180
H	5.6368930	0.3622520	-0.0004160
N	-0.3866680	0.5090320	-0.0002290
N	0.3869050	-0.5098040	0.0002420

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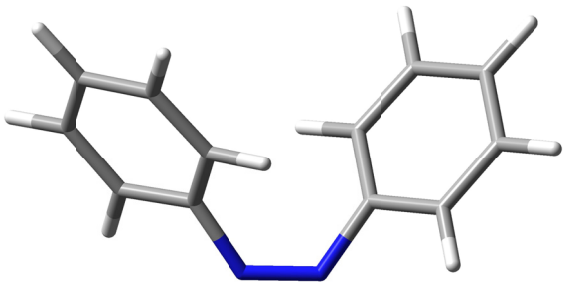

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –572.74987885 Hartrees
Gibbs Free Energy (298.15 K): –572.6034559 Hartrees

C	-2.2021330	-1.2664750	-1.1732570
C	-1.2613140	-0.2374410	-1.0435010
C	-1.4396740	0.7505020	-0.0490110
C	-2.5794320	0.7114830	0.7823620
C	-3.4897320	-0.3468600	0.6739080
C	-3.3070680	-1.3367440	-0.3070210
H	-2.0702450	-2.0219210	-1.9548780
H	-0.4010770	-0.1819960	-1.7161810
H	-2.7253830	1.5162800	1.5096020
H	-4.3575640	-0.3869870	1.3401330
H	-4.0327650	-2.1497330	-0.4090730
C	1.4399240	0.7512350	0.0477000
C	2.5782480	0.7096320	-0.7853560
C	1.2627590	-0.2338760	1.0452010
C	3.4884650	-0.3486700	-0.6750670
H	2.7235340	1.5120870	-1.5153200
C	2.2032850	-1.2629730	1.1763300
H	0.4034270	-0.1759670	1.7188560
C	3.3069950	-1.3358830	0.3087420
H	4.3552610	-0.3908740	-1.3425190
H	2.0722330	-2.0162690	1.9601670
H	4.0326220	-2.1487780	0.4119560
N	-0.6313810	1.9370080	0.0331410
N	0.6310990	1.9373610	-0.0344160

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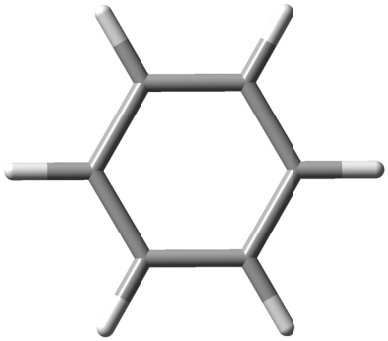

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –232.24708901 Hartrees
Gibbs Free Energy (298.15 K): –232.176951 Hartrees

C	-1.3908940	-0.1957900	0.0000010
C	-0.5257660	-1.3022380	0.0000590
C	0.8649700	-1.1064680	-0.0000310
C	1.3908860	0.1958420	0.0000110
C	0.5258150	1.3022180	0.0000330
C	-0.8650110	1.1064370	-0.0000440
H	-2.4752960	-0.3486330	-0.0000180
H	-0.9357410	-2.3177520	-0.0000200
H	1.5394110	-1.9692810	-0.0001060
H	2.4753080	0.3485340	-0.0000380
H	0.9356560	2.3177840	0.0000550
H	-1.5393340	1.9693440	-0.0000500

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –109.52669311 Hartrees
Gibbs Free Energy (298.15 K): –109.53981 Hartrees

N	0.0000000	0.0000000	0.5587680
N	0.0000000	0.0000000	-0.5587680

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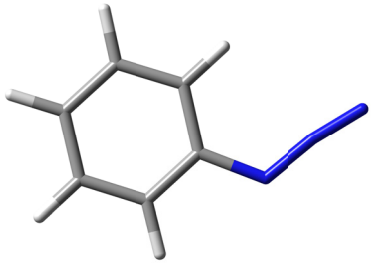

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -395.85954638 Hartrees
Gibbs Free Energy (298.15 K): -395.791068 Hartrees

C	0.1464350	-0.3599290	-0.0001210
C	-0.8867450	-1.3172800	-0.0001290
C	-0.1604020	1.0165440	0.0000370
C	-2.2218000	-0.8951930	-0.0000600
H	-0.6244430	-2.3789100	-0.0003560
C	-1.5010790	1.4231400	0.0000270
H	0.6444630	1.7591270	0.0000550
C	-2.5365350	0.4739790	0.0000250
H	-3.0212970	-1.6428470	-0.0001320
H	-1.7356550	2.4925230	0.0001180
H	-3.5809950	0.7998110	0.0001010
N	1.4734510	-0.8764850	0.0005140
N	2.4311190	-0.0821920	-0.0001320
N	3.4209560	0.5190660	-0.0001610

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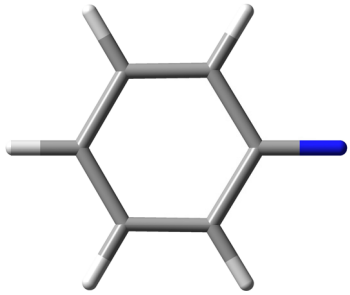

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -286.30615696 Hartrees
Gibbs Free Energy (298.15 K): -286.247434 Hartrees

C	1.0823430	-0.0000120	0.0000100
C	0.3379440	-1.2407910	-0.0000120
C	0.3379610	1.2407820	-0.0000190
C	-1.0524160	-1.2230580	0.0000000
H	0.8992170	-2.1790430	-0.0000250
C	-1.0523980	1.2230700	0.0000070
H	0.8992530	2.1790230	-0.0000390
C	-1.7577870	0.0000090	0.0000080
H	-1.6042000	-2.1688320	-0.0000130
H	-1.6041740	2.1688470	-0.0000010
H	-2.8519330	0.0000210	0.0000220
N	2.4125650	-0.0000020	0.0000130

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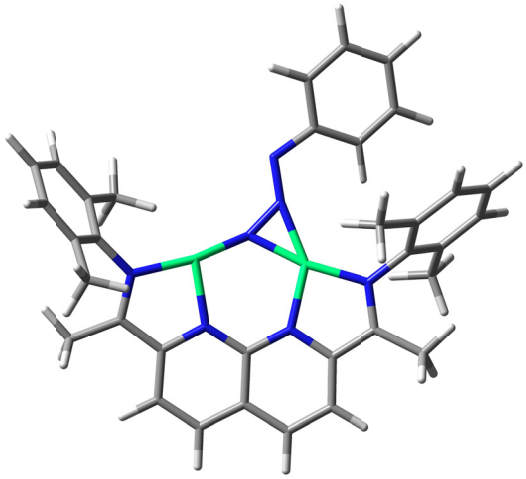

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -4715.65389915 Hartrees
Gibbs Free Energy (298.15 K): - 4715.14524 Hartrees

C	-5.7556480	1.3311260	0.5403860
H	-5.9253660	1.8181930	1.5168650
H	-6.3265260	0.3911890	0.5233920
H	-6.1745650	1.9998350	-0.2335020
C	-4.2881490	1.0627170	0.3227030
C	-3.3005680	2.1091060	0.4105810
C	-3.6369350	3.4658680	0.5872710
H	-4.6835140	3.7495570	0.7234130
C	-2.6392170	4.4261920	0.5571270
H	-2.8727430	5.4901250	0.6647560
C	-1.2882840	4.0377540	0.3555170
C	-0.9722020	2.6239300	0.2383240
C	-0.2460610	4.9941740	0.2399020
H	-0.4899900	6.0580400	0.3227560
C	1.0498450	4.5703690	-0.0013900
H	1.8639710	5.2898040	-0.1158820
C	1.3259030	3.1908780	-0.0753750
C	2.6431390	2.6658620	-0.3204380
C	3.7939260	3.5734200	-0.6755000
H	3.5097890	4.2624160	-1.4893130
H	4.6655540	2.9903640	-1.0047610
H	4.1058030	4.1960930	0.1830640
C	-4.5852690	-1.3065050	-0.1724210
C	-4.4867240	-2.4006610	0.7318790
C	-5.2327560	-3.5610950	0.4663180
H	-5.1628280	-4.4042330	1.1626400
C	-6.0459100	-3.6540790	-0.6717170
H	-6.6176040	-4.5671430	-0.8664500
C	-6.1013040	-2.5841130	-1.5743090
H	-6.7080160	-2.6659820	-2.4834150
C	-5.3734300	-1.3999750	-1.3534410
C	-3.5825940	-2.3070960	1.9371620
H	-2.6266690	-1.8232520	1.6471740

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C	-5.4032500	-0.2875790	-2.3786480
H	-4.4059510	0.1639990	-2.5142320
C	3.9770940	0.6729860	-0.4744620
C	5.0060340	0.7463900	0.5015660
C	6.2233900	0.0903040	0.2338180
H	7.0261730	0.1445920	0.9781850
C	6.4151310	-0.6295890	-0.9529160
H	7.3696930	-1.1308440	-1.1426890
C	5.3703320	-0.7314500	-1.8815790
H	5.5022230	-1.3219760	-2.7948190
C	4.1372980	-0.0968630	-1.6563370
C	4.8062600	1.4852900	1.8071930
H	3.7862000	1.3406210	2.2010120
C	2.9899500	-0.2321270	-2.6272590
H	2.0650770	-0.4620390	-2.0673490
C	2.1188210	-3.2015660	0.5096610
C	3.3293090	-2.5562210	0.8574190
H	3.3171930	-1.4978760	1.1300240
C	4.5290980	-3.2778940	0.8729520
H	5.4564240	-2.7626290	1.1428070
C	4.5500630	-4.6451870	0.5489400
H	5.4923190	-5.2023620	0.5671390
C	3.3480060	-5.2936400	0.2139390
H	3.3495690	-6.3608280	-0.0330690
C	2.1431090	-4.5842630	0.2019200
H	1.1960620	-5.0741990	-0.0445430
N	-3.7780330	-0.1564160	0.0761720
N	-1.9749600	1.6876680	0.2653920
N	0.3364380	2.2188510	0.0832350
N	2.7219200	1.3265680	-0.2613620
N	-0.2494020	-0.5739260	0.6071960
N	0.7871840	-1.3234360	0.4458270
Ni	-1.9434930	-0.2290950	0.1702100
Ni	1.0982770	0.4923950	0.1341670
H	-5.7453840	-0.6715770	-3.3531040
H	-6.0897110	0.5297570	-2.0919630
H	-3.3675730	-3.3005390	2.3597830
H	-4.0151590	-1.6757800	2.7346130
H	3.1769490	-1.0317730	-3.3604670
H	2.7969310	0.7064650	-3.1776820
H	5.5238860	1.1325780	2.5651580
H	4.9572560	2.5748810	1.6985780
N	0.8434420	-2.6131170	0.5287680

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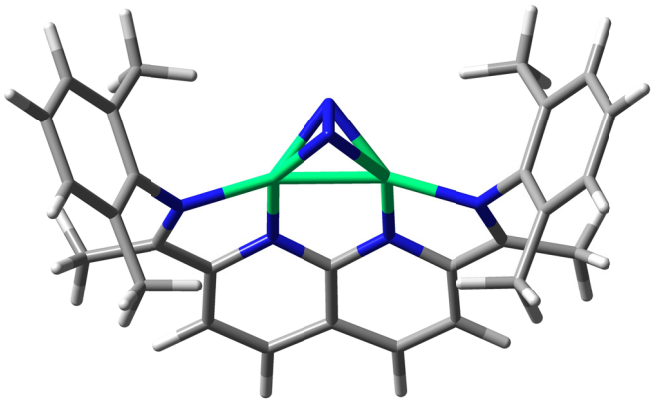

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -4429.29417922 Hartrees
Gibbs Free Energy (298.15 K): -4428.87177 Hartrees

Ni	1.1158880	-0.1712940	-0.4418070
Ni	-1.1158180	-0.1717840	-0.4411750
N	-2.9470540	-0.0004260	0.1071650
N	-1.1462980	1.6814140	-0.4069740
N	1.1466120	1.6816270	-0.4073090
N	2.9470700	-0.0004930	0.1066430
C	-4.8718140	1.6065720	0.1105810
H	-5.3581120	1.4168280	-0.8641890
H	-5.0294860	2.6669870	0.3577200
H	-5.3968980	0.9855530	0.8540520
C	-3.4077820	1.2646040	0.0455530
C	-2.3706120	2.2582680	-0.0849870
C	-2.4403130	3.6374670	0.1914890
H	-3.4089950	4.1030960	0.3948460
C	-1.2732850	4.4072880	0.2616100
H	-1.3291150	5.4724680	0.5059340
C	0.0001480	3.7936840	0.0973740
C	0.0001300	2.3888500	-0.2242810
C	1.2736200	4.4072950	0.2614710
H	1.3294400	5.4724710	0.5058210
C	2.4406760	3.6375290	0.1912560
H	3.4093390	4.1031900	0.3946440
C	2.3709890	2.2583380	-0.0853040
C	3.4079960	1.2645050	0.0452310
C	4.8720960	1.6061470	0.1105040
H	5.3590590	1.4134450	-0.8633410
H	5.3964250	0.9869620	0.8560510
H	5.0299840	2.6671690	0.3548470
C	-3.8616720	-1.0958120	0.2083460
C	-4.2539130	-1.5468030	1.4953260

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C	-5.1230010	-2.6499840	1.5778750
H	-5.4354110	-3.0035120	2.5671210
C	-5.5742030	-3.3054010	0.4239060
H	-6.2432340	-4.1678100	0.5084260
C	-5.1486730	-2.8664610	-0.8375020
H	-5.4802530	-3.3895630	-1.7416940
C	-4.2897540	-1.7609210	-0.9694930
C	-3.7975430	-1.2994000	-2.3219150
H	-2.7062970	-1.1259770	-2.2905930
C	-3.7281340	-0.8695650	2.7407130
H	-2.6243870	-0.8321390	2.7306700
C	3.8614750	-1.0959800	0.2083090
C	4.2896080	-1.7615150	-0.9692690
C	5.1483060	-2.8671730	-0.8368400
H	5.4799300	-3.3905930	-1.7408330
C	5.5735790	-3.3058170	0.4247580
H	6.2424360	-4.1683260	0.5096300
C	5.1223230	-2.6499810	1.5784680
H	5.4345090	-3.0032910	2.5678630
C	4.2534380	-1.5466720	1.4954810
C	3.7274580	-0.8691370	2.7406260
H	2.6237020	-0.8319390	2.7304950
C	3.7977600	-1.3002270	-2.3219060
H	4.2606580	-0.3445510	-2.6303750
H	-4.0507370	-1.4081340	3.6459260
H	-4.0741880	0.1762500	2.8302880
H	-4.0140660	-2.0458780	-3.1019670
H	-4.2602260	-0.3435930	-2.6302940
H	4.0143630	-2.0469020	-3.1017470
H	2.7065360	-1.1266100	-2.2909080
H	4.0500920	-1.4073820	3.6460210
H	4.0732820	0.1767740	2.8299360
N	-0.0000600	-1.2887620	-1.4287700
N	0.0006270	-1.7643590	-0.2786310

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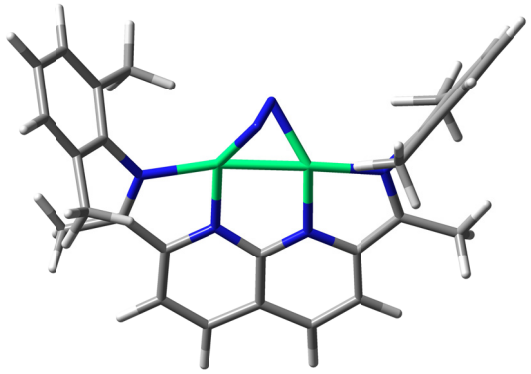

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -4429.27637992 Hartrees
Gibbs Free Energy (298.15 K: -4428.85774 Hartrees

Ni	1.1019100	-0.2191130	-0.1260400
Ni	-1.1018570	-0.2191870	0.1266690
N	-3.0306820	0.0098810	0.0764430
N	-1.1239320	1.6454840	0.1776910
N	1.1240610	1.6454790	-0.1767910
N	3.0307320	0.0098010	-0.0767460
C	-4.8703400	1.7131270	0.3908810
H	-5.2338580	2.2917540	-0.4784530
H	-4.9764910	2.3627390	1.2772610
H	-5.5269390	0.8397230	0.5154930
C	-3.4369290	1.2885900	0.2076930
C	-2.3615700	2.2545870	0.1809370
C	-2.4452550	3.6690720	0.1297990
H	-3.4261160	4.1530600	0.1243290
C	-1.2826640	4.4411450	0.0638990
H	-1.3486170	5.5336640	0.0382660
C	0.0000280	3.8138290	-0.0001640
C	0.0000480	2.3840340	0.0002260
C	1.2827330	4.4411320	-0.0646310
H	1.3486570	5.5336650	-0.0395720
C	2.4453340	3.6690780	-0.1303390
H	3.4261710	4.1531260	-0.1253820
C	2.3617120	2.2545550	-0.1807950
C	3.4370180	1.2885450	-0.2078850
C	4.8703580	1.7130880	-0.3916490
H	5.5274320	0.8396100	-0.5131390
H	5.2330640	2.2947770	0.4759600
H	4.9767080	2.3598630	-1.2801100
C	-3.9629100	-1.0709250	0.0704630
C	-4.0163200	-1.9258860	1.2037260
C	-4.8838150	-3.0311420	1.1724900
H	-4.9294440	-3.6917600	2.0456850

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C	-5.6744620	-3.2983910	0.0463540
H	-6.3421080	-4.1658890	0.0355880
C	-5.5894420	-2.4621680	-1.0749720
H	-6.1860810	-2.6813720	-1.9679600
C	-4.7340050	-1.3450310	-1.0915310
C	-4.6128850	-0.4838040	-2.3286830
H	-3.5550460	-0.3223900	-2.5995630
C	-3.1399380	-1.6427610	2.4004590
H	-2.1277290	-1.3583860	2.0567800
C	3.9628370	-1.0710850	-0.0707670
C	4.0156730	-1.9264570	-1.2037580
C	4.8829980	-3.0318330	-1.1724880
H	4.9281700	-3.6927740	-2.0454630
C	5.6740850	-3.2988030	-0.0465870
H	6.3415800	-4.1664160	-0.0357910
C	5.5896970	-2.4621480	1.0744550
H	6.1866980	-2.6810990	1.9672620
C	4.7344240	-1.3448720	1.0909850
C	4.6140870	-0.4831270	2.3278530
H	3.5564170	-0.3209340	2.5989090
C	3.1389410	-1.6435550	-2.4002860
H	3.5163960	-0.7956990	-3.0011880
H	-3.0608840	-2.5210630	3.0599200
H	-3.5174040	-0.7946460	3.0009870
H	-5.1208930	-0.9579650	-3.1835220
H	-5.0619980	0.5165350	-2.1913010
H	3.0595090	-2.5220440	-3.0594520
H	2.1269000	-1.3588630	-2.0563870
H	5.1219930	-0.9572940	3.1827500
H	5.0638220	0.5168730	2.1899920
N	-0.2337090	-1.6975870	-0.5683060
N	0.2338140	-1.6969350	0.5700510

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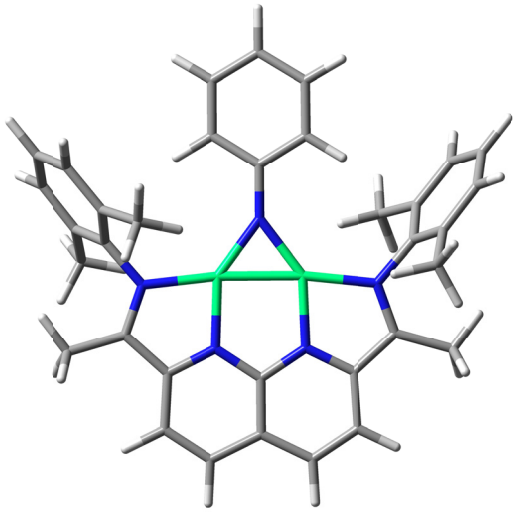

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -4606.18959433 Hartrees
Gibbs Free Energy (298.15 K): -4605.683989 Hartrees

Ni	-1.0690670	0.3255510	-0.0364870
Ni	1.0691340	0.3254460	0.0341410
N	2.9741230	0.5315910	0.1053030
N	1.1350600	2.1694830	0.0467710
N	-1.1349980	2.1695930	-0.0477930
N	-2.9740980	0.5317110	-0.1063940
N	0.0000380	-1.1106780	-0.0007570
C	4.8586510	2.2184690	0.3165550
H	4.9819060	2.8768470	1.1953840
H	5.2149080	2.7868270	-0.5628110
H	5.5128510	1.3443000	0.4461490
C	3.4202600	1.8041200	0.1622050
C	2.3529480	2.7812360	0.1132760
C	2.4399350	4.2102990	0.1294850
H	3.4212670	4.6899200	0.1823220
C	1.2858240	4.9768410	0.0701520
H	1.3458340	6.0700380	0.0753490
C	0.0000000	4.3405600	0.0014770
C	0.0000220	2.9257610	0.0001570
C	-1.2858410	4.9769050	-0.0658750
H	-1.3458870	6.0701090	-0.0691050
C	-2.4399840	4.2104570	-0.1261870
H	-3.4213360	4.6901770	-0.1777790
C	-2.3529460	2.7813840	-0.1124490
C	-3.4202710	1.8042810	-0.1619200
C	-4.8586870	2.2188570	-0.3153960
H	-4.9823210	2.8772740	-1.1941530
H	-5.2143070	2.7872880	0.5641740
H	-5.5131310	1.3448240	-0.4446540
C	3.9048420	-0.5535520	0.1145910

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C	4.7029300	-0.8368970	-1.0266240
C	5.5646360	-1.9490630	-0.9735530
H	6.1815610	-2.1788970	-1.8498860
C	5.6335000	-2.7637060	0.1645770
H	6.3112040	-3.6233180	0.1840230
C	4.8104980	-2.4900850	1.2662320
H	4.8351330	-3.1416880	2.1467030
C	3.9277810	-1.3967760	1.2578140
C	2.9716280	-1.1329380	2.3939390
H	1.9770850	-0.9062720	1.9631570
C	4.6056770	0.0002550	-2.2829060
H	3.5544720	0.2172500	-2.5390260
C	-3.9047960	-0.5534590	-0.1160230
C	-4.7029240	-0.8371560	1.0250890
C	-5.5645650	-1.9493610	0.9716650
H	-6.1815120	-2.1794850	1.8479080
C	-5.6332910	-2.7637310	-0.1666640
H	-6.3109340	-3.6233850	-0.1863650
C	-4.8101650	-2.4898340	-1.2681550
H	-4.8346370	-3.1412670	-2.1487550
C	-3.9275150	-1.3964770	-1.2594030
C	-2.9711910	-1.1324340	-2.3953250
H	-1.9767270	-0.9058230	-1.9642980
C	-4.6057780	-0.0004660	2.2816960
H	-5.1205890	0.9724030	2.1806470
C	-0.0001330	-2.4813600	0.0007200
C	-1.1933880	-3.2186180	0.2619510
H	-2.1144760	-2.6656430	0.4690150
C	-1.1856880	-4.6155940	0.2614930
H	-2.1168350	-5.1555990	0.4668830
C	-0.0003990	-5.3294190	0.0037720
H	-0.0005050	-6.4241690	0.0049650
C	1.1850160	-4.6163780	-0.2555350
H	2.1160530	-5.1569940	-0.4598160
C	1.1929640	-3.2194080	-0.2590250
H	5.0676720	-0.5249370	-3.1341030
H	5.1192100	0.9737030	-2.1810120
H	2.1141310	-2.6670410	-0.4673640
H	2.8948710	-2.0007230	3.0667540
H	3.2638310	-0.2516560	2.9938540
H	-5.0665890	-0.5266210	3.1329430
H	-3.5546690	0.2176380	2.5372180
H	-2.8942990	-2.0001140	-3.0682600
H	-3.2632680	-0.2510460	-2.9951430

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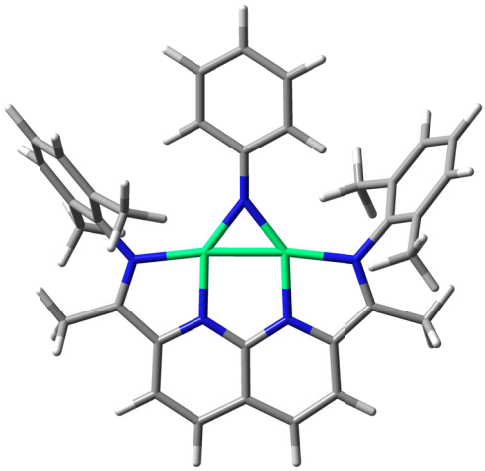

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -4606.19035728 Hartrees
Gibbs Free Energy (298.15 K): -4605.68853 Hartrees

Ni	-1.0832430	0.3040590	-0.0406100
Ni	1.0769070	0.3194590	0.0575880
N	3.0160600	0.5450520	0.1403940
N	1.1317140	2.1734810	-0.0484600
N	-1.1425610	2.1607350	-0.1374120
N	-3.0252380	0.5187260	-0.0523820
N	0.0084620	-1.1094980	0.0153710
C	4.8652320	2.2606760	0.2918490
H	4.9555020	3.0217420	1.0860040
H	5.2505900	2.7169440	-0.6382860
H	5.5124980	1.4095670	0.5483430
C	3.4308060	1.8257710	0.1411800
C	2.3588240	2.7931110	0.0404950
C	2.4305070	4.2024830	0.0455000
H	3.4039410	4.6983020	0.1056270
C	1.2598220	4.9701060	-0.0245420
H	1.3188230	6.0630520	-0.0245860
C	-0.0170520	4.3368510	-0.0866090
C	-0.0096900	2.9018840	-0.0872610
C	-1.3001640	4.9574750	-0.1414310
H	-1.3700910	6.0497600	-0.1469850
C	-2.4644480	4.1775100	-0.1767290
H	-3.4448350	4.6625700	-0.2031780
C	-2.3780810	2.7694120	-0.1596880
C	-3.4465970	1.7924620	-0.1526190
C	-4.8873090	2.2105170	-0.2931470

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H	-5.0139530	2.8752140	-1.1651640
H	-5.2318030	2.7726420	0.5941080
H	-5.5440590	1.3379580	-0.4207860
C	3.9481640	-0.5319190	0.1916750
C	4.7941760	-0.8333320	-0.9114280
C	5.6490430	-1.9476840	-0.8086320
H	6.3015100	-2.1896640	-1.6555830
C	5.6660210	-2.7518750	0.3386780
H	6.3394070	-3.6132660	0.3955660
C	4.7957440	-2.4657760	1.4003870
H	4.7798980	-3.1086530	2.2875910
C	3.9209620	-1.3681820	1.3427120
C	2.9219100	-1.0832350	2.4356340
H	1.9515090	-0.8374340	1.9591880
C	4.7577400	-0.0181830	-2.1856810
H	3.7296370	0.2917630	-2.4369640
C	-3.9578990	-0.5610610	-0.0385620
C	-4.7570750	-0.8276960	1.1060750
C	-5.6198730	-1.9397410	1.0697520
H	-6.2383150	-2.1549380	1.9488050
C	-5.6875990	-2.7738910	-0.0544630
H	-6.3658340	-3.6333190	-0.0600420
C	-4.8638120	-2.5186010	-1.1602100
H	-4.8893030	-3.1834160	-2.0309070
C	-3.9834820	-1.4230590	-1.1687310
C	-3.0304040	-1.1681120	-2.3097560
H	-2.0404520	-0.9107600	-1.8818490
C	-4.6604900	0.0306000	2.3478390
H	-5.1756690	1.0012120	2.2291360
C	0.0288740	-2.4752070	-0.0836770
C	-1.1659550	-3.2392470	0.0788800
H	-2.1006960	-2.7084590	0.2826760
C	-1.1373060	-4.6322600	-0.0103240
H	-2.0657180	-5.1985730	0.1216540
C	0.0706200	-5.3095820	-0.2656590
H	0.0868260	-6.4020170	-0.3357320
C	1.2582860	-4.5700830	-0.4266720
H	2.2034870	-5.0877040	-0.6230820
C	1.2463600	-3.1770610	-0.3350380
H	5.1588960	-0.6029880	-3.0290900
H	5.3650390	0.9027140	-2.1126810
H	2.1667680	-2.5982130	-0.4567660
H	2.7976600	-1.9466690	3.1071160
H	3.2027530	-0.2044910	3.0443630

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H	-5.1207570	-0.4799420	3.2088720
H	-3.6095830	0.2550260	2.5982550
H	-2.9335530	-2.0487950	-2.9630970
H	-3.3369220	-0.3055990	-2.9292500

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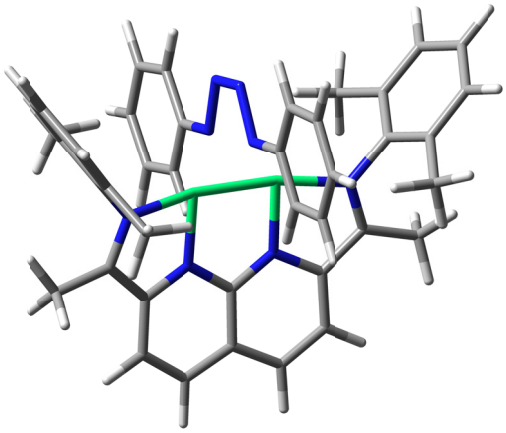

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -5002.07280163 Hartrees
Gibbs Free Energy (298.15 K): -5001.47934 Hartrees

Ni	-1.0961480	0.2078290	-0.0212110
Ni	1.0972000	0.1546250	-0.0529980
N	2.9820770	0.0330870	-0.4211610
N	1.1509670	1.3442950	-1.4988050
N	-1.1259520	1.3933570	-1.4696490
N	-2.9939760	0.1599230	-0.3555390
N	0.0375920	0.7203200	1.5711200
C	4.8868200	1.0169180	-1.7279670
H	5.3488760	1.7745970	-1.0678880
H	5.0290450	1.3519270	-2.7668290
H	5.4439540	0.0788530	-1.5797030
C	3.4279070	0.8420310	-1.4020590
C	2.3796050	1.5472670	-2.1004570
C	2.4544890	2.2985980	-3.2958550
H	3.4273100	2.4882810	-3.7584370
C	1.2917530	2.7754270	-3.9088500
H	1.3549920	3.3430490	-4.8424420
C	0.0114920	2.4899950	-3.3465990
C	0.0125000	1.7484960	-2.1196800
C	-1.2679990	2.8373520	-3.8729000
H	-1.3296900	3.4099730	-4.8035630
C	-2.4348650	2.4128360	-3.2278400
H	-3.4136290	2.6422660	-3.6594460
C	-2.3572980	1.6551240	-2.0384410
C	-3.4221740	0.9902380	-1.3245860
C	-4.8717250	1.2050960	-1.6737410
H	-5.5285130	0.7751920	-0.9037150
H	-5.1270200	0.7303370	-2.6391810
H	-5.0965880	2.2806460	-1.7703880
C	3.9104760	-0.7299110	0.3594670
C	4.3101790	-2.0127590	-0.1000560
C	5.1893400	-2.7624960	0.7027070

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H	5.5040380	-3.7531690	0.3556760
C	5.6525420	-2.2685100	1.9294260
H	6.3313130	-2.8696560	2.5429510
C	5.2375850	-1.0051940	2.3707860
H	5.5904500	-0.6160230	3.3324790
C	4.3643310	-0.2150640	1.6014090
C	3.9011140	1.1359200	2.0940570
H	2.8099390	1.1446080	2.2630990
C	3.7970360	-2.5636360	-1.4110440
H	2.6963020	-2.6528910	-1.4050330
C	-3.9262340	-0.6003970	0.4226530
C	-4.2967370	-0.1285800	1.7090720
C	-5.1703130	-0.9148910	2.4818230
H	-5.4607920	-0.5568200	3.4758620
C	-5.6615560	-2.1365070	2.0030250
H	-6.3369920	-2.7375100	2.6203490
C	-5.2790650	-2.5892030	0.7333380
H	-5.6541120	-3.5474920	0.3566610
C	-4.4080610	-1.8389260	-0.0776180
C	-3.9858490	-2.3493020	-1.4364930
H	-2.8886660	-2.4533660	-1.5032090
C	-3.7546000	1.1798550	2.2335510
H	-4.0257900	2.0306940	1.5835530
C	0.0827210	2.0133610	2.1692020
C	0.0914640	3.1414260	1.3199140
H	0.0619340	2.9861550	0.2397170
C	0.1366510	4.4335800	1.8570990
H	0.1426560	5.2944230	1.1799480
C	0.1742650	4.6282060	3.2477160
H	0.2097920	5.6390690	3.6660310
C	0.1651650	3.5069530	4.0937630
H	0.1935020	3.6409530	5.1807110
C	0.1196920	2.2079180	3.5703080
H	4.2184740	-3.5627280	-1.6048880
H	4.0574550	-1.9154390	-2.2670020
H	0.1123570	1.3347050	4.2248160
H	4.3943850	1.3984900	3.0430600
H	4.1105110	1.9395380	1.3663680
H	-4.1362900	1.3876390	3.2452860
H	-2.6516580	1.1599530	2.2787220
H	-4.4331680	-3.3357540	-1.6369730
H	-4.2938810	-1.6704160	-2.2518260
C	-0.0832350	-2.6754820	-0.0455110
C	-0.1302790	-3.8976230	0.6615600
C	-0.0863680	-2.6964000	-1.4598040
C	-0.1795720	-5.1080870	-0.0424140
H	-0.1268990	-3.8750100	1.7528350
C	-0.1363860	-3.9142910	-2.1514580
H	-0.0470380	-1.7458050	-2.0050400
C	-0.1834980	-5.1292270	-1.4473760
H	-0.2159860	-6.0486890	0.5178740
H	-0.1373560	-3.9114700	-3.2466650
H	-0.2224580	-6.0805630	-1.9872830

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N	0.0318340	-0.3151850	2.5167130
N	-0.0082080	-1.4751960	1.9875330
N	-0.0326340	-1.4074460	0.5913040

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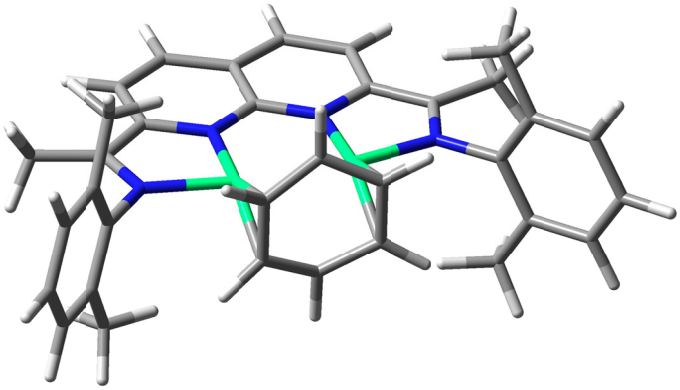

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: –4552.05572180 Hartrees
Gibbs Free Energy (298.15 K): –4551.54164 Hartrees

Ni	1.2394110	-0.1417820	0.0024180
Ni	-1.2394390	-0.1417680	-0.0025480
N	3.1257200	0.1682600	0.0010620
N	-3.1257150	0.1682270	-0.0014090
N	1.1468710	1.7125410	0.0020860
N	-1.1469150	1.7125390	-0.0020650
C	1.2456540	-1.9851430	0.7141420
H	2.1475310	-2.2486550	1.2717760
C	1.2405620	-1.9809700	-0.7244960
H	2.1388120	-2.2409400	-1.2896090
C	-0.0053080	-1.7547750	-1.3901430
H	-0.0093110	-1.6914860	-2.4824050
C	-1.2454140	-1.9848800	-0.7157750
H	-2.1473690	-2.2481180	-1.2734400
C	-1.2404240	-1.9811360	0.7228680
H	-2.1385720	-2.2415420	1.2879350
C	0.0055150	-1.7541000	1.3883220
H	0.0095310	-1.6909090	2.4805930
C	3.4843410	1.4750640	0.0016940
C	-3.4843700	1.4750130	-0.0016790
C	2.3877480	2.3756280	0.0021760
C	2.4365820	3.7828770	0.0018990
H	3.4058660	4.2891170	0.0021310
C	1.2630320	4.5328890	0.0010860
H	1.2992900	5.6267440	0.0008970
C	-0.0000340	3.8795900	-0.0000600
C	-1.2630990	4.5328740	-0.0012430
H	-1.2993630	5.6267300	-0.0012170
C	-2.4366530	3.7828540	-0.0019640
H	-3.4059320	4.2890910	-0.0022030
C	-2.3877920	2.3756110	-0.0021120
C	-0.0000160	2.4378020	-0.0000110
C	4.1526650	-0.8242410	0.0000310

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C	4.6400140	-1.3314240	1.2358460
C	5.6053180	-2.3558200	1.2106740
H	5.9821680	-2.7522470	2.1606020
C	6.0852220	-2.8689080	-0.0017070
H	6.8307730	-3.6707070	-0.0023930
C	5.6060400	-2.3530490	-1.2131730
H	5.9834930	-2.7472830	-2.1637740
C	4.6407840	-1.3285330	-1.2366540
C	-4.1526340	-0.8242960	0.0002370
C	-4.6401020	-1.3285940	1.2371530
C	-5.6054470	-2.3530460	1.2141520
H	-5.9823940	-2.7473190	2.1649390
C	-6.0853210	-2.8688370	0.0029330
H	-6.8309480	-3.6705660	0.0040200
C	-5.6060210	-2.3557600	-1.2096950
H	-5.9834030	-2.7521230	-2.1594360
C	-4.6406650	-1.3314320	-1.2353430
C	4.9270020	1.9090590	0.0019750
H	5.4645270	1.5216750	0.8856400
H	5.0179750	3.0044730	0.0043040
H	5.4639270	1.5255020	-0.8837160
C	-4.9270640	1.9088960	-0.0011760
H	-5.4653250	1.5205450	-0.8839440
H	-5.0181360	3.0042920	-0.0044810
H	-5.4631570	1.5261460	0.8853890
C	4.1623080	-0.7533300	2.5504050
H	3.0780350	-0.5526820	2.5351220
C	4.1644460	-0.7472840	-2.5503310
H	3.0805190	-0.5449180	-2.5352380
C	-4.1630450	-0.7474390	2.5506180
H	-3.0792320	-0.5445710	2.5347140
C	-4.1636540	-0.7532970	-2.5501390
H	-3.0793750	-0.5526540	-2.5354320
H	-4.3911550	-1.4244290	3.3897070
H	-4.6540300	0.2199840	2.7657050
H	-4.3939270	-1.4310660	-3.3879930
H	-4.6526300	0.2149260	-2.7661460
H	4.6550600	0.2204570	-2.7648100
H	4.3934850	-1.4239590	-3.3894190
H	4.3921180	-1.4311230	3.3883680
H	4.6511910	0.2148730	2.7666910

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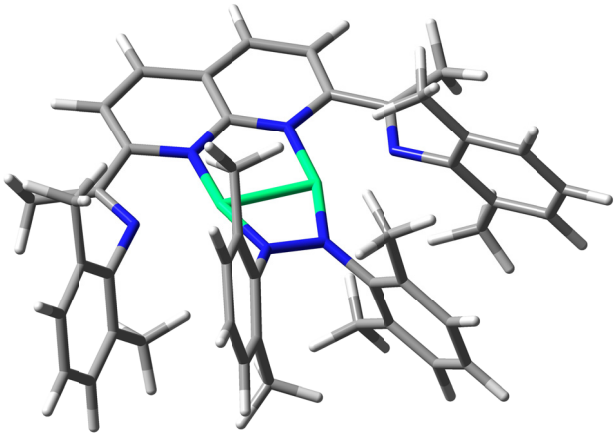

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -5049.84552013 Hartrees
Gibbs Free Energy (298.15 K): -5049.151627 Hartrees

Ni	-1.1221890	0.8434020	0.0555660
Ni	1.1328650	0.8326580	-0.0481760
N	-3.0787900	1.0783900	-0.0913570
N	3.1000990	1.0669950	0.0853710
N	-1.1339060	2.6627440	-0.0089500
N	1.1478540	2.6537000	0.0284130
N	-0.6790590	-0.8823550	0.1301530
N	0.6702910	-0.8934640	-0.1047670
C	-3.4550550	2.3705390	-0.1324600
C	3.4722330	2.3574570	0.1444200
C	-2.3720130	3.3067340	-0.0333010
C	-2.4287690	4.7131320	-0.0116210
H	-3.4007840	5.2147660	-0.0164540
C	-1.2569880	5.4747870	0.0232400
H	-1.3064640	6.5678140	0.0399010
C	0.0136600	4.8326500	0.0296320
C	0.0092190	3.3933360	0.0165460
C	1.2860280	5.4683420	0.0487970
H	1.3414090	6.5612150	0.0532250
C	2.4537920	4.6981790	0.0708140
H	3.4309630	5.1896070	0.0894710
C	2.3860680	3.2935680	0.0643270
C	-4.0615340	0.0704270	-0.3498270
C	-4.1416990	-0.4573270	-1.6690610
C	-5.0705380	-1.4767590	-1.9360190
H	-5.1362600	-1.8809600	-2.9528810
C	-5.9062030	-1.9750630	-0.9257010
H	-6.6206920	-2.7748940	-1.1462260
C	-5.8187690	-1.4460050	0.3664220
H	-6.4681600	-1.8321560	1.1608030

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C	-4.9067810	-0.4185930	0.6782020
C	4.0853210	0.0498610	0.2892600
C	4.9112430	-0.3899360	-0.7769500
C	5.8264820	-1.4308070	-0.5304690
H	6.4603720	-1.7806910	-1.3534540
C	5.9365220	-2.0185460	0.7357790
H	6.6526530	-2.8291060	0.9057620
C	5.1229540	-1.5649600	1.7832930
H	5.2086760	-2.0136770	2.7797860
C	4.1897610	-0.5333750	1.5807620
C	-1.4002310	-2.0410480	0.5815010
C	-1.8108040	-2.0458540	1.9468160
C	-2.5203060	-3.1567450	2.4336960
H	-2.8259110	-3.1693300	3.4862460
C	-2.8371660	-4.2358260	1.5962370
C	-2.4698610	-4.1939820	0.2476880
H	-2.7495250	-5.0154900	-0.4216680
C	-1.7610850	-3.1004140	-0.2888870
C	1.3704830	-2.0752420	-0.5290810
C	1.7768650	-2.1217550	-1.8947010
C	2.4702490	-3.2538020	-2.3549720
H	2.7761420	-3.2953430	-3.4066030
C	2.7710800	-4.3169570	-1.4922330
C	2.4024460	-4.2385090	-0.1456790
H	2.6668120	-5.0496190	0.5423640
C	1.7115620	-3.1214760	0.3651850
C	-4.8880210	2.8043280	-0.3051150
H	-5.3955290	2.1788580	-1.0577060
H	-4.9563030	3.8552140	-0.6222560
H	-5.4572130	2.6943680	0.6360740
C	4.8974580	2.8195130	0.3213400
H	5.5245290	2.0149070	0.7331540
H	4.9508490	3.6879380	0.9974010
H	5.3414460	3.1267700	-0.6437280
C	-3.2554900	0.0968130	-2.7609440
H	-2.2136290	0.1861340	-2.4048520
C	-4.8669590	0.1496700	2.0801850
H	-5.7450390	0.7931580	2.2769600
C	4.8408970	0.2587150	-2.1410980
H	3.8074680	0.5214990	-2.4148890
C	3.3289390	-0.0212590	2.7124440
H	2.2832590	0.0986410	2.3770470
H	5.2498870	-0.4104110	-2.9153000
H	5.4294050	1.1947860	-2.1750270
H	3.3580640	-0.7027290	3.5774740
H	3.6586170	0.9765720	3.0565940
H	-4.8865030	-0.6572520	2.8319010
H	-3.9650400	0.7563870	2.2466080
H	-3.5646730	1.1148970	-3.0621670
H	-3.2803430	-0.5421470	-3.6580760
H	-3.3908430	-5.0946570	1.9898690
H	3.3122850	-5.1928660	-1.8649950
C	1.3904440	-3.0673460	1.8399510

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H	1.2430680	-2.0310440	2.1781960
H	0.4696810	-3.6281100	2.0763320
H	2.2139410	-3.5083750	2.4259950
C	-1.4834930	-0.8898420	2.8628280
H	-1.6701950	0.0666090	2.3428100
H	-2.0868820	-0.9302720	3.7836160
H	-0.4178420	-0.8806150	3.1548030
C	-1.4467560	-3.0793250	-1.7657910
H	-1.2942240	-2.0503560	-2.1240830
H	-0.5315140	-3.6515270	-1.9960800
H	-2.2777120	-3.5241500	-2.3379460
C	1.4537700	-0.9903380	-2.8422690
H	1.6067370	-0.0202180	-2.3367280
H	2.0806390	-1.0389610	-3.7468080
H	0.3963090	-1.0086930	-3.1625440

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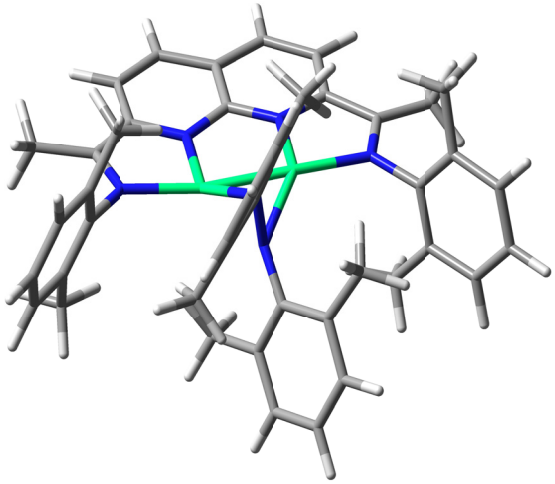

Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy: -5049.82111491 Hartrees
Gibbs Free Energy (298.15 K): -5049.128763 Hartrees

Ni	-1.1252930	0.7215630	-0.1302420
Ni	1.1251470	0.7215460	0.1305590
N	-3.0475500	0.9538160	-0.1213030
N	3.0473890	0.9538040	0.1219880
N	-1.1384720	2.5550440	-0.1175500
N	1.1383250	2.5550410	0.1177730
N	-0.1220260	-0.7042360	0.7045450
N	0.1219600	-0.7039660	-0.7049230
C	-3.4507570	2.2461130	-0.1167010
C	3.4505950	2.2461070	0.1171120
C	-2.3770050	3.1910580	-0.1296930
C	-2.4396320	4.6036720	-0.1137980
H	-3.4142570	5.0995300	-0.1404280
C	-1.2740740	5.3661210	-0.0651620
H	-1.3260620	6.4593320	-0.0605350
C	-0.0000800	4.7259020	0.0000700
C	-0.0000720	3.2949560	0.0000940
C	1.2739150	5.3661280	0.0653190
H	1.3259010	6.4593390	0.0607000
C	2.4394670	4.6036870	0.1140100
H	3.4140760	5.0995730	0.1406660
C	2.3768670	3.1910640	0.1299460
C	-4.0353720	-0.0765280	-0.0137780
C	-4.7551500	-0.5246390	-1.1532350
C	-5.6642510	-1.5893970	-0.9959300
H	-6.2161400	-1.9453370	-1.8738690
C	-5.8747260	-2.1889460	0.2516760
H	-6.5856790	-3.0156740	0.3520800
C	-5.1714570	-1.7228670	1.3722860
H	-5.3356270	-2.1817390	2.3538290
C	-4.2466990	-0.6703250	1.2626710

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C	4.0353430	-0.0764300	0.0145080
C	4.2472170	-0.6698220	-1.2620460
C	5.1721450	-1.7222090	-1.3716420
H	5.3367320	-2.1807720	-2.3532600
C	5.8750860	-2.1885140	-0.2509130
H	6.5861950	-3.0151090	-0.3513080
C	5.6641010	-1.5893420	0.9967810
H	6.2157560	-1.9454380	1.8748060
C	4.7547860	-0.5247580	1.1540760
C	-0.4215810	-1.8219120	1.5293100
C	0.1180960	-1.7409680	2.8515770
C	-0.1436110	-2.7787670	3.7580290
H	0.2936860	-2.7252080	4.7615200
C	-0.9543460	-3.8651370	3.3998610
C	-1.5309750	-3.8994550	2.1247420
H	-2.2026840	-4.7218610	1.8521720
C	-1.2935950	-2.8928920	1.1685790
C	0.4215920	-1.8212940	-1.5301200
C	-0.1179990	-1.7398020	-2.8524000
C	0.1438010	-2.7771890	-3.7592930
H	-0.2934220	-2.7231920	-4.7627930
C	0.9545510	-3.8636880	-3.4015540
C	1.5310910	-3.8985450	-2.1264110
H	2.2028170	-4.7210450	-1.8541640
C	1.2936090	-2.8924220	-1.1698120
C	-4.8993240	2.6566140	-0.0726900
H	-5.4828480	1.9734160	0.5653720
H	-5.3618100	2.6347350	-1.0769930
H	-5.0098820	3.6779380	0.3223040
C	4.8992080	2.6564070	0.0729290
H	5.4820930	1.9744620	-0.5670850
H	5.3624890	2.6321550	1.0768040
H	5.0097330	3.6785520	-0.3199120
C	-4.5959080	0.1284030	-2.5093930
H	-3.6440020	0.6724510	-2.5962300
C	-3.5064130	-0.1552160	2.4747330
H	-3.9058410	0.8211990	2.8067020
C	3.5073160	-0.1544190	-2.4742210
H	2.4420430	0.0056810	-2.2388080
C	4.5950450	0.1278890	2.5103770
H	3.6439760	0.6735310	2.5963220
H	3.5856840	-0.8585900	-3.3169390
H	3.9066130	0.8222500	-2.8056070
H	4.6406640	-0.6222100	3.3174520
H	5.4090460	0.8526270	2.7011840
H	-3.5842090	-0.8597670	3.3171860
H	-2.4412930	0.0052760	2.2388970
H	-5.4088380	0.8546900	-2.6988770
H	-4.6438010	-0.6212310	-3.3167580
H	-1.1528010	-4.6680730	4.1172220
H	1.1530920	-4.6662950	-4.1192590
C	2.0138210	-2.9856030	0.1572520
H	1.4633130	-3.6111380	0.8804130

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H	3.0101920	-3.4327140	0.0101060
H	2.1611920	-1.9985730	0.6193070
C	0.9521420	-0.5550000	3.2717110
H	1.6183260	-0.2295580	2.4551830
H	0.3134290	0.3189310	3.4998860
H	1.5470010	-0.7853230	4.1700970
C	-2.0138570	-2.9855000	-0.1584990
H	-1.4633720	-3.6107080	-0.8819610
H	-3.0102190	-3.4326860	-0.0115070
H	-2.1612510	-1.9982660	-0.6201120
C	-0.9520430	-0.5536770	-3.2721010
H	-1.6184620	-0.2287470	-2.4555580
H	-0.3133670	0.3204440	-3.4996460
H	-1.5466670	-0.7835750	-4.1707530

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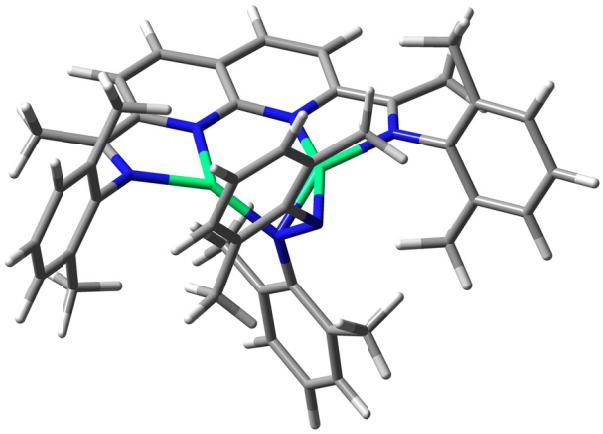

Charge: 0
Multiplicity: 3
Imaginary Frequencies: 0
Electronic Energy: -5049.81620498 Hartrees
Gibbs Free Energy (298.15 K): -5049.12748 Hartrees

Ni	-1.3132830	0.2406580	-0.0816570
Ni	1.2826640	0.2573250	0.0293080
N	-3.1798770	0.5261060	-0.5901670
N	3.1549970	0.6448480	-0.2691210
N	-1.2261810	2.1098740	-0.2361860
N	1.0885070	2.1384090	-0.2860950
N	-0.1043300	-0.6168170	1.0728580
N	-0.7270730	-1.5476490	0.2048000
C	-3.5447620	1.8198590	-0.5378930
C	3.4408820	1.9595080	-0.3554920
C	-2.4548290	2.7441630	-0.4030630
C	-2.5399920	4.1432920	-0.5127490
H	-3.5174580	4.6202530	-0.6257950
C	-1.3769980	4.9124160	-0.5168030
H	-1.4262620	6.0026820	-0.5994450
C	-0.1078510	4.2790080	-0.4478100
C	-0.0774740	2.8352990	-0.3324040
C	1.1381160	4.9594070	-0.4774010
H	1.1505960	6.0516740	-0.5449430
C	2.3261640	4.2350050	-0.4253480
H	3.2834410	4.7618400	-0.4501740
C	2.2999600	2.8285430	-0.3471900
C	-4.1921520	-0.4704150	-0.7746360
C	-4.6875810	-0.7577880	-2.0745170
C	-5.6149500	-1.8079780	-2.2194610
H	-5.9906320	-2.0442130	-3.2218570
C	-6.0596640	-2.5446680	-1.1146520
H	-6.7741680	-3.3630510	-1.2504730
C	-5.5931470	-2.2210590	0.1670210
H	-5.9556750	-2.7750490	1.0404410
C	-4.6663370	-1.1813910	0.3601950
C	4.2495750	-0.2717250	-0.3901510

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C	4.6060100	-0.7389460	-1.6832630
C	5.6674430	-1.6548430	-1.7964520
H	5.9493080	-2.0168010	-2.7918740
C	6.3555530	-2.1110120	-0.6629620
H	7.1733410	-2.8314250	-0.7680920
C	5.9944870	-1.6368060	0.6050530
H	6.5354030	-1.9820720	1.4937470
C	4.9501330	-0.7054760	0.7654480
C	-0.5049150	-0.7009090	2.4546070
C	-0.1832250	0.4030360	3.3056760
C	-0.4459580	0.3210700	4.6829820
H	-0.1879410	1.1804350	5.3120850
C	-1.0215110	-0.8190480	5.2488670
C	-1.3377710	-1.8937160	4.4132500
H	-1.7867180	-2.7958480	4.8439880
C	-1.0998680	-1.8811780	3.0233440
C	0.2356850	-2.0247020	-0.7414420
C	-0.1925580	-2.2882330	-2.0807960
C	0.6878980	-2.8902510	-2.9891820
H	0.3441480	-3.0595620	-4.0163240
C	1.9751900	-3.2882080	-2.6007850
C	2.3697830	-3.0995420	-1.2735380
H	3.3528090	-3.4516680	-0.9442030
C	1.5299140	-2.4926040	-0.3155070
C	-4.9760780	2.2852450	-0.6353210
H	-5.6656980	1.5026820	-0.2844780
H	-5.2545140	2.5236030	-1.6784530
H	-5.1388320	3.1924480	-0.0326620
C	4.8534190	2.4668760	-0.5034180
H	5.2841200	2.1588040	-1.4731250
H	5.5111740	2.0478380	0.2761380
H	4.9061540	3.5626430	-0.4431720
C	-4.2745890	0.0560310	-3.2824550
H	-3.2465900	0.4394020	-3.1931460
C	-4.2192140	-0.7778110	1.7439540
H	-4.6913280	0.1725970	2.0560110
C	3.8574490	-0.2587160	-2.9051330
H	2.7901680	-0.5369060	-2.8492240
C	4.6253780	-0.1500580	2.1351420
H	3.5385660	-0.0765870	2.3065860
H	4.2791560	-0.7013590	-3.8216370
H	3.8943880	0.8402480	-3.0087990
H	5.0608670	-0.7785010	2.9283790
H	5.0285590	0.8717840	2.2663740
H	-4.4812420	-1.5421400	2.4919890
H	-3.1299820	-0.6103270	1.7766440
H	-4.9372020	0.9315120	-3.4192160
H	-4.3448720	-0.5448810	-4.2038360
H	-1.2181720	-0.8732170	6.3242700
H	2.6517430	-3.7639950	-3.3176640
C	0.4054310	1.6805470	2.7706500
H	1.2042300	1.4880110	2.0343040
H	-0.3577820	2.2791560	2.2415820

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H	0.8121670	2.2943860	3.5900280
C	-1.5190390	-3.1371480	2.2757460
H	-2.3510730	-2.9508020	1.5801800
H	-0.7152160	-3.5708180	1.6617740
H	-1.8373520	-3.8986060	3.0089140
C	1.9859890	-2.5563230	1.1338880
H	2.2999530	-1.5797090	1.5343380
H	1.1893720	-2.9207330	1.8001440
H	2.8441940	-3.2416100	1.2183530
C	-1.5917080	-1.9369560	-2.4994140
H	-2.3253720	-2.6741540	-2.1253370
H	-1.8827870	-0.9720650	-2.0530040
H	-1.6856960	-1.8835930	-3.5956870

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