Supporting Information for:

Toward One-pot Olefin/Thiophene Block Copolymers using an in situ Ligand Exchange

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I. Materials

Flash chromatography was performed on SiliCycle silica gel (40–63 μm). Thin layer chromatography was performed on Merck TLC plates (pre-coated with silica gel 60 F254). iPrMgCl (2 M in THF) was purchased from Sigma-Aldrich and titrated using salicylaldehyde phenylhydrazone.[1] 2,5-Dibromo-3-decylthiophene (DB3DT) and 2,5-dibromo-3-hexylthiophene (DB3HT) were purchased from TCI America and purified by column chromatography with hexanes as the eluent. Methylmagnesium chloride (3 M in Et_2O) was purchased from Sigma-Aldrich. 5,5'-Dibromo-2,2'-bithiophene was purchased from Ark Pharm Inc. Compounds **S1**,[2] **C2**,[2] **S2**,[3] **S3**,[3] and **S4**[3] were prepared according to modified literature procedures. All other reagent grade materials and solvents were purchased from Sigma-Aldrich, Acros Organics, or Fisher and were used without further purification unless otherwise noted. Tetrahydrofuran (THF) and diethyl ether (Et_2O) were dried and deoxygenated using an Innovative Technology solvent purification system composed of activated alumina, copper catalyst, and molecular sieves. The glovebox in which specified procedures were carried out was an MBraun LABmaster 130 with an N_2 atmosphere.

II. General Experimental

NMR Spectroscopy Unless otherwise noted, ^1H and ^{13}C NMR spectra for all compounds were acquired at rt. Chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane (TMS) and referenced with residual solvent. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m), broad resonance (br). Residual water is denoted by an asterisk (*).

High Resolution Mass Spectrometry (HRMS) High-resolution mass spectrometry data were obtained on a Micromass AutoSpec Ultima Magnetic Sector mass spectrometer.

Size Exclusion Chromatography (SEC) Polymer molecular weights were determined by comparison with polystyrene standards (Varian, EasiCal PS-2 MW 580–377,400) at 40 °C and a flow rate of 1.0 mL/min in THF on a Malvern Viscotek GPCMax VE2001 equipped with two Viscotek LT- 5000L 8 mm (ID) × 300 mm (L) columns and analyzed with Viscotek TDA 305 (with RI, UV-PDA Detector Model 2600 (190–500 nm), RALS/LALS, and viscometer). Data presented correspond to the absorbance at 254 nm normalized to the highest peak. Peaks are normalized to the polymer peak. When traces are presented in series, the normalized peaks are offset vertically. The peak at ~21 min includes unreacted, quenched monomer and/or unactivated DB3HT or DB3DT (see monomer activation procedures).

Polymer work-up for SEC Polymerizations were quenched using aq. HCl (12 M). The organic layer was extracted with $CHCl_3$, dried over $MgSO_4$, and filtered through a PTFE filter (0.2 μm). The resulting solution was concentrated under reduced pressure, redissolved (~0.5 mg polymer/mL) in THF/toluene (99:1 v/v) with mild heating, and filtered through a PTFE filter (0.2 μm) into a SEC vial.

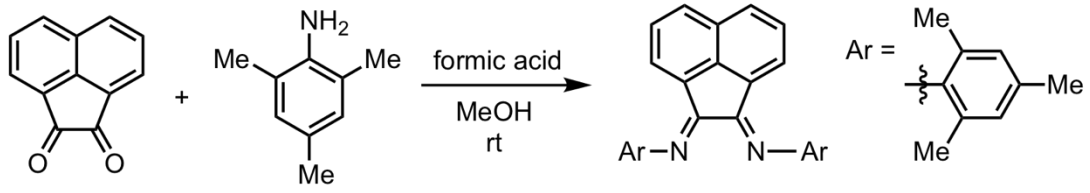
Gas Chromatography (GC) Gas chromatographic analysis was done using a Shimadzu GC 2010 containing a Shimadzu SHRX5 (crossbound 5% diphenyl – 95% dimethyl polysiloxane; 15 m, 0.25 mm ID, 0.25 µm df) column.

Polymer work-up for GC Polymerizations were quenched using aq. HCl (12 M). The organic layer was extracted with $CHCl_3$, dried over $MgSO_4$, and filtered through a PTFE filter (0.2 µm) into a GC vial.

Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry (MALDI-TOF/MS) Matrix-assisted laser desorption/ionization mass spectrometry was done on a Bruker AutoFlex Speed MALDI-TOF in positive-ion reflectron mode using *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as a matrix. Samples were prepared by mixing polymer dissolved in THF/toluene (99:1 v/v) (~1 mg polymer/1 mL THF) with DCTB dissolved in $CHCl_3$ (~1 M). Samples were made with varying polymer/DCTB ratios ([2.5–10 µL]/[2.5 µL] to ensure good signal/noise) and then spotted on a MALDI 96-well plate and air-dried. The data were analyzed using flexAnalysis. The MALDI-TOF/MS spectra shown represent the polymer distribution as well as a zoomed spectrum from the center of the curve unless otherwise noted.

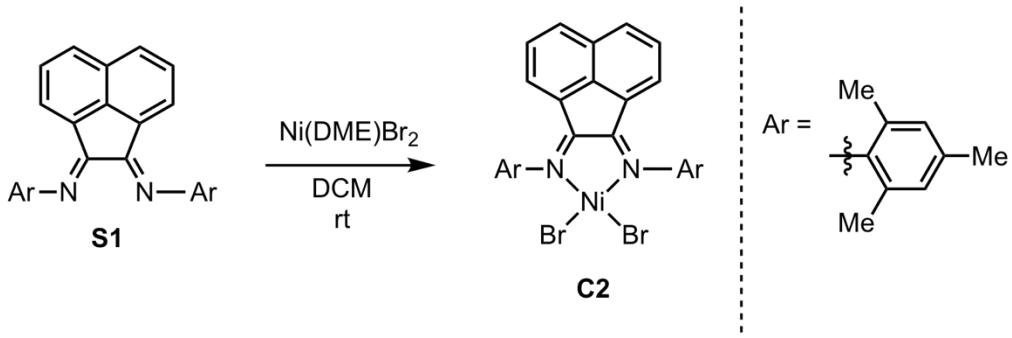
iPrMgCl titration[1] In a glovebox, a precise amount of salicylaldehyde phenylhydrazone (10–20 mg) was dissolved in a precise amount of THF (0.3–0.5 mL). For titration, iPrMgCl was added dropwise using a 100 µL syringe into the salicylaldehyde phenylhydrazone solution. Titration was complete when the solution turned bright orange.

III. Synthetic Procedures

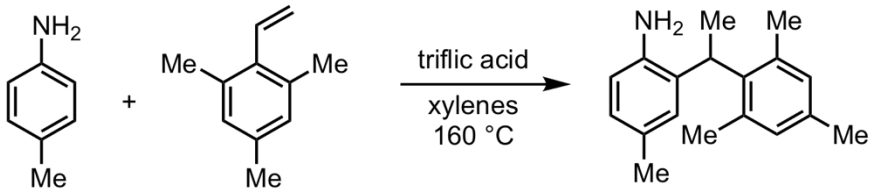


S1

ArN=(An)=NAr (Ar = 2,4,6-trimethylphenyl, An = acenaphthylene) (S1).[2] Acenaphthenequinone (100 mg, 0.549 mmol, 1.00 equiv) was added to a solution containing formic acid (11 µL, 0.29 mmol, 0.52 equiv) in MeOH (1.45 mL) in a 10 mL round-bottom flask equipped with a stir bar. Subsequently, 2,4,6-trimethylaniline (170 µL, 1.2 mmol, 2.2 equiv) was added to the stirring solution. After 18 h at rt, the reaction flask was placed in a –20 °C freezer where an orange solid precipitated from the solution over 24 h. The orange solid was collected via filtration over a fine frit, washed with cold MeOH (3 × 10 mL) and cold pentane (3 × 10 mL), then collected and dried under reduced pressure. The filtrate was transferred to a 100 mL round-bottom flask with DCM (10 mL), concentrated, re-dissolved in DCM (4 mL), filtered through glass wool, and cooled to –20 °C to recrystallize. The orange solid was collected by filtration over a fine frit, washed with cold MeOH (3 × 10 mL) and cold pentane (3 × 10 mL), and dried under reduced pressure. The solids from each crystallization were combined, resulting in **S1** as an orange powder (174 mg, 76%). HRMS (ESI+): Calcd. for $C_{30}H_{28}N_2$ $[M+H]^+$ 417.2325; found 417.2326.

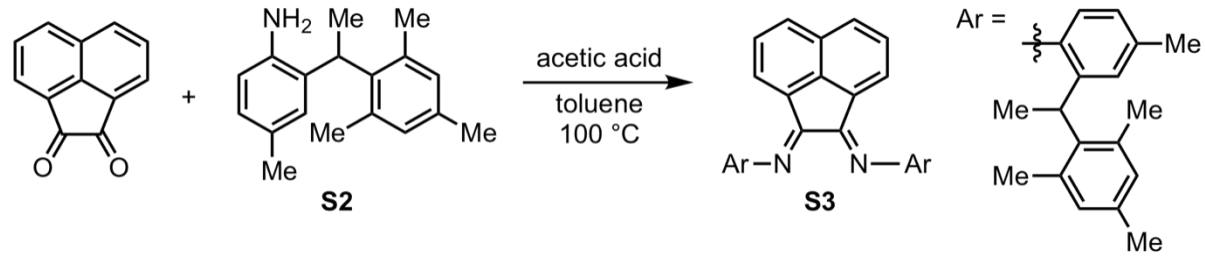


(ArN=(An)=NAr)NiBr$_2$ (Ar = 2,4,6-trimethylphenyl, An = acenaphthylene) (C2).[2] In a 50 mL round-bottom flask, **S1** (145 mg, 0.348 mmol, 1.00 equiv) was dissolved in DCM (9.5 mL). Then, Ni(DME)Br$_2$ (113 mg, 0.365 mmol, 1.05 equiv) was added and the reaction mixture was stirred for 20 h at rt. Overnight, a purple precipitate formed, which was collected by filtration over a fine frit and washed with cold MeOH (3 × 10 mL) and cold pentane (3 × 10 mL). The solid was collected and re-dissolved in DCM (3 mL), filtered through glass wool into a 20 mL vial, layered with pentanes (6 mL), and cooled to –20 °C. After 24 h, dark purple crystals were collected and washed with cold MeOH (3 × 10 mL) and cold pentanes (3 × 10 mL) to yield **C2** as dark purple crystals (116 mg, 53%).

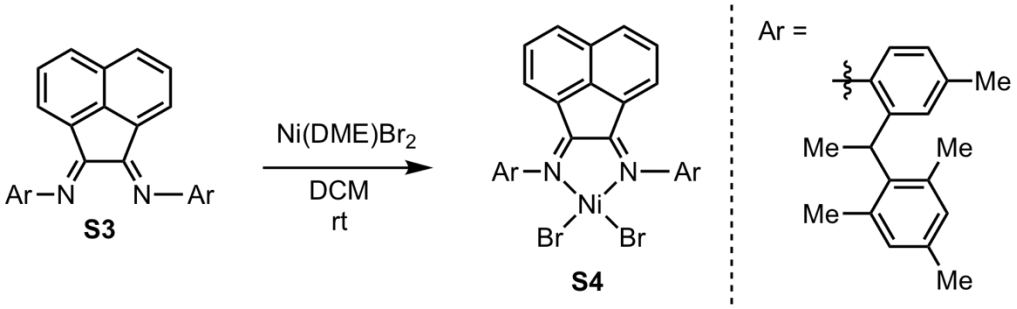


S2

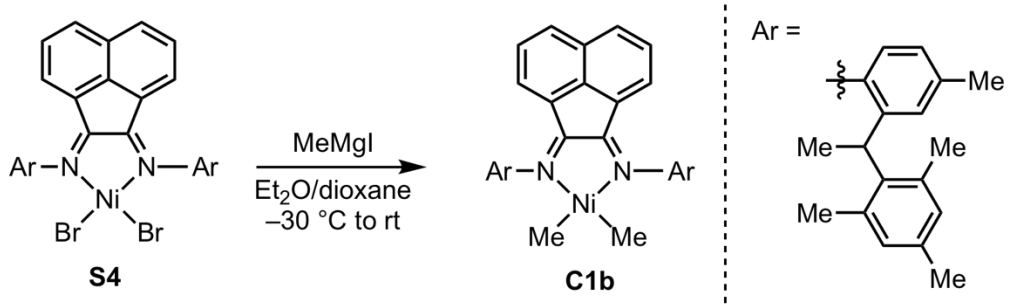
4-Methyl-2-(sec-(2,4,6-trimethylphenethyl)aniline (S2).[3] To a 15 mL bomb flask equipped with a stir bar, *p*-toluidine (1.36 g, 12.7 mmol, 1.46 equiv) was dissolved in xylenes (1.1 mL). Subsequently, 2,4,6-trimethylstyrene (1.40 mL, 8.67 mmol, 1.00 equiv) and triflic acid (200 µL, 2.25 mmol, 0.260 equiv) were added to the reaction flask, which was sealed and placed behind a blast shield. The solution was stirred for 17 h at 160 °C. Upon cooling to rt, the heterogeneous mixture was transferred to a 250 mL round-bottom flask with EtOAc (50 mL), concentrated, and purified via column chromatography on silica gel (100% hexanes to 80/20 hexanes/EtOAc) to give a brown oil, which was recrystallized in 10/1 hexanes/EtOAc to yield **S2** as a white solid (1.25 g, 57%). HRMS (ESI+): Calcd. for $C_{18}H_{23}N$ $[M+H]^+$ 254.1903; found 254.1899.



***Rac*-ArN=(An)=NAr (Ar = 4-methyl-2-(sec-(2,4,6-trimethylphenethyl)phenyl; An = acenaphthylene) (S3).**[3] To a 20 mL vial equipped with a stir bar, acenaphthenequinone (438 mg, 2.41 mmol, 0.490 equiv) and **S2** (1.25 mg, 4.92 mmol, 1.00 equiv) were dissolved in toluene (2.8 mL) and glacial acetic acid (5.5 mL, 96 mmol, 19 equiv). After 3 h at 100 °C, the resulting heterogeneous mixture was filtered over a fine frit, washed with cold MeOH (3 × 10 mL) and cold hexanes (3 × 10 mL), and dried under reduced pressure to yield **S3** as a yellow powder (1.13 g, 72%). HRMS (ESI+): Calcd. for $C_{48}H_{48}N_2$ $[M+H]^+$ 653.3890; found 653.3897.



***Rac*-(ArN=(An)=NAr)NiBr$_2$ (Ar = 4-methyl-2-(sec-(2,4,6-trimethylphenethyl)-phenyl; An = acenaphthylene) (S4).**[3] In a 50 mL Schlenk flask equipped with a stir bar, Ni(DME)Br$_2$ (156 mg, 0.505 mmol, 1.10 equiv) and **S3** (300 mg, 0.460 mmol, 1.00 equiv) were dissolved in DCM (15 mL) and stirred at rt under N_2 for 16 h. Then, the dark maroon liquid was concentrated, dissolved in DCM (20 mL), filtered through Celite, layered with pentane (60 mL), and cooled to –20 °C. The resulting solid was collected by filtration over a coarse frit, washed with cold pentane (3 × 10 mL), and dried under reduced pressure to yield **S4** as a dark maroon solid (338 mg, 90%).



***Rac*-(ArN=(An)=NAr)NiMe$_2$ (Ar = 4-methyl-2-(sec-(2,4,6-trimethylphenethyl)-phenyl; An = acenaphthylene) (C1b).** In a glovebox, **S4** (300 mg, 0.340 mmol, 1.00 equiv) and diethyl ether (40 mL) were added to a 100 mL Schlenk flask equipped with a stir bar. The red suspension was cooled in the freezer (–30 °C) for 10 min. Then, MeMgI (2.6 M in Et_2O, 0.28 mL, 0.72 mmol, 2.2 equiv) was added dropwise at –30 °C. The red suspension immediately turned dark purple. The Schlenk flask was placed back in the freezer for 10 min. Then dioxane (2.7 mL, 0.043 mmol, 0.13 equiv) was added and stirred for 2 h at rt after which time the solution was filtered through a frit, and the solvent was removed in vacuo until ~10 mL remained. Pentanes (~10 mL) were added to the solution, and the solvent was removed in vacuo until ~5 mL remained. The heterogeneous mixture was then filtered over a frit, washed with pentanes (3 × 5 mL), and dried under reduced pressure to yield **C1b** as a purple powder (130 mg, 52%).

IV. NMR Spectra

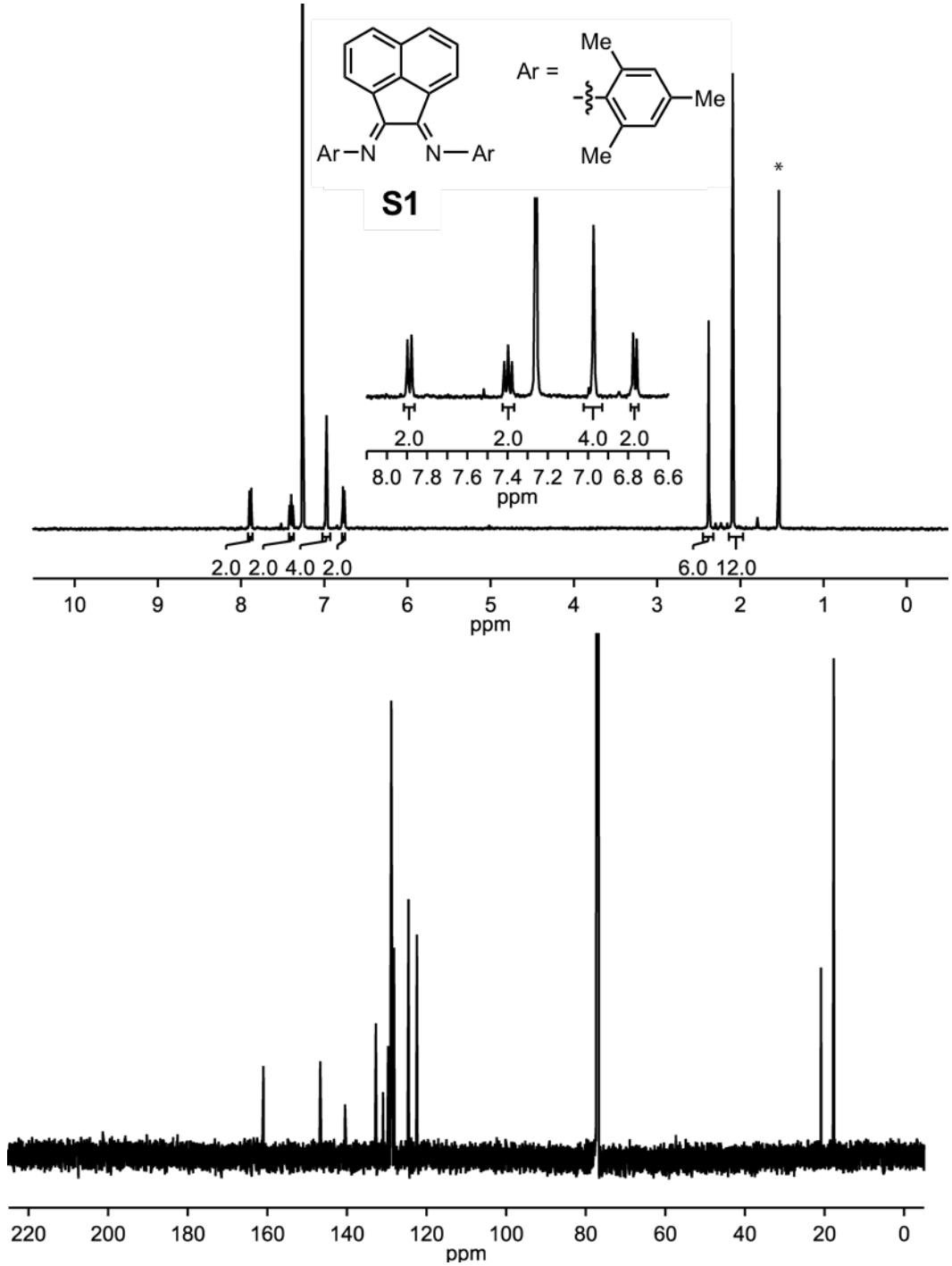


Figure S1. ^{1}H and ^{13}C NMR spectra of **S1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 2H), 6.96 (s, 4H), 6.75 (d, *J* = 7.3 Hz, 2H), 2.36 (s, 6H), 2.07 (s, 12H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 161.01, 146.73, 140.50, 132.76, 130.96, 129.67, 128.88, 128.72, 128.19, 124.55, 122.44, 20.92, 17.70.

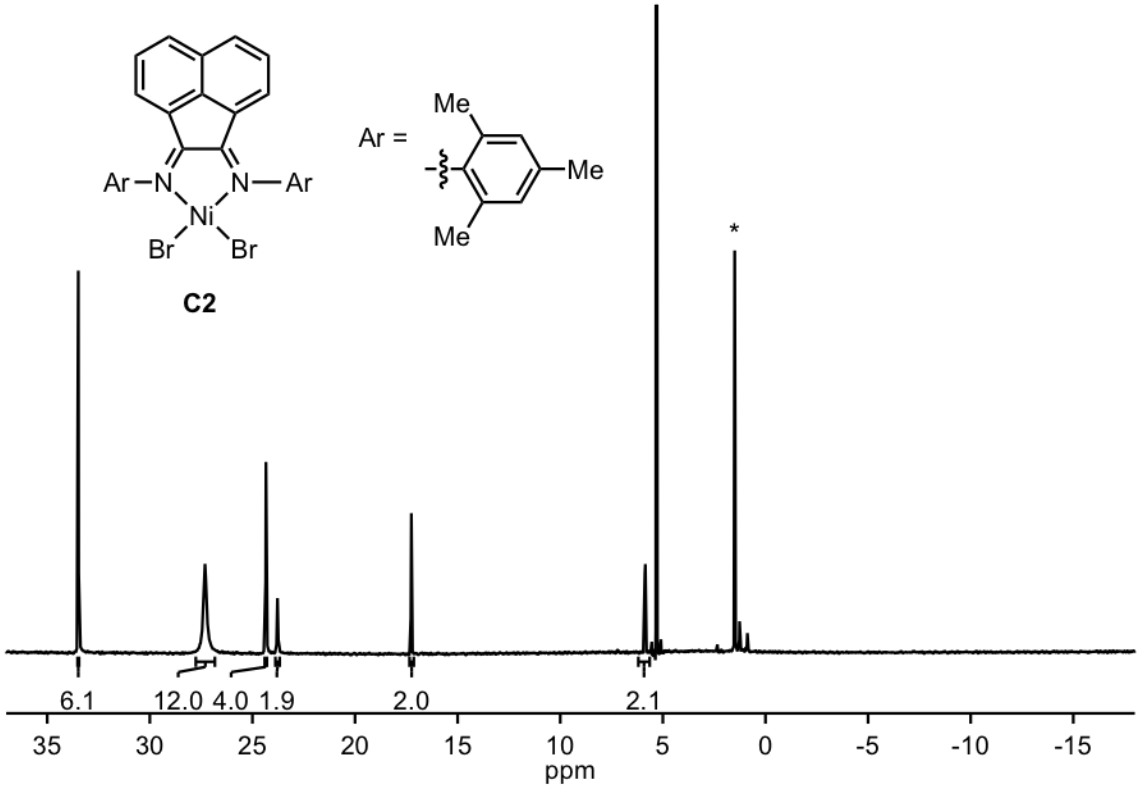


Figure S2. ^{1}H NMR spectrum of **C2**. ^{1}H NMR (400 MHz, CD_2Cl_2, rd = 0.005 s, at = 0.05 s) δ 33.77 (s, 6H), 27.54 (s, 12H), 24.49 (s, 4H), 23.93 (s, 2H), 17.35 (d, *J* = 7.9 Hz, 2H), 5.85 (s, 2H).

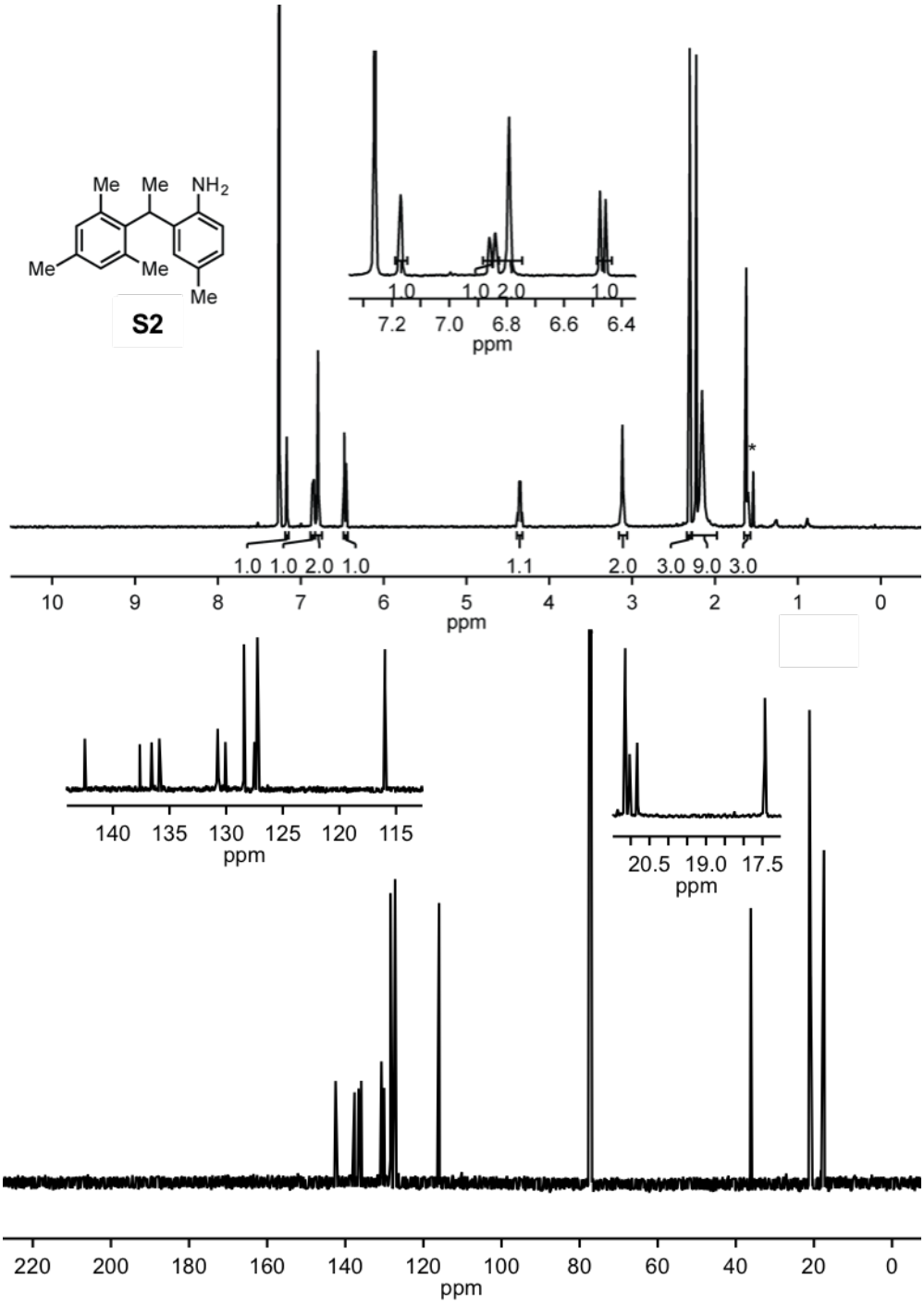


Figure S3. ^{1}H and ^{13}C NMR spectra of **S2**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (s, 1H), 6.85 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.80 (s, 2H), 6.47 (d, *J* = 7.9 Hz, 1H), 4.35 (q, *J* = 7.3 Hz, 1H), 3.12 (s, 2H), 2.30 (s, 3H), 2.19 (overlapping peaks, 9H), 1.61 (d, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.48, 137.63, 136.58, 135.90, 130.75, 130.07, 128.43, 127.50, 127.24, 115.98, 36.17, 21.15, 21.03, 20.83, 17.43.

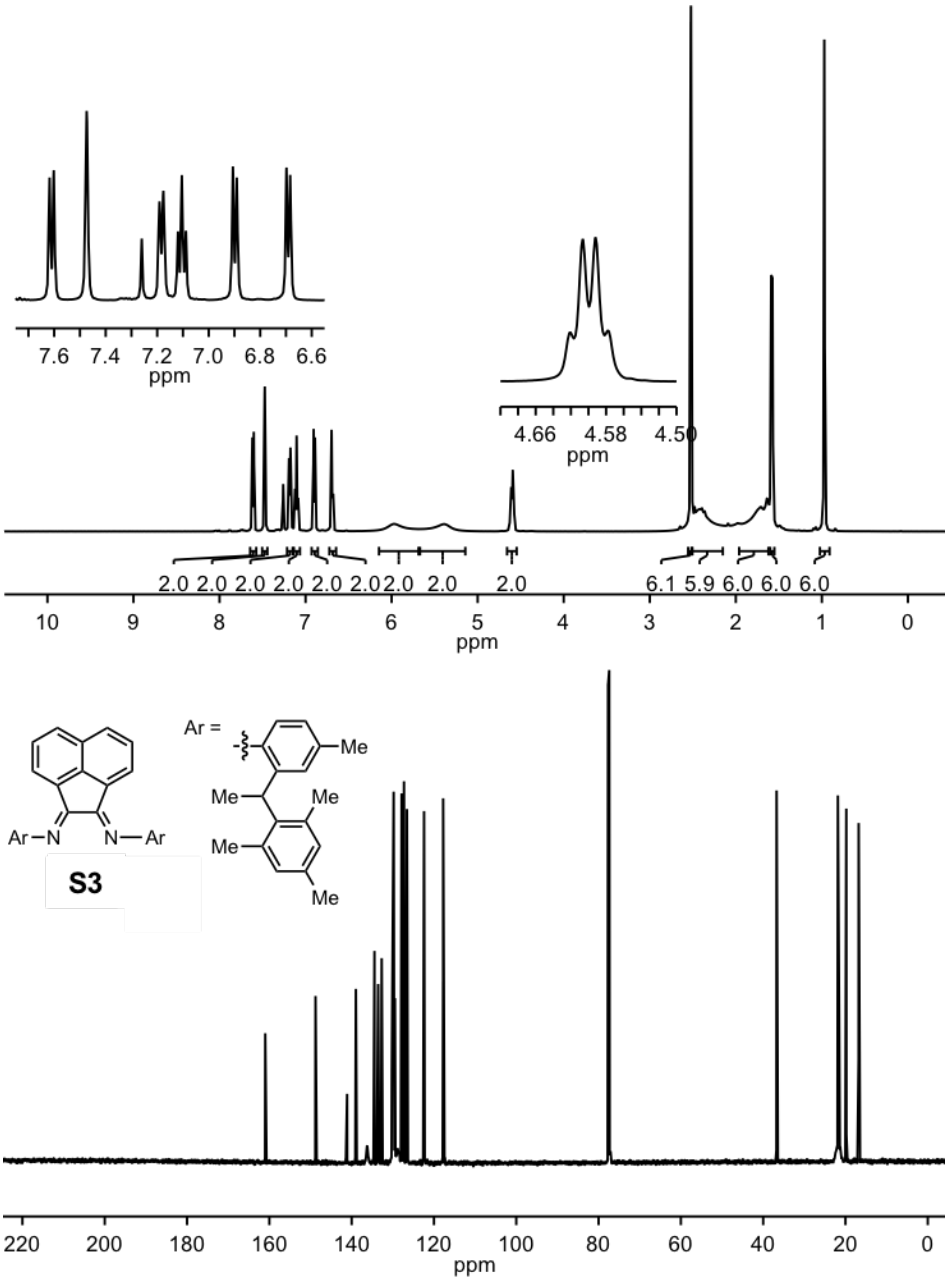


Figure S4. ^{1}H and ^{13}C NMR spectra of **S3**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.47 (s, 2H), 7.18 (d, *J* = 7.7 Hz, 2H), 7.10 (t, *J* = 7.7 Hz, 2H), 6.90 (d, *J* = 7.8 Hz, 2H), 6.69 (d, *J* = 7.2 Hz, 2H), 5.97 (br s, 2H), 5.39 (br s, 2H), 4.60 (q, *J* = 7.4 Hz, 2H), 2.52 (s, 6H), 2.41 (br s 6H), 1.62 (br s, 6H), 1.58 (d, *J* = 7.4 Hz, 6H), 0.97 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.00, 148.78, 141.11, 138.97, 136.22 (br), 134.46, 133.56, 132.70, 130.25, 129.80, 129.48, 128.78 (br), 127.85, 127.28, 126.57, 122.40, 117.77, 36.74, 21.84, 21.65 (br), 19.80, 16.80.

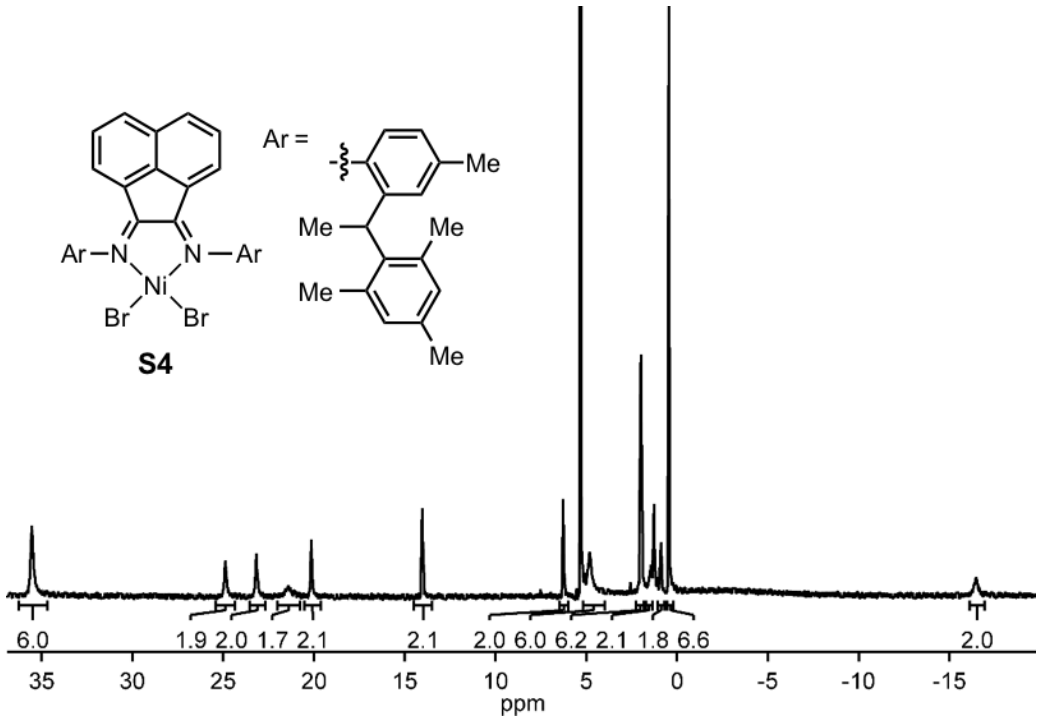


Figure S5. ^{1}H NMR spectrum of **S4**. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 35.53 (s, 6H), 24.88 (s, 2H), 23.17 (s, 2H), 21.45 (br s, 2H), 20.14 (s, 2H), 14.03 (s, 2H), 6.27 (s, 2H), 4.82 (br s, 6H), 1.99 (s, 6H), 1.44 (s, 2H) 0.87 (s, 2H), 0.45 (s, 6H), –16.43 (br s, 2H). Unaccounted for hydrogens (6H) due to peak broadening. Spectrum matches literature precedent.[3]

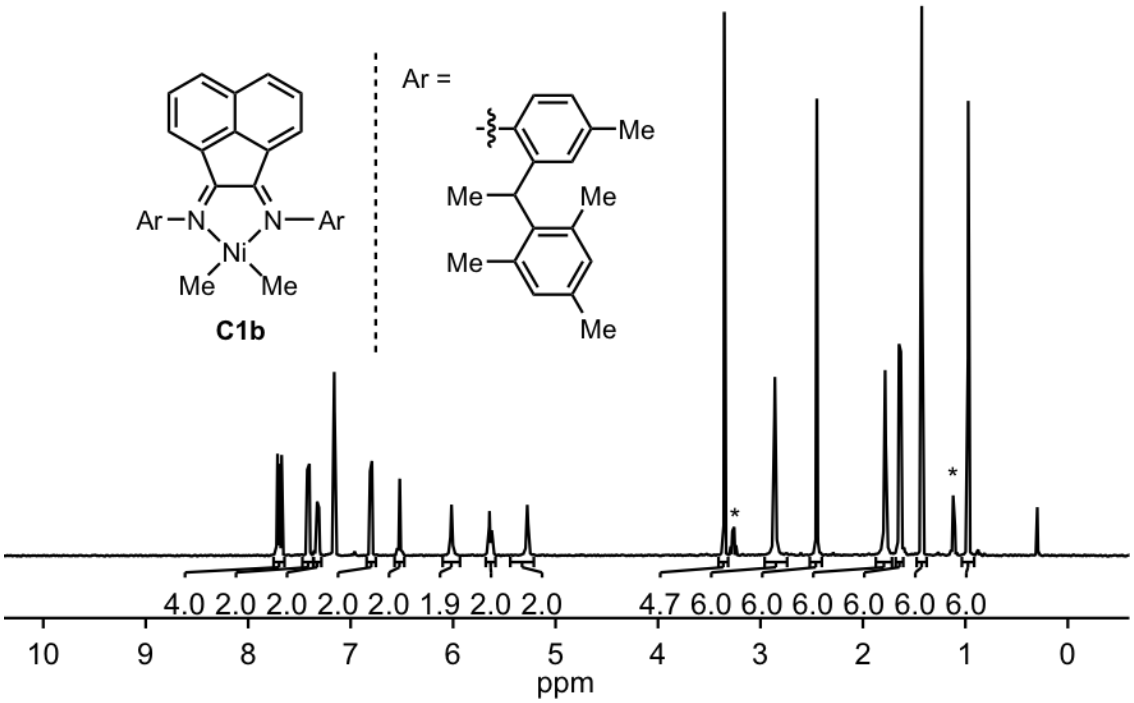
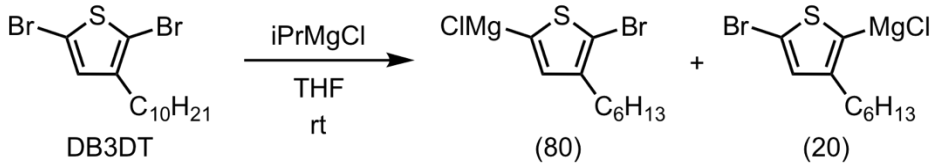


Figure S6. ^{1}H NMR spectrum of **C1b**: ^{1}H NMR (400 MHz, C_6D_6) δ 7.87–7.71 (m, 4H), 7.51 (d, *J* = 8.3 Hz, 2H), 7.42 (dd, *J* = 7.7, 1.7 Hz, 2H), 6.90 (d, *J* = 7.2 Hz, 2H), 6.69–6.54 (m, 2H), 6.12 (s, 2H), 5.74 (q, *J* = 7.4 Hz, 2H), 5.38 (s, 2H), 3.45 (s, 5H), 2.96 (s, 6H), 2.55 (s, 6H), 1.88 (s, 6H), 1.74 (d, J = 7.4 Hz, 6H), 1.53 (s, 6H), 1.07 (s, 6H).*indicates residual ether.

V. Me End-Capping Experiments

Precatalyst screen for ligand-exchange

Monomer activation:



DB3DT (80) (20)

In a glovebox, iPrMgCl (2.2 M in THF, 204 µL, 0.448 mmol, 0.800 equiv) was added to a stirring solution of DB3DT (214.0 mg, 0.5599 mmol, 1.000 equiv) in THF (5.40 mL) and stirred for 30 min at rt.

Preparing precatalysts:

$Ni(dppp)Cl_2$: $Ni(dppp)Cl_2$ (5.5 mg, 0.0101 mmol) was weighed into a 4 mL vial with a stir bar.

$Ni(IPr)(PPh_3)Cl_2$: $Ni(IPr)(PPh_3)Cl_2$ (5.5 mg, 0.0071 mmol) was weighed into a 4 mL vial and dissolved in THF (0.71 mL) for an overall concentration of 0.01 M.

$Pd(IPr)(3\text{-}Clpy)Cl_2$: $Pd(IPr)(3\text{-}Clpy)Cl_2$ (5.0 mg, 0.0074 mmol) was weighed into a 4 mL vial and dissolved in THF (0.74 mL) for an overall concentration of 0.01 M.

$Pd(IPent)(3\text{-}Clpy)Cl_2$: $Pd(IPent)(3\text{-}Clpy)Cl_2$ (2.6 mg, 0.0033 mmol) was weighed into a 4 mL vial and dissolved in THF (0.33 mL) for an overall concentration of 0.01 M.

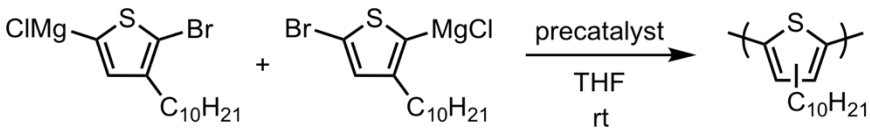
Preparing M(0) scavenger stock solution:

5,5'-Dibromo-2,2'-bithiophene (128 mg, 0.396 mmol) was dissolved in THF (5.27 mL) in a vial for an overall concentration of 0.075 M.

End-capping experiment vials:

5,5'-Dibromo-2,2'-bithiophene (0.075 M in THF, 0.80 mL, 0.060 mmol, 150 equiv – relative to the catalyst that will be added to this vial) and THF (0.36 mL) were added to a 20 mL vial equipped with a stir bar.

Polymerizations:



Polymerization procedure for precatalysts $Ni(IPr)(PPh_3)Cl_2$, $Pd(IPr)(3\text{-}Clpy)Cl_2$, and $Pd(IPent)(3\text{-}Clpy)Cl_2$: In a glovebox, to a 20 mL vial equipped with a stir bar was added THF (3.57 mL), Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv), and precatalyst

(0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv) and stirred at rt for the following times Ni(IPr)(PPh_3)Cl_2 (5 min), Pd(IPr)(3-Clpy)Cl_2 (15 min), and Pd(IPent)(3-Clpy)Cl_2 (30 min).

Polymerization procedure for precatalyst Ni(dppp)Cl_2: In a glovebox, Ni(dppp)Cl_2 (5.5 mg, 0.010 mmol) was preinitiated by stirring with activated monomer (0.08 M in THF, 0.38 mL, 0.030 mmol, 3.0 equiv) for 60 s. The preactivated catalyst solution ([Ni] = 0.027 M in THF, 0.068 mL, 0.0018 mmol, 1.0 equiv) was added to a 20 mL vial equipped with a stir bar containing THF (3.50 mL) and Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 22 equiv) and stirred at rt for 30 min.

In situ end-capping:
An aliquot (1.0 mL each containing 0.00040 mmol catalyst, *new* 1.0 equiv) was removed from the polymerization and added to the end-capping experiment reaction vial. Then MeMgI (0.24 M in Et_2O, 50. µL, 0.012 mmol, 30. equiv) was added to the end-capping reaction vial (note that adding MeMgI after the polymer was added was necessary to avoid forming a white precipitate, which forms if MeMgI is stirred in THF in the absence of catalyst). The remaining polymerization solution was removed from the glovebox, quenched with aq. HCl (12 M, 2 mL), and worked up for analysis by GC, SEC, and MALDI-TOF/MS analysis (see general experimental, "before end-capping" for Table S2). Unless otherwise noted, the end-capping experiment reactions were stirred for 1 h (the end-capping reaction with Ni(dppp)Cl_2 was stirred for 14 h) before treating outside the glovebox with aq. HCl (12 M, 1 mL) and working up for SEC and MALDI-TOF/MS ("after end-capping" for Table S2).

Table S1. GC data from the polymerization of 3-decylthiophene at rt via Ni and Pd precatalysts before end-capping experiments.

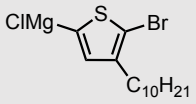
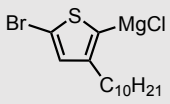
	 **(% conv.)**	 **(% conv.)**
Ni(dppp)Cl_2	72	0
Ni(IPr)(PPh_3)Cl_2	quant.	quant.
Pd(IPr)(3-Clpy)Cl_2	quant.	49
Pd(IPent)(3-Clpy)Cl_2	71	33

Table S2. SEC data from the polymerization of 3-decylthiophene at rt via Ni and Pd precatalysts before and after end-capping experiments.

	before end-capping		after end-capping	
	M_n (kg/mol)	Đ	M_n (kg/mol)	Đ
Ni(dppp)Cl_2	10.15	1.14	9.45	1.15
Ni(IPr)(PPh_3)Cl_2	8.42	1.17	8.94	1.15
Pd(IPr)(3-Clpy)Cl_2	7.34	1.18	7.38	1.24
Pd(IPent)(3-Clpy)Cl_2	5.26	1.35	4.73	1.76

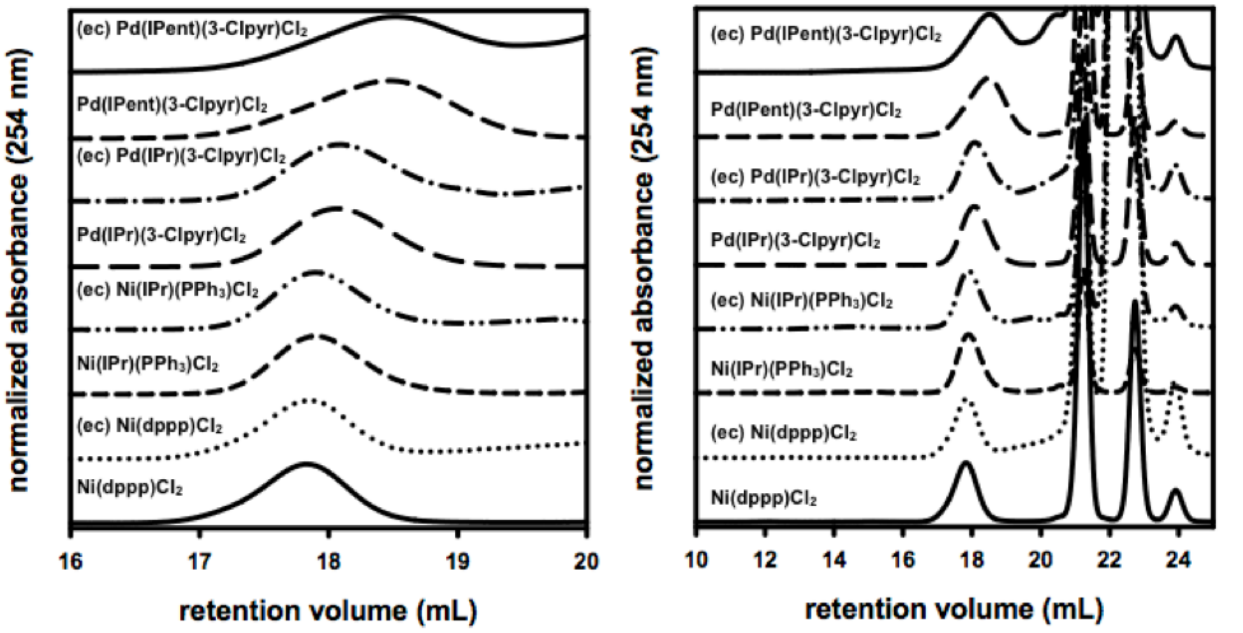


Figure S7. SEC data from the polymerization of 3-decylthiophene at rt via Ni and Pd precatalysts before and after end-capping experiments (ec). Zoomed (left) and full traces (right) of the same experiment are shown. Note that M(0) scavenging agent and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min, and BHT elutes at 23.8 min.

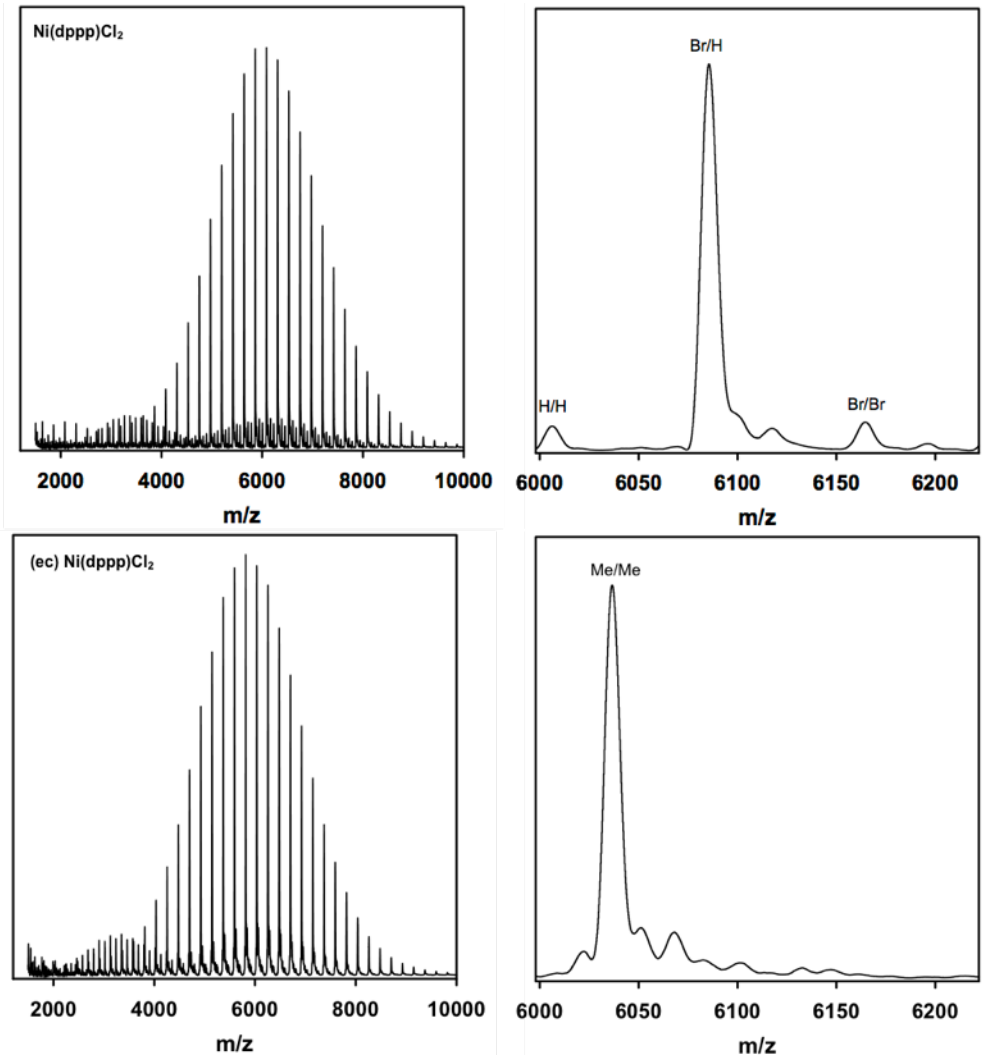


Figure S8. MALDI-TOF/MS spectra of the polymerization of 3-decylthiophene at rt via $Ni(dppp)Cl_2$ before and after end-capping experiments (ec). Full trace (left) zoomed image (right). Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 27.

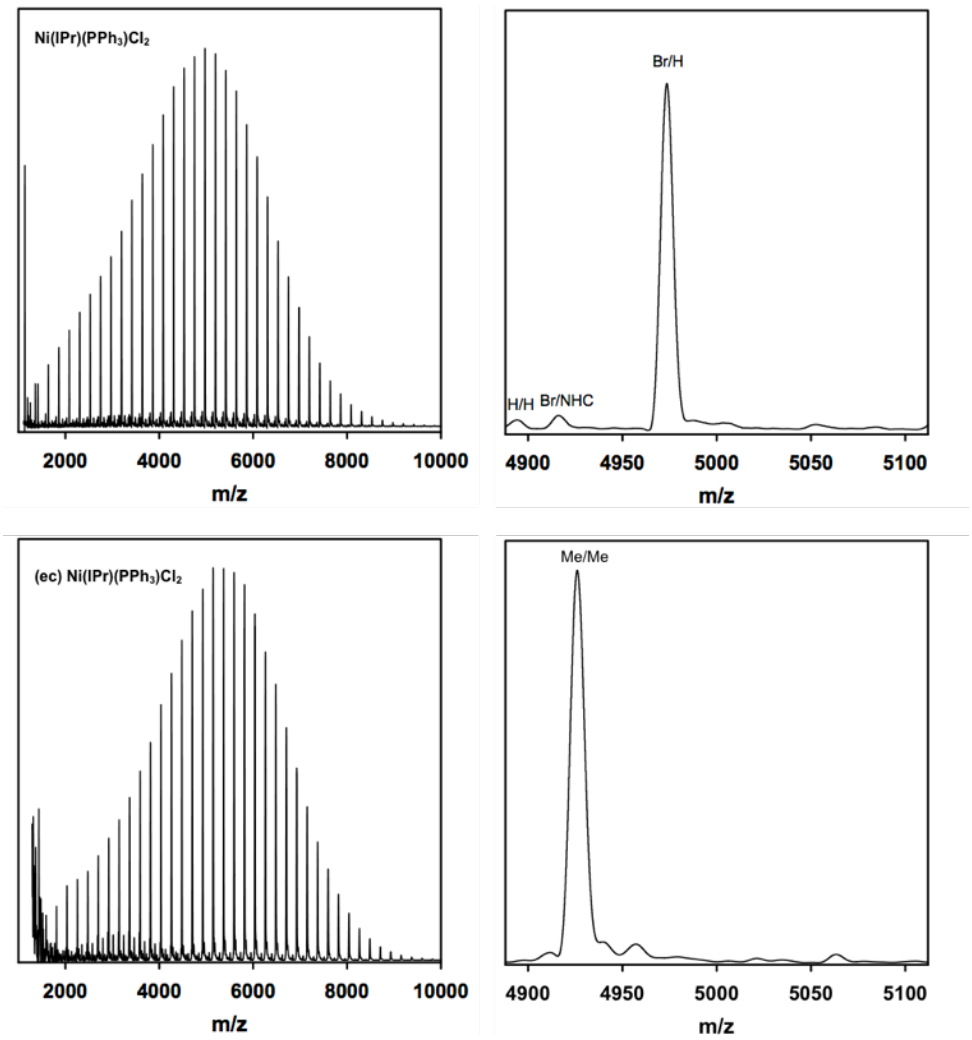


Figure S9. MALDI-TOF/MS spectra of the polymerization of 3-decylthiophene at rt via $Ni(IPr)(PPh_3)Cl_2$ before and after end-capping experiments (ec). Full trace (left) zoomed image (right). Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 22.

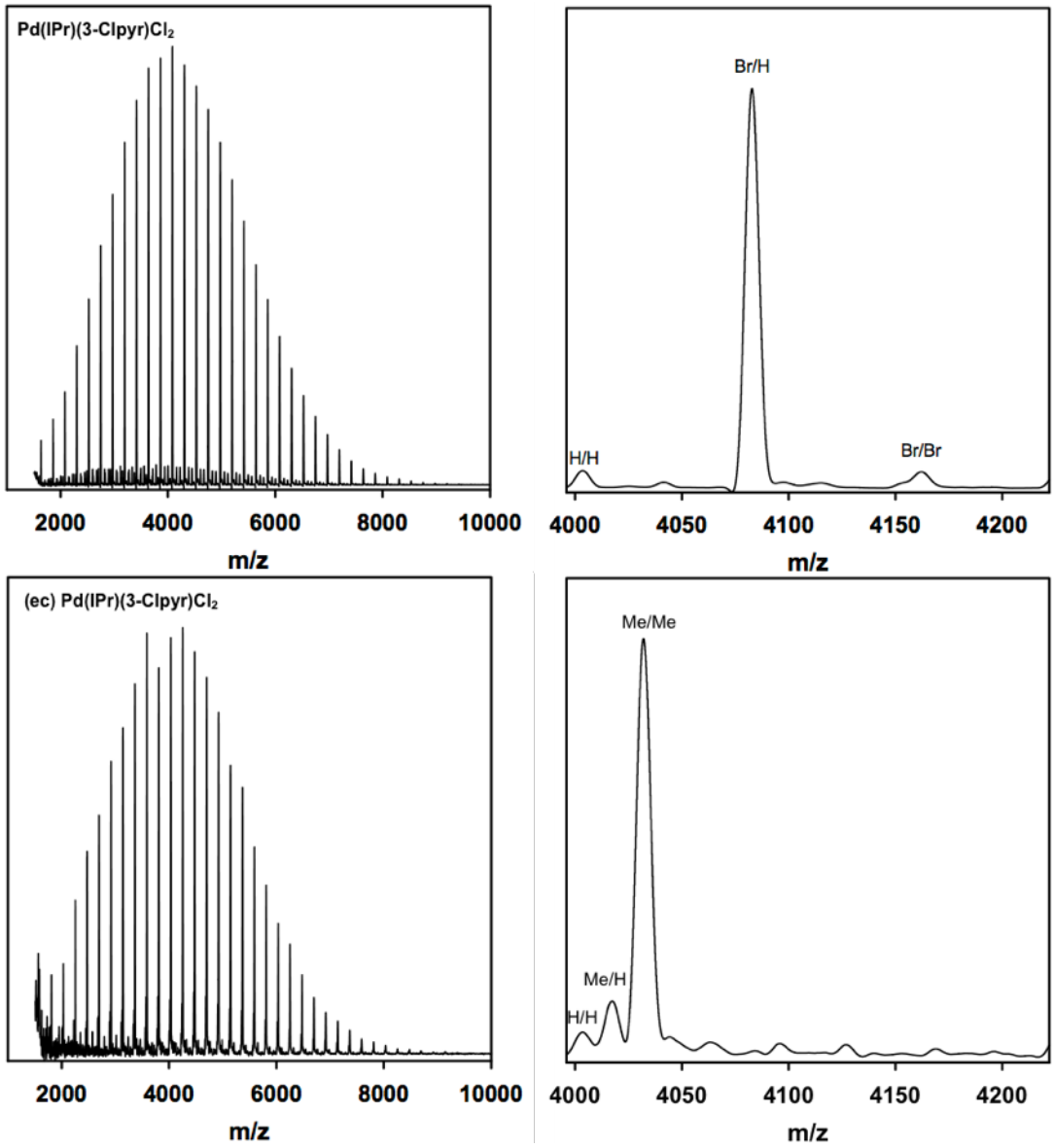


Figure S10. MALDI-TOF/MS spectra of the polymerization of 3-decylthiophene at rt via Pd(IPr)(3-Clpy)Cl_2 before and after end-capping experiments (ec). Full trace (left) zoomed image (right). Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 18.

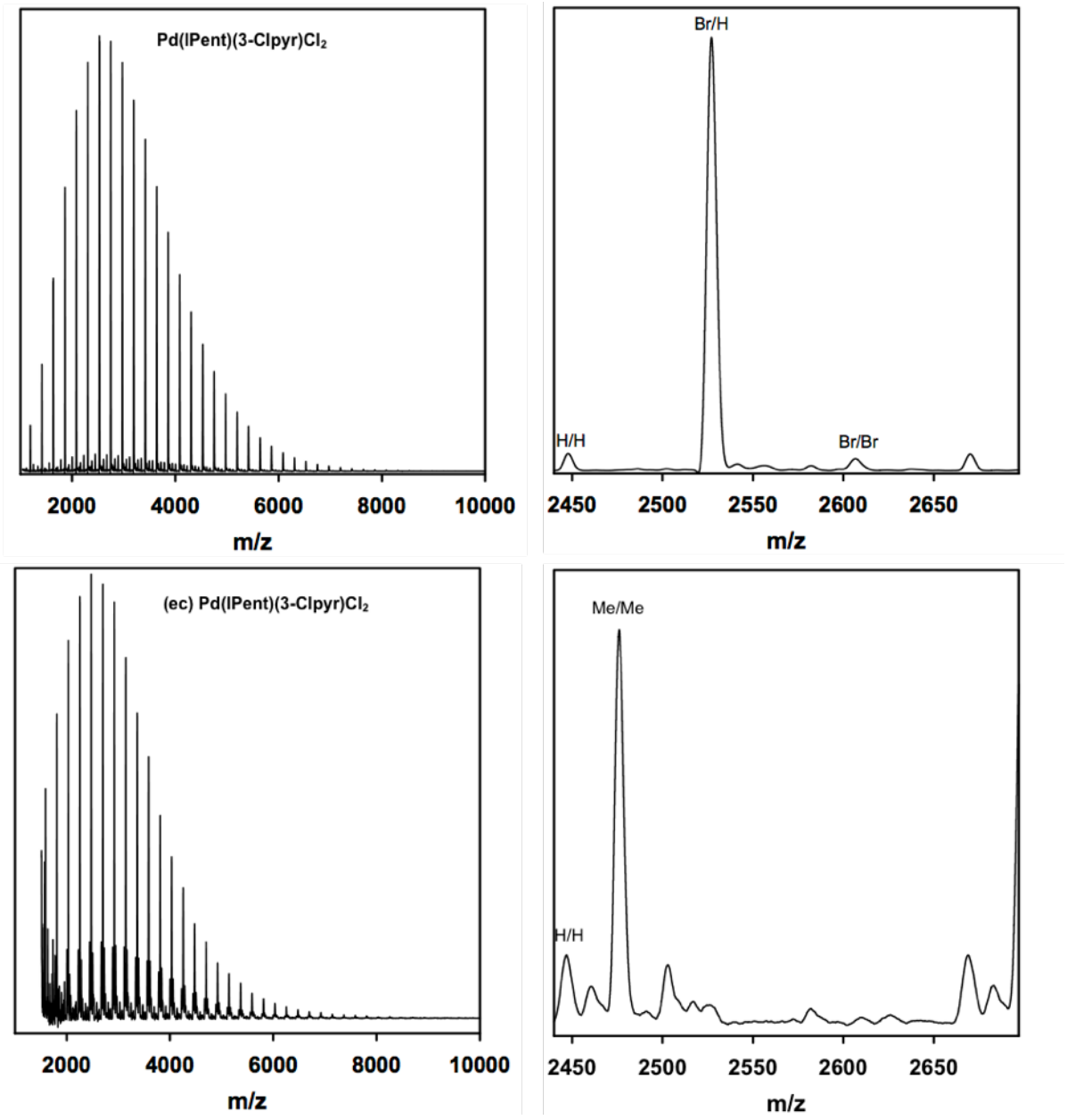
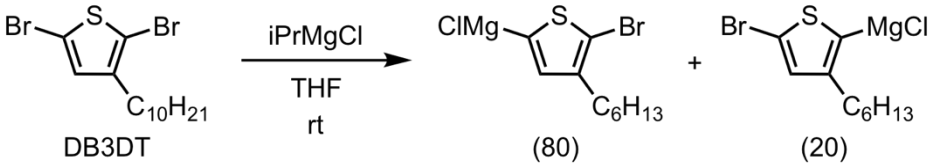


Figure S11. MALDI-TOF/MS spectra of the polymerization of 3-decylthiophene at rt via Pd(IPent)(3-Clpy)Cl_2 before and after end-capping experiments (ec). Full trace (left) zoomed image (right). Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 11.

Ligand exchange thiophene polymerization followed by end-capping

Monomer activation:



In a glovebox, iPrMgCl (2.2 M in THF, 140 µL, 0.307 mmol, 0.800 equiv) was added to a stirring solution of DB3DT (147 mg, 0.384 mmol, 1.00 equiv) in THF (3.7 mL) and stirred for 30 min at rt.

Preparing stock solutions:

C2: **C2** (11.0 mg, 0.0173 mmol) was weighed into a 4 mL vial and dissolved in THF (1.73 mL) for an overall concentration of 0.01 M.

IPr: IPr (6.0 mg, 0.018 mmol) was weighed into a 4 mL vial and dissolved in THF (1.8 mL) for an overall concentration of 0.01 M.

PPh_3: PPh_3 (4.3 mg, 0.016 mmol) was weighed into a 4 mL vial and dissolved in THF (1.6 mL) for an overall concentration of 0.01 M.

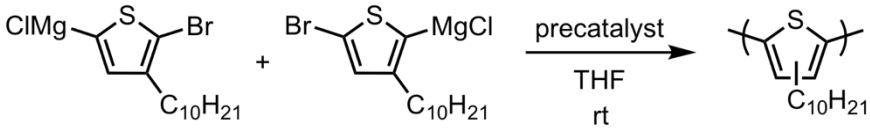
py: py (20 µL, 0.25 mmol) was weighed into a 4 mL vial and dissolved in THF (2.5 mL) for an overall concentration of 0.1 M.

M(0) scavenger: 5,5'-Dibromo-2,2'-bithiophene (111 mg, 0.342 mmol) was dissolved in THF (4.56 mL) in an 8 mL vial for an overall concentration of 0.075 M.

End-capping experiment vials:

5,5'-Dibromo-2,2'-bithiophene (0.075 M in THF, 0.80 mL, 0.060 mmol, 150 equiv – relative to the catalyst that will be added to this vial) and THF (0.36 mL) were added to a 20 mL vial equipped with a stir bar.

Polymerizations:



Polymerization procedure for **C2** only: In a glovebox, to a 20 mL vial equipped with a stir bar was added THF (3.57 mL) and **C2** (0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv) and stirred for 15 min (to be consistent with the following reactions). Then, Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv) was added and stirred at rt for 6 min.

Polymerization procedure for **C2** and IPr only: In a glovebox, to a 20 mL vial equipped with a stir bar was added THF (3.38 mL), **C2** (0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv) and IPr (0.01 M in THF, 0.192 mL, 0.00192 mmol, 1.20 equiv) and stirred for 15 min. Then, Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv) was added and stirred at rt for 6 min.

Polymerization procedure for **C2**, IPr, and PPh_3: In a glovebox, to a 20 mL vial equipped with a stir bar was added in the following order, THF (3.19 mL), **C2** (0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv), IPr (0.01 M in THF, 0.192 mL, 0.00192 mmol, 1.20 equiv), and PPh_3 (0.01 M in THF, 0.192 mL, 0.00192 mmol, 1.20 equiv) and stirred for 15 min. Then, Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv) was added and stirred at rt for 6 min.

Polymerization procedure for **C2**, IPr, and py: In a glovebox, to a 20 mL vial equipped with a stir bar was added in the following order, THF (3.36 mL), **C2** (0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv), py (0.1 M in THF, 0.0192 mL, 0.00192 mmol, 1.20 equiv), and IPr (0.01 M in THF, 0.192 mL, 0.00192 mmol, 1.20 equiv) and stirred for 15 min. Then, Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv) was added and stirred at rt for 6 min.

Polymerization procedure for **C2**, IPr, py, and 1-hexene: In a glovebox, to a 20 mL vial equipped with a stir bar was added in the following order, THF (2.86 mL), 1-hexene (0.5 mL, ~2500 equiv relative to Ni), **C2** (0.01 M in THF, 0.160 mL, 0.00160 mmol, 1.00 equiv), py (0.1 M in THF, 0.0192 mL, 0.00192 mmol, 1.20 equiv), and IPr (0.01 M in THF, 0.192 mL, 0.00192 mmol, 1.20 equiv) and stirred for 15 min. Then, Grignard monomer solution (0.080 M in THF, 0.50 mL, 0.040 mmol, 25 equiv) was added and stirred at rt for 6 min.

In situ end-capping:
An aliquot (1.0 mL containing 0.00040 mmol catalyst, 1.0 equiv) was removed from the polymerization and added to the end-capping experiment reaction vial. Then, MeMgI (0.24 M in Et_2O, 50. µL, 0.012 mmol, 30. equiv) was added (note that adding MeMgI after the polymer was necessary to avoid forming a white precipitate, which forms if MeMgI is stirred in THF in the absence of catalyst). The remaining polymerization solution was removed from the glovebox, quenched with aq. HCl (12 M, 2 mL), and worked up for analysis by GC, SEC, and MALDI-TOF/MS analysis (see general experimental). The end-capping experiments were stirred for 1 h before quenching outside the glovebox with aq. HCl (12 M, 1 mL) and working up for SEC and MALDI-TOF/MS.

Table S3. GC data from the polymerization of 3-decylthiophene to evaluate IPr ligand-exchange effectiveness. GC data is acquired from the polymerizations before end-capping is done.

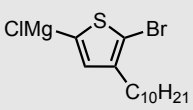
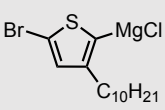
	 (% conv.)	 (% conv.)
C2	quant.	quant.
C2 and IPr	quant.	quant.
C2, IPr, and PPh_3	quant.	quant.
C2, IPr, and py	84	49
C2, IPr, py, and 1-hexene	59	38

Table S4. SEC data from the polymerization of 3-decylthiophene to evaluate IPr ligand-exchange effectiveness. SEC data is acquired from the polymerizations before and after end-capping is done.

	before end-capping		**after end-capping**	
	M_n (kg/mol)	**Đ**	**M_n (kg/mol)**	**Đ**
C2	9.99	1.72	8.58	1.68
C2 and IPr	11.04	1.92	8.88	1.82
C2, IPr, and PPh_3	5.64*	3.23*	5.01**	17.12**
C2, IPr, and py	5.52	1.22	4.29	1.23
C2, IPr, py, and 1-hexene	5.79	1.23	4.39	1.21

*bimodal or **trimodal SEC trace

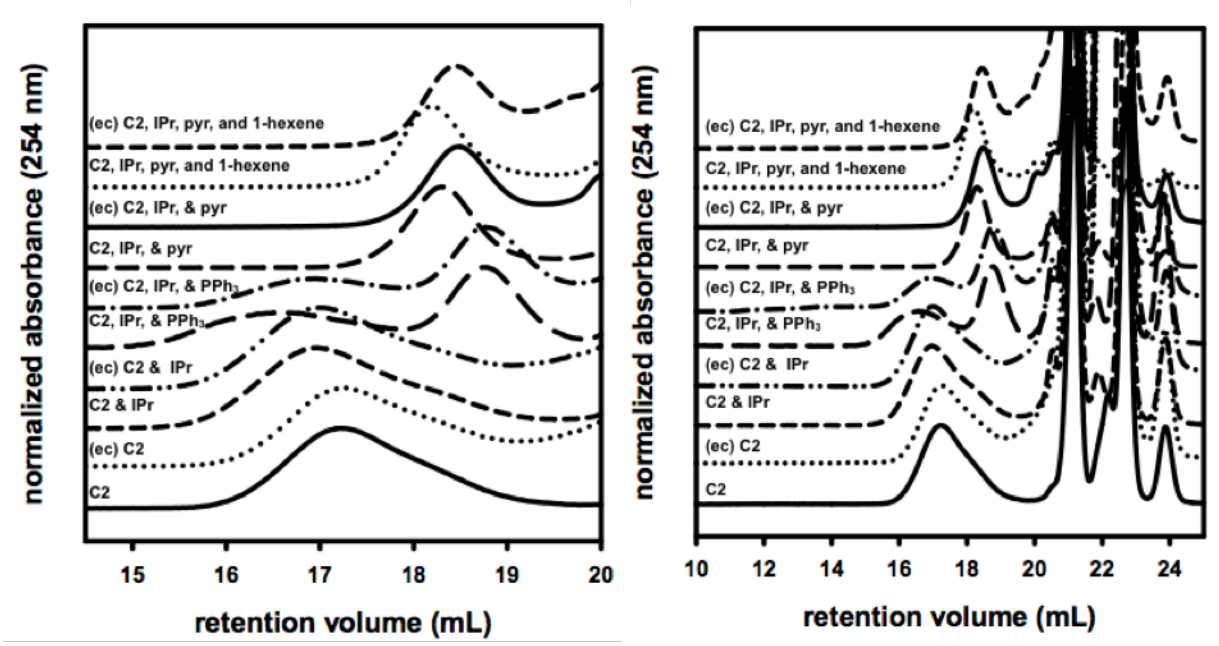


Figure S12. SEC data from the polymerization of 3-decylthiophene to evaluate IPr ligand-exchange effectiveness before and after (ec) end-capping experiments. Zoomed (left) and full traces (right) of the same experiment are shown. Note that M(0) scavenging agent and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

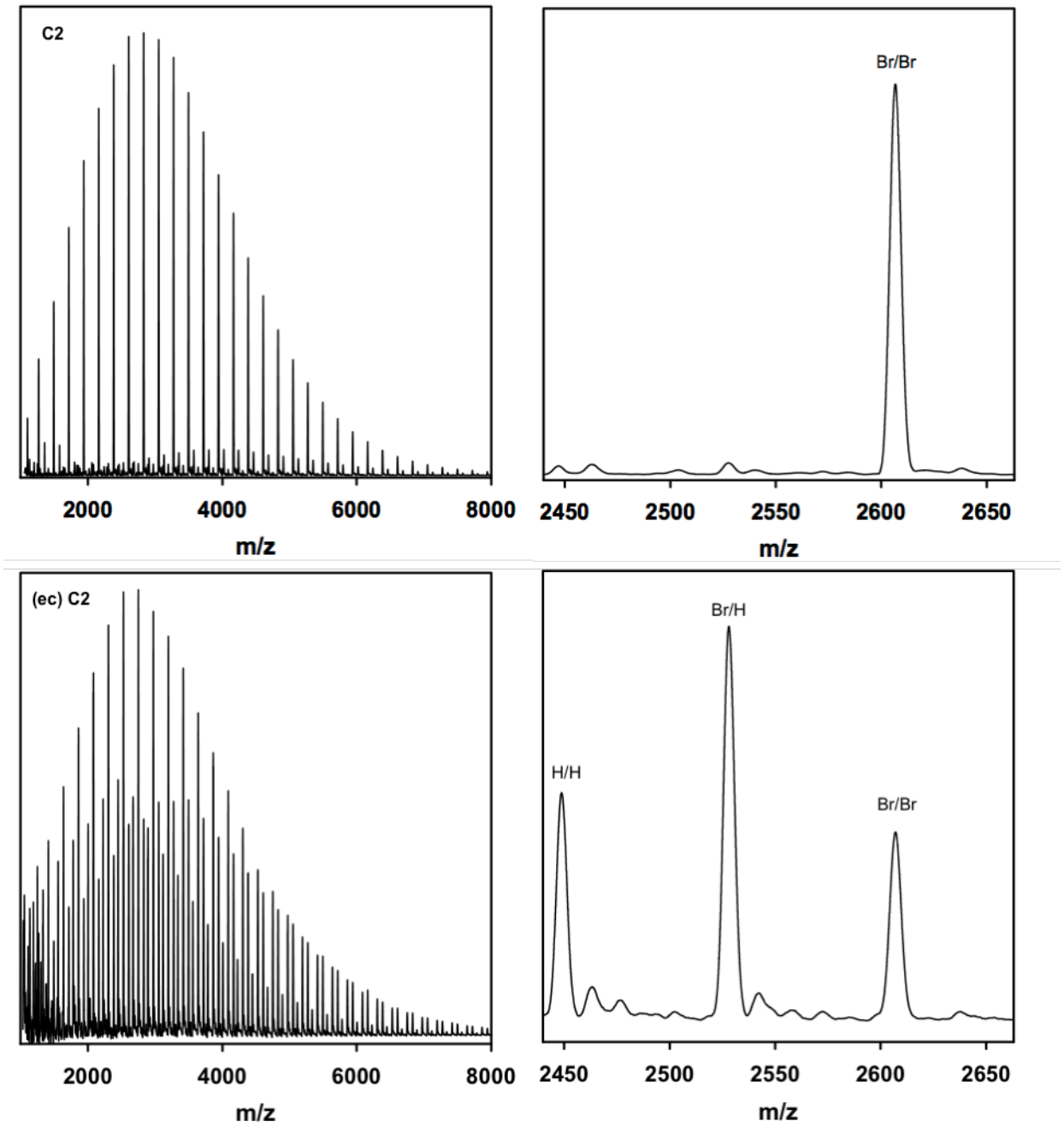


Figure S13. MALDI-TOF/MS data from the polymerization of 3-decylthiophene using precatalyst **C2** before and after (ec) end-capping experiments. Full traces (left) and zoomed (right) of the same experiment are shown. Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 11.

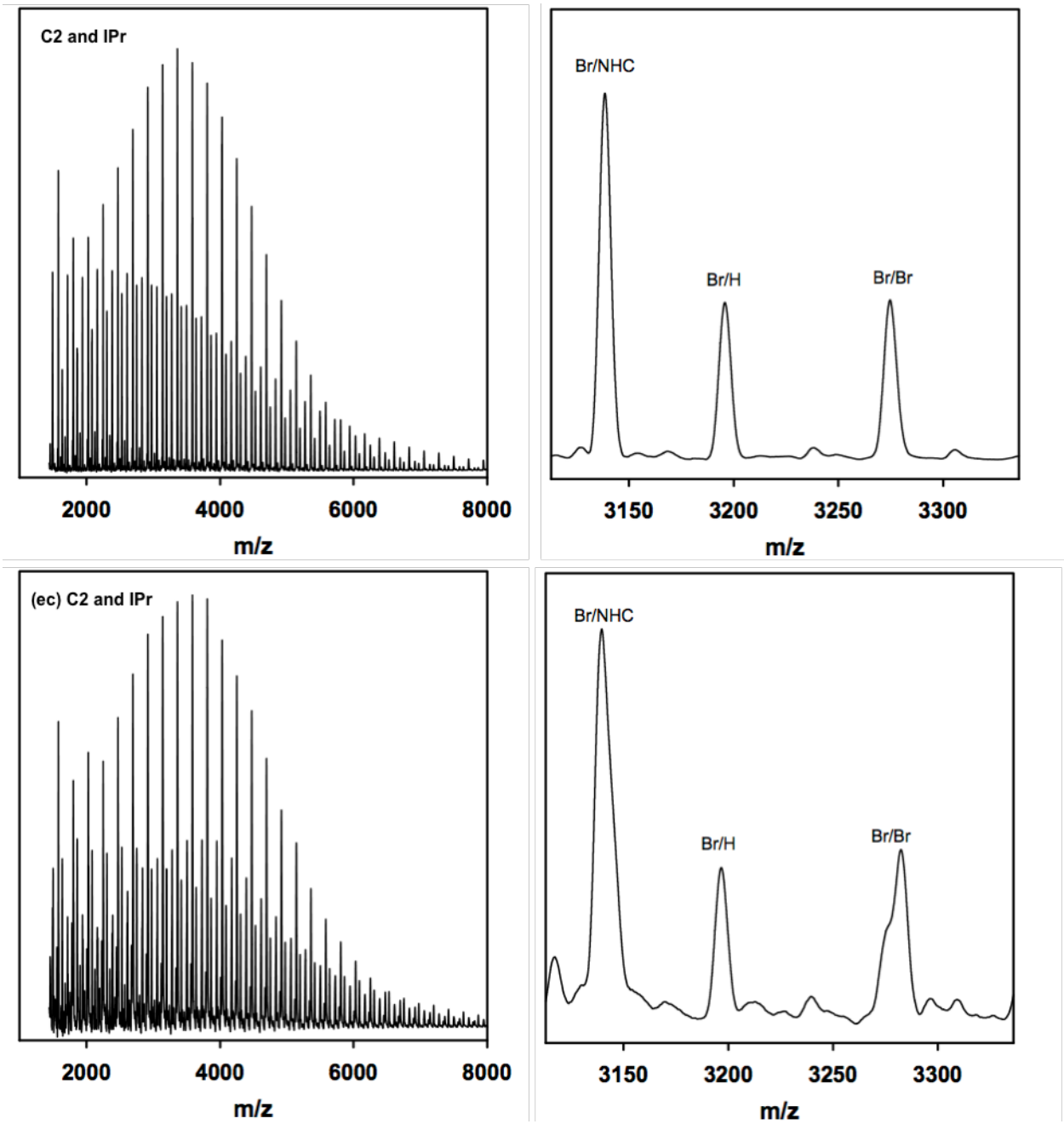


Figure S14. MALDI-TOF/MS data from the polymerization of 3-decylthiophene using precatalyst **C2** treated with IPr before and after (ec) end-capping experiments. Full traces (left) and zoomed (right) of the same experiment are shown. Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 14.

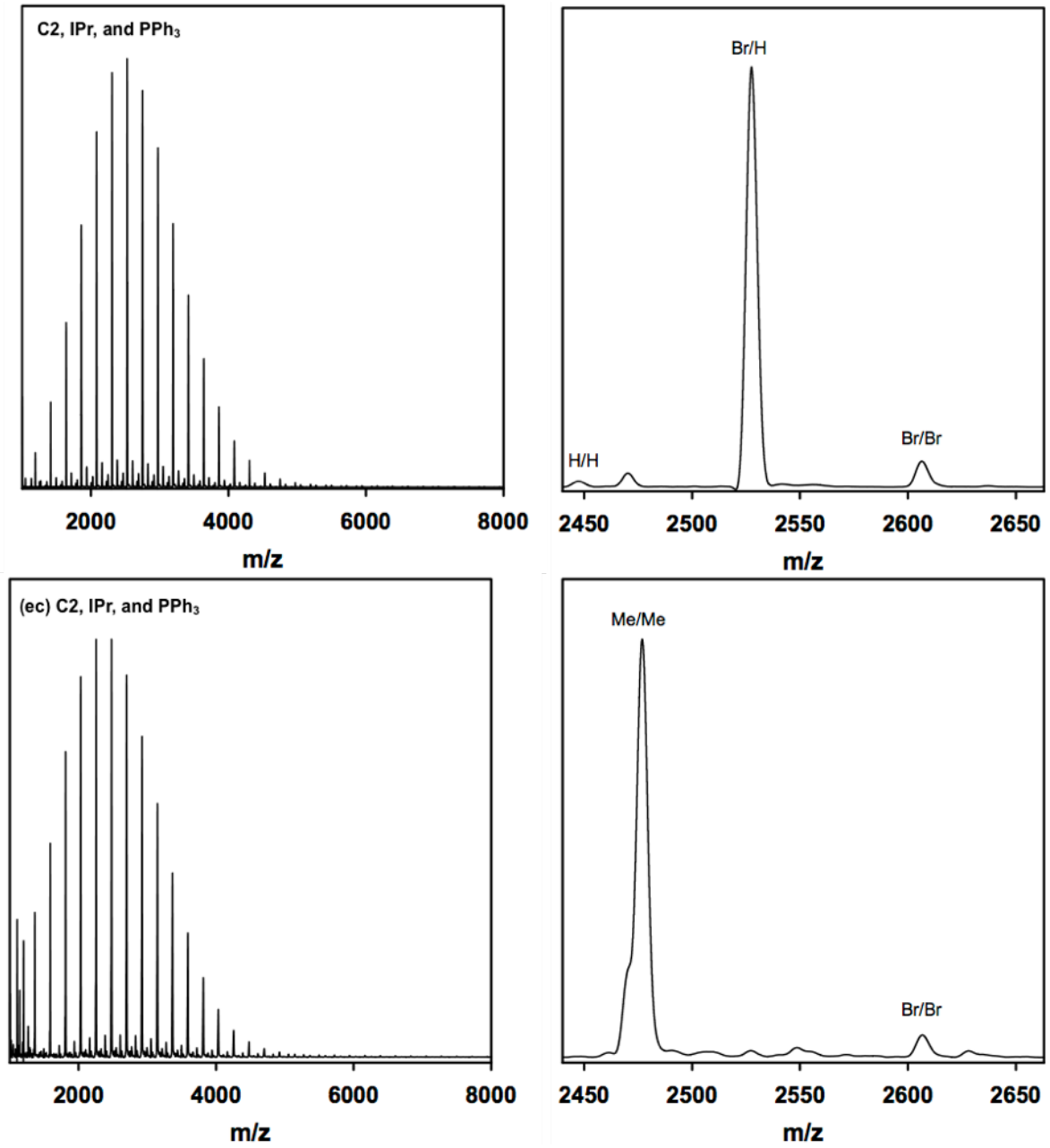


Figure S15. MALDI-TOF/MS data from the polymerization of 3-decylthiophene using precatalyst **C2** treated with IPr and PPh_3 before and after (ec) end-capping experiments. Full traces (left) and zoomed (right) of the same experiment are shown. Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 11. Note that the SEC trace indicates high molecular weight polymer was formed however these polymers did not ionize here.

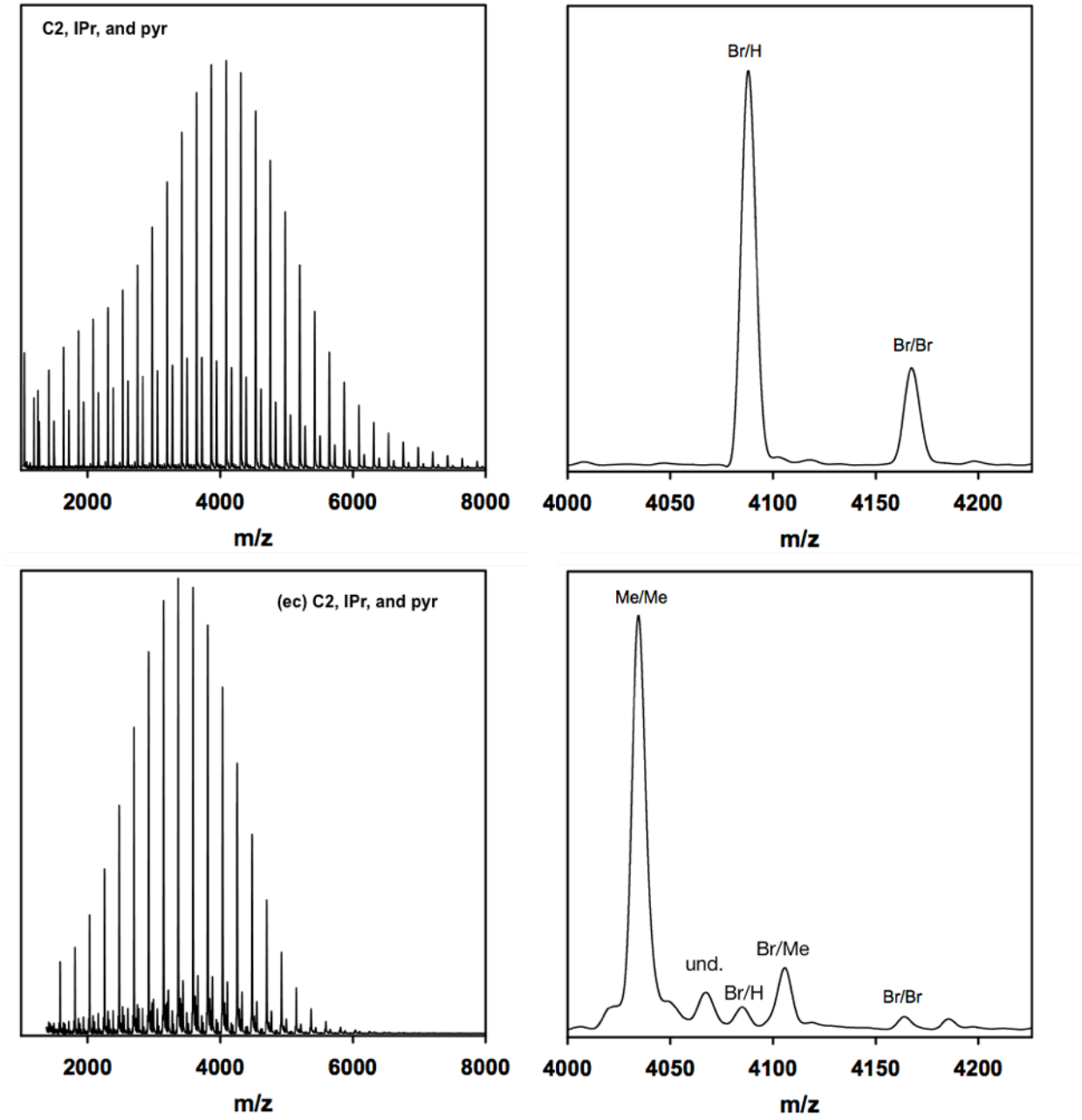


Figure S16. MALDI-TOF/MS data from the polymerization of 3-decylthiophene using precatalyst **C2** treated with py and IPr before and after (ec) end-capping experiments. Full traces (left) and zoomed (right) of the same experiment are shown. Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 18.

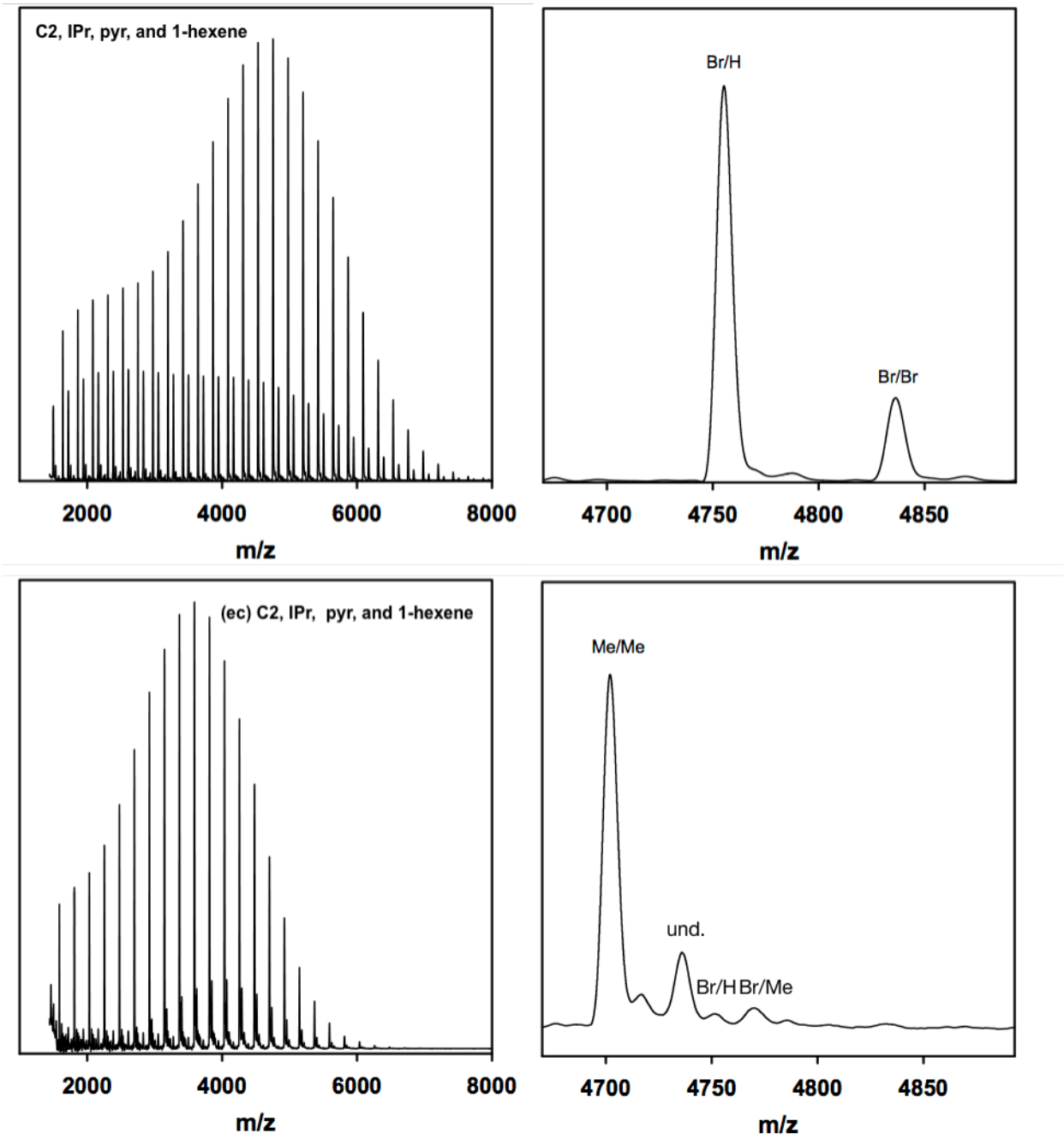
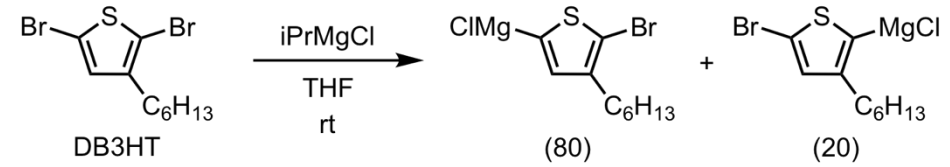


Figure S17. MALDI-TOF/MS data from the polymerization of 3-decylthiophene in the presence of 1-hexene using precatalyst **C2** treated with py and IPr before and after (ec) end-capping experiments. Full traces (left) and zoomed (right) of the same experiment are shown. Values calculated using average mass method, signal-to-noise = 2. The degree of polymerization shown is 21.

VI. Attempted Copolymerization

Standard copolymerization conditions

Thiophene monomer activation:



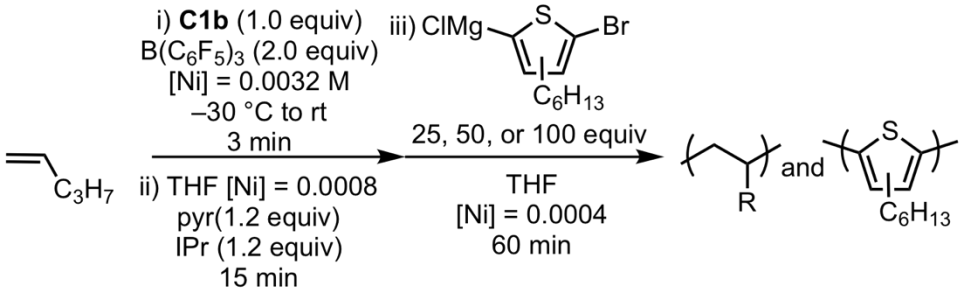
In a 20 mL vial equipped with a stir bar, DB3HT (92.7 mg, 0.284 mmol, 1.00 equiv) was dissolved in THF (2.73 mL) and reacted with iPrMgCl (2.1 M in THF, 108 µL, 0.227 mmol, 0.799 equiv) and stirred for 30 min at rt.

Preparing stock solutions:

IPr (4.8 mg, 0.012 mmol) was dissolved in THF (1.2 mL) for an overall concentration of 0.010 M, which is stored in the freezer (–30 °C).

Pyridine (20 µL, 0.25 mmol) was dissolved in THF (2.28 mL) for an overall concentration of 0.10 M.

Tris(pentafluorophenyl) borane (BCF, 14.0 mg, 0.0273 mmol) was dissolved in 1-pentene (3.79 mL) for an overall concentration of 0.00720 M, which was placed in the freezer (–30 °C).



Macroinitiator synthesis:

Precatalyst **C1b** (8.2 mg, 0.011 mmol) was dissolved in 1-pentene (0.40 mL) and placed in the freezer (–30 °C) for 2 min. Then, while both **C1b** and BCF were still cold, BCF (0.0072 M in 1-pentene, 3.06 mL, 0.0221 mmol, 2.00 equiv) was added to the stirring catalyst, which were stirred for 3 min at rt. Overall [Ni] = 0.0032 M in 1-pentene. Then, THF (10.42 mL) was added to stall the polymerization. Overall [Ni] = 0.0008 M in 1-pentene/THF (total volume = 13.88 mL). An aliquot (2.0 mL) was removed from the glovebox and immediately quenched with MeOH (5 mL).

Ligand-exchange:

To the remaining macroinitiator solution (0.0095 mmol Ni remain), py (0.10 M in THF, 114 µL, 0.0114 mmol, 1.20 equiv) and IPr (0.010 M in THF, 1.14 mL, 0.0114 mmol, 1.20 equiv) were

added and stirred for 15 min at rt. Overall [Ni] = 0.00072 M in 1-pentene/THF (total volume = 13.13 mL).

Thiophene addition:
Three aliquots (0.00072 M Ni in THF/1-pentene, 1.50 mL each, 0.00109 mmol Ni, *new* 1.00 equiv) from the ligand-exchanged macroinitiator solution were added to stirring Grignard thiophene monomer solutions and stirred for 1 h before quenching outside of the glovebox with aq. HCl (12 M, 2 mL) and working up for SEC and MALDI-TOF/MS.

Vial 1) thiophene monomer (0.080 M in THF, 0.34 mL, 0.027 mmol, 25. equiv) in THF (0.89 mL)
Vial 2) thiophene monomer (0.080 M in THF, 0.68 mL, 0.055 mmol, 50. equiv) in THF (0.54 mL)
Vial 3) thiophene monomer (0.080 M in THF, 1.36 mL, 0.109 mmol, 100. equiv)

Table S5. GC data from the ligand-exchange copolymerization experiments.

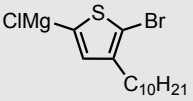
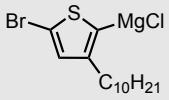
	 **(% conv.)**	 **(% conv.)**
Vial 1 (25 equiv thiophene)	6	0
Vial 2 (50 equiv thiophene)	19	4
Vial 3 (100 equiv thiophene)	20	6

Table S6. SEC data from the ligand-exchange copolymerization experiments.

	before ligand exchange		**after ligand exchange**	
	M_n **(kg/mol)**	**Đ**	M_n **(kg/mol)**	**Đ**
Poly(olefin) macroinitiator	21.10	1.31	21.27	1.33

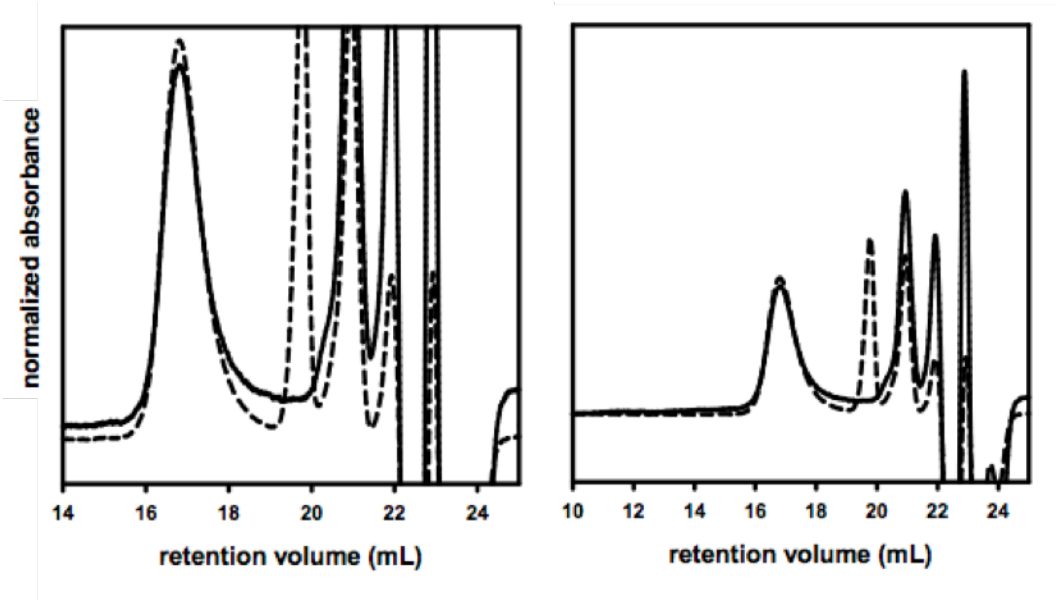


Figure S18. SEC data from the attempted ligand-exchange copolymerization. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents poly(1-pentene) macroinitiator before ligand-exchange. The dashed line represents poly(1-pentene) macroinitiator after ligand-exchange. The RI traces are shown, poly(olefin) does not absorb UV light. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

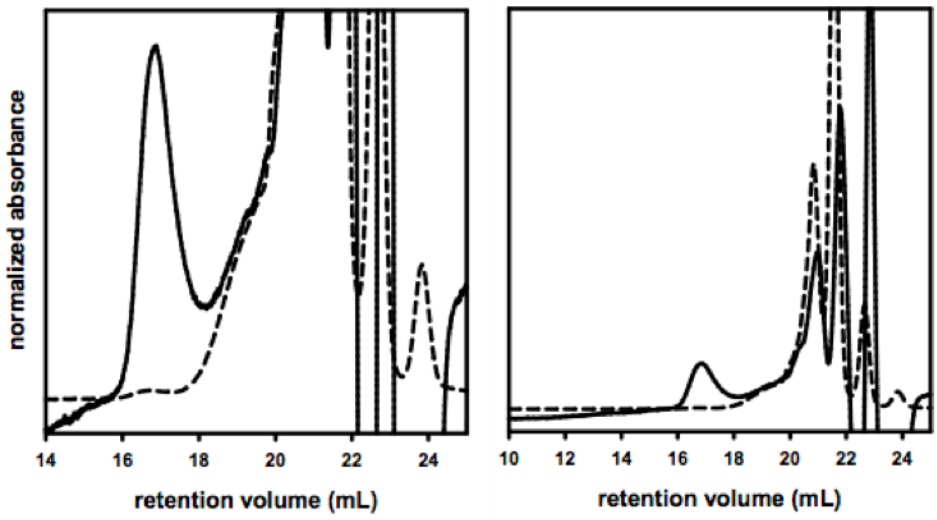


Figure S19. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (25 equiv). Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

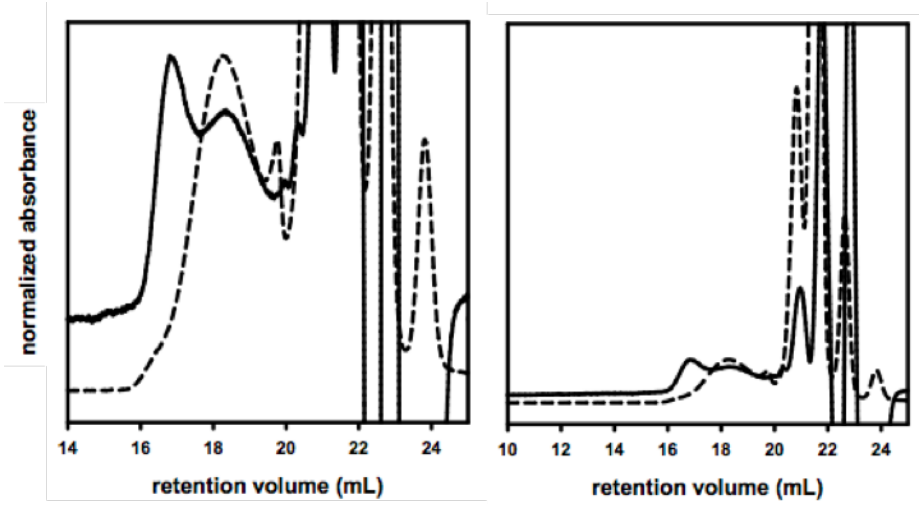


Figure S20. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (50 equiv). Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

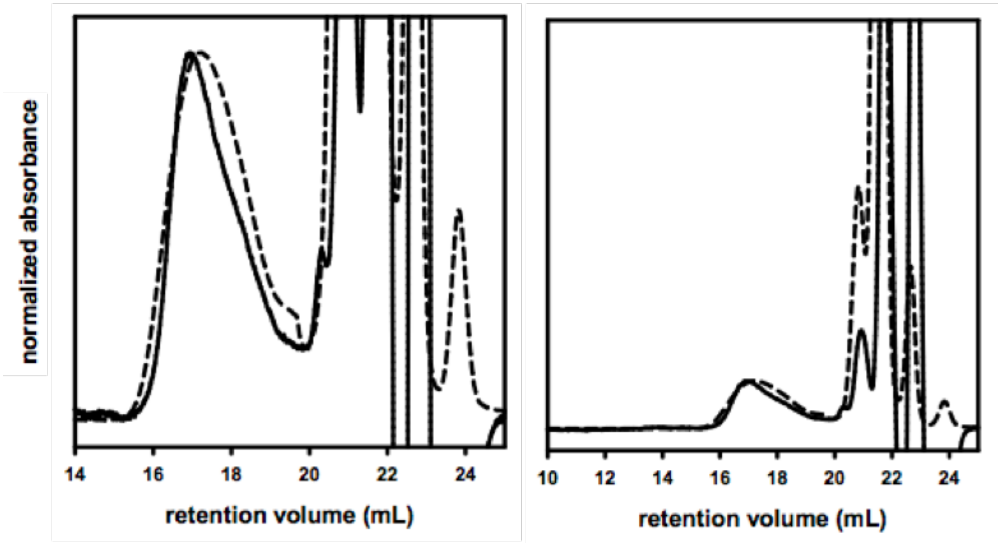


Figure S21. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (100 equiv). Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

Alternative reaction conditions

Several different reaction conditions were tested to investigate whether successful chain-extension can be observed. Modifications made from the "*standard copolymerization conditions*" are noted below.

Lower temperature CTP:

After ligand exchange, Grignard thiophene monomer solutions and the ligand-exchanged macroinitiator solution were cooled to –30 °C for 10 min. Three aliquots (0.00072 M Ni in THF/1-pentene, 1.50 mL each, 0.0011 mmol Ni, *new* 1.0 equiv) from the ligand-exchanged macroinitiator solution were added to stirring Grignard thiophene monomer solutions and stirred at –30 °C for 1 h, warmed to rt, and stirred at rt for 1 h before quenching outside of the glovebox with aq. HCl (12 M, 2 mL) and working up for SEC analysis.

Vial 1) thiophene monomer (0.080 M in THF, 0.34 mL, 0.027 mmol, 25. equiv) in THF (0.89 mL)
Vial 2) thiophene monomer (0.080 M in THF, 0.68 mL, 0.055 mmol, 50. equiv) in THF (0.54 mL)
Vial 3) thiophene monomer (0.080 M in THF, 1.36 mL, 0.109 mmol, 100. equiv)

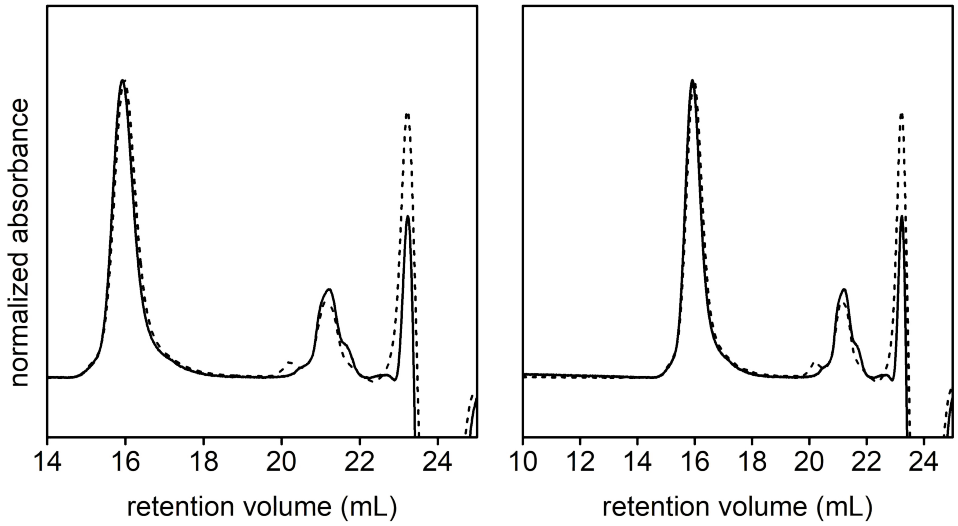


Figure S22. SEC data from the attempted ligand-exchange copolymerization. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents poly(1-pentene) macroinitiator before ligand-exchange. The dashed line represents poly(1-pentene) macroinitiator after ligand-exchange. The RI traces are shown, poly(olefin) does not absorb UV light. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

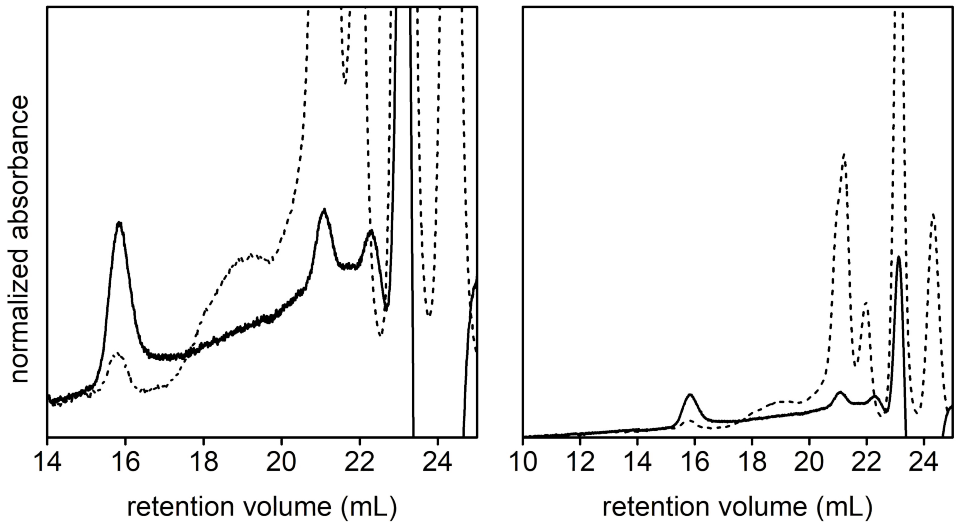


Figure S23. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (25 equiv) at a lower temperature. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

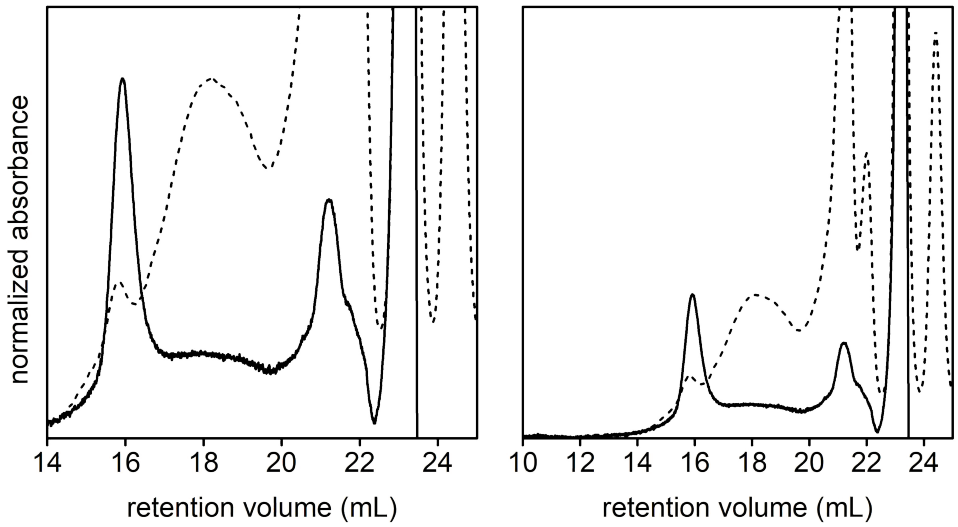


Figure S24. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (50 equiv) at a lower temperature. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

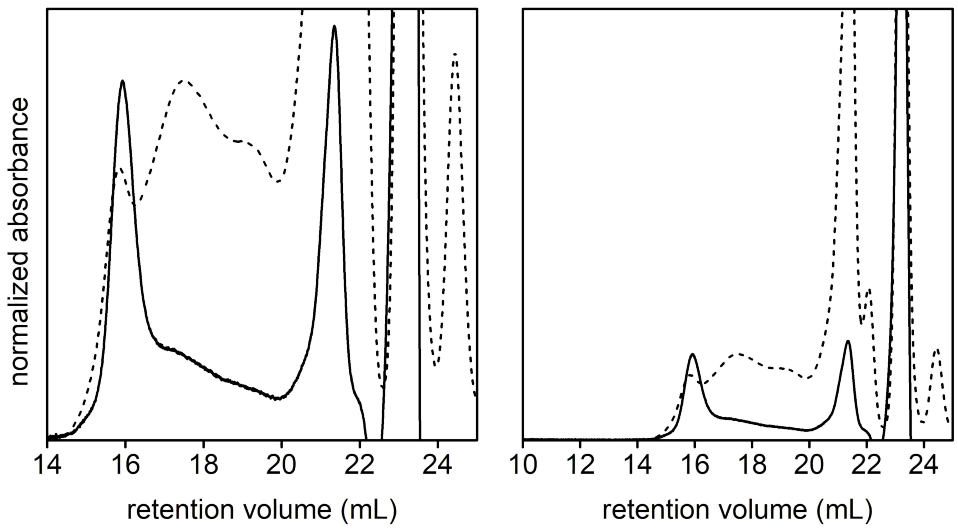


Figure S25. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (100 equiv) at a lower temperature. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

Alternative addition order:
After macroinitiator synthesis, three aliquots (0.0072 M Ni in THF/1-pentene, 1.50 mL each, 0.0011 mmol Ni, *new* 1.00 equiv) from the macroinitiator solution was added to stirring Grignard thiophene monomer solutions. Then py (0.10 M in THF, 114 µL, 0.0114 mmol, 1.20 equiv), and IPr (0.010 M in THF, 1.14 mL, 0.0114 mmol, 1.20 equiv) were added. The solutions were stirred at –30 °C for 1 h, warmed to rt, and stirred at rt for 1 h before quenching outside of the glovebox with aq. HCl (12 M, 2 mL) and working up for SEC analysis.

Vial 1) thiophene monomer (0.080 M in THF, 0.34 mL, 0.027 mmol, 25. equiv) in THF (0.89 mL)
Vial 2) thiophene monomer (0.080 M in THF, 0.68 mL, 0.055 mmol, 50. equiv) in THF (0.54 mL)
Vial 3) thiophene monomer (0.080 M in THF, 1.36 mL, 0.109 mmol, 100. equiv)

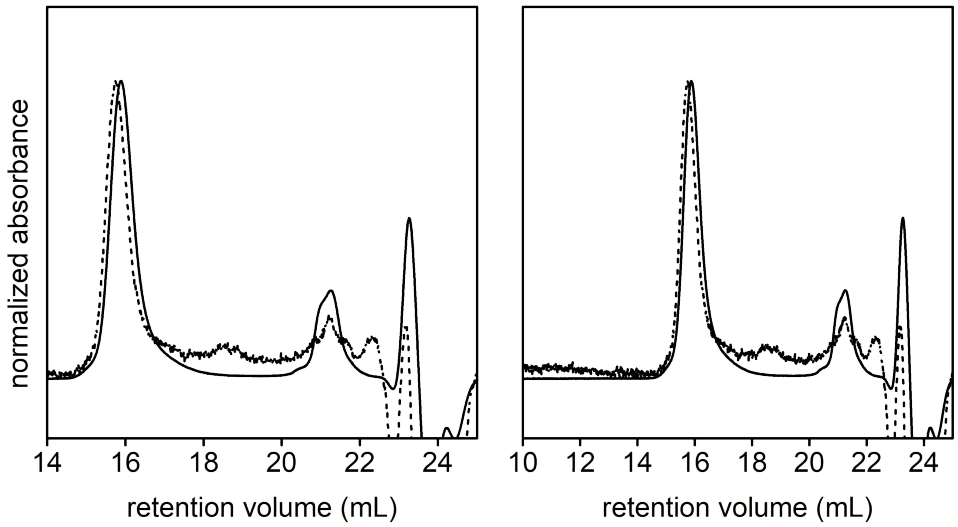


Figure S26. SEC data from the attempted ligand-exchange copolymerization. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents poly(1-pentene) macroinitiator before ligand-exchange. The dashed line represents poly(1-pentene) macroinitiator after ligand-exchange. The RI traces are shown, poly(olefin) does not absorb UV light. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

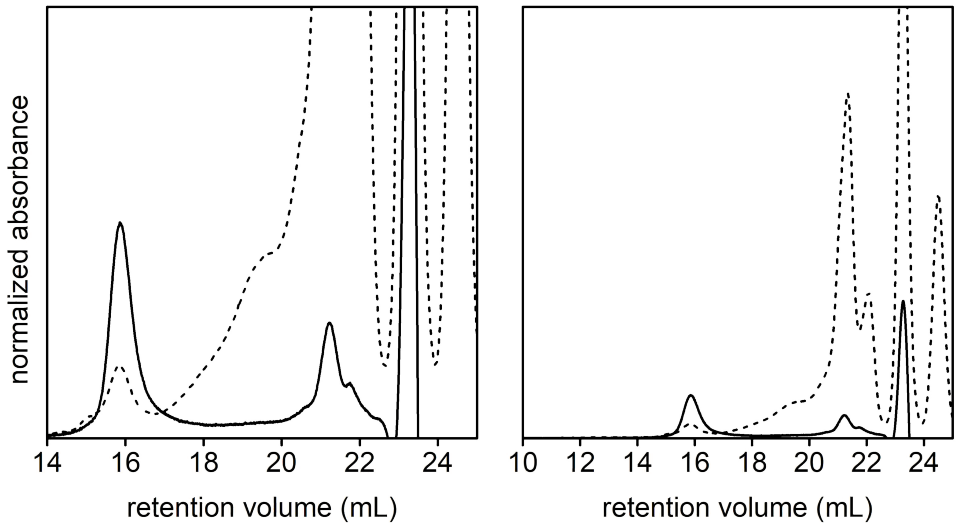


Figure S27. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (25 equiv) at a lower temperature with a different addition order. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

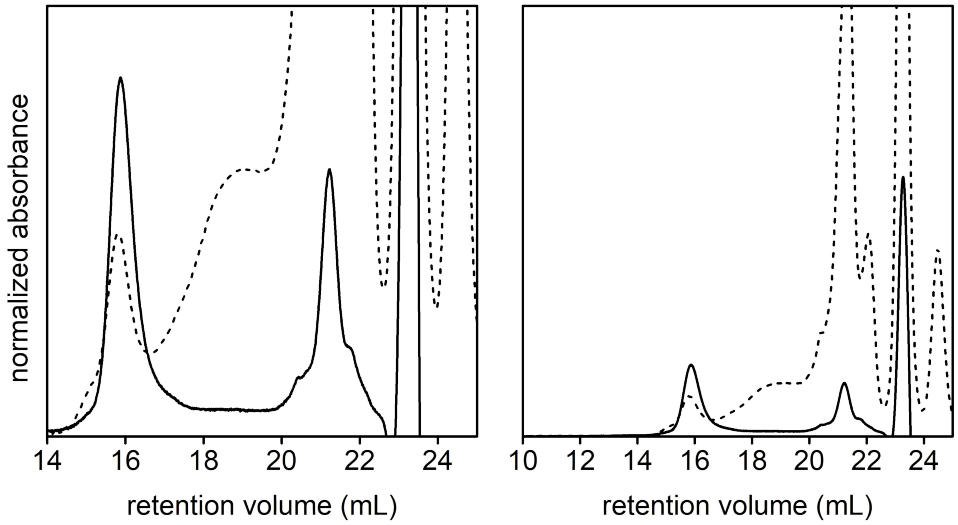


Figure S28. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (50 equiv) at a lower temperature with a different addition order. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

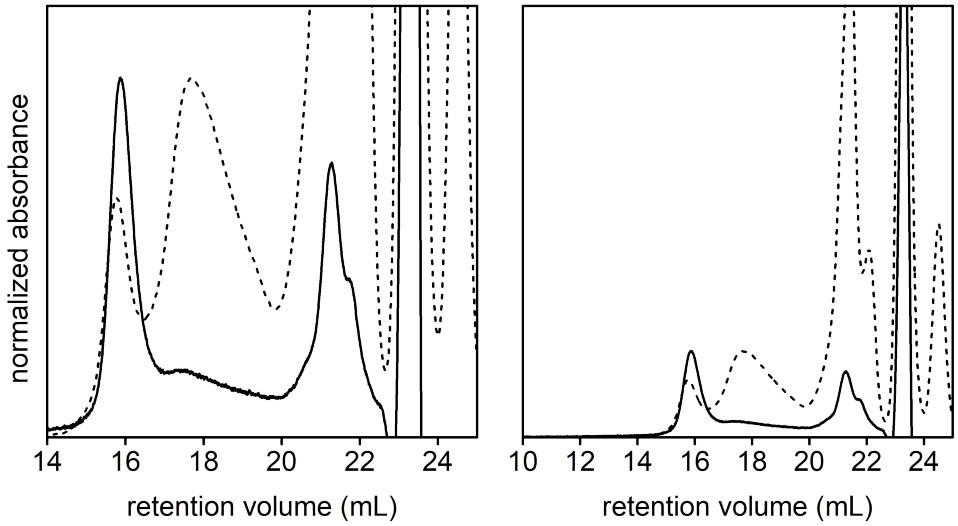


Figure S29. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (100 equiv) at a lower temperature with a different addition order. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

Addition of quaternary ammonium salt:
After ligand exchange, the Grignard monomer solution and the ligand-exchanged macroinitiator solution were cooled to –30 °C for 10 min. Three aliquots (0.00072 M Ni in THF/1-pentene, 1.50 mL each, 0.0011 mmol Ni, *new* 1.0 equiv) from the ligand-exchanged macroinitiator solution and tetrabutylammonium bromide solution (0.10 M in THF, 0.114 mL, 0.0114 mmol) were added to stirring Grignard thiophene monomer solutions and stirred at –30 °C for 1 h, warmed to rt, and stirred at rt for 1 h before quenching outside of the glovebox with aq. HCl (12 M, 2 mL) and working up for SEC analysis.

Vial 1) thiophene monomer (0.080 M in THF, 0.34 mL, 0.027 mmol, 25. equiv) in THF (0.89 mL)
Vial 2) thiophene monomer (0.080 M in THF, 0.68 mL, 0.055 mmol, 50. equiv) in THF (0.54 mL)
Vial 3) thiophene monomer (0.080 M in THF, 1.36 mL, 0.109 mmol, 100. equiv)

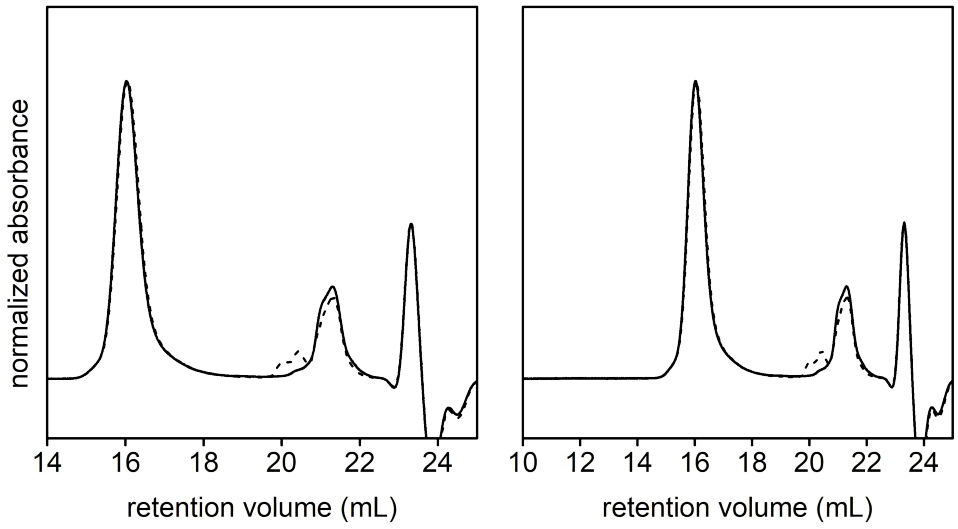


Figure S30. SEC data from the attempted ligand-exchange copolymerization. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents poly(1-pentene) macroinitiator before ligand-exchange. The dashed line represents poly(1-pentene) macroinitiator after ligand-exchange. The RI traces are shown, poly(olefin) does not absorb UV light. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

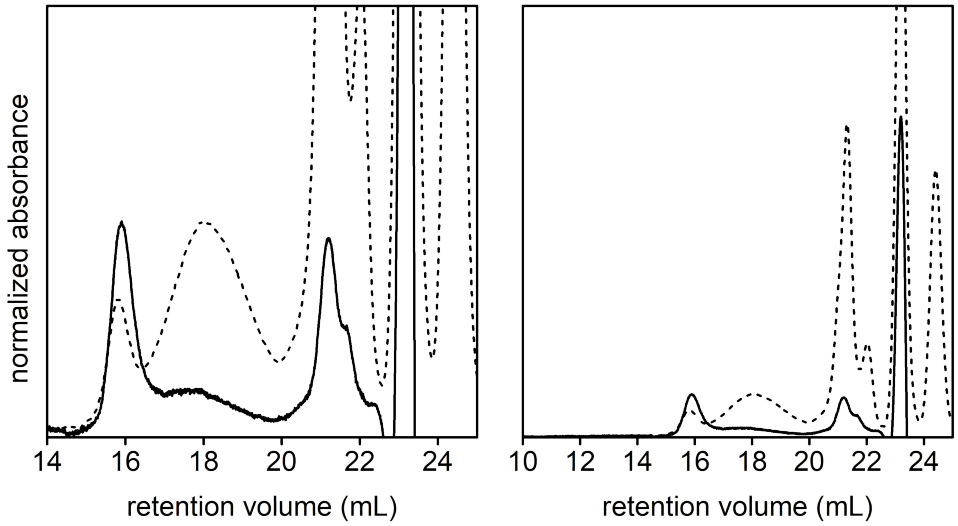


Figure S31. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (25 equiv) at a lower temperature with an addition of quaternary ammonium salt. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

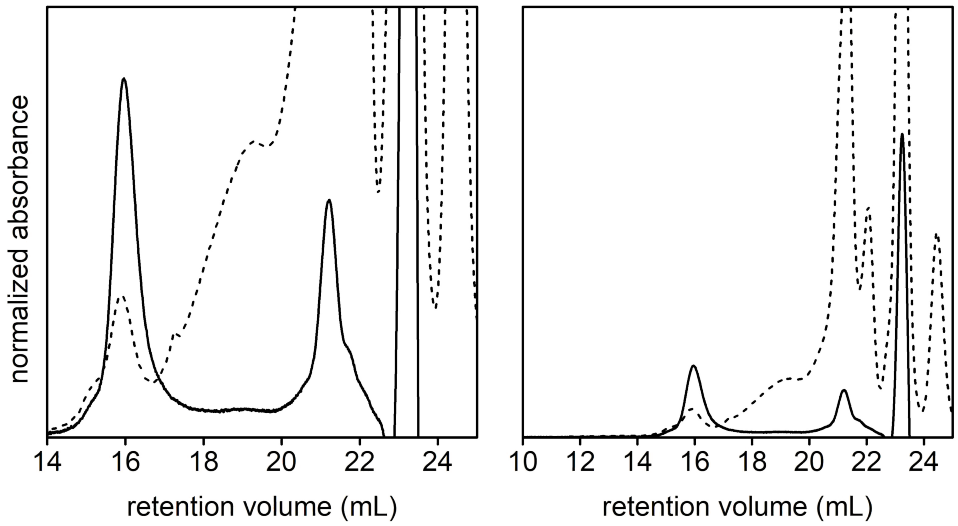


Figure S32. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (50 equiv) at a lower temperature with an addition of quaternary ammonium salt. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

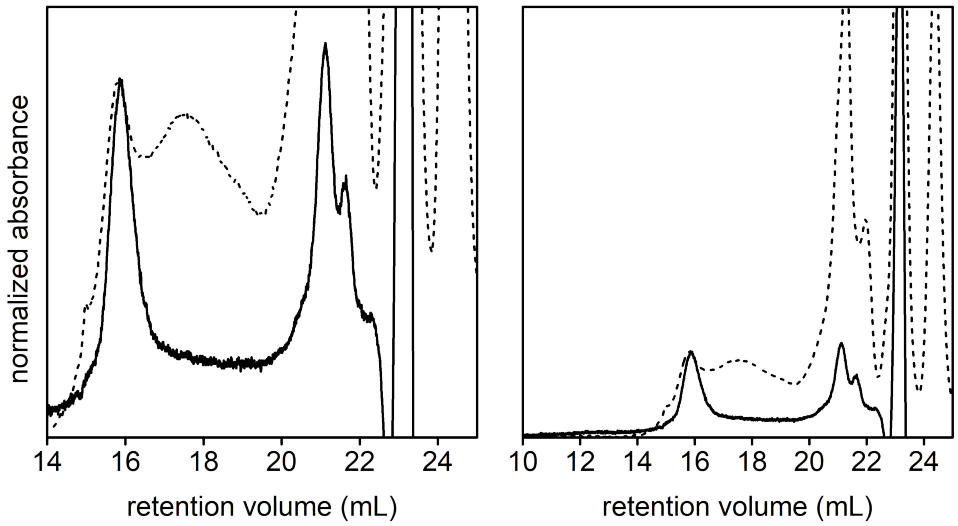


Figure S33. SEC data from the attempted ligand-exchange copolymerization with thiophene monomer added (100 equiv) at a lower temperature with an addition of quaternary ammonium salt. Zoomed (left) and full traces (right) of the same experiment are shown. The solid line represents the RI trace. The dashed line represents the UV trace. Note that BCF and residual monomer elute from 20.5–22 min, PhMe elutes at 23.1 min and BHT elutes at 23.8 min.

VII. Density Functional Simulations

Computational Details

Investigation of the β-hydride elimination pathway was performed using the single-ended growing string method,[4] developed within the Zimmerman Group. All initial geometries for intermediates and transition states were obtained using density functional theory (DFT) in the Q-Chem 4.3 quantum chemistry package.[5] Restricted B3LYP-D3[6] with a singlet spin and LANL2DZ basis set and corresponding effective core potentials[7] was used for optimization and frequency calculations. Energies for initial geometries, intermediates and transition states were refined by applying the ωB97X density functional,[8] the cc-pVTZ basis sets, [9] and the SMD implicit solvent model, with THF as the chosen solvent,[10] using the ORCA quantum chemistry package.[11] All energies listed are Gibbs free energies with enthalpy and entropy corrections, and all geometries were confirmed to have the appropriate number of imaginary frequencies.

Thermodynamic corrections to the enthalpy (H) and gas-phase entropy (S(g)) under catalytic conditions (298.15 K, 1 atm) were computed for all structures.

To avoid inaccuracies inherent in the harmonic oscillator approximation, corrections for enthalpies and entropies were calculated by replacing low frequencies (<50 cm^{-1}) with 50 cm^{-1}. Solvent-based enthalpies H(l) were derived by adding thermal corrections for the enthalpies to the corresponding solution-phase total energies E(l). Energies reported in this article are therefore solvent-phase Gibbs free energies GTΔS(l) at 1 atm and 298.15 K.

All intermediates and transition states were confirmed to have the appropriate number of imaginary frequencies, unless otherwise noted in the XYZ cartesian coordinates section of the ESI. All geometry optimizations, frequency calculations, and single point calculations were performed with an SCF convergence of 10^{-6}.

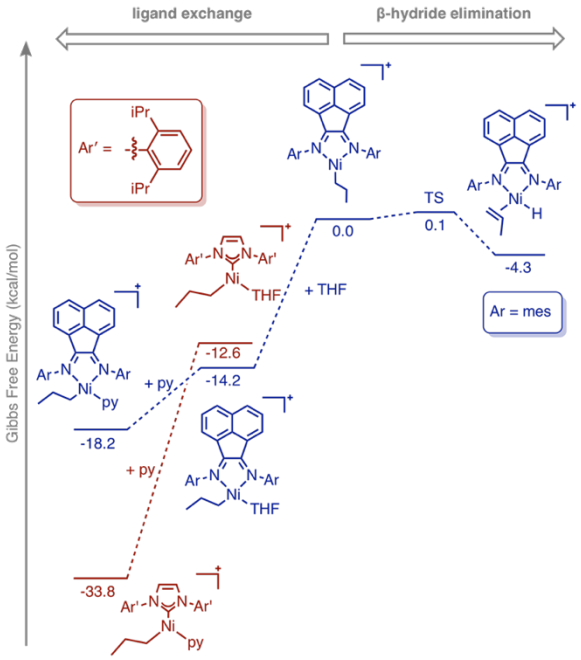


Figure S34. Energy diagram for Ni-diimine (**C2**) catalyst β-H elimination versus ligand exchange with the coordination of THF or Pyridine to Ni.

C2-C_6H_{13} β-H Elimination

To determine whether the β-H elimination pathway would still occur with a longer alkyl chain, the reaction was also modeled using the **C2** catalyst with a longer hexyl chain. A β-H elimination pathway was found, which has a 2.2 kcal/mol barrier and leads to intermediate, which is downhill -4.0 kcal/mol, Figure S22. Similar to the propyl model system, the Ni-H_β and C_α-H_β bond distances of 1.447 and 2.631 Å, respectively, as well as the H_β-Ni-C_α angle of 90.0° suggest the formation of a Ni-H species.

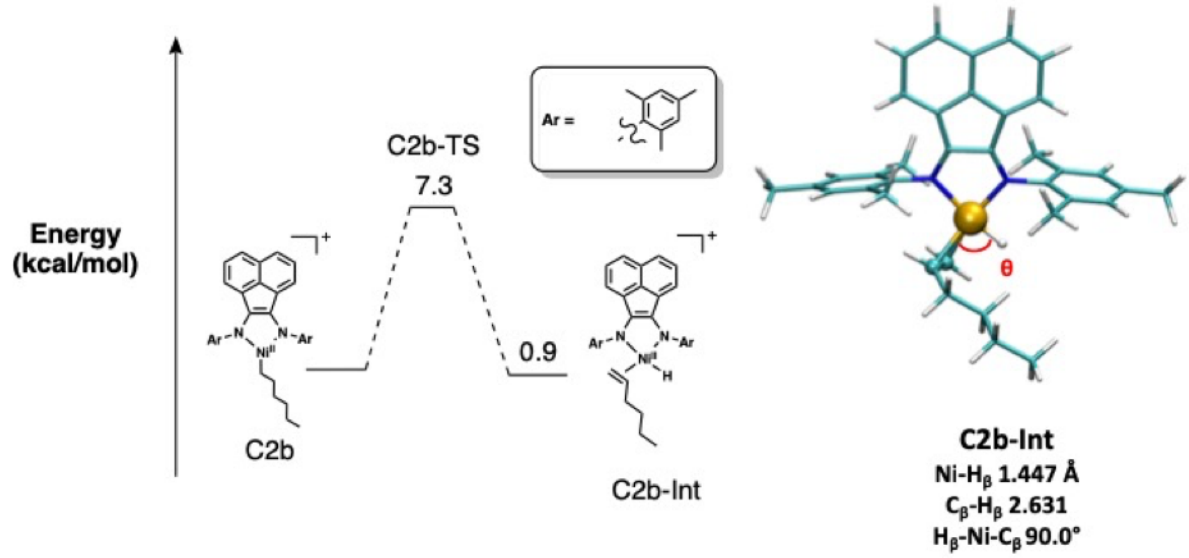
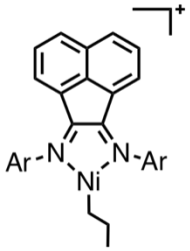


Figure S35. (Left) Energy diagram for β-hydride elimination from the Ni-diimine (**C2**) catalyst with longer alkyl chain. (Right) 3-D renderings of the intermediate C2b-Int.

XYZ cartesian coordinates

Structure C2



Ar = mes

Final Energy in solvent: -2896.489003 Ha

Frequency: i23.69 corresponds to Me group rotation replaced with 50 cm^{-1}

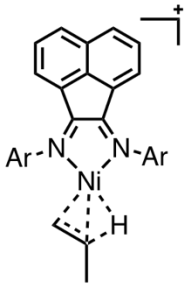
Entropy Correction: 208.521 replaced with 210.50 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.50513382	0.03895124	0.05189054
N	-0.19901290	-0.01746404	1.82526832
N	-1.12898101	1.09038566	-0.41546107
C	-1.30302594	0.66696451	1.92067054
C	-1.84169764	1.26946319	0.65606681
C	-2.29870446	0.86635228	2.97070912
C	-3.15117023	1.83600760	0.95911560
C	-3.37582781	1.56141606	2.34034034

C	-4.58871088	1.86225882	2.98953470
C	-2.43463576	0.46596110	4.29100527
C	-3.64825187	0.77171810	4.96637083
C	-4.69557555	1.44662912	4.34875565
C	-4.14351927	2.45519237	0.21466274
C	-5.59074099	2.50513417	2.20321015
C	-5.36224425	2.79370000	0.86251731
H	-4.01628456	2.66004644	-0.84209534
H	-1.65011693	-0.07816964	4.80158263
H	-5.61056491	1.64677682	4.89703678
H	-3.76009253	0.45521054	5.99690604
H	-6.54618923	2.75377153	2.65389376
H	-6.14253472	3.27396442	0.28262979
C	0.34972502	-0.71026470	2.95258599
C	-1.53448093	1.39999162	-1.75345689
C	0.17477819	-2.10497319	3.02397110
C	1.02820688	0.02439356	3.94337824
C	0.70758365	-2.76499298	4.13822820
C	1.39381010	-2.07595185	5.15028144
C	1.54145617	-0.68238108	5.03675628
C	1.17160794	1.52310622	3.81747938
H	0.57917469	-3.84024331	4.21976009
H	2.07101049	-0.13736653	5.81229163
C	-0.72723183	2.30965606	-2.47828192
C	-2.61003854	0.71994542	-2.37250235
C	-1.04851628	2.57359052	-3.81057112
C	-2.87777777	1.01195087	-3.71903478
C	-2.12430758	1.93583394	-4.45294473
H	-0.44145134	3.28270090	-4.36587655
H	-3.68868538	0.48174470	-4.21028530
C	-3.43611157	-0.33549149	-1.67088737
C	1.98228061	-2.81615635	6.32857259
H	1.54377103	-3.81250214	6.43722771
H	1.82272405	-2.27065197	7.26495155
H	3.06593779	-2.94360996	6.20833899
C	-2.44079838	2.23176637	-5.89990507
H	-3.18678640	1.53855003	-6.29916270
H	-1.54311188	2.15905970	-6.52462795
H	-2.83376891	3.24959092	-6.01821754
C	-0.61188594	-2.84365712	1.96632743
C	0.43779780	2.99838136	-1.80813174
H	0.98208831	3.62740445	-2.51659913
H	1.15425198	2.27452014	-1.39071447

H	0.10880905	3.62954338	-0.97429457
H	-3.79826688	-1.07343614	-2.39267068
H	-4.31725982	0.09488175	-1.17842302
H	-2.86532910	-0.87214168	-0.90639717
H	-0.29337791	-2.56089546	0.95558437
H	-1.68452571	-2.61607773	2.03479034
H	-0.49489987	-3.92514086	2.07300416
H	1.49604190	1.80523712	2.80912316
H	1.90070350	1.90969070	4.53295860
H	0.21733819	2.03339829	4.00380996
C	2.08000400	-0.97442789	0.22791535
C	3.19783399	-0.24214110	0.95700530
H	2.23541687	-1.00084057	-0.88119157
H	1.93695810	-1.99512706	0.59859760
C	4.57184541	-0.93181692	0.79429067
H	4.53520568	-1.95867864	1.17572205
H	5.34813498	-0.38924727	1.34526881
H	4.86780646	-0.97237476	-0.26034372
H	2.94558340	-0.19576014	2.02414898
H	3.27280343	0.79428058	0.59643986

Structure C2-Int-TS



Ar = mes

Final Energy in solvent: -2896.483354 Ha

Frequency: i643.88 (β-H Elimination). Me group rotations i31.14, i24.80 both replaced with 50 cm^{-1}

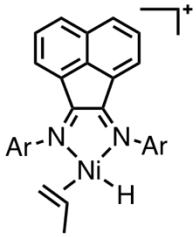
Entropy Correction: 208.6 replaced with 212.975 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.771948	0.039250	0.329424
N	-0.145601	-0.112826	2.094838
N	-0.776590	1.088456	-0.184010
C	-1.148717	0.716181	2.146516
C	-1.517703	1.367497	0.847664
C	-2.224068	0.999050	3.101344
C	-2.808974	2.019712	1.020015
C	-3.186994	1.761844	2.369981

C	-4.453023	2.110398	2.881086
C	-2.537081	0.585209	4.386830
C	-3.801912	0.948544	4.929184
C	-4.735605	1.687256	4.211959
C	-3.690210	2.669293	0.169030
C	-5.335298	2.793491	1.991873
C	-4.955153	3.063907	0.682847
H	-3.444790	2.850496	-0.870487
H	-1.853985	-0.020651	4.968815
H	-5.697168	1.925727	4.655340
H	-4.046714	0.620790	5.932634
H	-6.322676	3.082456	2.337528
H	-5.650088	3.569798	0.022381
C	0.243202	-0.911551	3.214817
C	-1.205384	1.345797	-1.537815
C	0.093688	-2.309632	3.095454
C	0.797532	-0.312503	4.365097
C	0.490671	-3.105004	4.176710
C	1.039600	-2.548945	5.342650
C	1.186706	-1.153674	5.414796
C	0.982592	1.185099	4.453068
H	0.367758	-4.181807	4.106758
H	1.622027	-0.711038	6.305812
C	-0.603698	2.398598	-2.256780
C	-2.155728	0.489004	-2.132358
C	-0.988119	2.596311	-3.586557
C	-2.499296	0.725011	-3.471663
C	-1.933135	1.768762	-4.215024
H	-0.535847	3.408093	-4.148364
H	-3.219016	0.065135	-3.947250
C	-2.791374	-0.658339	-1.379602
C	1.493393	-3.429878	6.483036
H	1.043201	-4.425235	6.426145
H	1.233913	-2.993592	7.453503
H	2.583131	-3.559641	6.467190
C	-2.323572	2.001818	-5.656818
H	-2.925823	1.177046	-6.048763
H	-1.439417	2.106300	-6.295887
H	-2.911051	2.922518	-5.764710
C	-0.512641	-2.917592	1.852753
C	0.414762	3.290696	-1.591919
H	0.823258	4.018121	-2.298196
H	1.244734	2.700151	-1.183890

H	-0.023639	3.845189	-0.752667
H	-3.151014	-1.421889	-2.074814
H	-3.653983	-0.322060	-0.789401
H	-2.086730	-1.136051	-0.691157
H	0.004286	-2.573273	0.946617
H	-1.567472	-2.636849	1.736805
H	-0.458313	-4.008890	1.882050
H	1.370666	1.595981	3.513817
H	1.680708	1.444244	5.252563
H	0.035998	1.698847	4.659788
C	2.416312	-1.099684	0.683864
C	2.889157	0.092120	0.080424
H	2.400070	-2.004710	0.077322
H	2.415883	-1.241853	1.759943
C	3.775184	0.127411	-1.154501
H	4.813522	-0.017581	-0.831098
H	3.713032	1.086153	-1.677608
H	3.519896	-0.672668	-1.854990
H	3.062608	0.926356	0.767311
H	1.570065	0.482234	-0.845980

Structure C2-Int



Ar = mes

Final energy in solvent: -2896.492634 Ha

Frequency: i10.51 Me group rotation replaced with 50 cm^{-1}

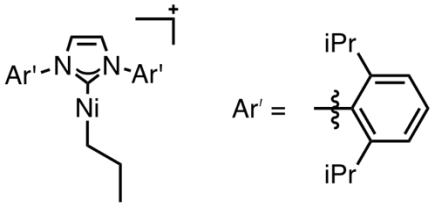
Entropy Correction: 215.756 replaced with 214.718 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.740520	-0.065599	0.148852
N	-0.062820	-0.072533	2.019281
N	-0.828505	0.963545	-0.310908
C	-1.119015	0.676389	2.048783
C	-1.542148	1.264877	0.734201
C	-2.175280	0.961006	3.020454
C	-2.828609	1.919134	0.929399
C	-3.164873	1.692788	2.298407
C	-4.412864	2.052730	2.842859
C	-2.432634	0.589583	4.330673
C	-3.677682	0.964919	4.906173

C	-4.642854	1.672343	4.196647
C	-3.740686	2.544172	0.091306
C	-5.328191	2.706285	1.963298
C	-4.991093	2.943667	0.635795
H	-3.527727	2.704693	-0.959528
H	-1.722559	0.008703	4.903535
H	-5.589562	1.920292	4.666709
H	-3.884109	0.672079	5.929343
H	-6.305290	3.000304	2.332003
H	-5.710012	3.429468	-0.015219
C	0.344701	-0.848149	3.154775
C	-1.254512	1.293083	-1.652407
C	0.019002	-2.219196	3.153453
C	1.064662	-0.242074	4.198673
C	0.457201	-2.990713	4.236266
C	1.195488	-2.432869	5.292141
C	1.482209	-1.056979	5.258979
C	1.336260	1.244983	4.173619
H	0.213682	-4.047724	4.256974
H	2.043326	-0.611124	6.073375
C	-0.628250	2.360834	-2.321079
C	-2.226773	0.487537	-2.279317
C	-1.021707	2.637287	-3.634939
C	-2.580375	0.801550	-3.598866
C	-1.996722	1.871621	-4.292755
H	-0.546741	3.460259	-4.161138
H	-3.317461	0.182610	-4.100787
C	-2.857362	-0.693233	-1.576692
C	1.689686	-3.292979	6.431588
H	1.165965	-4.253908	6.467199
H	1.552747	-2.795248	7.397521
H	2.762217	-3.505563	6.324936
C	-2.399557	2.191571	-5.715150
H	-2.998922	1.388392	-6.153053
H	-1.521371	2.342789	-6.353085
H	-2.994752	3.112334	-5.760874
C	-0.827183	-2.809751	2.045674
C	0.443543	3.166111	-1.629891
H	0.882956	3.902445	-2.307198
H	1.242805	2.506181	-1.268612
H	0.048265	3.702689	-0.757428
H	-3.349043	-1.351710	-2.296811
H	-3.618452	-0.377389	-0.850351

H	-2.110214	-1.284945	-1.034804
H	-0.441119	-2.549023	1.051000
H	-1.858288	-2.432866	2.088114
H	-0.869165	-3.899802	2.119649
H	1.711432	1.571928	3.195788
H	2.068734	1.525659	4.933388
H	0.418848	1.817310	4.365720
C	2.254864	-1.552907	0.410514
C	2.813747	-0.335016	0.735448
H	2.433219	-2.008191	-0.559391
H	1.830464	-2.187768	1.182946
C	3.700885	0.481208	-0.161374
H	4.730781	0.448388	0.220247
H	3.395085	1.534200	-0.173594
H	3.693610	0.106616	-1.187052
H	2.757015	-0.005867	1.773898
H	1.181138	-0.001155	-1.238440

Structure IPr



Final energy in solvent: -2786.973832 Ha

Frequency: No imaginary frequencies

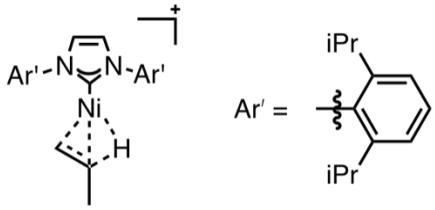
Entropy Correction: 215.686 replaced with 212.077 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

C	-1.42909312	-0.61997816	2.11627134
C	-0.07930606	-0.54413867	1.90938601
N	-2.01310013	-0.64785762	0.84301195
C	-1.05659425	-0.59772504	-0.12456983
N	0.13062541	-0.52872073	0.51564085
H	0.74356907	-0.50157670	2.60053308
H	-2.01074542	-0.65335601	3.02066080
Ni	-1.91352087	-0.61165803	-1.77703821
C	-3.39045358	-0.64000280	0.37872292
C	1.40042188	-0.45654961	-0.17694695
C	1.76878804	0.76943475	-0.77302764
C	2.98401639	0.78680741	-1.47295137
C	3.76770025	-0.36588798	-1.58424334
C	2.14003759	-1.64828793	-0.30968008

C	3.34755566	-1.57198058	-1.02008640
H	3.31741766	1.70096433	-1.94615377
H	4.70417025	-0.32607860	-2.13004917
H	3.95312675	-2.46061341	-1.14438959
C	1.59207015	-2.98123352	0.20820695
C	2.69092661	-3.97930482	0.62118323
H	3.24327594	-4.35158160	-0.24851537
H	2.23985973	-4.84702459	1.11403479
H	3.40649644	-3.52611531	1.31479632
C	0.64874785	-3.62941386	-0.84044637
H	0.98657449	-2.77752600	1.09972758
H	0.21378558	-4.55053773	-0.43514584
H	1.20475300	-3.88913571	-1.74837044
H	-0.17102707	-2.96204513	-1.12748629
C	0.85662139	1.99798312	-0.69662095
C	0.91310281	2.67590049	0.69250604
H	0.62985416	1.98790900	1.49438603
H	0.22633385	3.52961990	0.72126280
H	1.92373492	3.04429105	0.89909889
C	1.13260155	3.03378792	-1.80271157
H	-0.17184785	1.64366677	-0.84832991
H	1.13210209	2.57858761	-2.79966606
H	2.09685479	3.53398988	-1.65893342
H	0.35823173	3.80814686	-1.78398870
C	-4.02635721	0.61302518	0.17282389
C	-5.32219269	0.60468267	-0.36323674
C	-5.95828245	-0.59215395	-0.70004344
C	-5.30138939	-1.80955318	-0.52366231
C	-4.00380073	-1.86824148	0.01324808
C	-3.33028945	1.94260140	0.43604387
C	-3.31085853	-3.22251424	0.14244313
C	-4.09017728	-4.17098296	1.08217328
H	-4.24484569	-3.72044208	2.06797675
H	-3.53716481	-5.10698570	1.21452160
H	-5.07330400	-4.42079715	0.66762080
C	-3.11565755	-3.87639080	-1.24745993
H	-2.31743467	-3.06208004	0.57422060
H	-2.55297169	-4.81069893	-1.15196147
H	-2.55829301	-3.21766566	-1.92829280
H	-4.07840263	-4.10741168	-1.71613304
C	-3.08046141	2.68997414	-0.89681202
H	-2.50705394	2.06699620	-1.59603400
H	-2.51495180	3.61071068	-0.71787003

H	-4.02475171	2.96069620	-1.38201935
C	-4.13002739	2.81793600	1.42503133
H	-2.35158324	1.74002341	0.88219666
H	-3.58059783	3.73958414	1.64283195
H	-4.30689847	2.29012245	2.36819448
H	-5.10391299	3.09999399	1.00998976
H	-5.83111874	1.54647691	-0.53072567
H	-6.96105908	-0.57447410	-1.11353540
H	-5.79671508	-2.73124543	-0.80595153
C	-0.66787838	-0.27332729	-3.12248784
C	0.28728196	-1.37384078	-3.54138158
H	-0.17672978	0.69330869	-2.98501504
H	-1.53453974	-0.15566720	-3.82879661
C	1.00535030	-1.02603032	-4.86588840
H	1.69372715	-1.82912117	-5.15019000
H	1.58637494	-0.10303998	-4.75569386
H	0.29016336	-0.88527379	-5.68423516
H	-0.24766126	-2.32606664	-3.64620400
H	1.03843723	-1.50854648	-2.75836432

Structure IPr-Int-TS



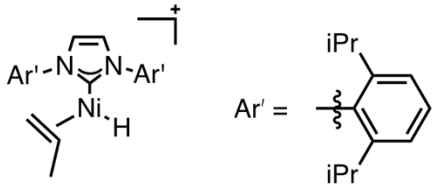
Final energy in solvent: -2786.952567 Ha
Frequency: i227.73 (β-H elimination). Me group rotations i25.24 and i7.41 replaced with 50 cm^{-1}
Entropy Correction: 208.578 replaced with 215.961 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

C	-1.463434	-0.745016	2.117355
C	-0.108535	-0.647445	1.957240
N	-2.020868	-0.692941	0.832675
C	-1.046555	-0.578245	-0.115273
N	0.126549	-0.542919	0.578104
H	0.691184	-0.645497	2.675387
H	-2.067728	-0.848826	3.001335
Ni	-1.308207	-0.344578	-2.068335
C	-3.418926	-0.697878	0.447968
C	1.396106	-0.388904	-0.104769
C	1.753341	0.896949	-0.575678
C	2.958606	1.002824	-1.286107

C	3.749793	-0.123963	-1.531047
C	2.151394	-1.548720	-0.370305
C	3.345994	-1.385561	-1.089767
H	3.280601	1.966911	-1.657456
H	4.679687	-0.018995	-2.080010
H	3.962851	-2.248667	-1.308549
C	1.644907	-2.938314	0.020990
C	2.773373	-3.926601	0.375392
H	3.360950	-4.202954	-0.507234
H	2.344467	-4.849317	0.780125
H	3.454302	-3.507904	1.123139
C	0.757174	-3.523244	-1.107168
H	1.011205	-2.835049	0.909717
H	0.392243	-4.518056	-0.828824
H	1.333272	-3.618422	-2.034507
H	-0.112946	-2.887490	-1.300081
C	0.845634	2.107097	-0.348403
C	0.973442	2.648534	1.094830
H	0.741604	1.879637	1.836618
H	0.283203	3.485586	1.249460
H	1.991992	3.006995	1.280108
C	1.060953	3.241861	-1.366766
H	-0.188549	1.762691	-0.479668
H	0.997228	2.880168	-2.399291
H	2.032191	3.731146	-1.235178
H	0.291279	4.008485	-1.227626
C	-4.032810	0.536040	0.135668
C	-5.366025	0.507840	-0.301018
C	-6.049717	-0.700878	-0.446347
C	-5.398935	-1.908245	-0.190660
C	-4.064342	-1.934692	0.245738
C	-3.265407	1.854756	0.148320
C	-3.339921	-3.270904	0.379021
C	-4.063858	-4.244109	1.334553
H	-4.205306	-3.798634	2.324646
H	-3.481468	-5.164623	1.450794
H	-5.050574	-4.523525	0.948168
C	-3.155484	-3.906729	-1.021278
H	-2.339596	-3.086070	0.784988
H	-2.572389	-4.831624	-0.949030
H	-2.631115	-3.221326	-1.699903
H	-4.124431	-4.149422	-1.471213
C	-2.953430	2.297829	-1.301372

H	-2.394332	1.513583	-1.854091
H	-2.336256	3.202442	-1.314196
H	-3.873226	2.484622	-1.865036
C	-4.014473	2.973380	0.904324
H	-2.309441	1.695462	0.657561
H	-3.401373	3.880029	0.946095
H	-4.244853	2.664114	1.928595
H	-4.956305	3.232415	0.409409
H	-5.868450	1.437510	-0.542170
H	-7.081135	-0.702592	-0.781745
H	-5.922777	-2.843515	-0.350652
C	-0.330109	0.297820	-3.583288
C	-0.474384	-1.122672	-4.017436
H	0.648971	0.589765	-3.195001
H	-0.803263	1.060155	-4.201536
C	0.820745	-1.784232	-4.560959
H	0.648866	-2.839468	-4.792158
H	1.627148	-1.709203	-3.825613
H	1.129206	-1.270339	-5.475059
H	-1.317431	-1.263496	-4.697929
H	-0.686724	-1.753178	-3.074391

Structure IPr-Int



Final energy in solvent: -2786.970726 Ha
Frequency: No imaginary frequencies
Entropy Correction: 220.162 replaced with 214.867 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

C	-1.422026	-0.834046	2.053527
C	-0.059755	-0.763147	2.017655
N	-1.876430	-0.611210	0.742668
C	-0.826012	-0.408453	-0.096922
N	0.290049	-0.509778	0.679603
H	0.677890	-0.869107	2.793312
H	-2.101881	-1.013351	2.867134
Ni	-0.702149	0.204628	-1.905170
C	-3.239298	-0.692566	0.256574
C	1.619723	-0.426734	0.111748
C	2.043123	0.777209	-0.508399

C	3.353689	0.808904	-1.006772
C	4.177872	-0.319646	-0.940498
C	2.382045	-1.610813	0.071465
C	3.685816	-1.524305	-0.442157
H	3.735786	1.710567	-1.466733
H	5.191674	-0.266123	-1.321919
H	4.308523	-2.409797	-0.468509
C	1.748280	-2.967106	0.391323
C	2.734024	-4.005333	0.957725
H	3.467777	-4.323741	0.208799
H	2.186497	-4.900013	1.273126
H	3.275917	-3.613159	1.824314
C	1.059543	-3.503982	-0.894355
H	0.959942	-2.826163	1.137136
H	0.562317	-4.458939	-0.690096
H	1.802961	-3.667707	-1.683665
H	0.307337	-2.800304	-1.271130
C	1.096857	1.970548	-0.720658
C	0.629057	2.633077	0.590942
H	0.129007	1.926207	1.255812
H	-0.064531	3.452489	0.375511
H	1.496669	3.045322	1.117721
C	1.618582	3.024560	-1.710572
H	0.137992	1.604009	-1.203132
H	1.927473	2.574843	-2.658188
H	2.468189	3.569177	-1.285132
H	0.828880	3.752486	-1.917074
C	-3.952151	0.498049	0.008543
C	-5.264299	0.382695	-0.475804
C	-5.834233	-0.867656	-0.720136
C	-5.086559	-2.028192	-0.514314
C	-3.768387	-1.967320	-0.036930
C	-3.333287	1.880903	0.181957
C	-2.946814	-3.251093	0.061217
C	-3.579358	-4.270414	1.034311
H	-3.715060	-3.838597	2.031390
H	-2.941195	-5.156227	1.125341
H	-4.560538	-4.602687	0.676250
C	-2.751256	-3.878910	-1.339979
H	-1.949566	-3.001984	0.440700
H	-2.104482	-4.761458	-1.272817
H	-2.286677	-3.165402	-2.030076
H	-3.707697	-4.195028	-1.771067

C	-3.168239	2.570524	-1.193420
H	-2.589101	1.945945	-1.887352
H	-2.656725	3.533589	-1.085999
H	-4.143777	2.753471	-1.657342
C	-4.154217	2.766660	1.143658
H	-2.334010	1.759080	0.613065
H	-3.649029	3.725903	1.302845
H	-4.282759	2.279418	2.116001
H	-5.150528	2.978605	0.739690
H	-5.840059	1.280730	-0.670707
H	-6.853432	-0.938068	-1.085031
H	-5.524602	-2.994338	-0.739263
C	-0.419188	0.637485	-3.807590
C	-1.422319	-0.406734	-3.870972
H	0.610558	0.359660	-4.043516
H	-0.672882	1.678747	-4.023103
C	-1.097307	-1.741925	-4.556232
H	-1.825906	-2.518269	-4.304775
H	-0.101048	-2.097024	-4.276286
H	-1.114112	-1.590969	-5.642634
H	-2.446081	-0.061900	-4.036011
H	-1.579715	-0.874116	-2.624428

THF structure

Final energy in solvent: -232.4741086 Ha
Frequency: No imaginary frequencies
Entropy Correction: 71.362 remained 71.362 after replacing frequencies < 50 cm $^{-1}$ with 50 cm^{-1}

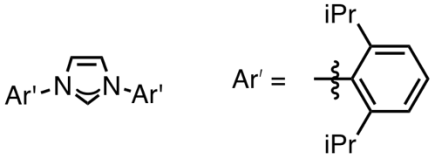
O	-1.14897858	2.55267097	0.06922179
C	-2.32454469	1.68731966	-0.13213098
C	-1.85159502	0.25519328	0.17337132
H	-2.66139445	1.78664702	-1.17265633
H	-3.12112503	2.03488532	0.53207762
C	-0.36140207	0.30460506	-0.23429624
H	-2.42011867	-0.50287310	-0.37382110
H	-1.94309406	0.04169087	1.24537493
C	0.05388896	1.71511739	0.21293588
H	-0.26443601	0.20273345	-1.32195382
H	0.23681954	-0.48149169	0.23642012
H	0.84618330	2.15328037	-0.40061747
H	0.37188678	1.72557140	1.26429428

Pyridine Structure

Final energy in solvent: -248.2970734 Ha
Frequency: No imaginary frequencies
Entropy Correction: 68.509 remained 68.509 after replacing frequencies < 50 cm $^{-1}$ with 50 cm^{-1}

C	-2.96780874	2.87324596	0.00121774
C	-2.92420845	1.47466481	-0.00055527
C	-1.76122866	3.58286462	-0.00227899
C	-0.55820792	2.86706219	-0.00737363
C	-0.60892552	1.46869374	-0.00879078
N	-1.76845079	0.77199141	-0.00547880
H	-3.92177568	3.38935677	0.00523299
H	-3.83709704	0.88790508	0.00201802
H	0.39819769	3.37844991	-0.01028317
H	-1.75890259	4.66802124	-0.00106523
H	0.30052770	0.87686426	-0.01268289

IPr Ligand Structure



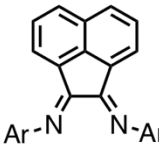
Final energy in solvent: -1160.140217 Ha
Frequency: i13.67 rocking motion frequency replaced with 50 cm^{-1}
Entropy Correction: 183.717 replaced with 186.672 after replacing frequencies < 50 cm $^{-1}$ with 50 cm^{-1}

C	-1.57413867	-0.68238231	2.05544689
C	-0.21614722	-0.65677653	2.07546940
N	-1.94864616	-0.69146026	0.69547831
C	-0.86346524	-0.66525271	-0.16812324
N	0.19525322	-0.64614062	0.72719274
H	0.48393136	-0.64567469	2.89316828
H	-2.29786391	-0.69767833	2.85241177
C	-3.31295488	-0.76191062	0.23929792
C	1.57666303	-0.64479423	0.31852921
C	2.24847823	0.58866309	0.20617371
C	3.60239555	0.56102652	-0.16094614
C	4.24742215	-0.65194481	-0.41642065
C	2.19557698	-1.88003389	0.04015927

C	3.54964852	-1.85874412	-0.32834056
H	4.15381530	1.48947243	-0.25467817
H	5.29603982	-0.65599822	-0.69786162
H	4.05986554	-2.78911907	-0.55041394
C	1.38605818	-3.17632363	0.05506080
C	2.18546302	-4.40156447	0.53660637
H	2.98168241	-4.67191179	-0.16758660
H	1.51940034	-5.26830209	0.61914022
H	2.64272603	-4.22475097	1.51675669
C	0.77313612	-3.42946179	-1.34563298
H	0.54877107	-3.03814395	0.75077879
H	0.15158952	-4.33333966	-1.33109669
H	1.56591466	-3.56830862	-2.09112565
H	0.14972530	-2.58053941	-1.64377134
C	1.48321500	1.89770939	0.37776935
C	2.33730585	3.04647744	0.94192485
H	2.84324707	2.75171133	1.86833783
H	1.70167706	3.91284832	1.15809995
H	3.10004214	3.37428330	0.22538603
C	0.83781356	2.29126577	-0.97472908
H	0.66392585	1.71812608	1.08442953
H	0.19078570	1.48686532	-1.33725731
H	1.61454588	2.48002077	-1.72595075
H	0.23648105	3.20205839	-0.86321832
C	-3.96222833	0.41855201	-0.18059643
C	-5.29562410	0.32099994	-0.60658052
C	-5.95836722	-0.90745459	-0.61895840
C	-5.28890929	-2.06557644	-0.22406218
C	-3.95419371	-2.01786345	0.20709370
C	-3.21628395	1.74304204	-0.28076297
C	-3.22337295	-3.31469058	0.54782272
C	-3.96055794	-4.13551081	1.62742770
H	-4.10636056	-3.54908903	2.54166926
H	-3.38355023	-5.03250175	1.88132189
H	-4.94671977	-4.46304162	1.27752902
C	-2.99976489	-4.15433673	-0.73251960
H	-2.23528140	-3.05826011	0.94218552
H	-2.43222840	-5.06353317	-0.49926038
H	-2.44110430	-3.57991704	-1.47803204
H	-3.95643157	-4.45500803	-1.17699995
C	-2.76175204	1.95240696	-1.74551814
H	-2.14385645	1.10819216	-2.06712795
H	-2.17708635	2.87455496	-1.84267797

H	-3.63303247	2.02290678	-2.40871201
C	-4.03582893	2.94271012	0.23250942
H	-2.31352043	1.66974953	0.33498028
H	-3.41309789	3.84472986	0.24164813
H	-4.40338436	2.76690312	1.24994785
H	-4.90118745	3.15082900	-0.40841796
H	-5.81572927	1.21084443	-0.94294603
H	-6.99031954	-0.96473750	-0.95185071
H	-5.80137562	-3.02155140	-0.26522713

C2 Ligand Structure



Ar = mes

Final energy in solvent: -1269.654455 Ha

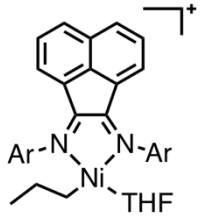
Frequency: No imaginary frequencies

Entropy Correction: 194.724 replaced with 187.337 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

N	-0.16861488	-0.34001606	2.02626850
N	-0.99902485	0.77688341	-0.47711934
C	-1.20198773	0.41596877	1.94114523
C	-1.63943355	1.01536026	0.60959183
C	-2.20936476	0.84049940	2.94947777
C	-2.88480751	1.77968555	0.87838811
C	-3.16872901	1.63327266	2.26335453
C	-4.31215928	2.18425387	2.88287029
C	-2.39216550	0.59030037	4.29953903
C	-3.53311917	1.14315748	4.94739433
C	-4.46850153	1.91650042	4.27383918
C	-3.76273383	2.50010420	0.08549597
C	-5.19314062	2.92694626	2.04354493
C	-4.91679728	3.07256846	0.69120414
H	-3.59338014	2.62871225	-0.97627726
H	-1.69553541	-0.01707404	4.86333388
H	-5.32970354	2.31370353	4.80295696
H	-3.67401372	0.94353665	6.00471873
H	-6.08889842	3.37211457	2.46645339
H	-5.60343876	3.63506790	0.06664854
C	0.27449024	-0.95650775	3.22569848
C	-1.36881846	1.26629916	-1.75838900
C	0.00932823	-2.33193578	3.40726829
C	1.06440697	-0.23944497	4.15258617

C	0.50935729	-2.96260837	4.55351464
C	1.28055519	-2.27687238	5.50286993
C	1.54953893	-0.91796920	5.27838908
C	1.37815811	1.22169660	3.92303122
H	0.29614707	-4.01854311	4.70182357
H	2.15621462	-0.36896660	5.99454085
C	-0.99707501	2.56763081	-2.16832023
C	-1.99152145	0.37501179	-2.66143123
C	-1.29675305	2.96529926	-3.47773954
C	-2.27689263	0.82323844	-3.95761272
C	-1.94537019	2.11583365	-4.38688639
H	-1.00545423	3.96358671	-3.79606549
H	-2.75808943	0.13765663	-4.65083933
C	-2.33842273	-1.02795872	-2.22283949
C	1.83925834	-2.99117709	6.71447450
H	1.24012768	-3.87223752	6.96897078
H	1.86347301	-2.33571776	7.59254680
H	2.86776726	-3.33622512	6.53930812
C	-2.27965398	2.58539653	-5.78626337
H	-2.43500580	1.73983017	-6.46469298
H	-1.47903889	3.20737867	-6.20289715
H	-3.19823899	3.18868108	-5.80094994
C	-0.80766125	-3.08630130	2.38428496
C	-0.27686717	3.49920449	-1.22041702
H	0.10755737	4.37307079	-1.75483410
H	0.56491267	2.99328369	-0.73327423
H	-0.93766203	3.86224855	-0.42171394
H	-2.60170640	-1.65383412	-3.08103880
H	-3.19034654	-1.04054411	-1.52900413
H	-1.49498968	-1.48804129	-1.69475696
H	-0.46243113	-2.85856735	1.36885112
H	-1.87067377	-2.81059127	2.42412270
H	-0.73896965	-4.16627653	2.54669569
H	1.75140098	1.38960499	2.90574464
H	2.13443072	1.57351433	4.63074041
H	0.48896728	1.85446807	4.04433538

C2-THF Structure



Ar = mes

Final energy in solvent: -3129.01292 Ha

Frequency: i20.13 THF-Ni rocking motion frequency replaced with 50 cm^{-1}

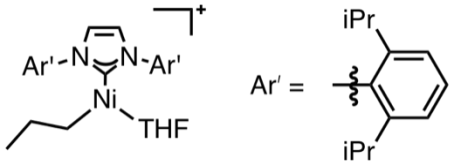
Entropy Correction: 237.332 replaced with 236.818 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.62507386	0.35172474	-0.06984907
N	-0.02660217	0.31428533	1.91166071
N	-1.04906641	1.28786406	-0.34941701
C	-1.12265145	0.99452478	2.03057413
C	-1.68878095	1.54155951	0.75908076
C	-2.13244040	1.17473659	3.07908808
C	-3.02480659	2.05719770	1.04774734
C	-3.24111819	1.79886780	2.43465626
C	-4.47827716	2.02706149	3.06900976
C	-2.25765545	0.78038304	4.40129652
C	-3.49143785	1.02403449	5.06687153
C	-4.57171651	1.62643300	4.43331127
C	-4.05770299	2.57955655	0.28225046
C	-5.51786384	2.57866558	2.26270301
C	-5.30215020	2.84397615	0.91594476
H	-3.94235504	2.77013278	-0.77740368
H	-1.45057990	0.27959128	4.92114923
H	-5.50301445	1.77633927	4.97017367
H	-3.59207999	0.71294034	6.10036912
H	-6.49096817	2.77186889	2.70295248
H	-6.11098013	3.25015916	0.31852339
C	0.52152095	-0.43294509	3.00147286
C	-1.67261427	1.57550417	-1.62449349
C	0.41679728	-1.83664060	2.94146190
C	1.17427906	0.22577641	4.06182344
C	0.99758912	-2.57969151	3.97627316
C	1.66915385	-1.96494155	5.04478805
C	1.74734768	-0.56243182	5.06870983
C	1.24987352	1.73512764	4.09644132
H	0.91663315	-3.66274001	3.95180693
H	2.26529155	-0.07239783	5.88788676
C	-1.63238451	2.87702677	-2.15972577

C	-2.26214173	0.50458133	-2.32436757
C	-2.21550098	3.09129958	-3.41517820
C	-2.83127641	0.76923654	-3.57687331
C	-2.81591507	2.05103423	-4.14270187
H	-2.18561327	4.08976820	-3.84191236
H	-3.28661038	-0.04999733	-4.12552103
C	-2.27502154	-0.89092604	-1.74803148
C	2.26233244	-2.79367813	6.16082202
H	2.50953832	-3.80451867	5.82156431
H	1.55370000	-2.89291902	6.99365042
H	3.17297314	-2.33756300	6.56249223
C	-3.39668476	2.30401611	-5.51506111
H	-4.00933860	1.46328966	-5.85386533
H	-2.60030077	2.45139736	-6.25596972
H	-4.01996288	3.20501839	-5.52761721
C	-0.37006775	-2.50723321	1.83879206
C	-0.97028260	4.00147647	-1.40222725
H	-0.88380516	4.89491496	-2.02533756
H	0.03498101	3.71304072	-1.07312087
H	-1.54354457	4.27345174	-0.50679034
H	-2.68512782	-1.60676270	-2.46514551
H	-2.88028795	-0.94746194	-0.83443545
H	-1.25990307	-1.21357342	-1.48328806
H	-0.11476999	-2.10207695	0.85366049
H	-1.44897181	-2.34707541	1.96884492
H	-0.19654053	-3.58703104	1.82949968
H	1.55307086	2.14772014	3.12620537
H	1.96147846	2.07641544	4.85174659
H	0.27392813	2.17749507	4.33376064
O	2.18334120	-0.69449311	0.38122204
C	3.29076328	-0.14914732	1.21308859
C	4.03007390	-1.40811497	1.64763420
H	2.82395502	0.41002544	2.01854096
H	3.89804156	0.51137756	0.58637427
C	3.98651676	-2.28252319	0.37154489
H	3.48692471	-1.88868433	2.46798970
H	5.05161738	-1.19940300	1.97544332
C	2.60911149	-1.98376224	-0.24454537
H	4.10862860	-3.34562779	0.59318954
H	4.78585415	-1.98744301	-0.31672163
H	1.84665473	-2.71714383	0.02116351
H	2.63163272	-1.84100377	-1.32486034
C	1.18512241	0.47905237	-1.92752355

C	2.57218419	1.11333825	-2.05639653
H	0.44446093	1.06402102	-2.47812690
H	1.16589474	-0.54937164	-2.32156369
C	2.95973234	1.36599399	-3.52908609
H	2.96131760	0.42673768	-4.09556132
H	3.95687979	1.81470385	-3.60922653
H	2.24227893	2.04282849	-4.00782768
H	3.33072354	0.47132332	-1.59147999
H	2.59481187	2.06807806	-1.51060358

IPr-THF Structure



Final energy in solvent: -3019.494507 Ha

Frequency: No imaginary frequencies

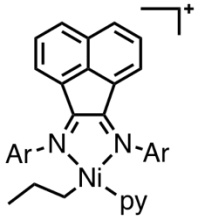
Entropy Correction: 246.37 replaced with 242.764 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

C	-1.37755146	-0.22859694	1.94404517
C	-0.06724724	-0.31360328	1.57978119
N	-2.12178453	-0.36634851	0.76487133
C	-1.30223888	-0.53028728	-0.32277527
N	-0.03465530	-0.48894537	0.18476182
H	0.83222499	-0.27627280	2.16555083
H	-1.84457070	-0.09733173	2.90415622
Ni	-2.22560143	-1.08426441	-1.87975171
C	-3.56010324	-0.49840481	0.64752235
C	1.17099908	-0.69941104	-0.58785543
C	2.05461292	0.38802819	-0.77168123
C	3.23301744	0.14597131	-1.49241083
C	3.50815922	-1.11699035	-2.02025341
C	1.41264267	-1.98276475	-1.12521003
C	2.60415325	-2.16464251	-1.84416079
H	3.93783499	0.95353154	-1.65010239
H	4.42622073	-1.28289324	-2.57388587
H	2.82704631	-3.14045970	-2.26086730
C	0.46355659	-3.16879986	-0.93953363
C	1.08401036	-4.25248454	-0.03016705
H	1.99995243	-4.66445703	-0.46897730
H	0.37737503	-5.07894849	0.11009156
H	1.33471916	-3.84407358	0.95474423
C	0.02559002	-3.76719199	-2.29531401

H	-0.44751700	-2.81649375	-0.44618869
H	-0.71726400	-4.55705055	-2.13163615
H	0.86998594	-4.20773908	-2.83561012
H	-0.41924032	-2.99433761	-2.93104413
C	1.76052127	1.78103465	-0.21577919
C	2.53096175	2.02742483	1.10335782
H	2.29095620	1.28184534	1.86706340
H	2.29103429	3.01768961	1.50539809
H	3.61138124	1.98271207	0.92506979
C	2.08865234	2.90348179	-1.22526514
H	0.68527322	1.83852129	-0.00434708
H	1.64693989	2.70707684	-2.20544943
H	3.16958817	3.01914020	-1.35797745
H	1.70134137	3.85934384	-0.85667659
C	-4.33323974	0.61611639	0.25439662
C	-5.72401437	0.44588349	0.17205604
C	-6.31958683	-0.78624214	0.44773305
C	-5.52798436	-1.88737275	0.77761047
C	-4.13253239	-1.77214623	0.87595702
C	-3.71379765	1.94799350	-0.14991613
C	-3.29293035	-3.01762680	1.15172545
C	-3.68497471	-3.69473842	2.48296844
H	-3.61599172	-2.99358022	3.32105992
H	-3.02202934	-4.54241286	2.68774609
H	-4.71144145	-4.07700957	2.44781011
C	-3.39948858	-4.01937675	-0.02490302
H	-2.24228399	-2.71926217	1.22923882
H	-2.74925916	-4.88325387	0.15260166
H	-3.10642257	-3.55818595	-0.97545645
H	-4.42637594	-4.38743717	-0.13427564
C	-4.06971616	2.27059435	-1.62033116
H	-3.75988978	1.45154151	-2.27994266
H	-3.56234593	3.18495646	-1.94568547
H	-5.14747647	2.42420859	-1.74319129
C	-4.14697516	3.08766990	0.79637532
H	-2.62500852	1.84990811	-0.09168841
H	-3.67827436	4.03101725	0.49639815
H	-3.85817904	2.87266826	1.83079400
H	-5.23348730	3.22924279	0.77274169
H	-6.34395678	1.28772617	-0.11510358
H	-7.39799294	-0.89245405	0.39016122
H	-5.99420326	-2.84931416	0.96041539
C	-1.42318036	-0.05158758	-3.28906784

C	-0.77410497	1.27832640	-2.95367725
H	-2.29053566	0.07367373	-3.95538746
H	-0.71339568	-0.76441465	-3.73489995
C	-0.37410711	2.04998281	-4.22948244
H	0.11260266	1.10084635	-2.34319659
H	-1.45812425	1.89110453	-2.35643286
O	-3.49852242	-1.99014467	-2.99140794
C	-4.96114590	-1.65636188	-2.91435814
C	-5.50806455	-2.06065509	-4.28297706
C	-4.58833847	-3.23212165	-4.70606684
C	-3.20800246	-2.78887511	-4.22091293
H	0.34326261	1.47443620	-4.82662756
H	0.08783173	3.01183699	-3.97943715
H	-1.24967071	2.25330172	-4.85806691
H	-5.03347955	-0.59292629	-2.68546956
H	-5.36879941	-2.23866129	-2.08547334
H	-5.41917809	-1.23036982	-4.99238564
H	-6.55960109	-2.35391813	-4.23313668
H	-2.69873261	-2.12365345	-4.92407922
H	-2.54401951	-3.59823345	-3.91902608
H	-4.60674119	-3.40797894	-5.78441851
H	-4.89065095	-4.15636871	-4.20205129

C2-Py Structure



Ar = mes

Final energy in solvent: -3144.842139 Ha

Frequency: i10.11 C2 rocking motion frequency replaced with 50 cm^{-1}

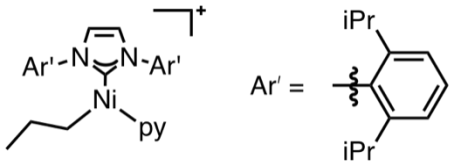
Entropy Correction: 232.834 replaced with 233.687 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

C	-1.51935059	-0.26806819	2.15660792
C	-0.18066787	-0.30996539	1.89178521
N	-2.16651616	-0.40863013	0.92192502
C	-1.26360786	-0.54193242	-0.10061576
N	-0.04335415	-0.46817551	0.50287878
H	0.67416661	-0.24660841	2.54144720
H	-2.06068167	-0.15684241	3.07959109
Ni	-2.05952323	-0.96030303	-1.78981620
C	-3.58425150	-0.42857770	0.62571301

C	1.19133286	-0.55557016	-0.24323670
C	1.87898096	0.64080560	-0.54062749
C	3.00031683	0.53910634	-1.37645068
C	3.40485380	-0.69709519	-1.89023917
C	1.58466395	-1.81869025	-0.72645073
C	2.71086161	-1.86251824	-1.56270834
H	3.55944119	1.42958694	-1.63577963
H	4.27084920	-0.75101249	-2.54143297
H	3.04527741	-2.81629363	-1.95614214
C	0.85235128	-3.10995101	-0.35245666
C	1.79901177	-4.10083281	0.36171163
H	2.59213339	-4.44729841	-0.31047710
H	1.23924746	-4.98051851	0.69864493
H	2.27329595	-3.63875449	1.23362794
C	0.18779314	-3.78040543	-1.57530123
H	0.04966244	-2.85936778	0.34995845
H	-0.32562272	-4.69943674	-1.27093695
H	0.93045159	-4.04091010	-2.33764509
H	-0.54748494	-3.10547830	-2.02630110
C	1.39556787	1.99393742	-0.01488853
C	2.55519880	2.96467417	0.28346537
H	3.31483871	2.49691262	0.91854690
H	2.17383830	3.85141542	0.80048502
H	3.04272319	3.30875388	-0.63533692
C	0.37589556	2.65104258	-0.97925895
H	0.87089925	1.82075643	0.93217838
H	-0.51921530	2.03630200	-1.11033611
H	0.82513022	2.81066780	-1.96635334
H	0.06371991	3.62535388	-0.58573075
C	-4.21930545	0.78053178	0.25995060
C	-5.57279191	0.72053200	-0.10574434
C	-6.26223119	-0.49393389	-0.12293036
C	-5.60725756	-1.67663436	0.21996641
C	-4.25513780	-1.67361878	0.59891287
C	-3.47929504	2.11012337	0.18543229
C	-3.56456989	-2.99414739	0.93289311
C	-4.24420702	-3.69855800	2.12867757
H	-4.27837587	-3.04814773	3.00867229
H	-3.69397356	-4.60809851	2.39229549
H	-5.27190225	-3.98884936	1.88295845
C	-3.52206455	-3.93217281	-0.29677434
H	-2.52775990	-2.77980232	1.21331963
H	-3.00929357	-4.86583454	-0.04087257

H	-2.98780383	-3.46996734	-1.13439420
H	-4.53232827	-4.18417721	-0.63912094
C	-3.40962164	2.59731601	-1.28060986
H	-2.93650618	1.84137017	-1.91704525
H	-2.82527913	3.52038198	-1.35141146
H	-4.41295249	2.80053905	-1.67338355
C	-4.12622284	3.17340227	1.09891787
H	-2.45170794	1.95475428	0.52911213
H	-3.55740402	4.10814754	1.05309522
H	-4.15342924	2.83624405	2.14060662
H	-5.15439626	3.39277588	0.78978611
H	-6.08756437	1.63282163	-0.38496947
H	-7.30930956	-0.51920900	-0.40680779
H	-6.14849751	-2.61616606	0.19280691
C	-0.82857698	-0.07408117	-3.00689440
C	-0.20618486	-0.97708366	-4.06727964
H	-0.05847213	0.38896555	-2.39311687
H	-1.47331356	0.69976489	-3.44738013
C	0.87151212	-0.21356549	-4.86987658
H	-0.97044821	-1.35102001	-4.75782214
H	0.26276767	-1.84671854	-3.59364423
N	-3.27996041	-1.53327055	-3.17421422
C	-3.08305212	-2.67014758	-3.89288133
C	-4.03286419	-3.14493001	-4.79305347
C	-5.22425400	-2.42916464	-4.96552017
C	-5.42784857	-1.26157222	-4.22180239
C	-4.43791272	-0.84006739	-3.33558882
H	-4.55466968	0.04916624	-2.73071054
H	-6.33747456	-0.68267680	-4.32480932
H	-5.97669780	-2.77465189	-5.66546985
H	-2.14417782	-3.18026967	-3.72788795
H	-3.83961491	-4.05436675	-5.34877623
H	0.44234835	0.66238800	-5.37054180
H	1.31618423	-0.85929434	-5.63582709
H	1.67206172	0.12951494	-4.20519652

IPr-Py Structure



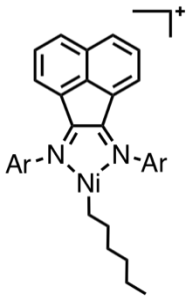
Final energy in solvent: -3035.334687 Ha
Frequency: No imaginary frequencies

Entropy Correction: 245.894 replaced with 241.17 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.92929147	0.55192724	0.03822612
N	0.14263765	0.40825891	1.84629577
N	-0.86248777	1.52381750	-0.35820249
C	-0.98757676	1.04785882	1.96564851
C	-1.54233729	1.68427514	0.73239841
C	-2.04558046	1.07936241	2.98615860
C	-2.90329062	2.12808282	1.02033641
C	-3.15582504	1.72934667	2.36384080
C	-4.42688607	1.84727233	2.96195555
C	-2.21427684	0.54873753	4.25686575
C	-3.48230420	0.68337365	4.88816334
C	-4.56021103	1.30757123	4.27362885
C	-3.92332296	2.68078061	0.26144985
C	-5.45585262	2.43471214	2.16798001
C	-5.20121300	2.83819786	0.86238225
H	-3.77206759	2.96374431	-0.77345829
H	-1.41711227	0.02276053	4.76420413
H	-5.51771204	1.36695119	4.78137147
H	-3.61062498	0.26428207	5.87966100
H	-6.45294739	2.54476668	2.58252308
H	-6.00415655	3.26718417	0.27303117
C	0.50551677	-0.46048350	2.93923490
C	-1.41900491	1.79287789	-1.66099094
C	0.17470859	-1.82129651	2.81424657
C	1.11441813	0.07097284	4.08520415
C	0.48764686	-2.66399054	3.88849629
C	1.10950296	-2.18104696	5.05005274
C	1.41137632	-0.81087646	5.13164815
C	1.40852685	1.54922053	4.16850360
H	0.24321084	-3.71956837	3.81475073
H	1.88908107	-0.42272473	6.02630612
C	-0.98425100	2.92155327	-2.38272963
C	-2.27564812	0.83461198	-2.24797666
C	-1.39748791	3.06456431	-3.71225566
C	-2.66828460	1.02751309	-3.57989729
C	-2.23011490	2.12213306	-4.33549590
H	-1.05715194	3.92898416	-4.27553985
H	-3.31775516	0.28897536	-4.04149106
C	-2.74996580	-0.38655943	-1.49322206
C	1.46917955	-3.11732138	6.18072450
H	0.88521560	-4.04172154	6.13754432

H	1.29767154	-2.65216247	7.15730680
H	2.53006978	-3.39578705	6.13521698
C	-2.61626456	2.27312758	-5.78927913
H	-3.40836910	1.57288208	-6.07065731
H	-1.75749336	2.08180047	-6.44633460
H	-2.96886022	3.28697565	-6.00873454
C	-0.49955386	-2.34556490	1.56581605
C	-0.12241297	3.96497628	-1.71786352
H	0.40263326	4.57605035	-2.45698942
H	0.61531372	3.50223301	-1.05545452
H	-0.72996020	4.63960765	-1.10064052
H	-3.13529467	-1.14391704	-2.18184948
H	-3.55985076	-0.13851218	-0.79532786
H	-1.94575470	-0.84075168	-0.90317731
H	0.07330196	-2.07806751	0.66731405
H	-1.50634151	-1.92483005	1.43829748
H	-0.59578826	-3.43388964	1.59991887
H	1.94709726	1.89265213	3.27695784
H	2.01168113	1.78361393	5.04852843
H	0.48255720	2.13627579	4.22955615
C	2.68308651	-0.31055959	0.23853985
C	4.69786273	-1.26281398	1.43773090
C	3.21747142	-0.84177572	1.56321629
H	3.34197548	0.49333640	-0.13226535
H	2.68279310	-1.10707304	-0.52155235
H	2.62949039	-1.70290204	1.89660675
H	3.12978939	-0.08051427	2.34581958
H	4.81834842	-2.04811621	0.68152907
H	5.08012523	-1.64700763	2.39086356
H	5.32336917	-0.41196863	1.13950091
N	1.35111740	0.62674274	-1.85190465
C	2.16645530	1.57657828	-2.37092885
C	2.33263221	1.73302403	-3.74526780
C	0.82604340	-0.11760831	-4.07693623
C	1.64737274	0.87836558	-4.61501150
H	2.98498812	2.51164882	-4.12087647
H	1.75580184	0.98228659	-5.68853829
C	0.70189699	-0.21790826	-2.69335061
H	0.06717882	-0.96213515	-2.23372996
H	0.28075920	-0.80210710	-4.71438019
H	2.67210761	2.21187418	-1.65865243

Structure C2b



Ar = mes

Final energy in solvent: -3014.443302 Ha

Frequency: i12.36 rocking motion frequency replaced with 50 cm^{-1}

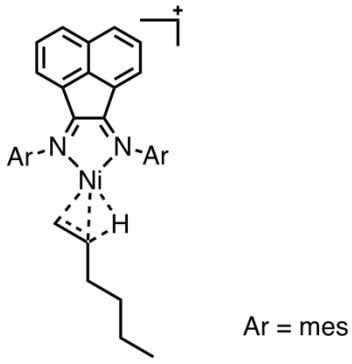
Entropy Correction: 236.933 replaced with 235.638 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.53604527	-0.03059083	-0.02203237
N	-0.18439566	-0.11528011	1.75133070
N	-1.13302336	0.97653406	-0.49434181
C	-1.32427329	0.51237800	1.83162183
C	-1.87123167	1.11322061	0.56619741
C	-2.30130876	0.74073223	2.89505800
C	-3.16712358	1.71052798	0.88710874
C	-3.37018419	1.46013792	2.27749352
C	-4.53236319	1.85735014	2.96650051
C	-2.39947973	0.40477534	4.23770502
C	-3.56693559	0.79561942	4.94764680
C	-4.60324910	1.49960555	4.34497682
C	-4.13917671	2.39346697	0.17170053
C	-5.51498275	2.55765721	2.20537914
C	-5.31175276	2.81588010	0.85500855
H	-4.02813257	2.59916123	-0.88642680
H	-1.61668760	-0.14359202	4.74664099
H	-5.47783957	1.77626869	4.92490445
H	-3.64769670	0.53092071	5.99569978
H	-6.43134664	2.88477348	2.68593999
H	-6.07375713	3.34755430	0.29627171
C	0.41442949	-0.75015470	2.89527319
C	-1.50666546	1.35436337	-1.82593753
C	0.27528427	-2.14470599	3.03932612
C	1.13866740	0.03479326	3.81843765
C	0.87788181	-2.74700397	4.15240184
C	1.60179673	-2.00648642	5.09833550
C	1.72002397	-0.61837035	4.91261833
C	1.28536732	1.52822974	3.63283763
H	0.77811938	-3.82053546	4.28154159

H	2.28440553	-0.02987288	5.62999667
C	-0.71439022	2.33110909	-2.47584422
C	-2.55098013	0.68288284	-2.50530385
C	-1.02203336	2.66560103	-3.79712198
C	-2.80548754	1.04928729	-3.83557552
C	-2.06720211	2.03919920	-4.49746015
H	-0.42741743	3.42728654	-4.29349999
H	-3.59475795	0.53028275	-4.37152557
C	-3.35056673	-0.43619888	-1.87349796
C	2.24532112	-2.68205386	6.28750628
H	2.08054141	-3.76293035	6.27025039
H	1.84181135	-2.29713702	7.23213854
H	3.32791802	-2.50869474	6.30516113
C	-2.36919712	2.41193222	-5.93005527
H	-3.16951647	1.79223753	-6.34380858
H	-1.48542615	2.28941447	-6.56755603
H	-2.68121815	3.46056282	-6.01124275
C	-0.52175439	-2.96083379	2.04826490
C	0.41418735	3.02464680	-1.74768549
H	0.98385503	3.65933711	-2.43075932
H	1.11635452	2.30668641	-1.29897337
H	0.04563206	3.65572017	-0.92946822
H	-3.83549526	-1.03710538	-2.64739147
H	-4.14147244	-0.06060730	-1.21223050
H	-2.71936968	-1.10686333	-1.27959729
H	-0.21855655	-2.75117572	1.01537198
H	-1.59644269	-2.74453072	2.11590256
H	-0.38931684	-4.03010475	2.23114359
H	1.61467894	1.77540505	2.61693766
H	2.01932550	1.93349188	4.33334884
H	0.33891172	2.05733053	3.80472557
C	2.13885995	-1.00184435	0.06160831
C	3.28933400	-0.52148433	0.92696076
H	2.26204891	-0.74328281	-1.02839607
H	1.96396240	-2.08020795	0.15913428
C	4.61914079	-1.29387775	0.71767402
H	2.99261188	-0.64117471	1.97759498
H	3.47476699	0.54997237	0.76339080
C	5.28811216	-1.05024254	-0.64676170
H	4.43132953	-2.36937154	0.85320025
H	5.31658016	-0.99719848	1.51418750
C	6.64187107	-1.77103287	-0.78571933
H	5.44002989	0.03170444	-0.78668509

H	4.62198199	-1.37893165	-1.45925478
C	7.33456748	-1.49547395	-2.12946626
H	7.53244014	-0.42403083	-2.25913966
H	6.71175314	-1.82417990	-2.97105955
H	8.29292471	-2.02167836	-2.19895229
H	6.48838218	-2.85318357	-0.66410781
H	7.30014165	-1.45946667	0.03847323

Structure C2b-Int-TS



Final energy in solvent: -3014.437765 Ha

Frequency: i582.21 (β-H eliminiation). Me group rotation frequency of i26.63 replaced with 50 cm^{-1}

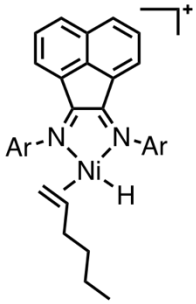
Entropy Correction: 232.044 replaced with 229.235 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	1.171724	-0.043215	0.657745
N	-0.009661	-0.319750	2.255676
N	-0.308251	1.029573	-0.011311
C	-0.979669	0.551089	2.228181
C	-1.180128	1.265716	0.924584
C	-2.126018	0.866824	3.086092
C	-2.460903	1.963876	0.987363
C	-2.976572	1.694965	2.290633
C	-4.248991	2.128061	2.712012
C	-2.561422	0.468801	4.341578
C	-3.837019	0.909547	4.789560
C	-4.661419	1.712567	4.011315
C	-3.217251	2.706031	0.092792
C	-5.000901	2.899616	1.776205
C	-4.490439	3.176406	0.513459
H	-2.868516	2.912184	-0.911183
H	-1.961680	-0.172885	4.975156
H	-5.633101	2.015010	4.386650
H	-4.177447	0.596369	5.770816
H	-5.987070	3.259854	2.050164

H	-5.085809	3.755453	-0.183472
C	0.232359	-1.159974	3.391645
C	-0.557142	1.341846	-1.399600
C	0.012713	-2.545076	3.230350
C	0.723780	-0.619283	4.601062
C	0.260559	-3.382944	4.324981
C	0.732061	-2.884327	5.547787
C	0.965009	-1.503052	5.660049
C	1.007539	0.859561	4.747308
H	0.080587	-4.448437	4.217926
H	1.352194	-1.104024	6.593274
C	0.121442	2.424959	-1.995545
C	-1.424213	0.510844	-2.142566
C	-0.091999	2.671652	-3.356952
C	-1.595868	0.798188	-3.504915
C	-0.944094	1.868873	-4.132401
H	0.424568	3.507173	-3.821374
H	-2.248006	0.157682	-4.090968
C	-2.143135	-0.667810	-1.523484
C	0.993633	-3.806288	6.715647
H	0.799577	-4.849950	6.452434
H	0.356419	-3.553579	7.572120
H	2.033745	-3.733627	7.055455
C	-1.143659	2.150289	-5.603768
H	-1.787663	1.399619	-6.070886
H	-0.187866	2.152781	-6.141634
H	-1.604910	3.132373	-5.763897
C	-0.507913	-3.099940	1.927200
C	1.032008	3.312267	-1.180972
H	1.517763	4.057751	-1.815656
H	1.812115	2.727792	-0.678220
H	0.481410	3.848542	-0.396957
H	-2.565270	-1.308327	-2.302450
H	-2.972909	-0.349793	-0.879407
H	-1.471499	-1.282772	-0.914074
H	0.100548	-2.762021	1.078721
H	-1.536522	-2.773118	1.727696
H	-0.502486	-4.192962	1.938539
H	1.561822	1.250915	3.886252
H	1.599298	1.051319	5.645050
H	0.085449	1.448093	4.828978
C	2.645379	-1.350128	1.073608
C	3.325995	-0.143087	0.783391

H	2.657248	-2.113309	0.296147
H	2.483770	-1.695292	2.089276
C	4.381322	0.030917	-0.305273
H	3.451727	0.552156	1.616792
H	2.188776	0.547107	-0.253137
C	4.122032	-0.707006	-1.626422
H	5.325936	-0.325656	0.136513
H	4.518392	1.101823	-0.502266
C	5.212446	-0.435032	-2.679910
H	3.143789	-0.393065	-2.026028
H	4.055368	-1.789368	-1.449913
C	4.933154	-1.141157	-4.014714
H	3.977971	-0.811089	-4.442144
H	4.884273	-2.229611	-3.883563
H	5.719079	-0.928096	-4.746789
H	6.186516	-0.759001	-2.287568
H	5.290741	0.649340	-2.844708

Structure C2b-Int



Ar = mes

Final energy in solvent: -3014.446888 Ha

Frequency: i48.53 Me group rotation frequency replaced with 50 cm^{-1}

Entropy Correction: 232.617 replaced with 230.966 after replacing frequencies < 50 cm^{-1} with 50 cm^{-1}

Ni	0.80451543	-0.59882452	0.21412156
N	-0.00893192	-0.43175491	2.07800205
N	-0.57350746	0.67368550	-0.28656778
C	-0.93914386	0.47320870	2.07004047
C	-1.24996392	1.10522737	0.73913629
C	-1.90712362	0.98809395	3.04090359
C	-2.39429582	1.99486281	0.92597818
C	-2.74646157	1.87894189	2.30594322
C	-3.86018817	2.53043305	2.87091135
C	-2.17934293	0.75103903	4.37993839
C	-3.28919699	1.41372513	4.97131916
C	-4.10834577	2.27591336	4.25185877

C	-3.16985547	2.78757685	0.09203320
C	-4.63258559	3.34584201	1.99142648
C	-4.28977492	3.46144044	0.64950396
H	-2.94576572	2.89492440	-0.96220406
H	-1.57730775	0.07305254	4.97238096
H	-4.95262083	2.75213727	4.73992088
H	-3.50521195	1.22936681	6.01747774
H	-5.50187556	3.87138609	2.37336294
H	-4.89798088	4.07964198	-0.00126284
C	0.30188983	-1.20518680	3.25288211
C	-0.82843277	1.11933180	-1.63590081
C	-0.23018035	-2.50915386	3.34897682
C	1.16371222	-0.67628729	4.23564457
C	0.12412254	-3.28053206	4.46355150
C	0.98032745	-2.79375419	5.46333472
C	1.48893565	-1.49284089	5.32825492
C	1.71011170	0.73085616	4.12902010
H	-0.27975510	-4.28511712	4.55047253
H	2.15891564	-1.10207159	6.08848827
C	-0.40997827	2.40056515	-2.05248847
C	-1.44350116	0.21233922	-2.52437431
C	-0.65560673	2.76751826	-3.38265541
C	-1.67298509	0.63382920	-3.84003416
C	-1.29364747	1.90688196	-4.28966644
H	-0.32526950	3.74579261	-3.72001623
H	-2.15189640	-0.05438402	-4.53014624
C	-1.84440945	-1.17356814	-2.07778310
C	1.32795891	-3.64146946	6.66560275
H	1.34404637	-4.70644127	6.41357280
H	0.59134610	-3.50837060	7.46907184
H	2.30743041	-3.37456492	7.07393629
C	-1.56695466	2.34383414	-5.71046323
H	-1.71207165	1.48525020	-6.37271632
H	-0.74322439	2.94438715	-6.11030686
H	-2.47457266	2.95940777	-5.76728518
C	-1.19251038	-3.04318752	2.31004490
C	0.32207157	3.34264656	-1.12236922
H	0.72855661	4.18882851	-1.68179944
H	1.15686680	2.84019609	-0.61877387
H	-0.33239712	3.75050674	-0.34170308
H	-2.26261419	-1.74368521	-2.91130558
H	-2.59625599	-1.15021107	-1.27878491
H	-0.97837167	-1.72815030	-1.69035813

H	-0.82292793	-2.89421959	1.28827894
H	-2.16736262	-2.54087503	2.36836158
H	-1.36622911	-4.11254338	2.45529301
H	2.12986737	0.93503594	3.13679756
H	2.49607707	0.89672815	4.86984884
H	0.92971252	1.48321032	4.30359878
C	2.08963348	-2.29919959	0.36902399
C	2.79890790	-1.23639318	0.88253874
H	2.26799757	-2.67341063	-0.63220157
H	1.51083035	-2.93880026	1.03015495
C	3.87452033	-0.43771306	0.18678296
H	2.70059400	-1.04064491	1.94995287
H	1.26116658	-0.60882704	-1.16531914
C	4.20876136	-0.81687424	-1.26277739
H	4.78173237	-0.53082767	0.80706612
H	3.60779791	0.63056074	0.23794723
C	5.31224990	0.07741056	-1.86009449
H	3.30586962	-0.73391348	-1.88303313
H	4.52988410	-1.86761000	-1.30750404
C	5.63056428	-0.26890379	-3.32248149
H	4.74320286	-0.15251354	-3.95701487
H	5.97694398	-1.30527782	-3.41757701
H	6.41508545	0.38280116	-3.72144686
H	6.22459882	-0.01291207	-1.25274645
H	4.99840932	1.12986543	-1.79168674

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