Supporting Information for

Trials and Tribulations of Designing Multitasking Catalysts for Olefin/Thiophene Block Copolymerizations

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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 (2M in THF) was purchased in 25 mL quantities from Aldrich. All other reagent grade materials and solvents were purchased from Aldrich, Acros, ArkPharm, or Fisher and used without further purification unless otherwise noted. 3HT was purified via flash chromatography with hexanes as the eluent. THF was dried and deoxygenated using an Innovative Technology solvent purification system composed of activated alumina, a copper catalyst, and molecular sieves. The glovebox in which specified procedures were carried out was an MBraun LABmaster 130 with a N_2 atmosphere and H_2O levels below 4 ppm. Compounds **S1**,[1] **S2**,[1] **C1**,[1] **C2**,[2] **C3**[2] were prepared using modified literature procedures.

II. General Experimental

NMR Spectroscopy: Unless otherwise noted, ^{1}H and ^{13}C spectra for all compounds were acquired at rt in CD_2Cl_2, $CDCl_3$, C_6D_6 on a Varian vnmrs 700 operating at 700 and 176 MHz or a Varian vnmrs 500 operating at 500 and 126 MHz, respectively. For ^{1}H and ^{13}C spectra in deuterated solvents, the 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), apparent doublet, (ad), doublet of doublets (dd), apparent doublet of doublets (add), triplet (t), apparent triplet (at), quartet (q), multiplet (m), and broad resonance (br). * denotes Si grease.

Mass Spectrometry: HRMS data were obtained on a Micromass AutoSpec Ultima Magnetic Sector mass spectrometer.

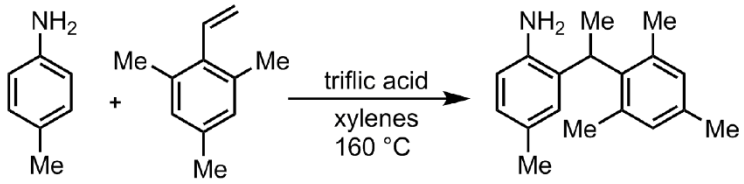
MALDI-TOF-MS: MALDI-TOF mass spectra were recorded using a Bruker AutoFlex Speed in linear or reflectron mode. The matrix trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB), was prepared at a concentration of 0.1M in $CHCl_3$. The instrument was calibrated with a sample of polythiophene with H/Br endgroups. The polymer sample was dissolved in THF or CH_2Cl_2 to obtain an approx.1 mg/mL solution. A 2.5 μL aliquot of polymer solution was mixed with 2.5 μL of the DCTB. This mixture (1 μL) was placed on the target plate and then air-dried. The data was analyzed using flexAnalysis.

Gel-Permeation Chromatography: Polymer molecular weights were determined by comparison with polystyrene standards (Varian, EasiCal PS-2 MW 580–377,400) 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 R.I., UV-PDA detector model 2600 (190–500 nm), RALS/LALS, and viscometer). Samples were dissolved in THF (with mild heating) and passed through a 0.2 μm PTFE filter prior to analysis. The RI detector was used for determining poly(olefin) MWs while the UV-PDA detector was used for determining poly(thiophene) and poly(olefin)-*b*-poly(thiophene) MWs.

Titrations of the Grignard Reagents: An accurately weighed sample of salicylaldehyde phenylhydrazone[3] (typically between 90–100 mg) was dissolved in 5.00 mL of THF. An aliquot (0.25 mL) of this solution was stirred at rt while the Grignard of interest was added dropwise using a 500 μL syringe. The initial solution is yellow and turns bright orange at the end-point.

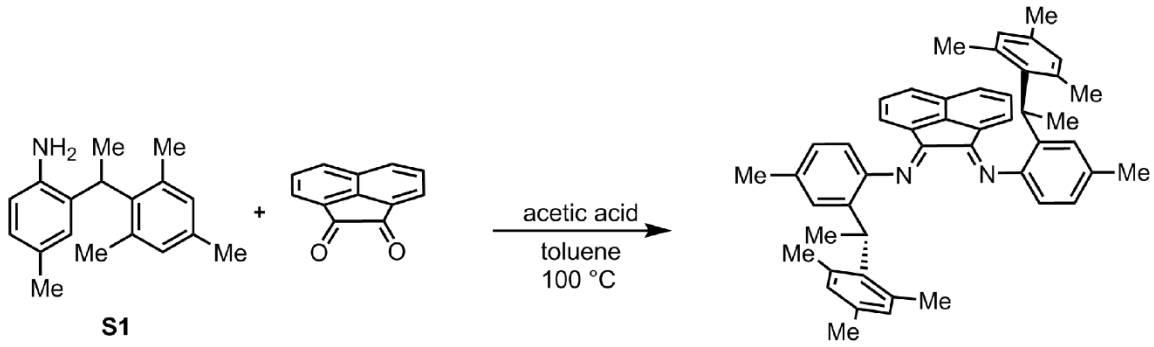
Gas Chromatography: Gas chromatography was carried out using a Shimadzu GC 2010 containing a Shimadzu SHRX5 (crossbound 5% diphenyl – 95% dimethyl polysiloxane; 15 m, 0.25 mm ID, 0.25 μm df) column.

III. Synthetic Procedures of S1, S2, C1, C2, C3



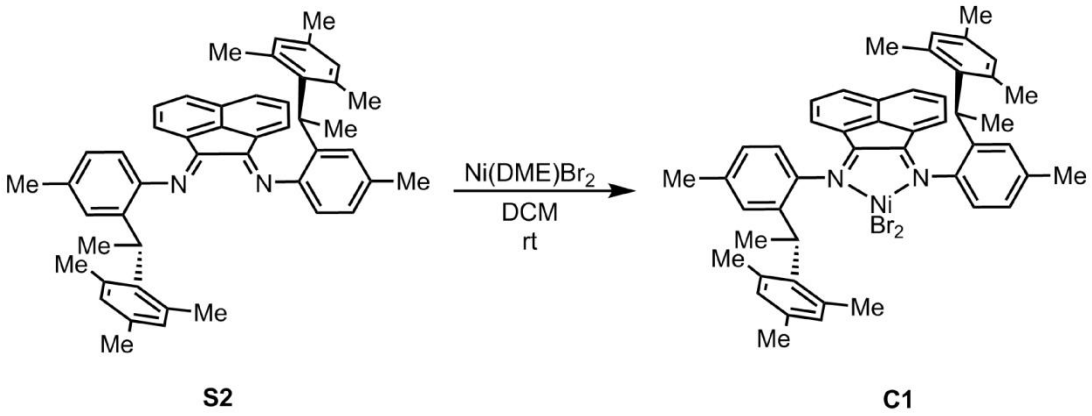
S1

2-(1-mesitylethyl)-4-methylaniline (S1): To a 50 mL bomb flask equipped with a stir bar were added 2,4,6-trimethylstyrene (1.07 mL, 6.62 mmol, 1.0 equiv), ρ-toluidine (1.06 g, 9.93 mmol, 1.5 equiv) and xylenes (1.73 mL). To the stirring solution was added triflic acid (0.12 mL, 1.3 mmol, 0.2 equiv). The flask was sealed and stirred at 160 °C for 18 h. After 18 h the reaction solution was cooled to rt, diluted with EtOAc (10 mL), transferred to a round-bottom flask, concentrated *in vacuo*, and subjected to flash chromatography with hexanes/EtOAc (90:10) as the eluent to produce 709 mg of **S1** as a white solid (42% yield). HRMS (EI): Calcd. for $C_{18}H_{23}N$ [M] 253.1830, found 253.1835.



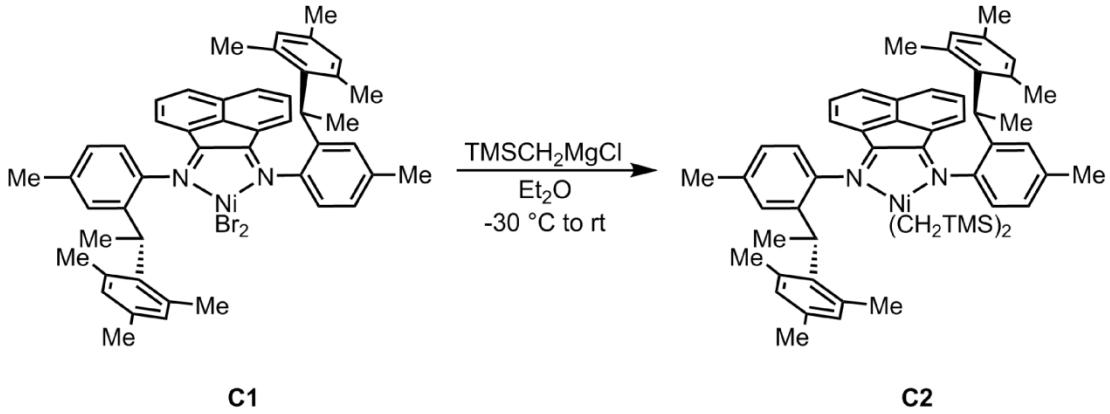
S1 **S2**

(1E,2E)-N1-N2-bis(2-(1-mesitylethyl)-4-methylphenyl)acenaphthylene-1,2-diimine (S2): To a 20 mL vial equipped with a stir bar were added **S1** (171 mg, 0.675 mmol, 2.05 equiv), acenaphthylenequinone (60.1 mg, 0.329 mmol, 1.0 equiv), glacial acetic acid (0.75 mL, 13 mmol, 40 equiv), and toluene (0.39 mL). The reaction was stirred at 100 °C for 3 h and then cooled to rt. The yellow precipitate that formed after cooling was then collected by vacuum filtration, washed with MeOH (10 mL) and hexanes (10 mL), and dried under vacuum to produce 144 mg of **S2** as a yellow solid (77% yield). HRMS (EI): Calcd. for $C_{48}H_{48}N_2$ [M] 652.3817, found, 652.3829.



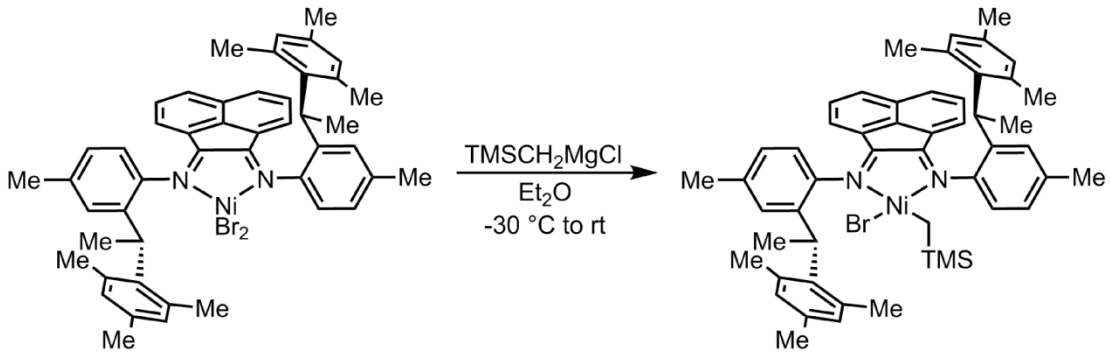
S2 **C1**

(1E,2E)-N1-N2-bis(2-(1-mesitylethyl)-4-methylphenyl)acenapythylene-1,2-diimine nickel dibromide (C1): To a 50 mL Schlenk flask equipped with a stir bar was added **S2** (152 mg, 0.233 mmol, 1.00 equiv), Ni(DME)Br_2 (75.0 mg, 0.244 mmol, 1.05 equiv) and DCM (4.7 mL). The flask was sealed with a rubber septum and the reaction stirred for 16 h at rt under an N_2 atmosphere. The dark red solution was then filtered through celite and concentrated *in vacuo*. The crude product was redissolved in a minimal amount of DCM (3 mL), layered with pentanes (20 mL), and recrystallized in a -20 °C freezer to afford 126 mg of **C1** as dark red crystals (62% yield).



C1 **C2**

(1E,2E)-N1-N2-bis(2-(1-mesitylethyl)-4-methylphenyl)acenaphthylene-1,2-diimine nickel bismethylenetrimethylsilyl (C2): In the glovebox were added **C1** (119 mg, 0.137 mmol, 1.0 equiv) and Et_2O (3.7 mL) to a 20 mL vial equipped with a stir bar. The vial was sealed with a teflon cap and placed in the freezer (-30 °C) for 15 min. After 15 min, the vial was removed and to the stirring mixture was added $TMSCH_2MgCl$ (340 µL, 0.850 M in Et_2O, 3.00 equiv). The reaction was warmed to rt and stirred for 30 min after which the initial dark green solution turned dark purple. The Et_2O was removed under high vac until 0.5 mL remained, then cold MeOH (5 mL) was added and the solution was passed through a syringe equipped with a 0.2 µm PTFE filter into a 20 mL vial. The solvent was removed under vacuum giving 55 mg of **C2** as a purple solid (45% yield).



C1 **C3**

(1E,2E)-N1-N2-bis(2-(1-mesitylethyl)-4-methylphenyl)acenaphthylene-1,2-diimine nickel monomethylenetrimethylsilyl monobromide (C3): In the glovebox were added **C1** (14.0 mg, 0.0169 mmol, 1.00 equiv) and Et_2O (0.45 mL) to a 20 mL vial equipped with a stir bar. The vial was sealed with a teflon cap and placed in the freezer (-30 °C) for 15 min. After 15 min, the vial was removed and to the stirring mixture was added $TMSCH_2MgCl$ (17.0 µL, 0.0145 mmol, 0.850 M in Et_2O, 0.900 equiv). The reaction was warmed to rt and stirred for 30 min, turning a dark green over time. After 30 min, the Et_2O solution was filtered through a glass wool plug to remove unreacted **C1**. The glass wool plug was rinsed with additional Et_2O (2.0 mL). The solvent was removed under high vac to produce a dark green solid. The solid was then dissolved in cold MeOH (1.0 mL) and filtered through a glass wool plug to produce a dark green filtrate. The solvent was removed under vacuum giving a green solid. The solid was dissolved in a minimal amount of Et_2O (0.5 mL) and pentane (5 mL) was added to the vial, producing a green precipitate. The mixture was filtered through a glass wool plug, leaving behind the solid at the top of the plug. This solid was rinsed with additional pentanes (1 mL). The solid was then redissolved in THF (1 mL) by passing the solvent through the glass wool plug into a new 20 mL vial. The solvent was then removed under vacuum to yield 7 mg of **C3**. (50% yield).

IV. NMR spectra of S1, S2, C1, C2, C3

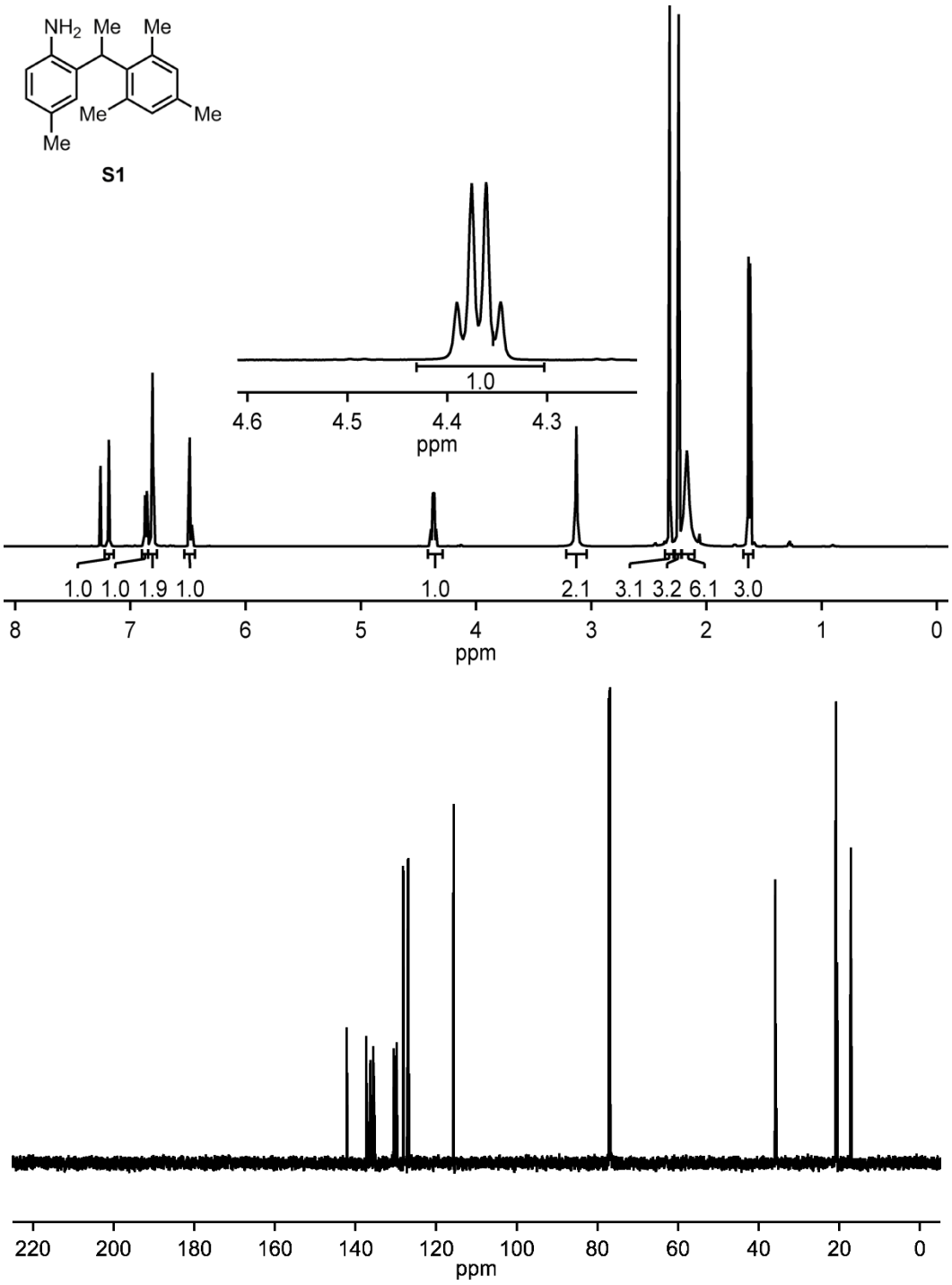


Figure S1. ^{1}H and ^{13}C NMR spectra of **S1**
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (s, 1H), 6.86 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.81 (s, 2H), 6.48 (d, *J* = 7.9 Hz, 1H), 4.37 (q, *J* = 7.3 Hz, 1H), 3.13 (s, 2H), 2.32 (s, 3H), 2.24 (s, 3H), 2.17 (br s, 6H), 1.63 (d, *J* = 7.3 Hz, 3H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 142.21, 137.36, 136.32, 135.64, 130.49, 129.80, 128.17, 127.23, 126.98, 115.72, 35.91, 20.89, 20.77, 20.57, 17.17

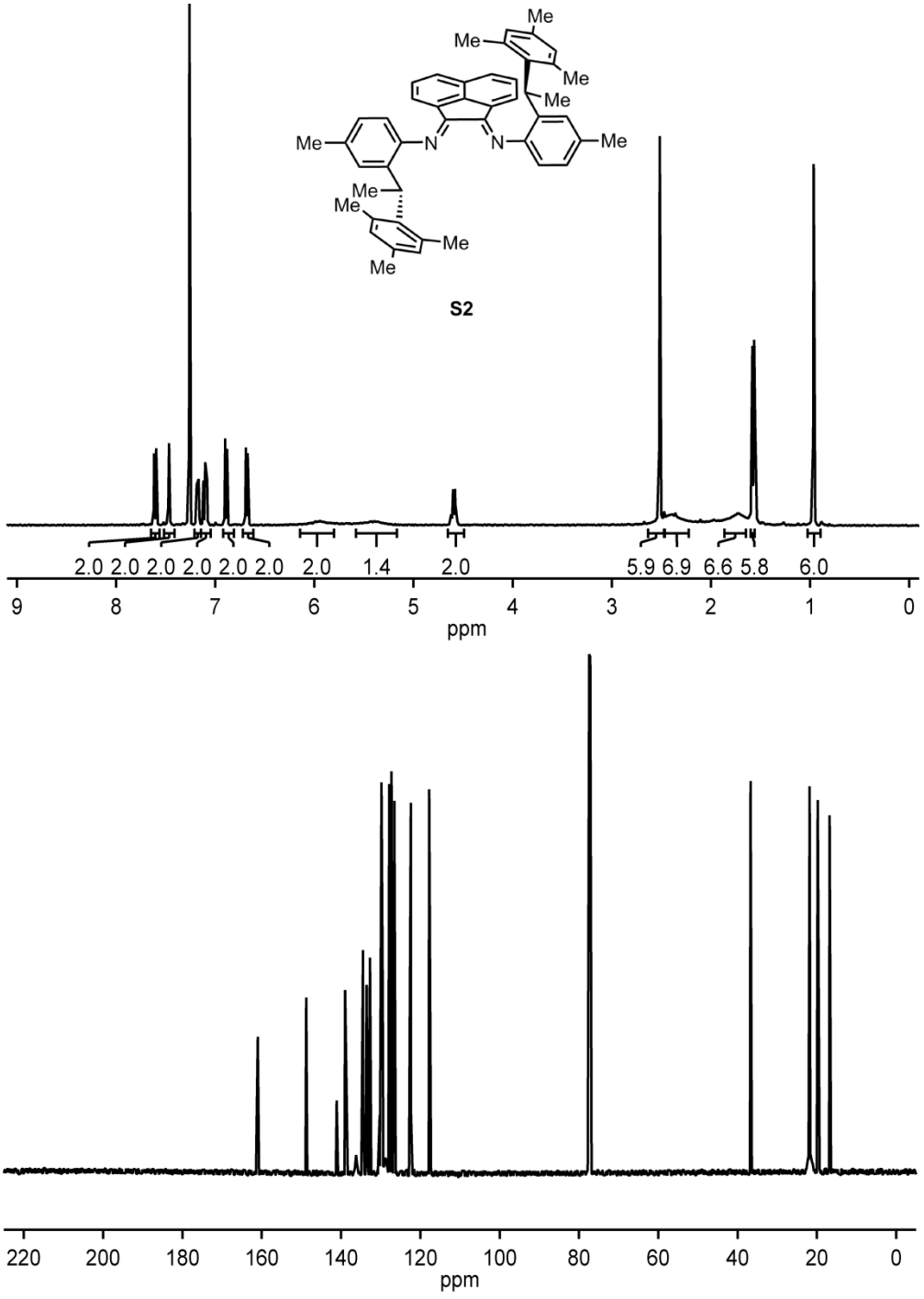


Figure S2. ^{1}H and ^{13}C NMR spectra of **S2**
^{1}H NMR (500 MHz $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.46 (d, *J* = 1.8 Hz, 2H), 7.18 (dd, *J* = 8.2, 1.8 Hz, 2H), 7.10 (dd, *J* = 8.2, 7.2 Hz, 2H), 6.89 (d, *J* = 7.8 Hz, 2H), 6.68 (d, *J* = 7.2 Hz, 2H), 5.95 (br s, 2H), 5.40 (br s, 2H), 4.59 (q, *J* = 7.4 Hz, 2H), 2.52 (s, 6H), 2.38 (br s, 6H), 1.73 (br s, 6H), 1.57 (d, *J* = 7.4 Hz, 6H), 0.96 (s, 6H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.75, 148.55, 140.87, 138.74, 136.7 (br), 134.21, 133.32, 132.45, 130.02, 129.56, 129.25, 127.60, 127.03, 126.33, 122.16, 117.53, 36.50, 25.77, 21.60, 19.55, 16.56

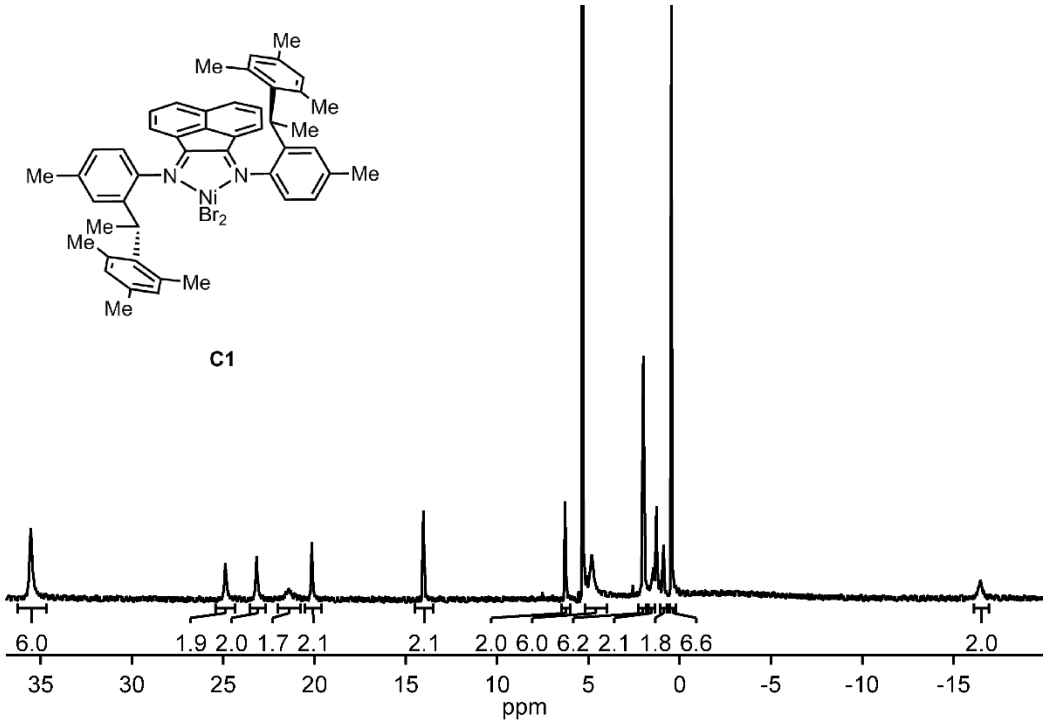


Figure S3. ^{1}H NMR spectrum of **C1**

^{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) (One Ar-CH_3 (6H) is unaccounted for. Spectrum matches literature[1])

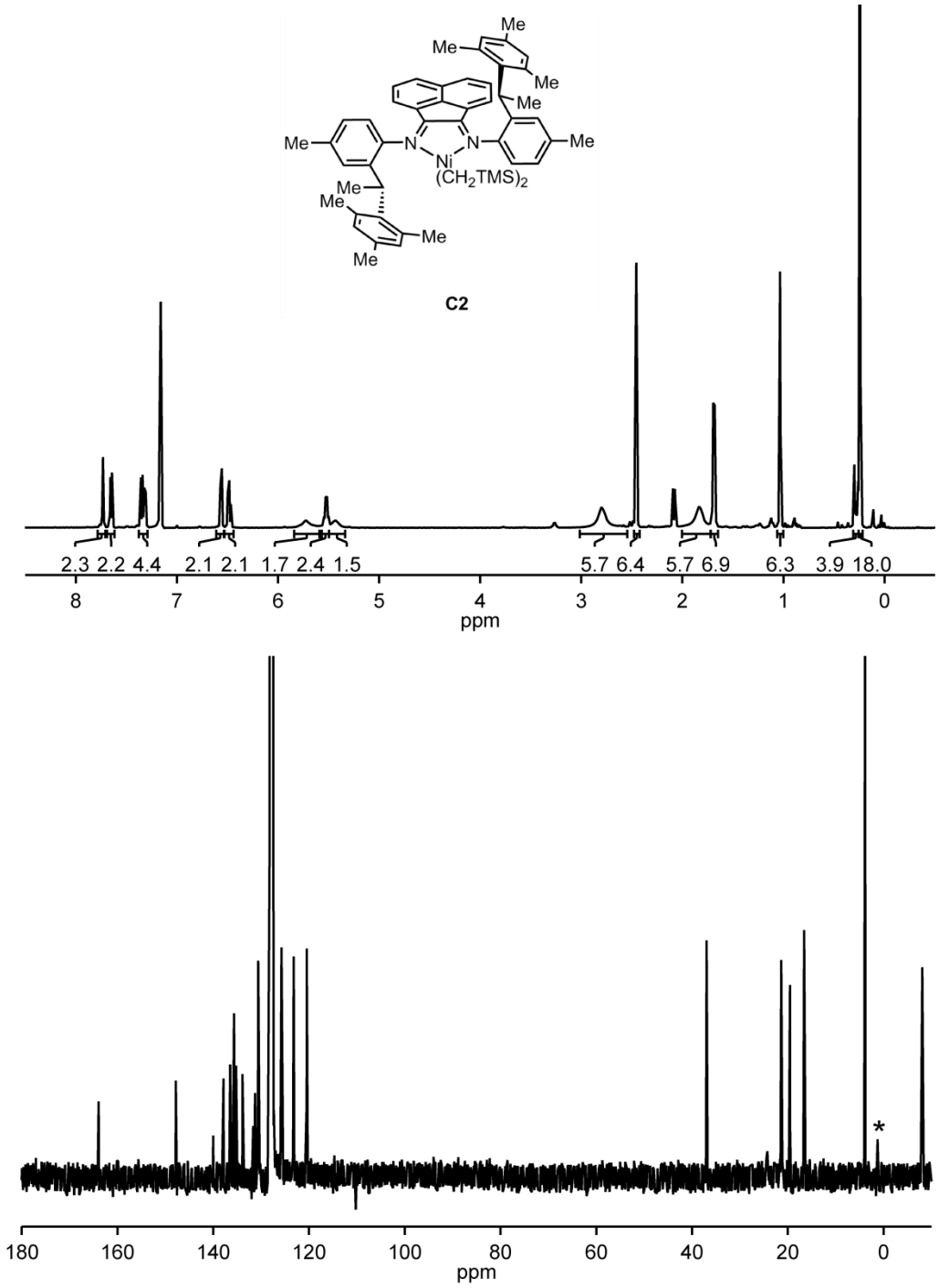


Figure S4. ^{1}H and ^{13}C NMR spectra of **C2**
^{1}H NMR (700 MHz, C_6D_6) δ 7.73 (s, 2H), 7.65 (d, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 6.56 (ad, J = 7.2 Hz, 2H), 6.48 (dd, *J* = 7.8, 7.7 Hz, 2H), 5.72 (br s, 2H), 5.52 (q, *J* = 7.4 Hz, 2H), 5.43 (br s, 2H), 2.80 (s, 6H), 2.46 (s, 6H), 1.83 (s, 6H), 1.69 (d, *J* = 7.4 Hz, 6H), 1.03 (s, 6H), 0.33 (m, 4H), 0.24 (s, 18H)
^{13}C NMR (176 MHz, C_6D_6) δ 163.93, 147.81, 140.02, 137.85, 136.46, 135.65, 135.22, 133.89, 131.66, 131.26, 130.60, 127.33, 123.19, 120.47, 36.96, 24.07, 21.37, 19.54, 16.59, 3.85, –8.09 (* denotes Si grease)

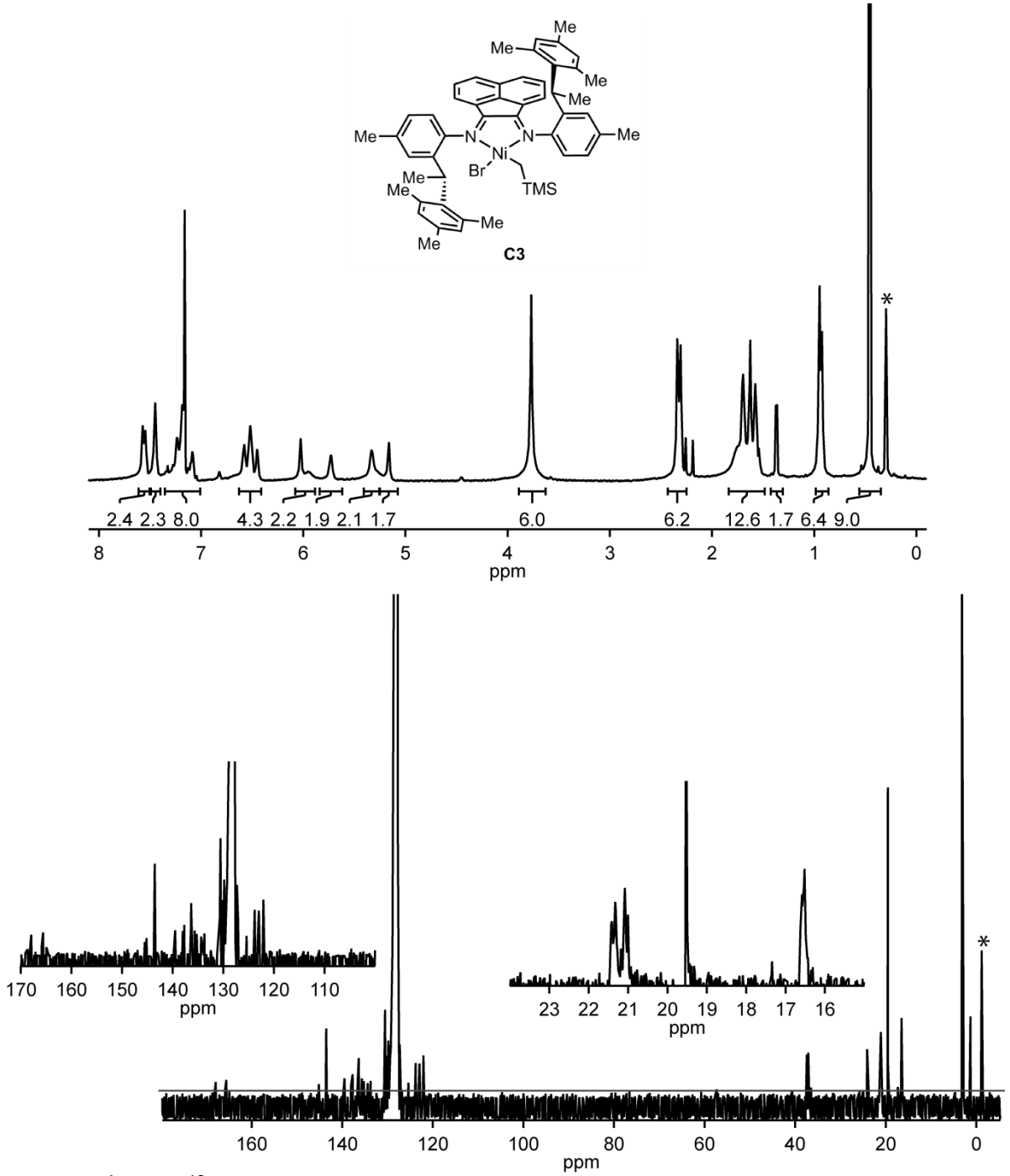


Figure S5. ^{1}H and ^{13}C NMR spectra of **C3**

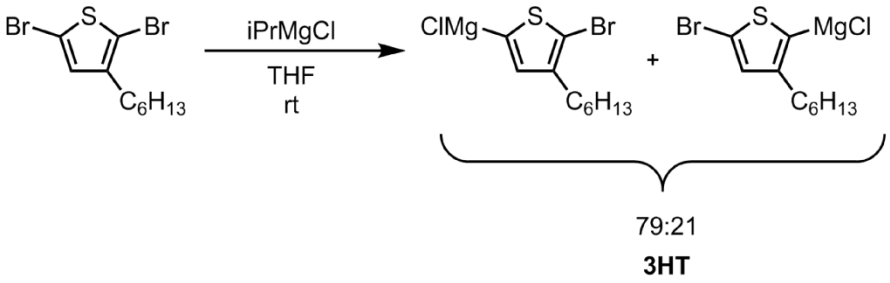
^{1}H NMR (700 MHz, C_6D_6) δ 7.56 (ad, 2H), 7.45 (s, 2H), 7.36 – 7.00 (m, 2H(C3), 6H (C_6D_6)), 6.52 (at, 4H), 6.14 – 5.87 (m, 2H), 5.73 (br s, 2H), 5.33 (br s, 2H), 5.16 (br s, 2H), 3.77 (s, 6H), 2.32 (ad, 6H), 1.87– 1.47 (m, 12H), 1.37 (d, *J* = 9.4 Hz, 2H), 0.94 (add, 6H), 0.46 (s, 9H)

^{13}C NMR(176 MHz, C_6D_6) δ 167.95, 165.59, 143.54, 139.54, 138.06, 138.00, 137.70, 136.55, 136.52, 136.12, 136.09, 136.08,135.65, 135.62, 135.23, 135.21, 135.19, 134.36, 134.34, 133.76, 133.72, 130.66, 130.55, 130.21, 127.25, 127.07, 125.38, 123.79, 122.95, 122.09, 121.93, 37.43, 37.10, 24.11, 21.43, 21.41, 21.33, 21.09, 21.00, 19.53, 16.51, 3.19, 1.30

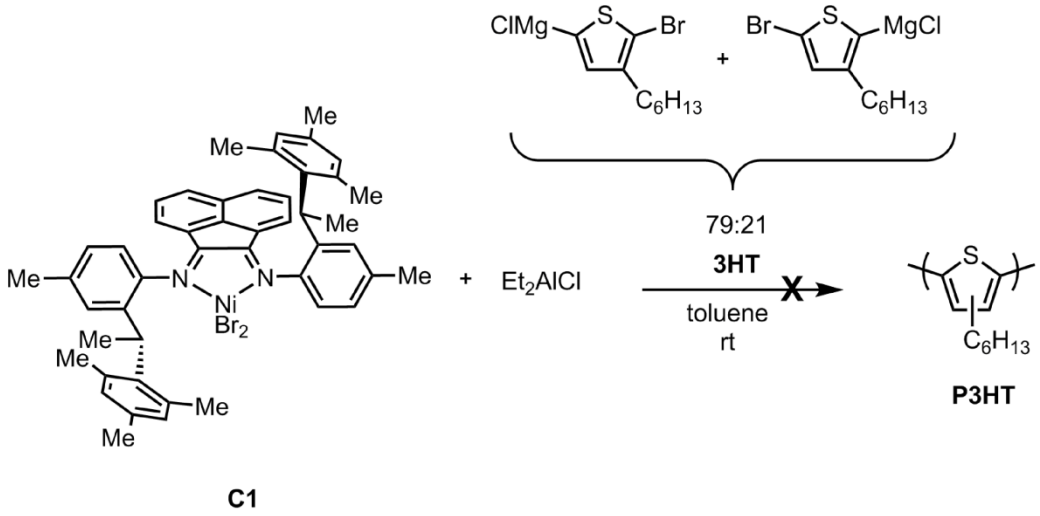
(⸻ = baseline used, * denotes Si grease)

V. Polymerization of 3HT monomer with precatalyst C1 and Et_2AlCl

General Procedure: Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl



In the glovebox 2,5-dibromo-3-hexylthiophene (169 mg, 0.518 mmol, 1 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane (approx. 4.0 mg) and THF (4.99 mL). To the stirring solution was added iPrMgCl (196 µL, 0.363 mmol, 2.00 M in THF, 0.900 equiv) and stirred for 30 min. **3HT** was titrated to be 0.071 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of **3HT** was quenched with aq. HCl (0.50 mL, 12 M) outside of the box. The quenched monomer was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).



In the glovebox to a 20 mL vial equipped with a stir bar were added Et_2AlCl (0.14 mL, 1.6 M in toluene, 200 equiv), toluene (2.5 mL), and **C1** (2.8 mg, 0.0060 mmol, 1 equiv) in 0.5 mL DCM to yield a purple opaque solution. To the stirring solution was added **3HT** (1.00 mL, 0.0720 mmol, 100 equiv). After 30 min the reaction was taken out of the box and quenched with aq. HCl (2 mL, 12 M). The reaction mixture was extracted with $CHCl_3$ (5 mL), dried over $MgSO_4$, filtered through a glass wool plug and split into two portions. The first portion was analyzed by GC showing 24% conversion of **3HT**. All solvent was removed from the other portion under reduced pressure. The oil was then dissolved in THF:PhMe (99:1) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.

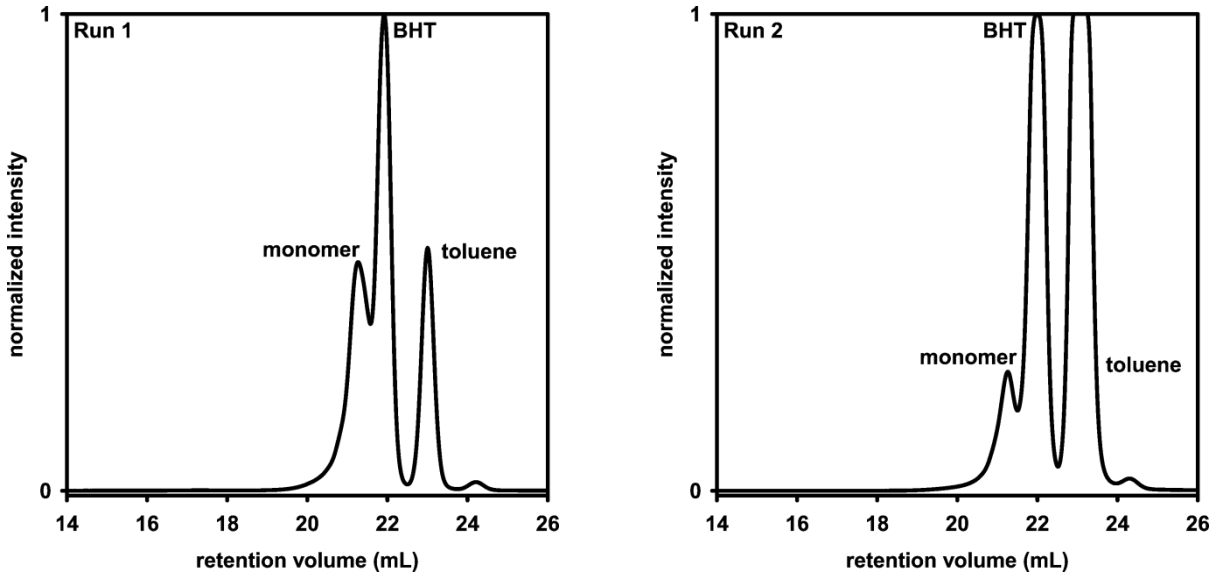
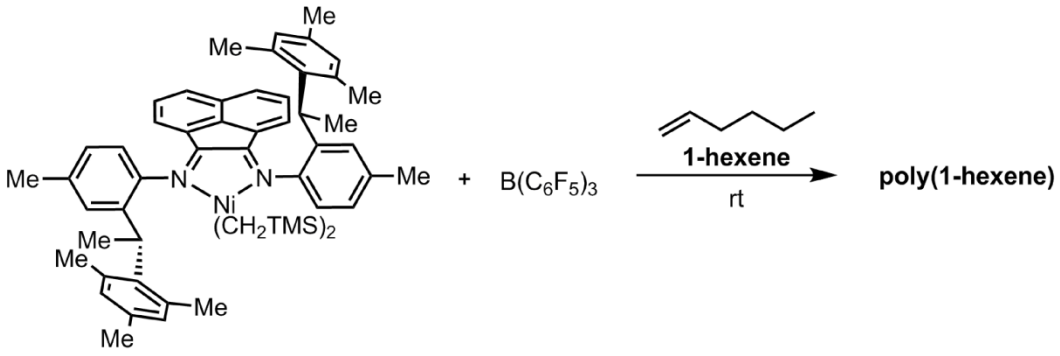


Figure S6. GPC trace for polymerization of **3HT** monomer with catalyst **C1** and **Et_2AlCl**. (BHT (Butylated hydroxytoluene) = THF stabilizer)

VI. Polymerization of 1-hexene monomer with precatalyst C2 and $B(C_6F_5)_3$



C2

To a 4 mL vial in the glovebox were added **C2** (2.7 mg, 0.0030 mmol, 1.0 equiv) and 1-hexene (1.00 mL). This solution was then passed through a syringe fitted with a PTFE filter (0.2 µm) into a 20 mL vial equipped with a stir bar. In another 4 mL vial were added **$B(C_6F_5)_3$** (3.1 mg, 0.0061 mmol, 2.0 equiv) and 1-hexene (0.50 mL). The **$B(C_6F_5)_3$** solution was then injected into the **C2** solution. The solution immediately turned dark green and then transitioned to a light pink. The polymerization was stirred for 5 min, turning slightly viscous, before being quenched outside of the box with MeOH (3 mL), precipitating **poly(1-hexene)** as a white solid (13.0 mg). The solvent was removed by decanting and the polymer was dissolved in THF:PhMe (99:1) (1.5 mL), and after mild heating passed through a PTFE filter (0.2 µm) to be analyzed by GPC. Integrated area on GPC trace is from retention volume of 14 mL to 20 mL.

Run 1: M_n **=** 78.2 kDa, **Đ =** 1.60 (13.0 mg)
Run 2: M_n **=** 64.1 kDa**, Đ =** 1.59 (8.0 mg)

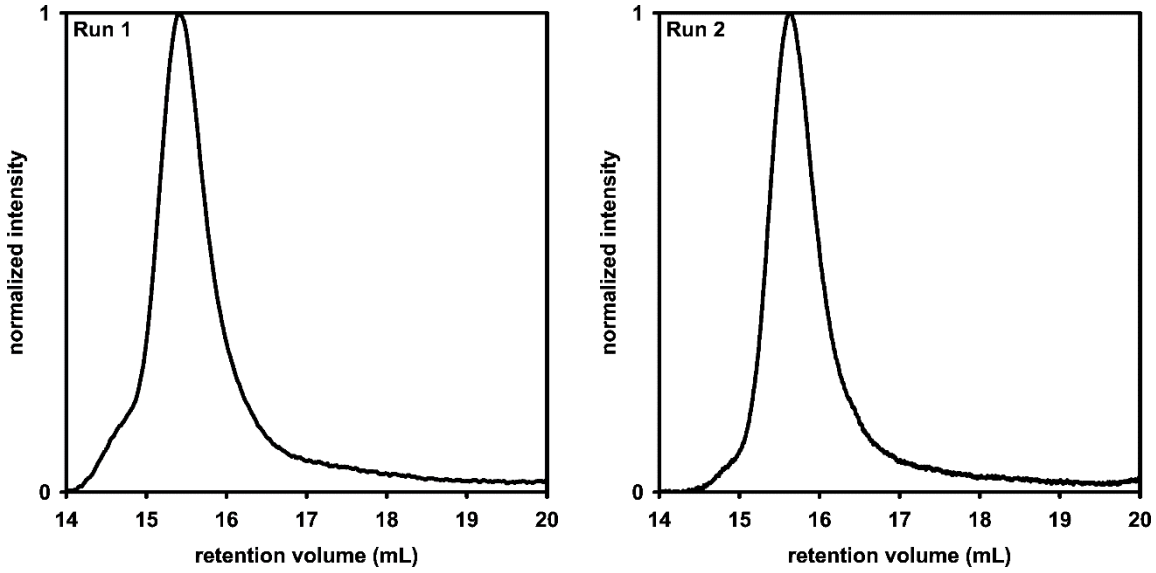


Figure S7. GPC trace for polymerization of **1-hexene** monomer with catalyst **C2** and **$B(C_6F_5)_3$.**

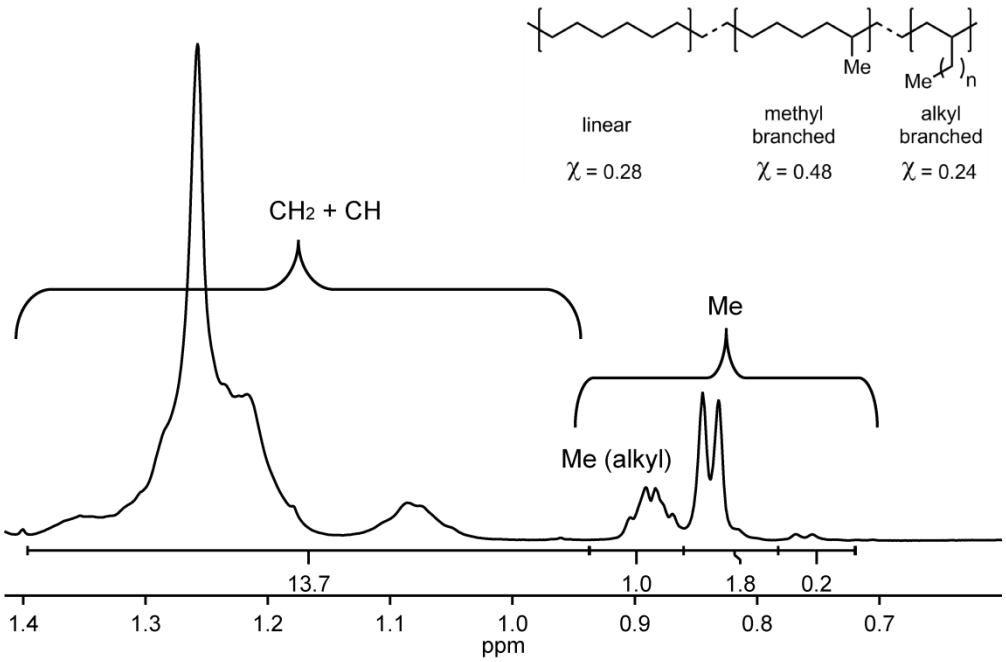


Figure S8. ^{1}H NMR spectrum of **poly(1-hexene)** generated with catalyst **C2** and **B(C_6F_5)$_3$**

$$R = \frac{[CH_3]}{[CH_2]} = \frac{(3/3)}{(13.7-1)/2} = 0.157$$

$$\chi_{linear} = \frac{[1-(\omega-2)R]}{[1+2R]} = 0.280$$

carbons in 1-hexene = $\omega = 6$

$$\chi_{alkyl} + \chi_{methyl} = 1 - \chi_{linear} = 0.717$$

$$\frac{\chi_{alkyl}}{\chi_{methyl}} = \frac{CH_3\,(Me\,(alkyl))}{CH_3\,(Me)} = \frac{1.0}{2.0} = 0.500$$

$$\chi_{alkyl} = (0.50)\,\chi_{methyl}$$

$$(0.50)\,\chi_{methyl} + \chi_{methyl} = 0.717$$

$$\chi_{methyl} = 0.480$$

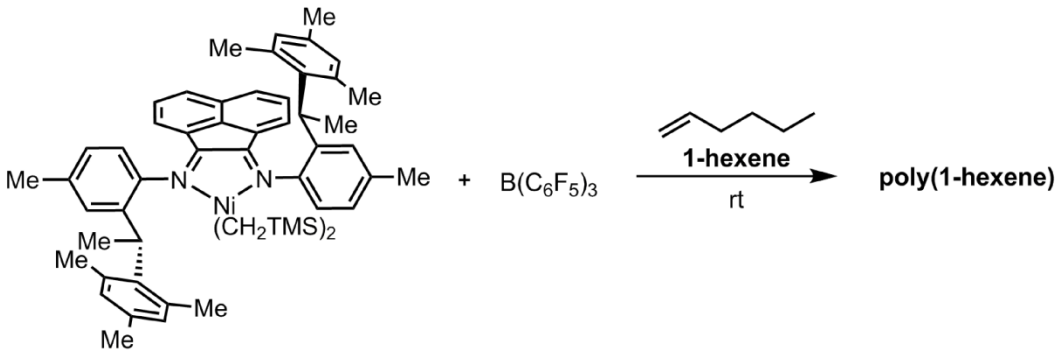
$$\chi_{alkyl} = 0.240$$

Equation S1. Calculating br/1000C of **poly(1-hexene)** using ^{1}H NMR spectroscopy[3]

Procedure: M_n versus time of 1-hexene polymerization with precatalyst C2 and $B(C_6F_5)_3$

C2 and $B(C_6F_5)_3$ stock solutions

In the glovebox were added **C2** (12.0 mg, 0.014 mmol, 0.50 mM) and 1-hexene (2.71 mL) to a 20 mL vial. In another 20 mL vial were added **$B(C_6F_5)_3$** (19 mg, 0.0074 mmol, 0.50 mM) and 1-hexene (7.42 mL).



C2

In the glovebox to a 20 mL vial equipped with a stir bar were added **C2** (0.50 mL, 0.0025 mmol, 0.50 mM solution in 1-hexene, 1.0 equiv) and **$B(C_6F_5)_3$** (1.0 mL, 0.0050 mmol, 0.50 mM solution in 1-hexene, 2.0 equiv). Aliquots were taken at 125, 210, 290, 385, and 530 s. Each aliquot was taken out of the glovebox and quenched with MeOH. If polymer did not precipitate, the solvent was removed under reduced pressure. If polymer did precipitate after quenching, the solvent was removed by decanting. The aliquots were then dissolved in THF:PhMe (99:1) (1.5 mL) and after mild heating were passed through a PTFE filter (0.2 µm) to be analyzed by GPC.

Run 1

aliquot (sec)	M_n (kDa)	Đ
125	27.2	1.27
210	39.2	1.34
290	49.6	1.38
385	60.0	1.41
530	69.0	1.45

Run 2

aliquot (sec)	M_n (kDa)	Đ
180	30.8	1.57
255	37.3	1.59
360	46.9	1.53
480	57.8	1.51

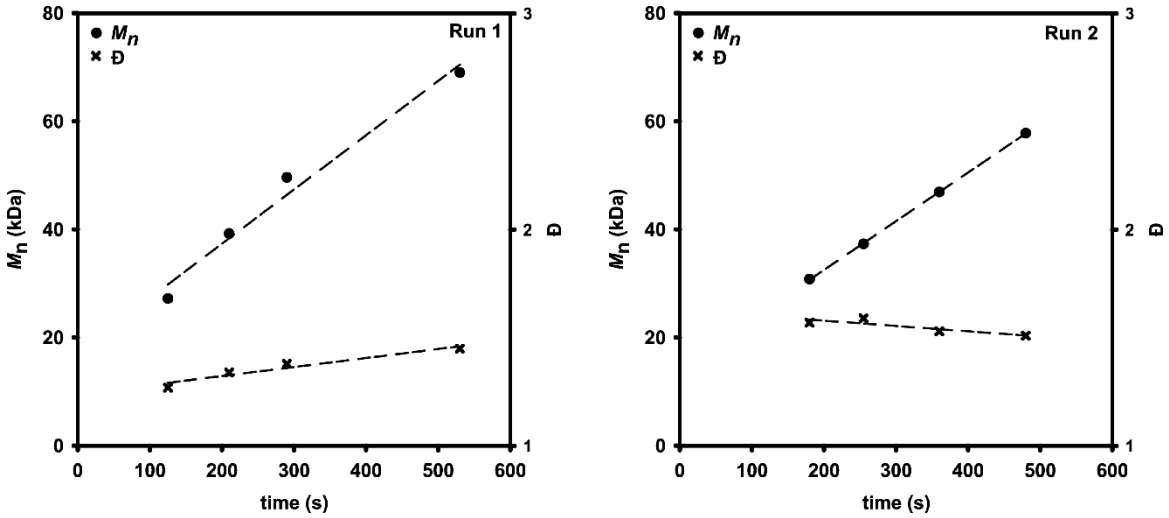
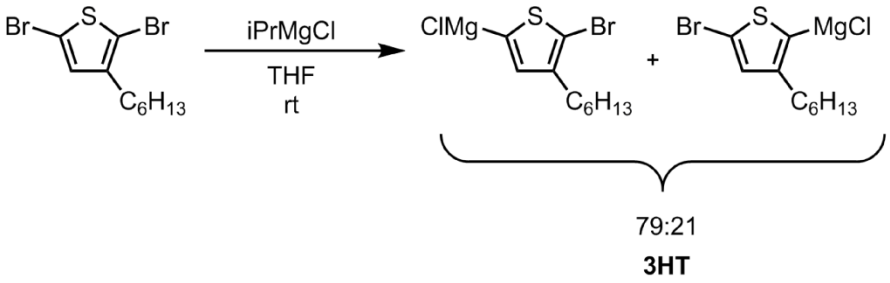


Figure S9. M_n versus time for polymerizing **1-hexene** monomer with precatalyst **C2** and **$B(C_6F_5)_3$**.

VII. Polymerization of 3HT monomer with precatalyst C2 and $B(C_6F_5)_3$

Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl

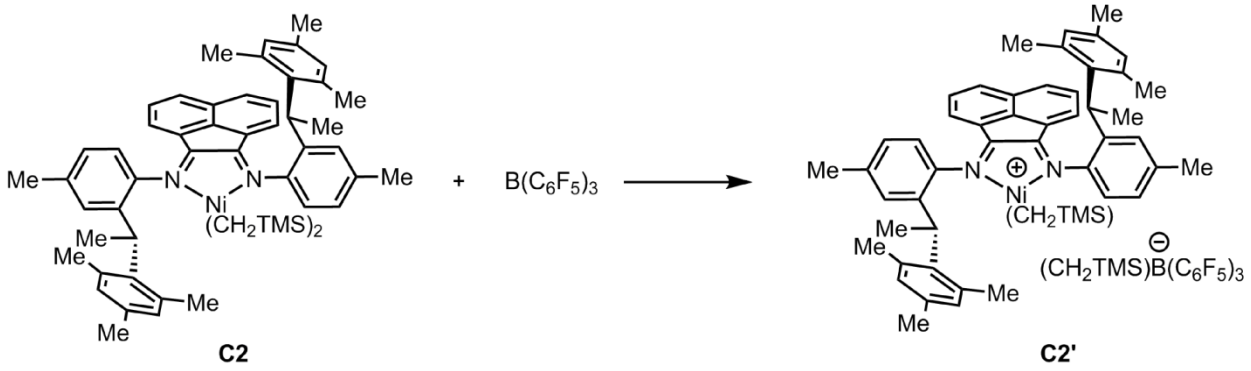


In the glovebox 2,5-dibromo-3-hexylthiophene (90.0 mg, 0.276 mmol, 1.00 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane std. (approx. 4 mg) and THF (2.66 mL). To the stirring solution was added iPrMgCl (100 µL, 0.193 mmol, 1.89 M in THF, 0.700 equiv) and stirred for 30 min. **3HT** was titrated to be 0.071 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of the Grignard solution was quenched with aq. HCl (0.5 mL, 12M) outside of the glovebox. The quenched monomer was extracted with $CHCl_3$ (2 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).

C2 and $B(C_6F_5)_3$ stock solutions

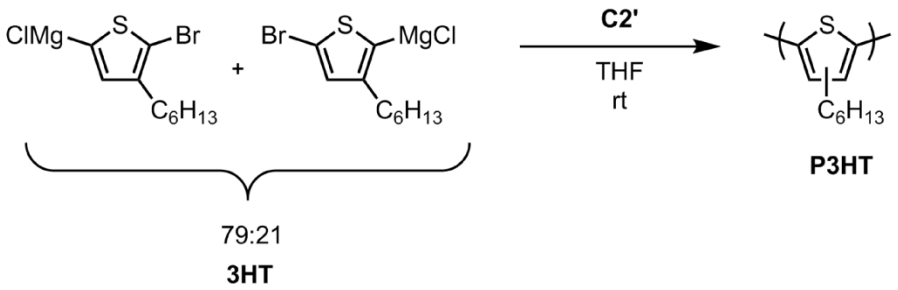
In the glovebox were added **C2** (5.2 mg, 0.0059 mmol, 0.50 mM) and toluene (1.18 mL) to a 4 mL vial. In another 4 mL vial were added **$B(C_6F_5)_3$** (3.8 mg, 0.0074 mmol, 0.50 mM) and toluene (1.48 mL). **C2** solutions were made fresh for each **3HT** polymerization

Activation of precatalyst C2 with $B(C_6F_5)_3$



C2 (0.11 mL, 0.50 mM in toluene, 1.0 equiv) and **$B(C_6F_5)_3$** (0.11 mL, 0.50 mM in toluene, 1.0 equiv) were added to a 4 mL vial equipped with a stir bar and stirred for 5 min. **C2'** solution must be made fresh for each **3HT** polymerization.

Procedure: Polymerization of 3HT monomer with catalyst C2'



In the glovebox to a 20 mL vial equipped with a stir bar was added **3HT** (1.00 mL, 0.0700 mmol, 125 equiv relative to **C2'**) and THF (1.63 mL) to give an overall [**3HT**] of 0.02 M. To the stirring solution was added **C2'** (0.22 mL, 0.57 µmol, 1.0 equiv). The polymerization was stirred for 1 h before being quenched outside of the box with aq. HCl (2.0 mL, 12 M). The reaction mixture was extracted with $CHCl_3$ (5.0 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two equal portions. The first portion was diluted with additional $CHCl_3$ (2.0 mL) and analyzed by GC to show 70% conversion. The other portion was concentrated in vacuo and then redissolved in THF:PhMe (99:1) (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC. After GC and GPC analysis, both portions were recombined and the solvent removed *in vacuo* to yield a purple solid. The solid was dissolved in a minimum amount of $CHCl_3$ (0.5 mL), and precipitated with MeOH (15.0 mL). The mixture was then centrifuged, the solvent decanted, and the solid dried under vacuum to afford **P3HT** as a purple solid. Regioregularity of P3HT was calculated to be 75%.

Run 1: M_n **=** 23.5 kDa, **Đ =** 1.98 (6.7 mg, 58% yield)
Run 2: M_n **=** 19.5 kDa, **Đ =** 2.05 (5.5 mg, 47% yield)

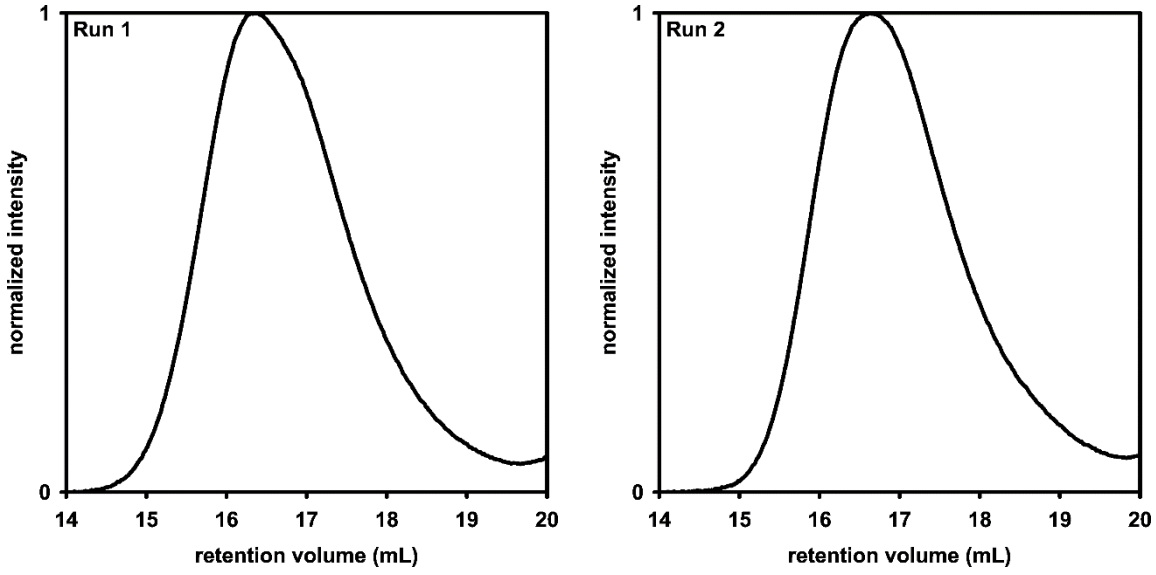


Figure S10. GPC trace of **P3HT** generated with catalyst **C2'**

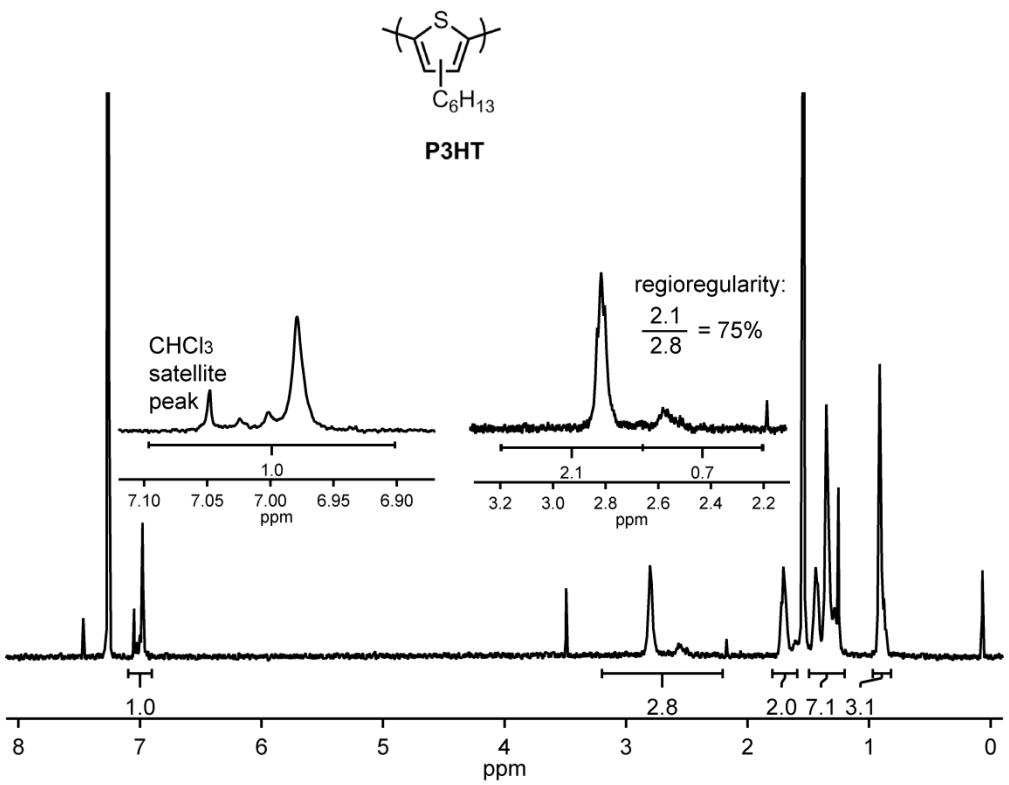


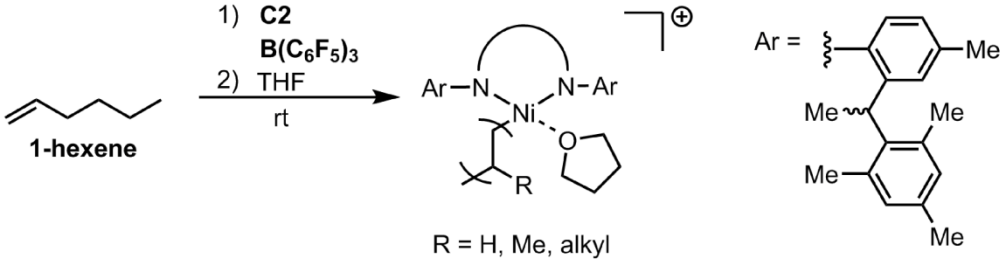
Figure S11. ^{1}H NMR spectrum of **P3HT** generated with **C2'**.

VIII. THF impact on 1-hexene polymerization

$B(C_6F_5)_3$ solution preparation

In a 4 mL vial were added **$B(C_6F_5)_3$** (2.5 mg, 0.0050 mmol, 2.0 equiv) and **1-hexene** (0.5 mL).

Procedure



In the glovebox was added **C2** (2.2 mg, 0.0025 mmol, 1 equiv) and **1-hexene** (1.0 mL) to a 4 mL vial. This solution was then passed through a syringe fitted with a PTFE filter (0.2 µm) into a 20 mL vial equipped with a stir bar. The **$B(C_6F_5)_3$** solution was then injected into the 20 mL vial. Upon adding the activator, the solution immediately turned dark green and then transitioned to a light pink. The reaction stirred for 3 min and THF (3.0 mL) was added to the vial. An aliquot (0.3 mL) was taken and quenched outside of the box with MeOH (2.0 mL). After 1 h the reaction was quenched outside of the box with MeOH (5.0 mL). The solvent was removed under reduced for both the first aliquot and final polymer. The resulting residues were dissolved in THF:PhMe (99:1) (1.5 mL), and after mild heating, passed through a PTFE filter (0.2 µm) to be analyzed by GPC.

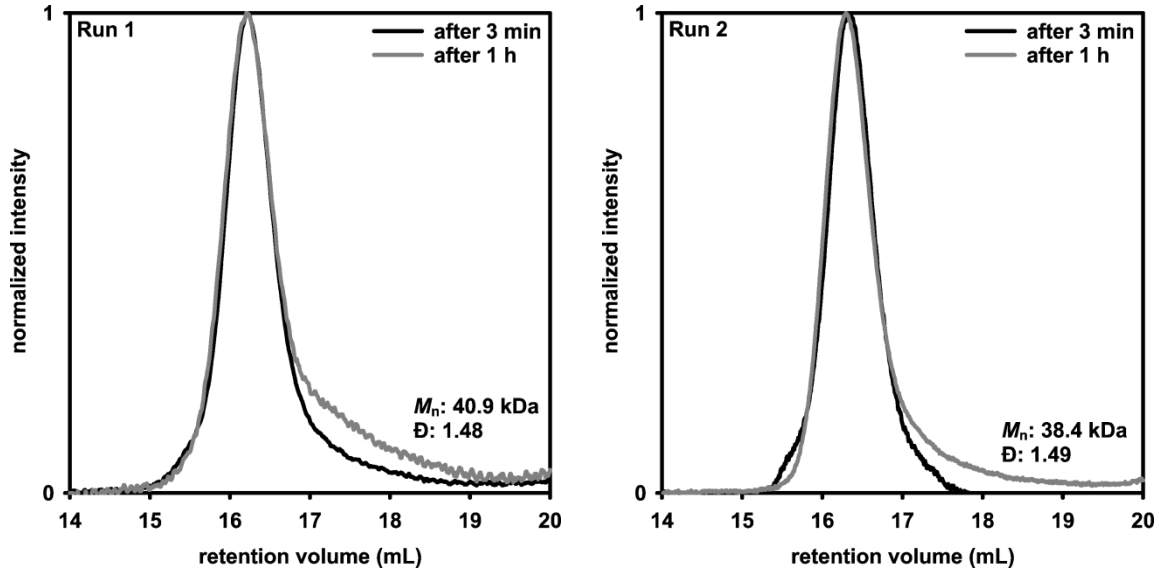


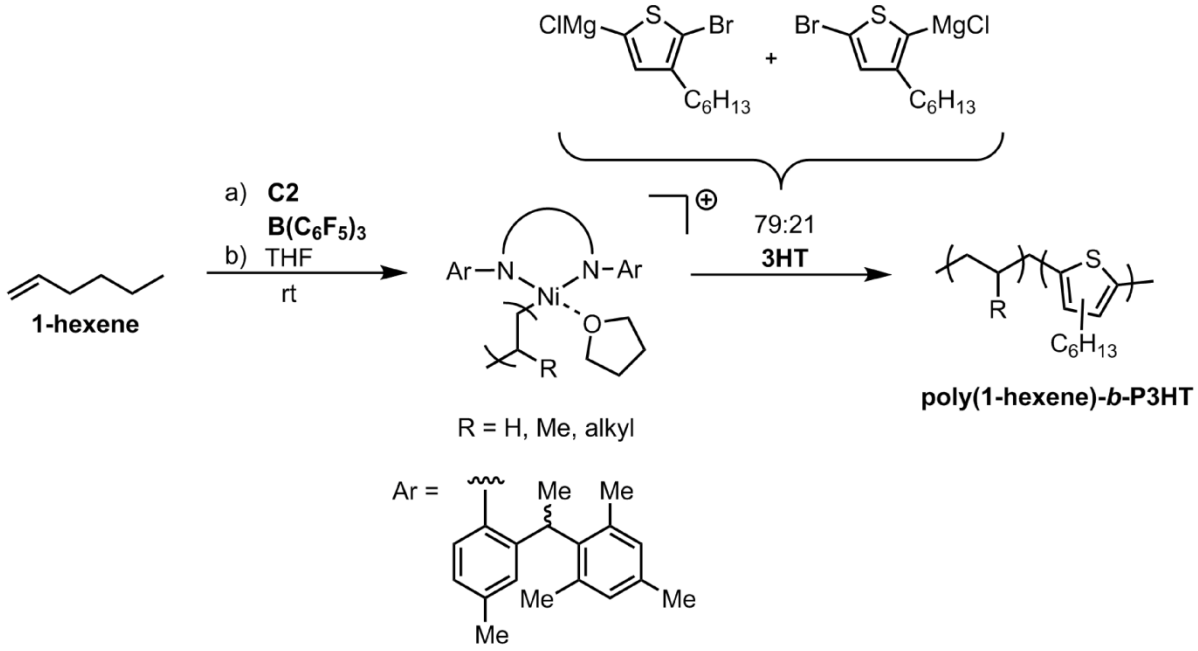
Figure S12. GPC trace of **1-hexene** polymerization at 3 min and 1 h after THF addition.

IX. Copolymerization of 3HT and 1-hexene monomers with precatalyst C2 and $B(C_6F_5)_3$

$B(C_6F_5)_3$ stock solution prep

In a 4 mL vial was added **$B(C_6F_5)_3$** (3.1 mg, 0.0062 mmol, 2.0 equiv) and **1-hexene** (0.5 mL).

Procedure



In the glovebox was added **C2** (2.8 mg, 0.0031 mmol, 1.0 equiv) and **1-hexene** (1.0 mL) to a 4 mL vial. This solution was then passed through a syringe fitted with a PTFE filter into a 20 mL vial equipped with a stir bar. The **$B(C_6F_5)_3$** solution was then injected into the **C2** solution. Upon adding the activator, the solution immediately turned dark green and then transitioned to a light pink. The reaction stirred for 3 min at rt and THF (3.00 mL) was added to the vial. Then an aliquot (0.5 mL) was taken and quenched outside of the glovebox with neutral MeOH (2 mL). To the remaining reaction was added **3HT** (1.0 mL, 0.070 mmol, 23 equiv). After 1 h the polymerization was quenched with aq HCl (2.00 mL, 12 M) outside of the glovebox. The mixture was extracted with $CHCl_3$ (5.00 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two portions. The first portion was analyzed by GC to show 11% conversion. The solvent was removed under reduced pressure from the second portion. The resulting solid was dissolved in THF:PhMe (99:1) (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.

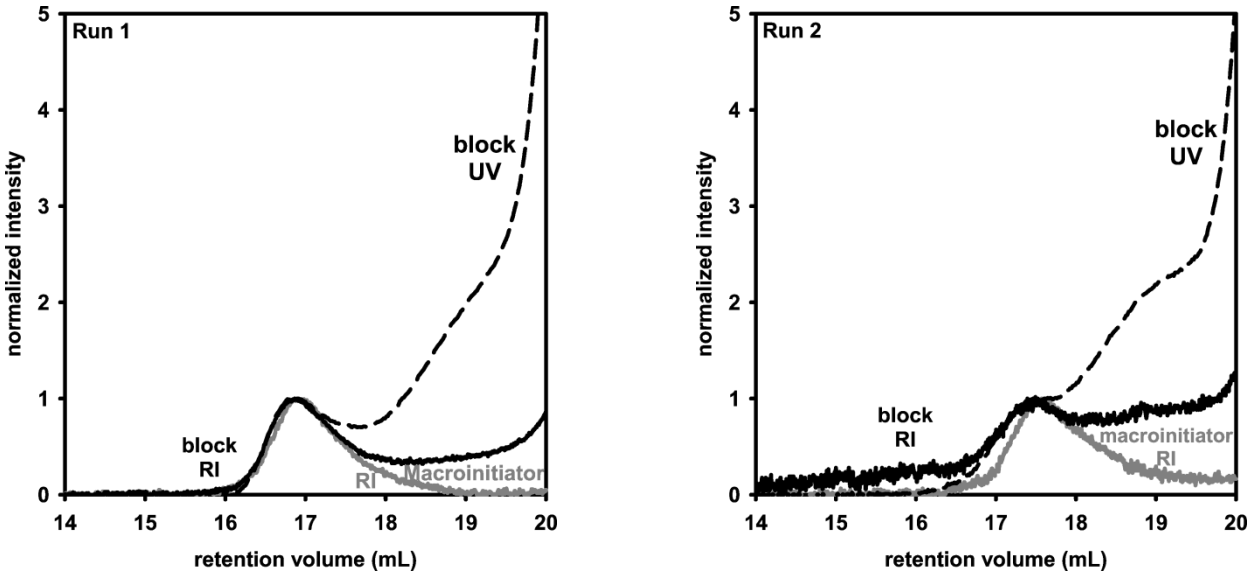
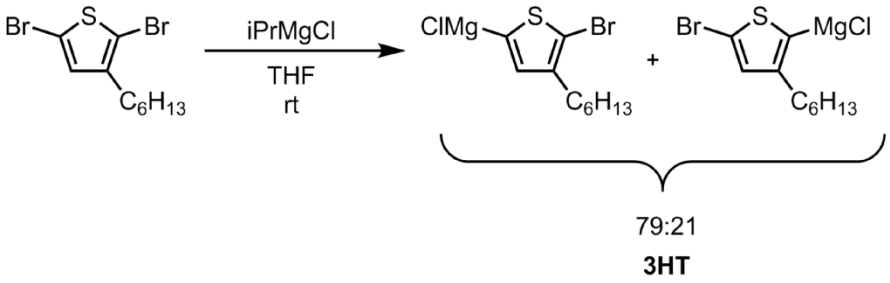


Figure S13. GPC trace of copolymerization of **1-hexene** and **3HT** product mixture.

X. Polymerization of 3HT monomer with varying amounts of 1-hexene

Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl

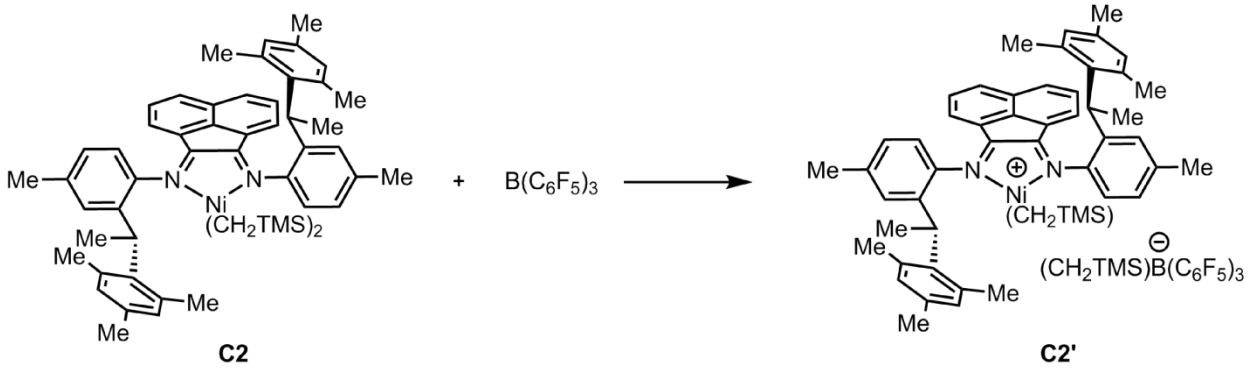


In the glovebox 2,5-dibromo-3-hexylthiophene (45.0 mg, 0.138 mmol, 1.00 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane (approx. 4.0 mg) and THF (1.33 mL). To the stirring solution was added iPrMgCl (48.0 µL, 0.0966 mmol, 2.00 M in THF, 0.700 equiv) and stirred for 30 min. **3HT** was titrated to be 0.070 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of **3HT** was quenched with aq HCl (0.50 mL, 12 M) outside of the box. The quenched monomer was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).

C2 and $B(C_6F_5)_3$ stock solutions

In the glovebox were added **C2** (6.0 mg, 0.0068 mmol, 0.50 mM) and toluene (1.35 mL) to a 4 mL vial. In another 4 mL vial were added **$B(C_6F_5)_3$** (7.0 mg, 0.014 mmol, 0.50 mM) and toluene (2.73 mL). **C2** solutions were made fresh for each **3HT** polymerization

Activation of precatalyst C2 with $B(C_6F_5)_3$



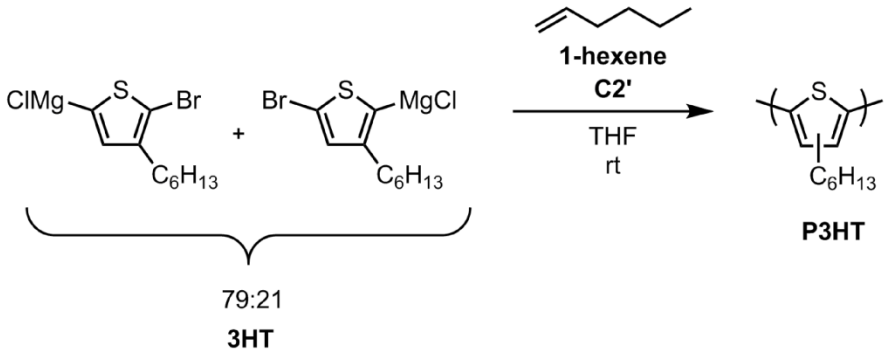
C2 (0.10 mL, 0.50 mM in toluene, 1.0 equiv) and **$B(C_6F_5)_3$** (0.10 mL, 0.50 mM in toluene, 1.0 equiv) were added to a 4 mL vial equipped with a stir bar and stirred for 5 min. **C2'** solution must be made fresh prior to use in **3HT** polymerization.

3HT stock solution preparation

In the glovebox to four separate 20 mL vials equipped with a stir bar was added **3HT** (100 equiv rel. to cat.), THF (X mL, 0.02 M), **1-hexene**

Vial 1: 3HT (1 mL, 0.07 M), THF (2.4 mL), **1-hexene** (0 mL, 0 equiv)
Vial 2: 3HT (1 mL, 0.07 M), THF (1.65 mL), **1-hexene** (0.75 mL, 12000 equiv)
Vial 3: 3HT (1 mL, 0.07 M), THF (2.34 mL), **1-hexene** (60 µL, 1000 equiv)
Vial 4: 3HT (1 mL, 0.07 M), THF (2.39 mL), **1-hexene** (10 µL, 50 equiv)

Procedure



To each vial was added the **C2'** solution (0.20 mL, 0.50 µmol, 1 equiv). The reactions were stirred at rt for 1 h before being quenched outside of the box with aq HCl (2.0 mL, 12 M). Each vial was extracted $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two portions The first portion was analyzed by GC. The solvent was removed under reduced pressure from the second portion. The resulting solid was then dissolved in THF (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.

Table S1: P3HT synthesis with varying equiv of **1-hexene**

Run 1:

X equiv 1-hexene	% conversion 3HT	M_n P3HT kDa	Đ
12000	12.6	5.87	1.85
1000	22.1	14.6	1.96
50	35.9	20.3	2.05
0	71.1	26.5	1.89

Run 2:

X equiv 1-hexene	% conversion 3HT	M_n P3HT kDa	Đ
12000	7.5	6.67	1.80
1000	13.7	15.8	2.02
50	35.0	24.2	2.02
0	93.6	24.8	2.03

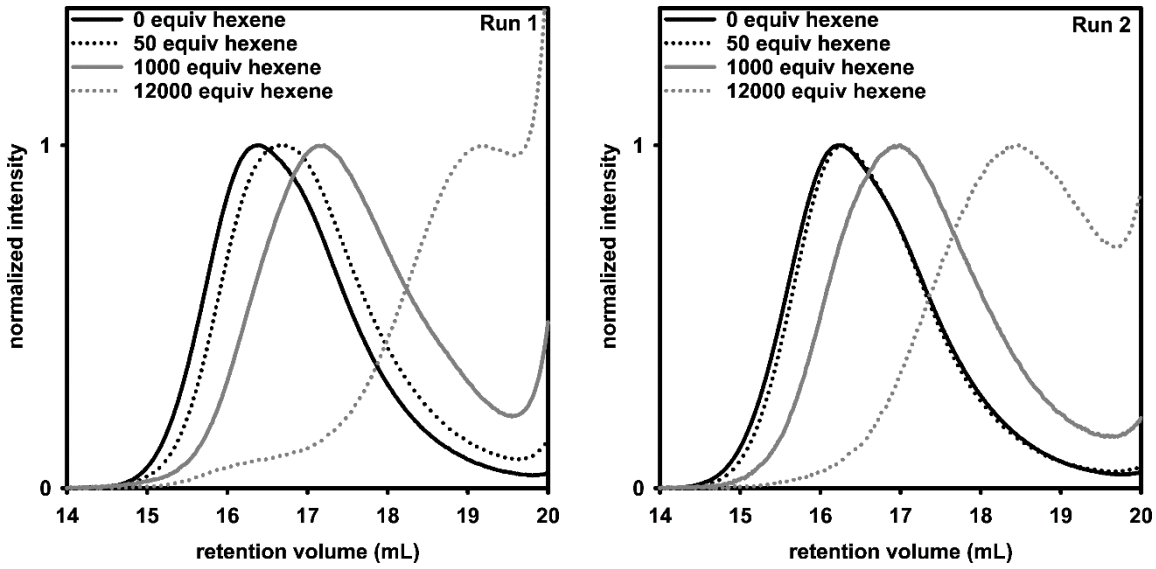
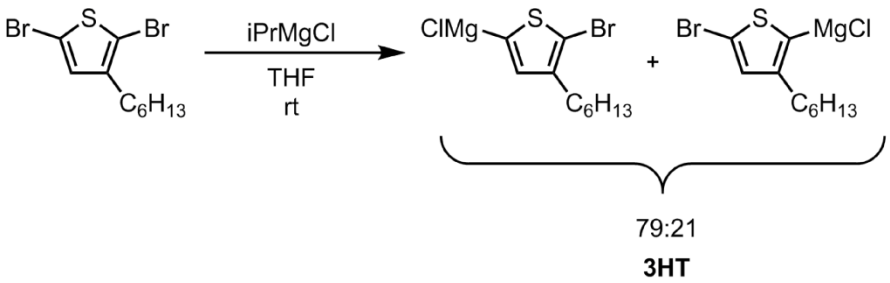


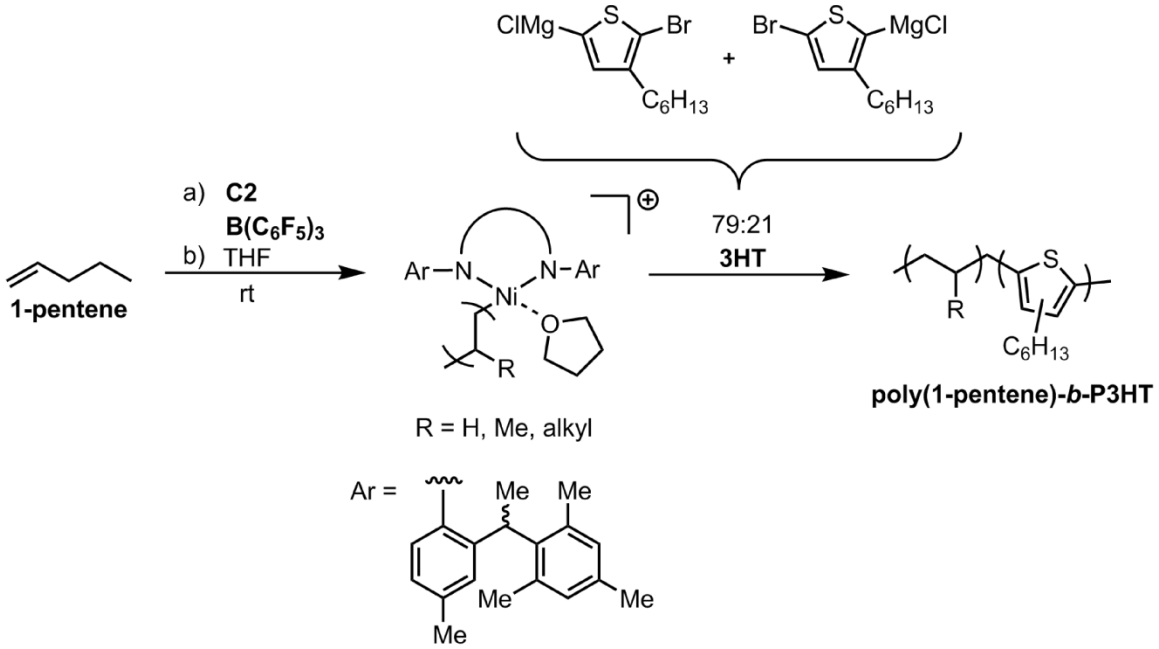
Figure S14. GPC trace of **P3HT** synthesis with varying equiv of **1-hexene**.

XI. Copolymerization of 1-pentene and 3HT monomers with precatalyst C2 and $B(C_6F_5)_3$

Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl



In the glovebox, 2,5-dibromo-3-hexylthiophene (250 mg, 0.768 mmol, 1 equiv), n-dodecane (approx. 4 mg), and tetrahydrofuran (THF, 7.40 mL) were added sequentially to a 20 mL vial equipped with a stir bar. To this solution iPrMgCl (268 µL, 0.537 mmol, 2.00 M in THF, 0.7 equiv) was added. The resulting thiophene Grignard solution was stirred for 30 min at rt and then titrated using salicylaldehyde phenylhydrazone.[i] An aliquot of the Grignard solution (0.3 mL, 0.070 M) was quenched with aq. HCl (0.5 mL, 12 M) outside the glovebox, extracted with $CHCl_3$ (2 mL), dried over $MgSO_4$, and analyzed by gas chromatography (GC) to show a mixture of regioisomers (79:21).



Copolymerization procedure

In the glovebox, precatalyst **C2** (15.7 mg, 0.0177 mmol, 1.0 equiv) and cold 1-pentene (2.00 mL, kept at -30 °C) were added to a 4 mL vial while stirring. After 2 min, the mixture was filtered through a PTFE filter (0.2 µm) into a 50 mL round-bottom flask equipped with a stir bar. A solution of $B(C_6F_5)_3$ (18.0 mg, 0.0354 mmol, 2.0 equiv) in cold 1-pentene (1 mL) was added and the reaction stirred for 20 s. Then, THF (5.0 mL) and toluene (3.0 mL) were added. The flask was then held under reduced pressure for 30 min (until ~2 mL solvent remained).

An aliquot (0.50 mL) of the remaining solution was added to a J-Young tube and analyzed by ^{1}H NMR spectroscopy (**Figure S15**) before quenching with MeOH (2 mL) and concentrating in vacuo. The residue was redissolved in THF (1.5 mL), passed through a PTFE syringe filter (0.2 µm), and analyzed by gel permeation chromatography (GPC) to estimate the macroinitiator molecular weight. THF (8.0 mL) and thiophene Grignard (4.0 mL) were added to the remaining macroinitiator solution. After 2 h, the reaction was quenched with aq. HCl (10 mL, 12 M). The resulting polymer was extracted with $CHCl_3$ (2 x 15 mL), dried over $MgSO_4$, and filtered using a Buchner funnel. An aliquot (0.5 mL) of this solution was split into two equal portions. The first portion was diluted with $CHCl_3$ (2.0 mL) and analyzed by GC to determine the thiophene conversion. The second portion was concentrated in vacuo and then redissolved in THF/toluene (99:1; 1.5 mL) with mild heating, passed through a PTFE filter, and analyzed by GPC. After analysis, both portions were recombined with the mother liquor and the solvent was removed in vacuo, yielding a maroon solid (25 mg).

Block Copolymer Purification

The maroon solid was dissolved in $CHCl_3$ (0.5 mL) and precipitated with MeOH (15.0 mL). The mixture was spun in a centrifuge for 10 min. The supernatant was decanted and saved. The precipitate was dried under reduced pressure, yielding 15 mg of polymer. ^{1}H NMR spectroscopic analysis revealed that this solid resembled P3HT homopolymer (**Figure S18**). The supernatant was concentrated under reduced pressure to generate a purple solid (10 mg). MeOH (10 mL) was added followed by sonication for 1 min. The resulting mixture was spun in the centrifuge for 10 min, and then supernatant was removed and saved. This process was repeated 3 times. Hexanes (10 mL) was added to the remaining solid, followed by centrifugation (10 min). The resulting yellow supernatant was collected, passed through a PTFE syringe filter (0.2 µm), and concentrated in vacuo to yield a solid (4 mg). ^{1}H NMR spectroscopic analysis revealed that the solid contains a mixture of the desired copolymer and poly(1-pentene) homopolymer (Figure S20).

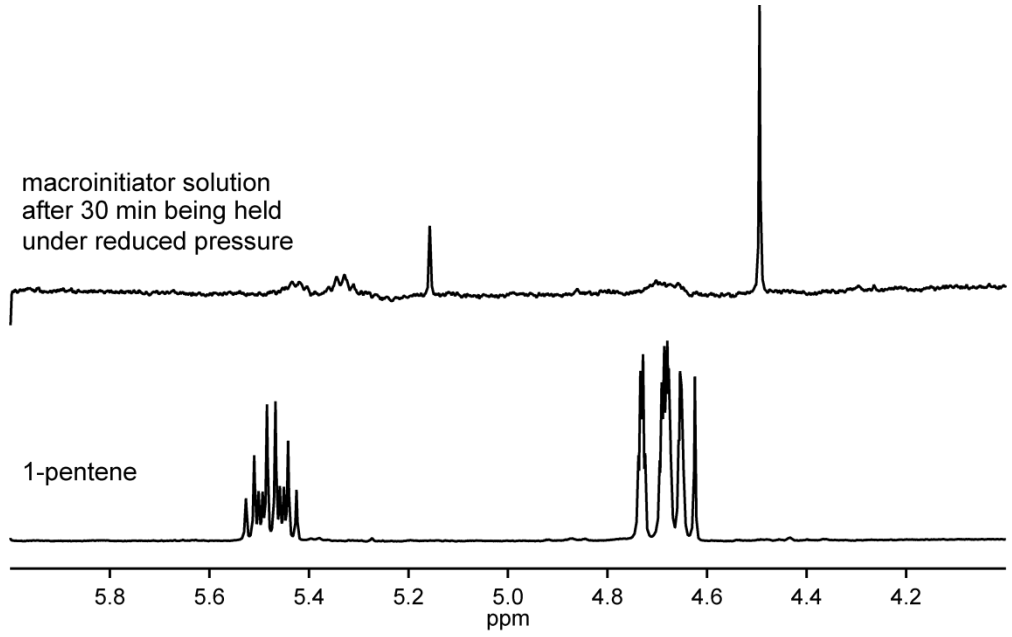


Figure S15. ^{1}H NMR spectrum of the poly(1-pentene) macroinitiator from glovebox after being held reduced pressure for 30 min.

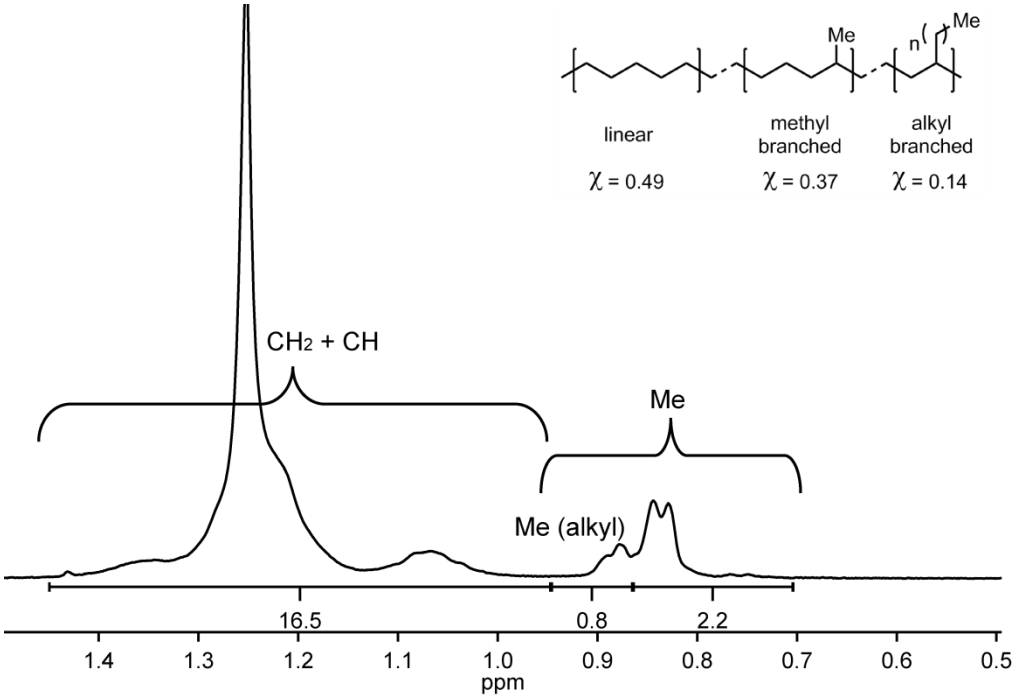


Figure S16. ^{1}H NMR spectrum of **poly(1-pentene)** macroinitiator

$$R = \frac{[CH_3]}{[CH_2]} = \frac{(3/3)}{(16.5\text{-}1)/2} = 0.129$$

$$\chi_{linear} = \frac{[1-(\omega-2)R]}{[1+2R]} = 0.487$$

carbons in 1-pentene = $\omega = 5$

$$\chi_{alkyl} + \chi_{methyl} = 1 - \chi_{linear} = 0.513$$

$$\frac{\chi_{alkyl}}{\chi_{methyl}} = \frac{CH_3\,(Me\ (alkyl))}{CH_3\,(Me)} = \frac{0.8}{2.2} = 0.364$$

$$\chi_{alkyl} = (0.364)\chi_{methyl}$$

$$(0.364)\chi_{methyl} + \chi_{methyl} = 0.513$$

$$\chi_{methyl} = 0.376$$

$$\chi_{alkyl} = 0.137$$

Equation S2. Calculating br/1000C of **poly(1-pentene)** using ^{1}H NMR spectroscopy.[3]

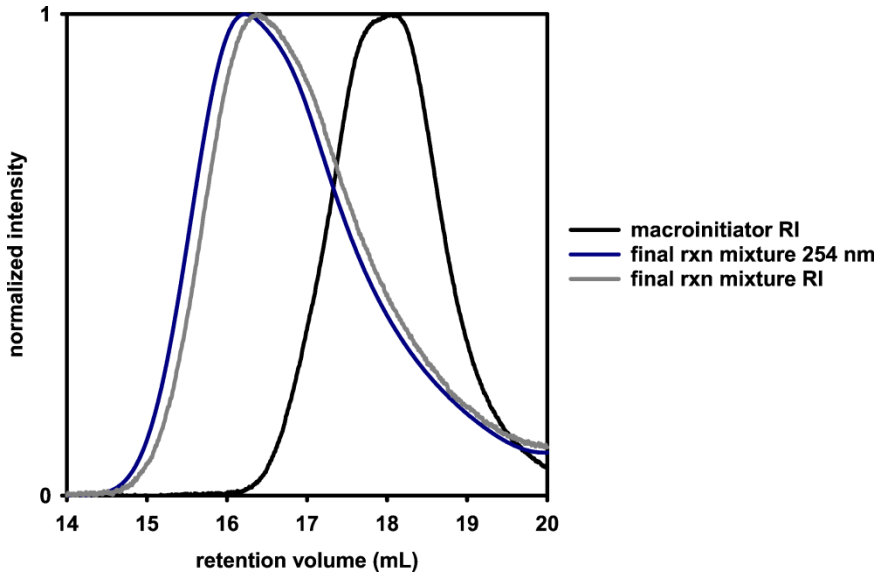


Figure S17. GPC trace of product mixture from copolymerization between **1-pentene** and **3HT** monomers using catalyst **C2** and **$B(C_6F_5)_3$**.

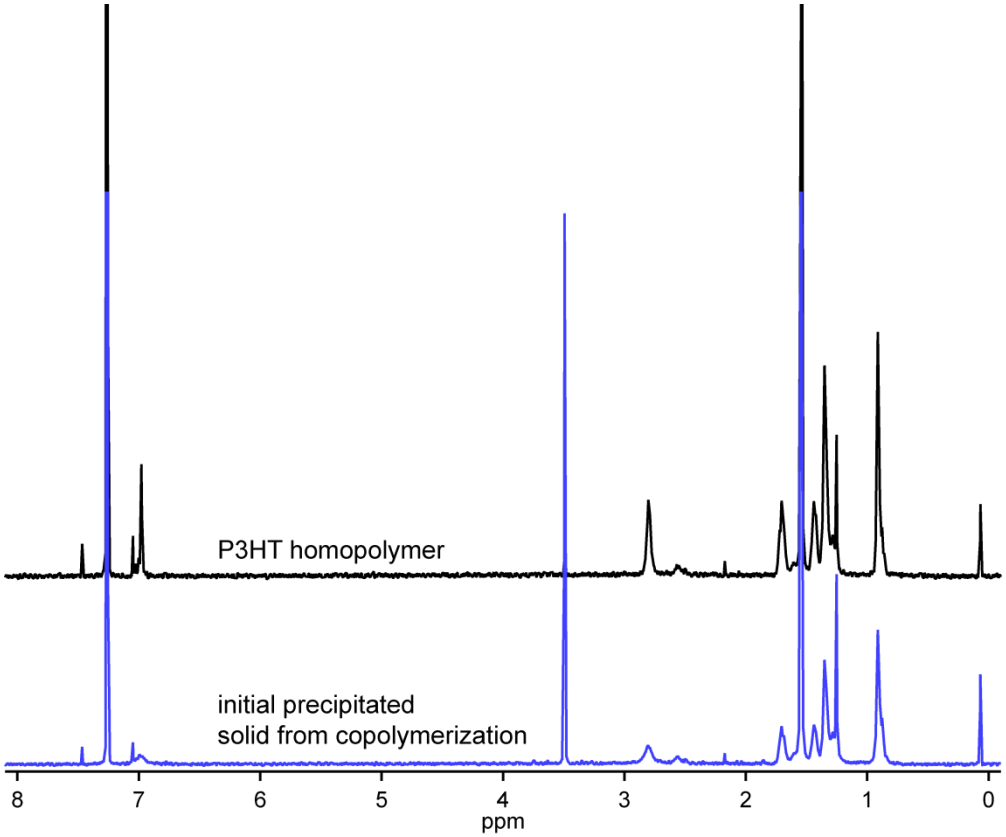


Figure S18. ^{1}H NMR spectrum after initial precipitation from copolymerization

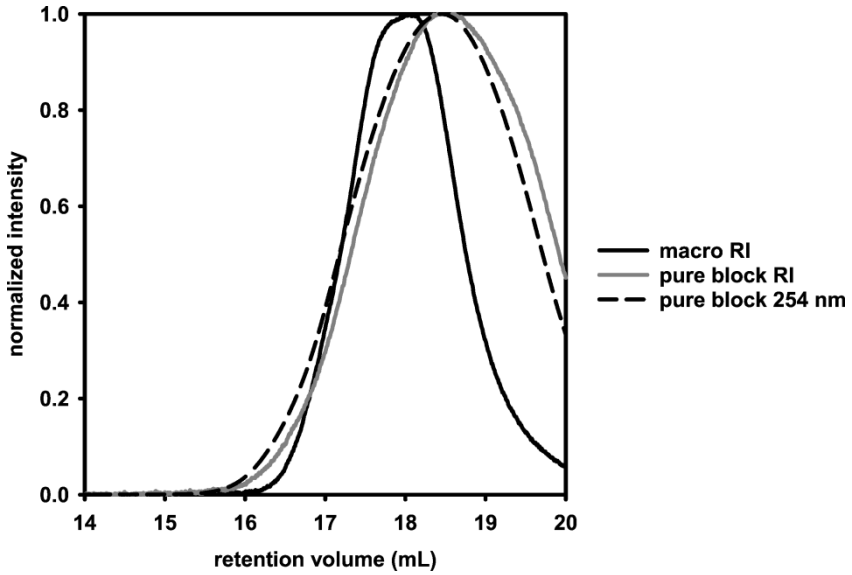


Figure S19. GPC trace of block copolymer (**poly(1-pentene)-*b*-P3HT**) after purification from copolymerization between **1-pentene** and **3HT** monomers using catalyst **C2** and **$B(C_6F_5)_3$**

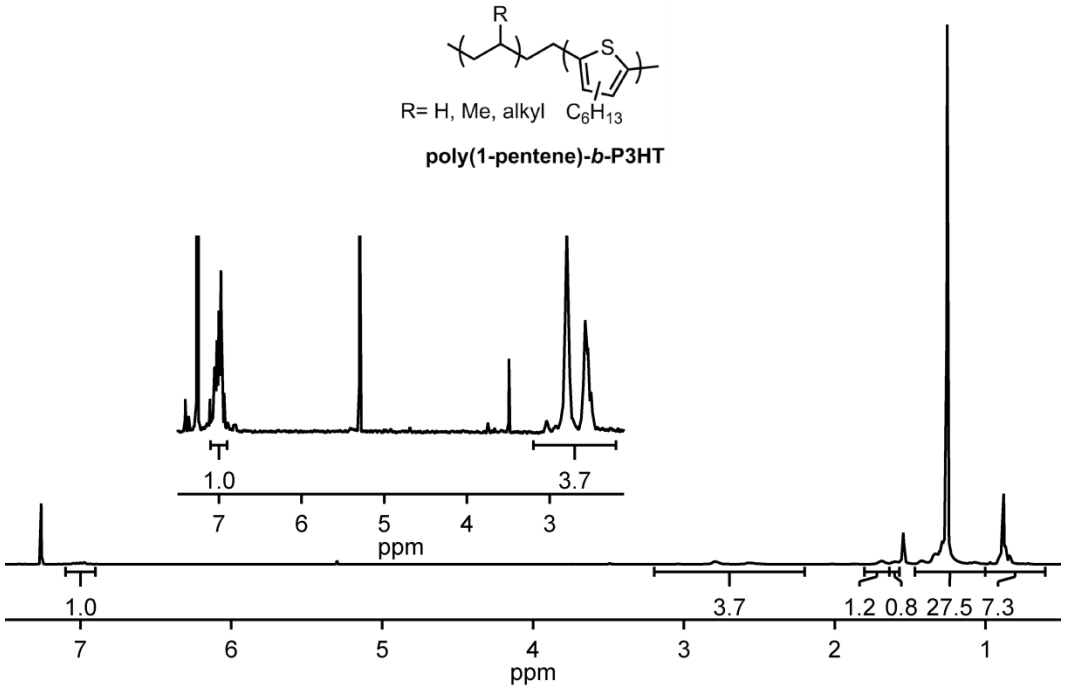


Figure S20. ^{1}H NMR spectrum of purified **poly(1-pentene)-*b*-P3HT**.

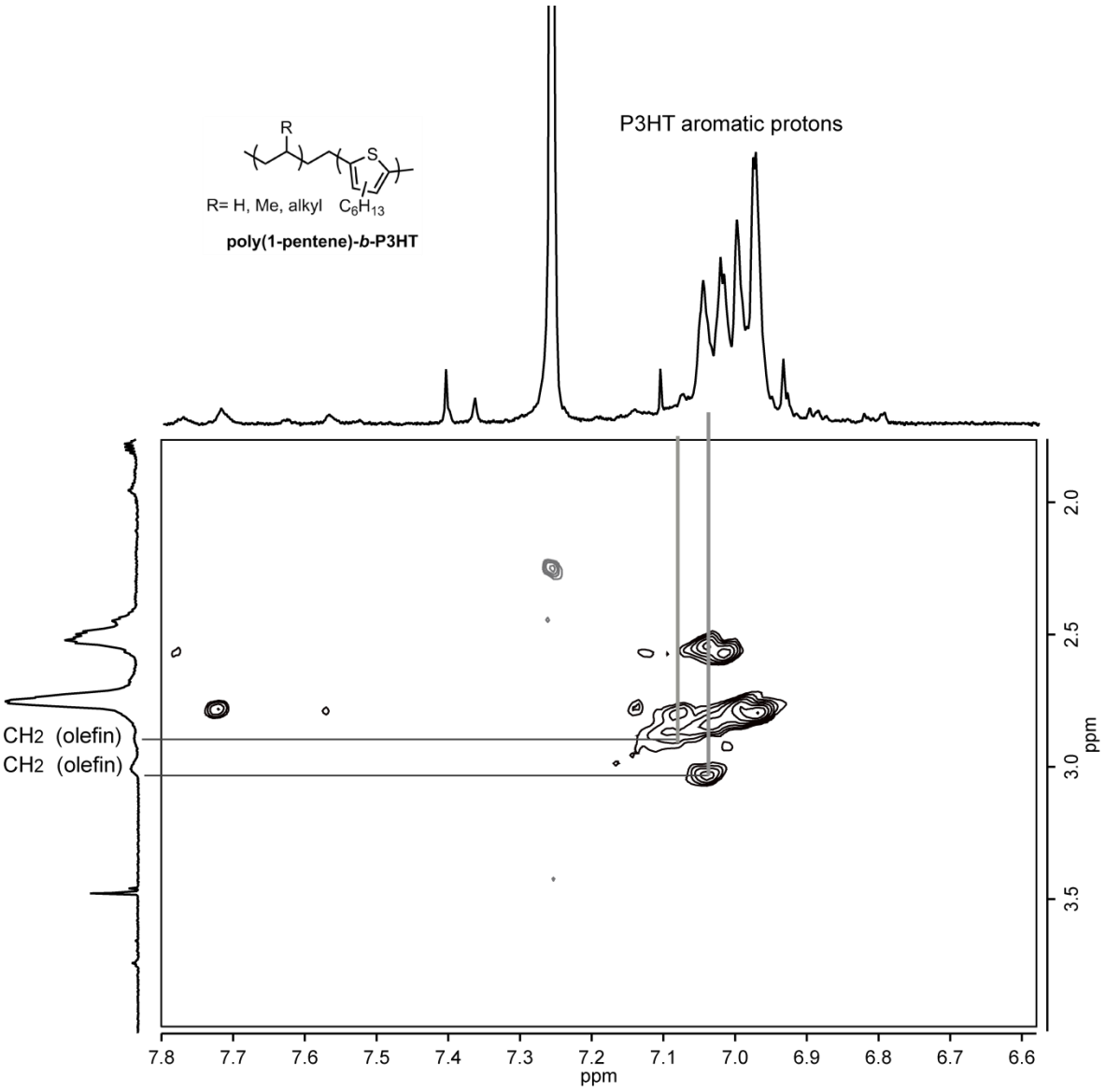
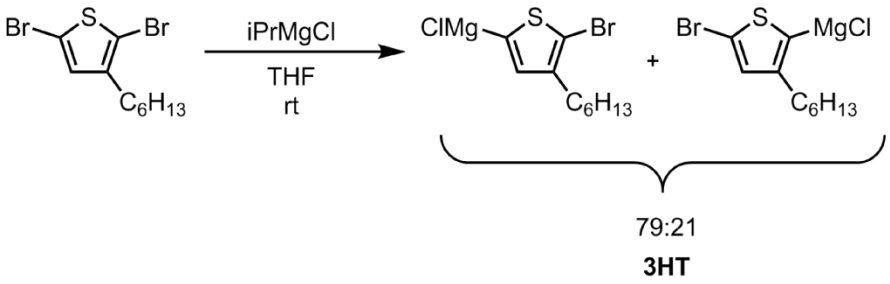


Figure S21. $^{1}H/^{1}H$ NOESY spectrum of purified **poly(1-pentene)-*b*-P3HT**.

XII. M_n versus percent conversion in polymerization of 3HT monomer with precatalyst C2 and $B(C_6F_5)_3$

Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl

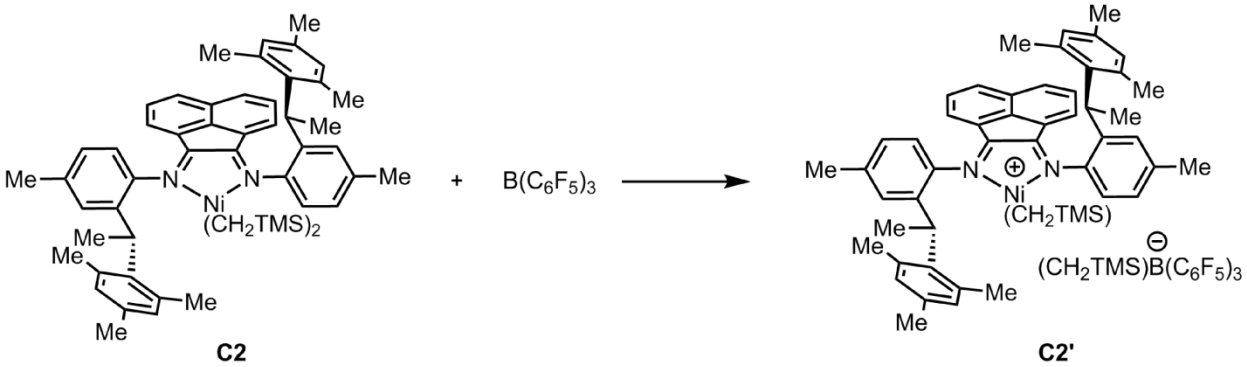


In the glovebox 2,5-dibromo-3-hexylthiophene (70.0 mg, 0.215 mmol, 1.00 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane (approx. 4.0 mg) and THF (2.07 mL). To the stirring solution was added iPrMgCl (80.0 µL, 0.150 mmol, 2.00 M in THF, 0.700 equiv) and stirred for 30 min. **3HT** was titrated to be 0.070 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of **3HT** was quenched with aq HCl (0.50 mL, 12 M) outside of the box. The quenched monomer was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).

C2 and $B(C_6F_5)_3$ stock solutions

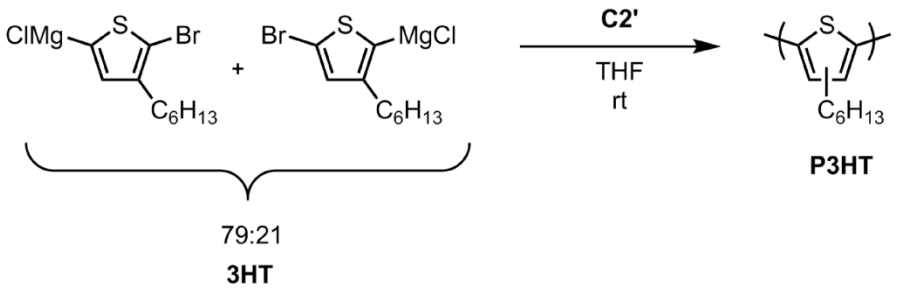
In the glovebox were added **C2** (6.0 mg, 0.0068 mmol, 0.50 mM) and toluene (1.35 mL) to a 4 mL vial. In another 4 mL vial were added **$B(C_6F_5)_3$** (7.0 mg, 0.014 mmol, 0.50 mM) and toluene (2.73 mL). **C2** solutions were made fresh for each **3HT** polymerization

Activation of precatalyst C2 with $B(C_6F_5)_3$



C2 (0.11 mL, 0.50 mM in toluene, 1.0 equiv) and **$B(C_6F_5)_3$** (0.11 mL, 0.50 mM in toluene, 1.0 equiv) were added to a 4 mL vial equipped with a stir bar and stirred for 5 min. **C2'** solution must be prepared fresh for each **3HT** polymerization.

Procedure



In the glovebox to a 20 mL vial equipped with a stir bar were added **3HT** (1.00 mL, 0.07 mmol, 125 equiv relative to **C2'**) and THF (1.63 mL) to give an overall [**3HT**] of 0.02 M. To the stirring solution was added **C2'** (0.22 mL, 0.57 µmol, 1 equiv). Aliquots were taken at 2 min, 4 min, 6 min, 8 min, and 10 min and quenched with aq. HCl (2.0 mL, 12 M) outside of the box. Each aliquot was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two equal portions. The first portion was diluted with additional $CHCl_3$ (2.0 mL) and analyzed by GC. The second portion was concentrated in vacuo and then redissolved in THF (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.

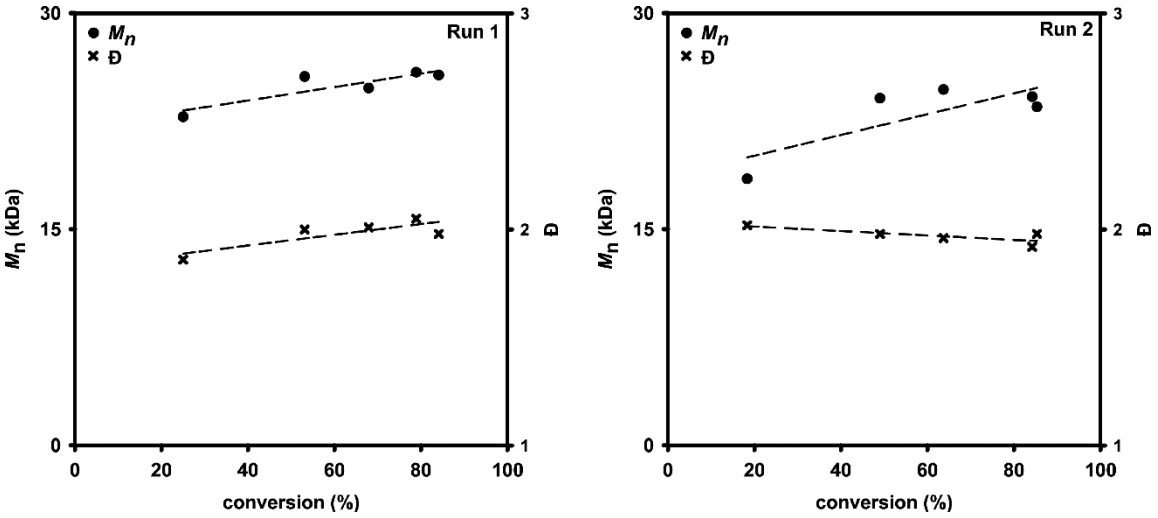
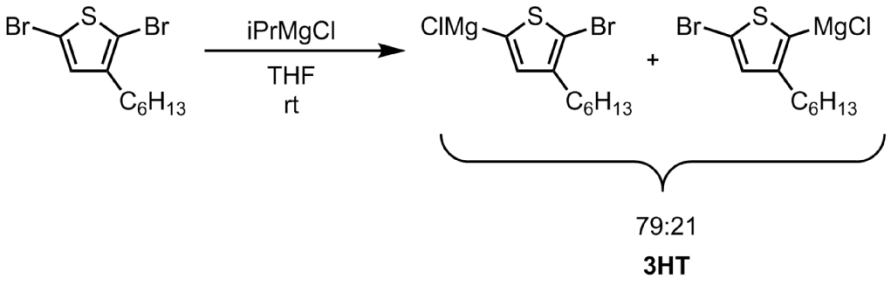


Figure S22. M_n versus percent conversion for polymerization of **3HT** monomer with catalyst **C2'**.

XIII. Polymerizations of 3HT monomer with precatalyst C3

Procedure: M_n versus percent conversion for polymerization of 3HT monomer with catalyst C3

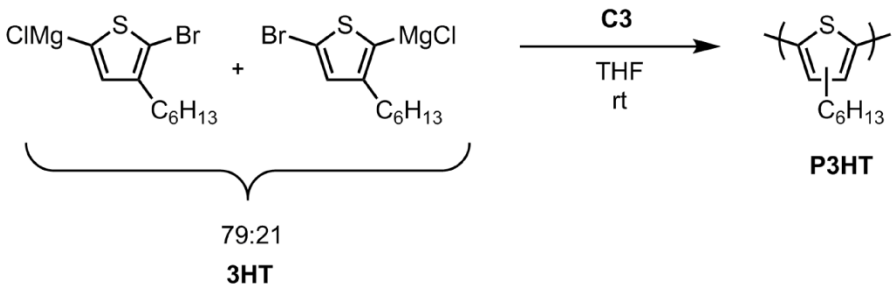
Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl



In the glovebox 2,5-dibromo-3-hexylthiophene (68.0 mg, 0.209 mmol, 1.00 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane (approx. 2.0 mg) and THF (2.01 mL). To the stirring solution was added iPrMgCl (73.0 µL, 0.146 mmol, 2.00 M in THF, 0.700 equiv) and stirred for 30 min. **3HT** was titrated to be 0.070 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of **3HT** was quenched with aq HCl (0.50 mL, 12 M) outside of the box. The quenched monomer was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).

C3 stock solution: C3 (2.0 mg, 0.0023 mmol, 0.50 mM) was added to a 4 mL vial equipped with a stir bar, followed by THF (0.46 mL). The solution was stirred for 5 min before using.

Procedure



In the glovebox, to a 20 mL vial equipped with a stir bar was added **3HT** (0.50 mL, 0.035 mmol, 117 equiv relative to **C3**) and THF (5.00 mL) to give an overall [**3HT**] of 0.005 M. To the stirring solution was added the **C3** solution (60.0 µL, 0.300 µmol, 1.00 equiv). Aliquots were taken at 2, 4, 6, 8, and 10 min and quenched with aq. HCl (0.5 mL, 12 M) outside of the box. Each aliquot was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two equal portions. The first portion was diluted with $CHCl_3$ (2.0 mL) and analyzed by GC. The second portion was concentrated in vacuo and redissolved in THF (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.

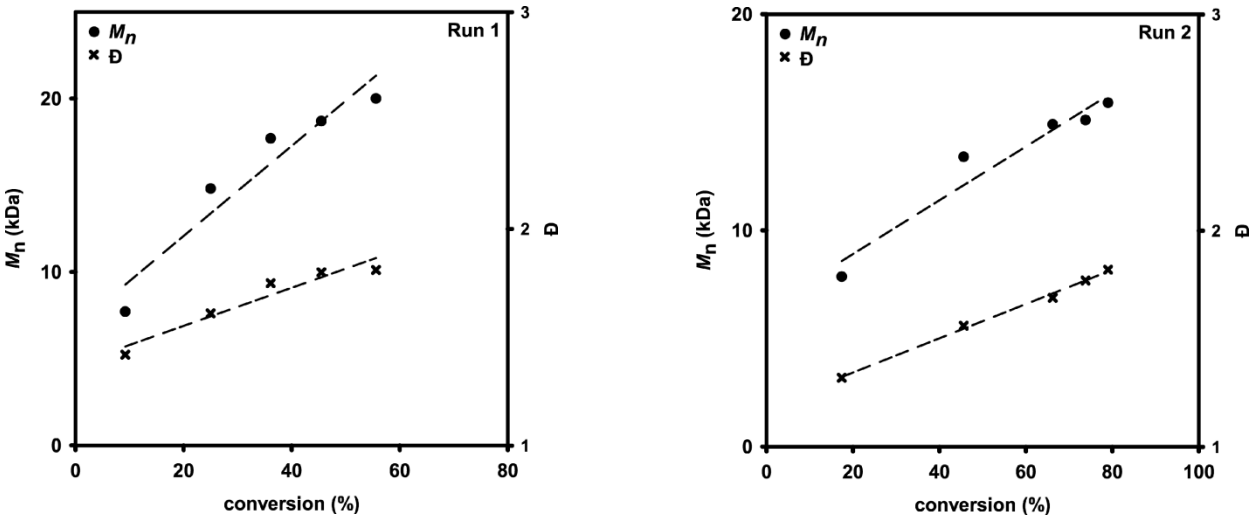


Figure S23. M_n versus percent conversion for polymerization of **3HT** monomer with precatalyst **C3**.

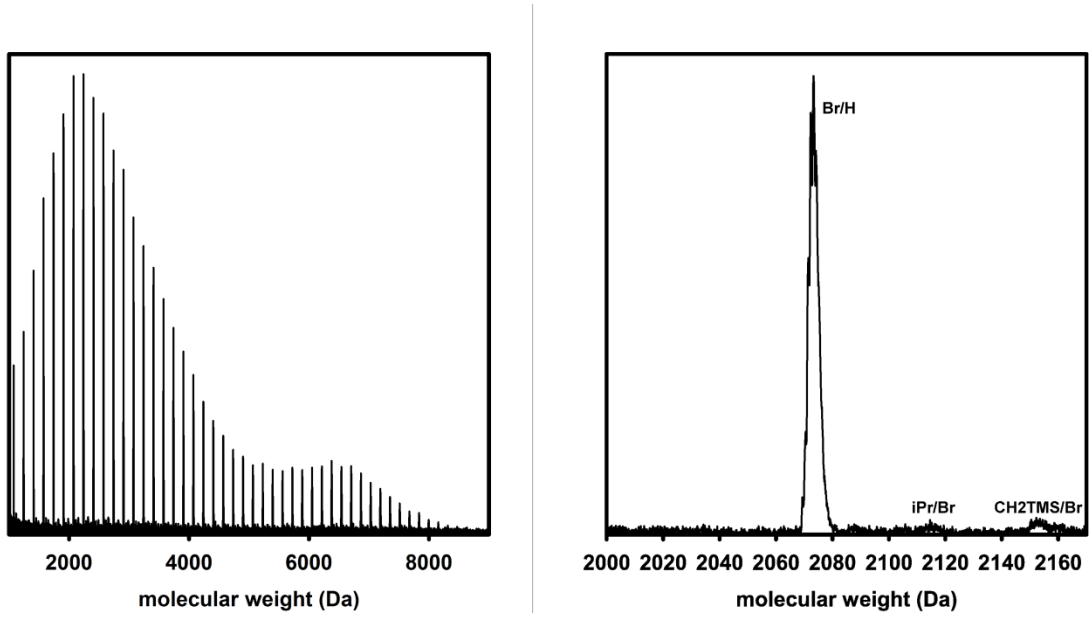
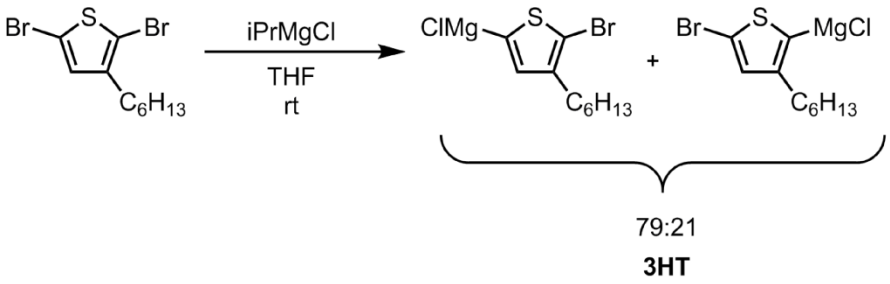


Figure S24. MALDI-TOF spectrum of the aliquot taken at 2 min in the polymerization of **3HT** monomer with precatalyst **C3**.

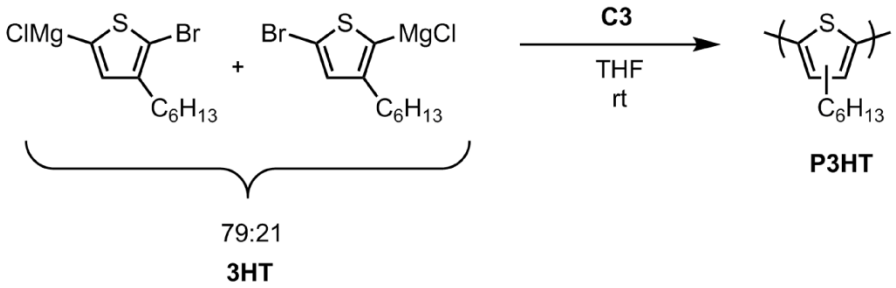
Procedure: M_n vs varying monomer:catalyst ratio in polymerization of 3HT monomer with catalyst C3

Activation of 2,5-dibromo-3-hexylthiophene with iPrMgCl



In the glovebox 2,5-dibromo-3-hexylthiophene (73.0 mg, 0.224 mmol, 1.00 equiv) was added to a 20 mL vial equipped with a stir bar, n-docosane (approx. 2.0 mg) and THF (2.16 mL). To the stirring solution was added iPrMgCl (78.0 µL, 0.157 mmol, 2.00 M in THF, 0.700 equiv) and stirred for 30 min. 3HT was titrated to be 0.070 M using salicylaldehyde phenylhydrazone. An aliquot (0.3 mL) of 3HT was quenched with aq HCl (0.50 mL, 12 M) outside of the box. The quenched monomer was extracted with $CHCl_3$ (2.0 mL), dried over $MgSO_4$, and analyzed by GC to show a mixture of regioisomers (79:21).

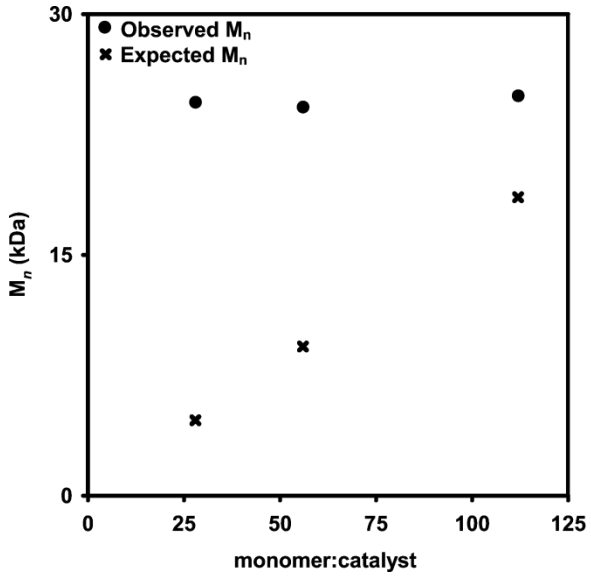
C3 stock solution: C3 (1.7 mg, 0.0019 mmol, 0.50 mM) was added to a 4 mL vial equipped with a stir bar, followed by THF (0.39 mL). The solution was stirred for 5 min before using.



To three 4 mL vials equipped with stir bars were added the **C3** solution (50 µL, 0.25 µmol) and the respective amounts of THF and **3HT** listed below.

Vial 1: THF (0.2 mL), **3HT** (0.10 mL, 0.0070 mmol, 28 equiv)
Vial 2: THF (0.4 mL), **3HT** (0.20 mL, 0.014 mmol, 56 equiv)
Vial 3: THF (0.8 mL), **3HT** (0.40 mL, 0.028 mmol, 112 equiv)

The polymerizations were stirred for 1 h at rt, after which each vial was removed from the box and quenched with aq. 12 M HCl (0.5 mL). Each vial was extracted with $CHCl_3$ (1.0 mL), dried over $MgSO_4$, and filtered through glass wool. The organic layer was then split into two equal portions. The first portion was diluted with $CHCl_3$ (2.0 mL) and analyzed by GC. The second portion was concentrated in vacuo and redissolved in THF (1.5 mL) with mild heating, passed through a PTFE filter (0.2 µm), and analyzed by GPC.



ratio 3HT:C3	% conversion 3HT	M_n (kDa)	Đ
28:1	98.3	24.5	1.91
56:1	98.2	24.2	1.86
112:1	93.3	24.9	2.07

Figure S25. Plot of M_n versus monomer:catalyst ratio in polymerization of **3HT** monomer with precatalyst **C3**.

XIV. Computational Details

All quantum chemical calculations were performed using density functional theory (DFT) in the Q-Chem quantum chemistry package.[4] The restricted B3LYP density functional[5-6] with singlet spin was used with the LANL2DZ basis set and core potential[7-8] to acquire geometries for all intermediates and transition states. The growing string method was used to optimize reaction paths and transition states,[9-11] followed by eigenvector optimization to fully refine these structures. The ωB97X-D density functional[12] and the triple-zeta, polarized cc-pVTZ basis set[13] were used to calculate energies with the SMD solvation model[14] using THF as the implicit solvent. The long alkyl chain of the polyolefin macroinitiator and the hexyl group of the 3-hexylthiophene Grignard monomer were substituted with methyl groups to reduce computational cost. Thermodynamic corrections were applied to the solvated energies at a temperature of 298 K.

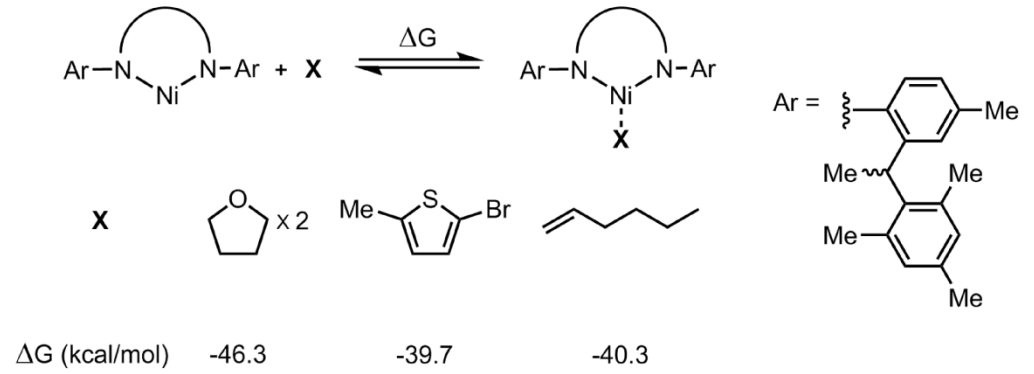


Figure S26a. Binding energy calculations of Ni(0) to species in copolymerization

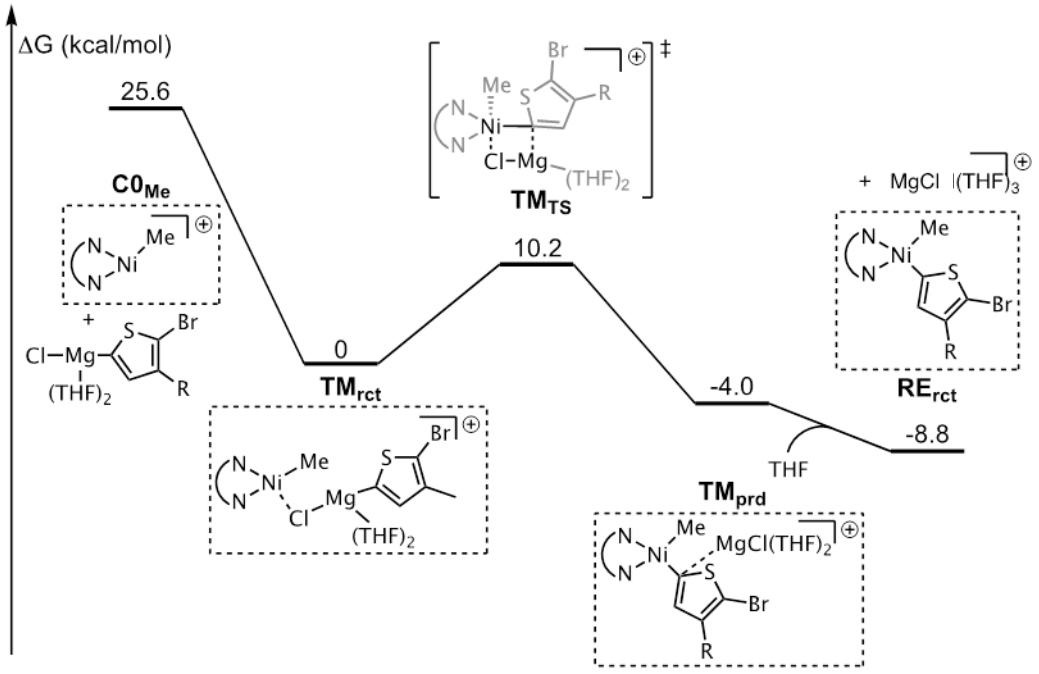
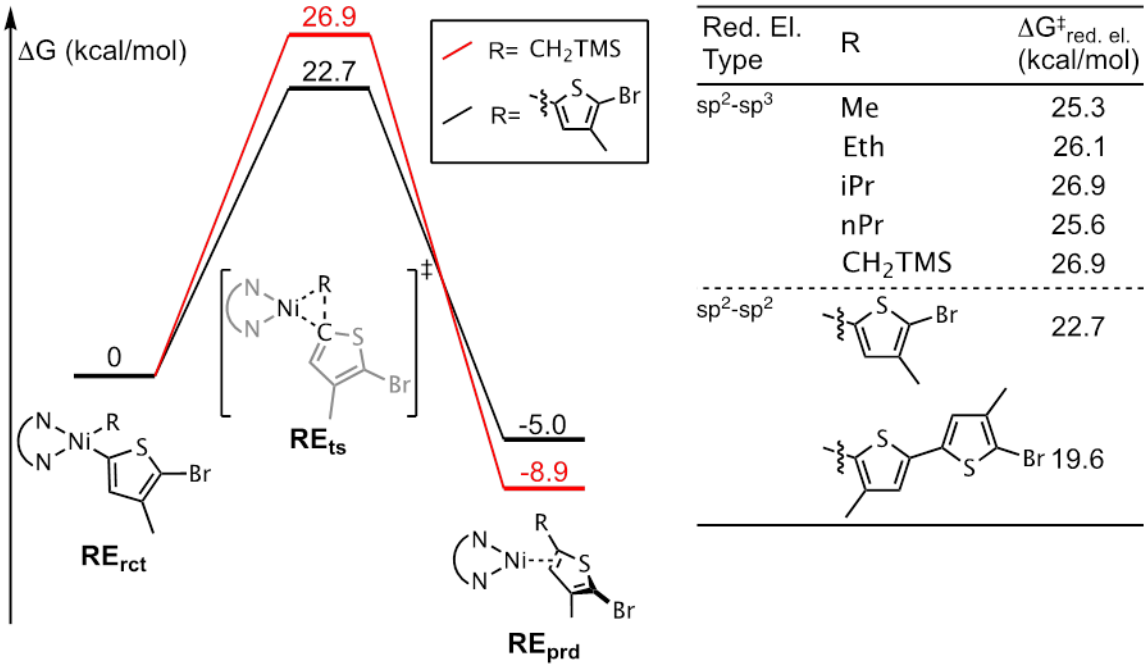


Figure S26b. The potential energy surface for transmetalation with thiophene at the cationic nickel center

After borane activation of **C2** and olefin enchainment, the resulting cationic macroinitiator must undergo transmetalation via thiophene monomer to begin thiophene polymerization. This reaction, which transforms the active nickel complex from cationic to neutral, is shown in Figure S26b. Transmetalation at the cationic macroinitiator, $\mathbf{C0_{Me}}$, begins after a thiophene monomer binds to the catalyst to form $\mathbf{TM_{rct}}$. In $\mathbf{TM_{rct}}$, the chloride of the thiophene monomer acts as a bridging ligand between the monomer and catalyst with a strong binding energy (over 25 kcal/mol). A facile transmetalation occurs via $\mathbf{TM_{TS}}$ with a barrier of 10.2 kcal/mol. The transmetalation product, $\mathbf{TM_{prd}}$, exhibits a lingering interaction between the nucleophilic carbon atom of thiophene and the electrophilic magnesium. Alkyl – aryl reductive elimination at $\mathbf{TM_{prd}}$ was performed but proved to be kinetically infeasible with a barrier over 30 kcal/mol. Upon addition of THF to $\mathbf{TM_{prd}}$, the MgCl complex dissociates from the nickel complex as cationic $MgCl(THF)_3$. This dissociation results in the neutral nickel species, $\mathbf{RE_{rct}}$, which can undergo reductive elimination.



Red. El. Type	R	$\Delta G^{\ddagger}_{red.\ el.}$ (kcal/mol)
sp^2-sp^3	Me	25.3
	Eth	26.1
	iPr	26.9
	nPr	25.6
	CH_2TMS	26.9
sp^2-sp^2		22.7
		19.6

Figure S26c. The potential energy surfaces for sp^2-sp^3 and sp^2-sp^2 reductive elimination

The relative rates of sp^2-sp^3 reductive elimination, (Figure S26b, red pathway) compared to thiophene homopolymerization (sp^2-sp^2 reductive elimination, black pathway) were computed for catalyst **C2**. The reaction begins at RE_{rct} and proceeds through the three-membered transition state, RE_{ts} to form the π-complex intermediate RE_{prd}. The calculated difference between the two reductive elimination pathways predicts slow sp^2-sp^3 reductive elimination and fast thiophene homocoupling. At room temperature, the 4.2 kcal/mol preference for the black pathway would result in a switching step that is approximately 1,000 times slower than thiophene homocoupling. This is in good agreement with experiments that exhibited slow switching (main text, eq 3 and eq 4).

The reductive elimination barriers for other alkyl and thiophene ligands were examined in the ligand survey in Figure S26b. These calculations showed that sp^2-sp^3 reductive elimination barriers slightly decrease with decreasing size of the alky reactive ligand. Reductive elimination involving two thiophene ligands remains fast in comparison, and the activation barrier decreases by about 3 kcal/mol for the dithiophene reactive ligand.

XYZ coordinates and Gibbs Free Energy (in Hartree) for all reported structures

All XYZ coordinates for structures used to calculate binding energies (Figure S26a), tranmetalation (Figure S26b), and reductive elimination barriers (Figure S26c) are provided below. Total electronic energies and free energy corrections are provided in Hartree.

C0 -3475.9730+0.7517

Ni	0.23029165	0.20543233	0.12986747
N	-0.56022459	-0.24632949	1.81146242
N	-1.22562073	1.37102767	-0.29216024
C	-1.68718922	0.50914517	1.89448022
C	-2.12496430	1.19670696	0.71166203
C	-2.71839012	0.67157133	2.93596514
C	-3.48754259	1.70796337	0.94724905
C	-3.78713872	1.38132185	2.30597729
C	-4.99005811	1.71767248	2.94632818
C	-2.88133298	0.28604846	4.25660801
C	-4.09606068	0.61439236	4.92719425
C	-5.12517204	1.30764665	4.30817137
C	-4.43714152	2.40629899	0.21931827
C	-5.94967803	2.43362264	2.16685071
C	-5.66612265	2.76038948	0.84936111
H	-4.27500182	2.67717577	-0.81669773
H	-2.10610251	-0.24511207	4.79536151
H	-6.03393284	1.54326712	4.85428635
H	-4.20965469	0.30892666	5.96294799
H	-6.90031528	2.71654204	2.60943062
H	-6.40399878	3.30381424	0.26690795
C	0.17472576	-0.61875500	2.97344535
C	-1.63910826	1.66266753	-1.62446084
C	0.61412173	-1.95877363	3.13510404
C	0.54085522	0.35678151	3.91977175
C	1.42294044	-2.25000626	4.24341506
C	1.79815291	-1.28268161	5.19077834
C	1.33641407	0.03172358	5.01700994
H	0.20146006	1.37664433	3.76849702
H	1.76932094	-3.26719007	4.38878363
H	1.60872663	0.80108693	5.73415450
C	-1.00598253	2.70513450	-2.35002942
C	-2.60524393	0.85590765	-2.25449854
C	-1.36782729	2.87585398	-3.69458967
C	-2.94777064	1.05694330	-3.59038524
C	-2.32355390	2.06997899	-4.33572566
H	-0.90205071	3.66927315	-4.26880957
H	-3.69299235	0.42086154	-4.05962762
H	-3.06741850	0.05981678	-1.67931965
C	2.69882245	-1.64551286	6.35059541
H	2.56428769	-2.68987044	6.65213352
H	2.50172830	-1.01303935	7.22290332
H	3.75821308	-1.51651612	6.08841155
C	-2.64992660	2.27153390	-5.79884926
H	-3.69316424	2.01738708	-6.01582230
H	-2.02140928	1.63593697	-6.43819530
H	-2.48236771	3.30875339	-6.10817336
C	0.24429638	-3.02322634	2.09298788
H	0.56330856	-2.58337660	1.14215208
C	-1.26232499	-3.31274972	1.93305444
C	1.03143350	-4.34911373	2.24000750
C	0.06803232	3.56865976	-1.67684566
C	-0.40416193	4.40718163	-0.47067544
C	0.87548997	4.44823761	-2.66218842
H	0.26525497	5.24169116	-3.10585140
H	1.30146308	3.84775072	-3.47456770
H	1.69822680	4.93361635	-2.12723424
H	2.11337392	-4.17149773	2.25828255
H	0.80778341	-5.00056755	1.38873259
H	0.75839837	-4.89785490	3.14760892
C	-2.11228627	-3.60564650	3.03012575
C	-1.80529775	-3.36666629	0.62174765
C	-3.46743165	-3.89487624	2.79677965
C	-3.16359542	-3.66128510	0.43685722
C	-4.02014542	-3.91658645	1.51301986
H	-3.55767160	-3.69430813	-0.57616953
H	-4.10525818	-4.11286751	3.65013258
C	-1.54178711	5.25150656	-0.51364679
C	-1.89023107	6.00083941	0.62348388
C	-1.14708280	5.95924963	1.80582179
C	-0.00338266	5.15279914	1.82262542
C	0.38052820	4.38543901	0.71447416
C	-1.56813213	6.74373431	3.02874533
H	-2.77093314	6.63616801	0.57516062
H	0.60892736	5.12003567	2.72060902
H	0.77256656	2.83781709	-1.26604871
C	-1.64171483	-3.63337497	4.47268598
C	-0.96436522	-3.11560241	-0.61464838
C	-2.42824267	5.40895989	-1.73604105
C	1.63848821	3.54728329	0.83508649
H	-1.55700543	-3.28188549	-1.51972841
H	-0.08832951	-3.77389602	-0.66938853
H	-0.59915577	-2.07605045	-0.64117063
H	-0.75109095	-4.25388113	4.61376530
H	-2.43016311	-4.04057663	5.11379963
H	-1.39307678	-2.63463561	4.84694071
H	-2.25415660	7.55595798	2.76594759
H	-0.70450049	7.18214802	3.54250979
H	-2.08448164	6.10044121	3.75437290
H	-2.96385140	4.48694178	-1.98312592
H	-1.86487523	5.69629433	-2.63053958
H	-3.17353193	6.19018440	-1.55599953
H	2.37698011	3.78032445	0.05737526
H	1.40859448	2.47339851	0.75997929
H	2.11889116	3.71655089	1.80396415
C	-5.49216397	-4.18838286	1.29584516
H	-5.66958274	-4.70313431	0.34483375
H	-6.06971025	-3.25381972	1.27255950
H	-5.90789942	-4.80734224	2.09844657

$C0(THF)_2$ -3940.9972+0.9782

Ni	0.75369123	0.52732481	0.02458177
N	-0.15560096	-0.16661593	1.58280089
N	-0.85178486	1.55784032	-0.32937429
C	-1.38095287	0.45017069	1.70141569
C	-1.80935532	1.22087604	0.60993155
C	-2.46533407	0.38039603	2.69796853
C	-3.21180522	1.61889745	0.82722362
C	-3.56033777	1.09135486	2.11226584

C	-4.81015816	1.25271967	2.72047161
C	-2.65526108	-0.18704218	3.94631759
C	-3.92296536	-0.03880231	4.58765968
C	-4.97529424	0.65308908	4.00945132
C	-4.17531837	2.34585233	0.14786290
C	-5.78523660	2.00271015	1.98853812
C	-5.45939651	2.52594467	0.74741554
H	-3.98128704	2.77619046	-0.82764860
H	-1.86651400	-0.73240153	4.45109593
H	-5.92401562	0.74565866	4.53095754
H	-4.05834407	-0.48811341	5.56756036
H	-6.77453122	2.15974104	2.40927530
H	-6.20469305	3.09658223	0.20020590
C	0.50128992	-0.70620772	2.72675597
C	-1.25493990	1.95394007	-1.63879871
C	0.78173611	-2.09831282	2.80227363
C	0.93918984	0.13631508	3.76641793
C	1.56641308	-2.56035447	3.87106698
C	2.03658129	-1.71659559	4.89158537
C	1.69172330	-0.35678960	4.83463384
H	0.67786546	1.18944211	3.71788360
H	1.80567859	-3.61749204	3.93061331
H	2.01414772	0.31519788	5.62609278
C	-0.76680500	3.15862219	-2.20991181
C	-2.08850017	1.12055746	-2.41214468
C	-1.06178559	3.42020288	-3.55831138
C	-2.39916323	1.42607177	-3.73755937
C	-1.86983552	2.57942923	-4.34053128
H	-0.68188483	4.32811882	-4.01560226
H	-3.04412376	0.76331753	-4.30945054
H	-2.47769171	0.21848076	-1.94993391
C	2.89258037	-2.26153397	6.01545745
H	2.63762084	-3.30205152	6.24512860
H	2.76798327	-1.67476225	6.93221449
H	3.96152532	-2.23971745	5.75945869
C	-2.19674070	2.92831499	-5.77697746
H	-3.21446715	3.33162048	-5.87036948
H	-2.14062635	2.04816740	-6.42877875
H	-1.50889177	3.68384853	-6.17126232
C	0.24773052	-3.03350931	1.70968381
H	0.43020897	-2.47684510	0.78702391
C	-1.27864653	-3.27883074	1.73840750
C	1.01450946	-4.37210825	1.58531811
C	0.05688093	4.12659169	-1.35114303
C	-0.72620700	4.83384198	-0.21994551
C	0.86387567	5.16925294	-2.16377167
H	0.21859955	5.90227749	-2.65871075
H	1.48412838	4.69081308	-2.93298772
H	1.52533374	5.72489797	-1.49024098
H	2.09614436	-4.20767909	1.49483151
H	0.67425670	-4.90463803	0.69051041
H	0.84699666	-5.03647817	2.43829964
C	-1.97393221	-3.74221273	2.88585324
C	-2.01261873	-3.08911607	0.53728309
C	-3.36186591	-3.94880786	2.81850970
C	-3.39763264	-3.30754214	0.51759438
C	-4.09933996	-3.72165012	1.65353394
H	-3.93968937	-3.13994354	-0.40991162
H	-3.87760237	-4.29223557	3.71197083
C	-1.93797882	5.54012513	-0.43432636
C	-2.55911663	6.19430090	0.64373113
C	-2.02796600	6.18513596	1.93551449
C	-0.81711244	5.51186938	2.12873979
C	-0.16210892	4.84622200	1.08363062
C	-2.74260834	6.85665211	3.08681892
H	-3.49147320	6.72261857	0.45937869
H	-0.36759703	5.49702375	3.11909523
H	0.78449372	3.48530487	-0.84741636
C	-1.30819176	-4.03327534	4.21812749
C	-1.35516262	-2.64720040	-0.75565199
C	-2.63327337	5.63622638	-1.77923465
C	1.14475848	4.14866463	1.40393982
H	-2.08841774	-2.64421364	-1.56897175
H	-0.53678580	-3.31439932	-1.05896972
H	-0.94235496	-1.63469310	-0.66402966
H	-0.45878066	-4.71875874	4.12737699
H	-2.02802274	-4.49780855	4.89989708
H	-0.93198634	-3.12519928	4.70015317
H	-3.47514630	7.58893033	2.73087818
H	-2.03988493	7.37559038	3.74971820
H	-3.28345345	6.12210736	3.69885759
H	-3.01541791	4.66706246	-2.11448463
H	-1.97754889	6.00945819	-2.57322738
H	-3.48380343	6.32256517	-1.71027506
H	1.98512655	4.54052914	0.81417680
H	1.07016851	3.07253874	1.20345389
H	1.39680109	4.28377243	2.46095161
C	-5.60218257	-3.88795758	1.63100307
H	-5.96068949	-4.17349727	0.63567102
H	-6.10401978	-2.94898910	1.90209273
H	-5.93257256	-4.65220406	2.34346846
H	5.44932769	-0.44435955	0.18606114
H	3.84126821	1.88896840	0.98013700
H	3.35098754	-1.31407783	-0.67524951
C	4.79592967	-0.87907544	0.95227900
C	3.45230047	1.03929672	1.55182827
H	5.46163901	0.69355887	2.35694959
O	2.68598502	0.18352419	0.60870764
C	3.38591746	-1.10626675	0.39543720
C	4.55890309	0.13179353	2.09921838
H	5.25441279	-1.80871355	1.30159718
H	2.75704178	1.38847560	2.31368779
H	2.84257561	-1.87870722	0.94507549
H	4.20713409	-0.38597789	2.99788116
H	3.29459272	1.47299198	-1.66195436
H	2.04966146	2.33967850	-2.61174936
H	3.38834736	1.40870845	-4.43987163
C	2.52255127	1.37122229	-2.42539313
C	2.98499726	0.69305869	-3.71744104
H	3.76257495	-0.05058645	-3.50468151
O	1.49875030	0.45288168	-1.87606098
C	1.69717582	0.00053180	-4.22194416
H	1.05781696	0.72186646	-4.74194483
C	1.01392133	-0.47543904	-2.93272424
H	1.90609118	-0.82632408	-4.90702403
H	1.31350685	-1.48582289	-2.63586409
H	-0.07241601	-0.40259924	-2.96401062

C0(thiophene) -6681.3772+0.8576

Ni	0.56698066	-0.20341874	-0.57553832
N	0.10890385	-0.59161890	1.35056169
N	-1.37557346	-0.62987040	-0.84341601
C	-1.13834483	-0.94858734	1.49612866
C	-1.94031839	-1.07024781	0.25068038

C	1.54393691	-0.93215583	-3.30591793
C	-2.00007661	-1.33411248	2.62450280
C	-3.25123550	-1.63052686	0.61580794
C	-3.23419037	-1.74765931	2.03915956
C	-4.32412680	-2.22813342	2.79181591
C	-1.86067852	-1.38954724	4.00082072
C	-2.95264441	-1.86599115	4.77880244
C	-4.14817664	-2.27714227	4.20605430
C	-4.38899465	-2.02410009	-0.06949182
C	-5.48299274	-2.61603351	2.05688535
C	-5.49943641	-2.51524449	0.67291537
H	-4.44788905	-1.97548442	-1.14927674
H	-0.94977109	-1.07383572	4.49321096
H	-4.95684218	-2.63794504	4.83466065
H	-2.83880361	-1.90844770	5.85709421
H	-6.35226213	-2.99485366	2.58603421
H	-6.38780883	-2.82083446	0.12972306
C	0.97317299	-0.32939709	2.46263854
C	-2.02466028	-0.69734134	-2.12078326
C	2.05053722	-1.19568901	2.76793458
C	0.78944486	0.86181455	3.18349675
C	2.93459797	-0.78985116	3.78008923
C	2.77789573	0.40571929	4.50057135
C	1.67971589	1.22367041	4.19451567
H	-0.03956219	1.51103659	2.92129485
H	3.77675735	-1.42650843	4.03104599
H	1.52660616	2.15311746	4.73541659
C	-2.46770780	0.48196346	-2.76689883
C	-2.12512133	-1.94373096	-2.75814320
C	-2.97656351	0.34569400	-4.06800780
C	-2.64695501	-2.04098338	-4.04868078
C	-3.07743781	-0.89068711	-4.72682646
H	-3.31065473	1.23268597	-4.59454249
H	-2.70492961	-3.01093148	-4.53405424
H	-1.75937446	-2.82660736	-2.24376366
C	3.78212595	0.80730065	5.55856139
H	4.26298664	-0.06830344	6.00763698
H	3.31008621	1.38265507	6.36234070
H	4.57841959	1.43488285	5.13522727
C	-3.65770716	-0.97749834	-6.12145950
H	-3.22108650	-1.80879941	-6.68535275
H	-3.47930688	-0.05646232	-6.68676053
H	-4.74469737	-1.13719501	-6.09480497
C	2.23958143	-2.49117253	1.97070073
H	2.12974843	-2.16983184	0.93005087
C	1.15983642	-3.57482320	2.19177064
C	3.65751060	-3.09978830	2.08554551
C	-2.32802951	1.84473709	-2.07598339
C	-3.14658921	2.03370417	-0.78052080
C	-2.53575665	3.05143427	-3.02219038
H	-3.56863235	3.13272307	-3.37800198
H	-1.87052734	2.99045353	-3.89040347
H	-2.30268131	3.97636209	-2.48574090
H	4.42535274	-2.34895691	1.86615123
H	3.76342593	-3.91605523	1.36347345
H	3.85777057	-3.51793416	3.07724487
C	0.76774560	-4.03086462	3.47714264
C	0.58229193	-4.19403440	1.04994820
C	-0.21265756	-5.03129460	3.58794014
C	-0.39522865	-5.18768485	1.20945324
C	-0.82170377	-5.61260855	2.47188713
C	0.99522189	-3.82932285	-0.36329393
H	-0.82618193	-5.64317831	0.32106827
H	-0.50291130	-5.36435990	4.58156645
C	1.36232752	-3.50839603	4.77200595
C	-1.90849628	-6.65338672	2.62449696
H	-1.93601824	-7.33405359	1.76649314
H	-2.89948898	-6.18483819	2.70051456
H	-1.76350650	-7.25496634	3.52877567
H	0.47186026	-4.46312664	-1.08655629
H	2.07152723	-3.96671874	-0.52866701
H	0.76416856	-2.78153363	-0.60471323
H	2.45651831	-3.53104351	4.76973801
H	1.02395959	-4.12315196	5.61214591
H	1.07053998	-2.47353700	4.97762529
C	-4.52874572	1.73396971	-0.68108764
C	-5.19939868	1.95098296	0.53568947
C	-4.55759846	2.47229993	1.66248678
C	-3.20581927	2.81225127	1.53656273
C	-2.49510589	2.61107419	0.34413314
C	-5.35548610	1.20295874	-1.83805474
C	-5.29220444	2.65879141	2.97195725
H	-6.25765019	1.70817765	0.59510178
H	-2.68880109	3.25870552	2.38301612
C	-1.04366803	3.04754236	0.30132026
H	-1.27531531	1.87740444	-1.77729422
H	-5.06837659	0.18717400	-2.12679941
H	-5.26316035	1.82297220	-2.73579497
H	-6.41476799	1.18363699	-1.56223315
H	-0.85096519	3.78256030	-0.48904533
H	-0.36125765	2.20642571	0.12187356
H	-0.75817415	3.51112777	1.25092824
H	-6.37255559	2.74738548	2.81482707
H	-4.95111651	3.55797793	3.49732816
H	-5.12771825	1.80661909	3.64594260
C	3.89320842	1.52914201	0.55663028
C	2.98563500	1.38967377	-0.63450127
C	2.47641685	0.07307460	-1.06282567
Br	2.89325631	4.31685046	-1.18292092
C	2.55322549	2.39733656	-1.43154035
C	1.58659489	0.10695461	-2.20813617
H	3.09969243	-0.80082092	-0.87007082
S	1.48880910	1.90437071	-2.82505164
H	3.37857413	1.23757479	1.47999291
H	4.25187168	2.55469035	0.67228164
H	4.76740667	0.87222662	0.45206013
H	1.68907496	-1.92935200	-2.87226878
H	2.33287547	-0.76982414	-4.05374376
H	0.57877854	-0.93765633	-3.82349664

C0(hexene) -3711.9239+0.9155

Ni	1.57018201	-1.05165307	-0.12341925
N	0.37509456	-1.16435770	1.48760589
N	0.12696310	0.14726702	-0.79036686
C	-0.72493107	-0.47343093	1.33356426
C	-0.90392282	0.18625488	0.01840510
C	-1.92573638	-0.20173420	2.14015355
C	-2.24590186	0.78875166	-0.00417478
C	-2.79879707	0.53969438	1.28900677
C	-4.07756572	0.97766984	1.68506949
C	-2.34375811	-0.50775629	3.42392806
C	-3.63212489	-0.07296608	3.84348672
C	-4.48042642	0.64505263	3.01211874
C	-3.00382540	1.49117847	-0.92633183

C	-4.83001366	1.70321243	0.71435779
C	-4.29884314	1.94298211	-0.54519713
H	-2.63672145	1.69413537	-1.92451266
H	-1.71355328	-1.06141335	4.10837346
H	-5.45712742	0.95716743	3.37022398
H	-3.95694428	-0.31505744	4.85034553
H	-5.82254769	2.06535636	0.96536273
H	-4.88718684	2.49375445	-1.27217840
C	0.74318121	-1.78237705	2.72529816
C	0.08649655	0.69313859	-2.11465585
C	0.75151845	-3.19272135	2.86149514
C	1.19205496	-0.96503564	3.77495076
C	1.26062511	-3.72092406	4.05709437
C	1.72973243	-2.91926615	5.11117467
C	1.67626627	-1.52689666	4.95722119
H	1.18088621	0.11180490	3.64174276
H	1.28819884	-4.79781266	4.18379874
H	2.02572068	-0.87929243	5.75625187
C	0.83818509	1.84524156	-2.44450370
C	-0.63030373	0.00277097	-3.10639875
C	0.84392334	2.24742541	-3.79015760
C	-0.60848562	0.43688100	-4.43118692
C	0.13501301	1.57093145	-4.79460367
H	1.41642965	3.12379034	-4.07274830
H	-1.15986468	-0.11587701	-5.18666810
H	-1.17617638	-0.89323570	-2.82923552
C	2.29446260	-3.54989375	6.36548228
H	1.72931618	-4.44318755	6.65466403
H	2.27499343	-2.85058163	7.20793208
H	3.33857750	-3.85976246	6.22142668
C	0.16271372	2.05786909	-6.22705806
H	-0.79029894	2.52411160	-6.51211739
H	0.34032752	1.23385293	-6.92820940
H	0.95095601	2.80236448	-6.37839194
C	0.26348710	-4.08188069	1.71168493
H	0.78554395	-3.68138333	0.83729707
C	-1.24410792	-3.98871255	1.38468385
C	0.70119686	-5.56144592	1.83264306
C	1.66073686	2.56376894	-1.36760911
C	0.84917418	3.23315643	-0.23816522
C	2.71606446	3.54409902	-1.93451839
H	2.26349602	4.42195706	-2.40780932
H	3.35712703	3.04690431	-2.67136976
H	3.35192616	3.90644557	-1.12018103
H	1.78522836	-5.64053506	1.97458869
H	0.43780922	-6.09570629	0.91397130
H	0.20736352	-6.08002134	2.66076070
C	-2.26332473	-4.11688642	2.36459348
C	-1.62762105	-3.84626023	0.02352906
C	-3.61111753	-4.03770404	1.97578083
C	-2.98718444	-3.77282415	-0.31702810
C	-3.99868637	-3.84872511	0.64565003
H	-3.25885061	-3.66245631	-1.36416002
H	-4.37718748	-4.12992030	2.74217936
C	-0.24155267	4.10728420	-0.47641944
C	-0.92276448	4.67720356	0.61316972
C	-0.55998167	4.42523287	1.93900286
C	0.54945231	3.60136367	2.16029628
C	1.26053454	3.01193283	1.10501124
C	-1.34187828	5.01306312	3.09271558
H	-1.76155300	5.33903561	0.41138619
H	0.87851279	3.41674351	3.18028988
H	2.22289615	1.75430008	-0.88965280
C	-1.98888677	-4.36395591	3.83698821
C	-0.61285106	-3.78676631	-1.10252192
C	-0.71805337	4.49359990	-1.86467393
C	2.46618571	2.15905106	1.45103140
H	-1.12223254	-3.74967102	-2.07088876
H	0.04597369	-4.66420185	-1.11547914
H	0.03482724	-2.90190520	-1.02926050
H	-1.37963340	-5.25958806	4.00241615
H	-2.93294043	-4.50858920	4.37187507
H	-1.45844043	-3.53354501	4.31173032
H	-1.91363705	5.89319794	2.77971238
H	-0.68261137	5.31389393	3.91522390
H	-2.05701107	4.28478799	3.49961852
H	-1.14189793	3.64750605	-2.41382057
H	0.09039999	4.89658569	-2.48398673
H	-1.49047623	5.26599054	-1.79282169
H	3.38045750	2.51151862	0.95779203
H	2.32556919	1.10892377	1.15839865
H	2.64998092	2.18120722	2.52990915
C	-5.45727983	-3.71928166	0.26563125
H	-5.62562344	-4.00692803	-0.77768053
H	-5.80685170	-2.68398151	0.38105795
H	-6.09419635	-4.34868698	0.89747396
C	3.11013486	-2.27917699	-0.21242088
C	3.03405360	-1.47587298	-1.39395520
H	3.86500589	-2.05777780	0.54503875
H	2.79683563	-3.32291155	-0.22964522
C	4.05967911	-0.39978553	-1.72056504
H	2.59140412	-1.93208893	-2.28572685
H	4.43083203	0.06341681	-0.79346380
H	3.58812397	0.40238460	-2.30825269
C	5.26384680	-0.94652442	-2.52189140
H	5.74796280	-1.74222896	-1.93656100
C	6.30113560	0.13082501	-2.88770476
H	4.89224214	-1.42238497	-3.44273195
H	6.68274924	0.59346774	-1.96504016
H	5.80284232	0.93497757	-3.45073437
C	7.47633122	-0.41637800	-3.71331556
H	8.02054860	-1.19241930	-3.15993865
H	8.19089284	0.37454468	-3.97087658
H	7.12043708	-0.86572414	-4.64926950

THF -232.4617+0.0998

O	-3.39477556	0.84318443	4.28666425
C	-3.72906647	-0.41843870	4.96874426
C	-5.25172592	-0.39400288	5.17821176
H	-5.68810389	-1.39698221	5.21297443
H	-5.50162794	0.11721481	6.11578815
C	-5.74285775	0.43538659	3.97012269
H	-6.72742713	0.88432675	4.13315660
H	-5.80237657	-0.19659021	3.07564665
H	-3.16023047	-0.45820277	5.90192563
H	-3.42222455	-1.25800359	4.33106135
C	-4.63168170	1.48711368	3.81283959
H	-4.82556188	2.37513143	4.42903276
H	-4.47354015	1.80412265	2.77820188

thiophene -3205.3128+0.0778

C	4.19134825	-2.44452926	-2.53041092
C	2.78893502	1.92174086	-0.15734575
C	2.73353322	0.85459369	-1.21636970

C	3.61812191	-0.29391361	-1.21889325
Br	0.51322535	2.13272529	-2.74584390
C	1.88484227	0.82545577	-2.28435112
C	3.45694713	-1.17358988	-2.24779691
H	4.36298275	-0.44421801	-0.44486582
S	2.12000533	-0.61157815	-3.35643662
H	2.81886829	1.47650867	0.84403258
H	1.92003203	2.58115732	-0.21116707
H	3.68861819	2.54108133	-0.26835382
H	4.96813537	-2.59570227	-1.77333339
H	4.67864620	-2.42813189	-3.51294045
H	3.52599867	-3.31660987	-2.50695386

hexene -235.8582+0.1354

C	-0.69545024	3.26197349	1.13844467
C	-1.59722418	4.19936015	0.82360699
H	-0.98434159	2.30274025	1.55789102
H	0.37003397	3.41953398	0.98530564
C	-1.27894932	5.55708757	0.25031536
H	-2.65646279	3.99882530	0.99681565
C	-1.75599657	6.71936915	1.15211773
H	-1.76061833	5.66273653	-0.73534545
H	-0.19671384	5.64461225	0.08146190
C	-1.47720709	8.10696225	0.54794653
H	-1.26389474	6.63687592	2.13202005
H	-2.83584481	6.61448761	1.33907135
C	-1.94835629	9.26023457	1.44814637
H	-1.43954257	9.23477261	2.41984324
H	-3.02766403	9.19748325	1.63619160
H	-1.74488782	10.23468228	0.98901782
H	-1.97116165	8.18064575	-0.43262626
H	-0.39866813	8.20818709	0.35626578

$C0_{Me}$ -3515.7598+0.7926

Ni	-0.59389769	-1.04576817	-0.18936625
N	-1.47394492	-1.19690973	1.59719620
N	-2.36485142	-1.19336439	-0.91346746
C	-2.75226508	-1.37913439	1.44812924
C	-3.24045842	-1.43434512	0.02521040
C	0.41811690	-0.89561974	-1.78190551
C	-3.90896517	-1.59276923	2.32096029
C	-4.67338627	-1.72175713	0.05724287
C	-5.01382838	-1.80455353	1.44264872
C	-6.31582377	-2.09032836	1.89948609
C	-4.11001602	-1.67564566	3.68997993
C	-5.41681943	-1.96353471	4.16878723
C	-6.49259782	-2.16177179	3.31238218
C	-5.66131642	-1.93253261	-0.89337201
C	-7.31047146	-2.28921583	0.89794884
C	-6.98142953	-2.21168118	-0.44991681
H	-5.44835920	-1.90071795	-1.95363888
H	-3.30149973	-1.52514664	4.39422310
H	-7.47560758	-2.37696620	3.71874880
H	-5.57308107	-2.02852442	5.23969361
H	-8.33089668	-2.51147754	1.19331877
H	-7.75311462	-2.37560556	-1.19355744
C	-0.79499408	-0.92758106	2.82277285
C	-2.69232505	-1.18155474	-2.31540791
C	0.36093942	-1.67226007	3.16607093
C	-1.20387436	0.16897703	3.60164171
C	1.09292498	-1.24031229	4.27860485
C	0.71575447	-0.13301792	5.05987549
C	-0.45537502	0.55882857	4.71175331
H	-2.08055975	0.73439118	3.30216933
H	1.98237662	-1.78937358	4.56339360
H	-0.76954978	1.41658183	5.29703265
C	-2.76123932	0.03712561	-3.02956103
C	-2.87304158	-2.41628635	-2.95756690
C	-3.01130768	-0.05521527	-4.40926809
C	-3.12677488	-2.46360330	-4.32691207
C	-3.19096009	-1.27707197	-5.07705893
H	-3.07020469	0.85601093	-4.99247836
H	-3.26173362	-3.42297922	-4.81633711
H	-2.79231386	-3.33178910	-2.38025780
C	1.56135671	0.30044245	6.23445320
H	1.82244221	-0.54940240	6.87516091
H	1.04356908	1.04152793	6.85003803
H	2.50344765	0.75143768	5.89680752
C	-3.42171350	-1.31837285	-6.57008557
H	-4.19249537	-2.04940909	-6.83734608
H	-2.50483039	-1.60755946	-7.10024868
H	-3.73075262	-0.34302450	-6.95699751
C	0.76886356	-2.90435030	2.34568240
H	0.80200323	-2.55059320	1.30066628
C	-0.24169240	-4.07475277	2.35898639
C	2.19611130	-3.41473588	2.66209441
C	-2.50596921	1.38417010	-2.33556970
C	-3.48062100	1.76036238	-1.19986612
C	-2.33244256	2.56994959	-3.31629993
H	-3.25708092	2.81055348	-3.84923230
H	-1.55142233	2.36210417	-4.05591704
H	-2.03914285	3.46306323	-2.75648136
H	2.94085190	-2.61701802	2.56181599
H	2.46225228	-4.21867103	1.97015934
H	2.26379427	-3.82754931	3.67371381
C	-0.85470096	-4.55710334	3.54595643
C	-0.50164842	-4.75342277	1.13750460
C	-1.74071541	-5.64470852	3.46944213
C	-1.39450983	-5.83582650	1.11224433
C	-2.03875350	-6.29313161	2.26637032
C	0.18310235	-4.38270793	-0.16387872
H	-1.57058746	-6.34614135	0.16880613
H	-2.19430149	-6.00617528	4.38855963
C	-0.58661994	-3.99405650	4.93051234
C	-3.01276011	-7.44869363	2.22026499
H	-2.82451025	-8.09657556	1.35817700
H	-4.05000539	-7.09485202	2.14380088
H	-2.94652616	-8.06260570	3.12460116
H	-0.09564762	-5.08617405	-0.95390902
H	1.27633780	-4.40120773	-0.08428467
H	-0.09595182	-3.37786098	-0.51889368
H	0.48238593	-3.93458148	5.15811422
H	-1.04135150	-4.63996141	5.68721468
H	-0.99804127	-2.98804736	5.06546218
C	-4.88990052	1.74297678	-1.35274142
C	-5.70563771	2.13206736	-0.27505810
C	-5.18219928	2.55916758	0.94902259
C	-3.78793580	2.61570603	1.07107799
C	-2.93419190	2.23511152	0.02480665
C	-5.58557147	1.36620891	-2.64763632
C	-6.08454260	2.95725933	2.09565622
H	-6.78386513	2.11591820	-0.41044795
H	-3.35078363	2.99435195	1.99209782
C	-1.44071322	2.40010165	0.23697337

H	-1.52957228	1.25249546	-1.85690723
H	-5.34761874	0.35195939	-2.97963698
H	-5.31197681	2.03764522	-3.46967676
H	-6.67029900	1.43352657	-2.52461235
H	-0.98663105	3.06360158	-0.50893901
H	-0.89740416	1.44383731	0.18234222
H	-1.23960051	2.83152172	1.22155420
H	-7.10108757	3.16659984	1.74863460
H	-5.71203262	3.85279056	2.60508700
H	-6.15218706	2.16011350	2.84884160
H	0.24221474	0.03736072	-2.32101770
H	0.28535193	-1.75039709	-2.44993933
H	1.43566249	-0.89995295	-1.34266851

TM_{rct} -7806.6058+1.0730

Ni	-0.13041907	-1.34434761	-0.80166470
N	-0.45530007	-1.54627026	1.23487218
N	-2.08153347	-1.17628419	-0.86137329
C	-1.72527334	-1.46653116	1.48902685
C	-2.63818195	-1.32183067	0.30783904
C	0.03276638	-1.26603993	-2.72563795
C	-2.56402896	-1.51264677	2.69253430
C	-4.01694695	-1.36305344	0.80297178
C	-3.90926007	-1.46512232	2.22255691
C	-5.02716069	-1.51364118	3.07922589
C	-2.32846354	-1.58693380	4.05542482
C	-3.44313204	-1.62762288	4.93646812
C	-4.75297134	-1.59662104	4.47595007
C	-5.27585163	-1.33195850	0.22411480
C	-6.30778546	-1.47294512	2.45405933
C	-6.41509759	-1.39010175	1.07185164
H	-5.40581310	-1.27151464	-0.84800168
H	-1.32377658	-1.60558587	4.45631529
H	-5.57667481	-1.63182136	5.18205104
H	-3.25819107	-1.68528612	6.00346961
H	-7.20361768	-1.51074548	3.06589808
H	-7.39942634	-1.36564649	0.61767936
C	0.51932601	-1.65516141	2.29008027
C	-2.89715569	-1.03496680	-2.04883226
C	1.18623201	-2.87666612	2.53758296
C	0.83815973	-0.49779739	3.01504866
C	2.17715111	-2.86958438	3.53378254
C	2.50679244	-1.72665407	4.28171999
C	1.82331723	-0.53236746	4.00391874
H	0.32743143	0.43057857	2.78283855
H	2.70289800	-3.79209484	3.75457176
H	2.05537947	0.37015096	4.56166749
C	-3.10218305	0.22596034	-2.65029676
C	-3.42350984	-2.20500009	-2.61620029
C	-3.83269252	0.24201296	-3.85148324
C	-4.15729523	-2.14507440	-3.79960972
C	-4.36493881	-0.91326771	-4.44294751
H	-3.99698216	1.19176447	-4.34584050
H	-4.55640763	-3.05765433	-4.23160324
H	-3.23374797	-3.15778311	-2.13253780
C	3.54384233	-1.79634321	5.38149778
H	4.29323596	-2.56874438	5.17911003
H	3.08202049	-2.04225467	6.34707842
H	4.06158936	-0.83949603	5.50931237
C	-5.12485635	-0.84087757	-5.74835938
H	-6.04753753	-1.43076009	-5.70743707
H	-4.52515842	-1.23775662	-6.57782381
H	-5.39354257	0.18932228	-6.00006269
C	0.87597479	-4.12264944	1.69769028
H	0.92367801	-3.75747030	0.66705114
C	-0.53628349	-4.72237375	1.87330392
C	1.95131760	-5.23099741	1.80329314
C	-2.49239306	1.50121530	-2.04890375
C	-3.10327049	1.98199789	-0.71349656
C	-2.38418235	2.67354648	-3.05585622
H	-3.35966790	3.08971066	-3.32472641
H	-1.87972431	2.35739604	-3.97624167
H	-1.80079531	3.48443243	-2.60903834
H	2.94977891	-4.83615293	1.58328028
H	1.73169988	-6.01915951	1.07685754
H	1.97370383	-5.70017818	2.79159330
C	-1.10440527	-5.01631767	3.14032165
C	-1.26430992	-5.07334616	0.70432684
C	-2.39152307	-5.57552856	3.20755718
C	-2.54565876	-5.63453844	0.82155885
C	-3.13873964	-5.88010928	2.06479631
C	-0.69593240	-4.89811532	-0.69197904
H	-3.08392936	-5.90359787	-0.08397087
H	-2.81175289	-5.79098758	4.18657961
C	-0.38231696	-4.79051495	4.45601661
C	-4.53283384	-6.45646999	2.16983993
H	-4.80800667	-7.00467558	1.26299530
H	-5.28181095	-5.66589085	2.31475052
H	-4.62024997	-7.14353905	3.01852757
H	-1.38964663	-5.30163853	-1.43617208
H	0.25883789	-5.42206025	-0.82281095
H	-0.51688680	-3.84396406	-0.94885832
H	0.59352629	-5.28746497	4.48380797
H	-0.97454640	-5.19611713	5.28175554
H	-0.20301090	-3.73108179	4.66373479
C	-4.49536452	2.17435120	-0.51585714
C	-4.95902875	2.62805594	0.73100347
C	-4.09753003	2.92211779	1.79284908
C	-2.72433510	2.77680208	1.56832189
C	-2.21371010	2.32700209	0.34107768
C	-5.53710439	1.95104163	-1.59667389
C	-4.62953518	3.38474535	3.13070616
H	-6.02840414	2.77033954	0.86465708
H	-2.02510819	3.04132055	2.35763835
C	-0.70687914	2.27477733	0.18233092
H	-1.46190438	1.21611606	-1.81420483
H	-5.61424552	0.90355281	-1.90311831
H	-5.32232667	2.52832953	-2.50214657
H	-6.52150575	2.26611312	-1.23799526
H	-0.35313411	2.90974271	-0.63835839
H	-0.33151745	1.26202328	-0.01591188
H	-0.20949542	2.63154110	1.08777291
H	-5.58963972	3.90002470	3.02240393
H	-3.93216098	4.07103262	3.62285597
H	-4.78959976	2.53861222	3.81351256
H	-0.13910437	-0.23250860	-3.05205557
H	-0.73374295	-1.92181122	-3.14696337
H	1.02963216	-1.60586998	-3.01062911
Cl	2.19048296	-1.49272613	-0.58909156
H	2.72414113	2.21498182	2.58610353
H	2.47857276	0.56003557	-3.32081255
H	1.25466555	4.48729484	3.62260252
H	2.97543283	4.79656316	3.88498818
H	4.48724185	-2.09407872	1.59283868

H	3.70732523	2.19956742	-4.60725934
C	2.75213997	2.86477783	1.71419299
C	2.15239636	4.92959648	3.17157086
Mg	3.57648478	0.50407134	-0.32408530
C	3.53924197	0.35904127	-3.47187103
C	4.19696972	1.22143175	-4.54860585
H	5.93982024	-0.43825701	3.47422730
C	5.35167133	-1.72891784	1.03337960
H	6.68556260	-2.58063654	2.54061986
H	4.14146871	0.75313336	-5.53483297
C	3.03892491	2.36638340	0.46062648
C	2.47228126	4.28265303	1.85093079
O	4.25149579	0.74164379	-2.20794163
C	6.64170705	-1.72947315	1.85571333
O	5.10175623	-0.27877108	0.73390035
H	1.97671694	6.00110155	3.05700831
C	6.59719158	-0.37501341	2.59996180
H	5.42393453	-2.25007678	0.07811012
H	3.69583613	-0.71225906	-3.61902157
H	5.32103005	2.55065944	-2.21783813
C	6.01440059	0.58120393	1.55919989
C	5.65164596	1.37413822	-4.04910925
H	5.40727823	1.39267337	1.96156821
C	5.49373173	1.51863410	-2.53380566
H	6.15410435	2.24024336	-4.48752931
H	7.58462783	-0.05282413	2.94104621
C	2.54439701	4.91772097	0.64317620
H	7.51912885	-1.77839510	1.20117189
S	2.95858767	3.80431994	-0.71357521
H	6.23709148	0.48082863	-4.29331860
H	6.30892613	1.07688141	-1.95703210
H	6.77752573	0.98493529	0.88676972
Br	2.24717714	6.81381721	0.28883276

TMTS -7806.5962+1.0797

Ni	0.40257399	-0.70536797	-0.61924363
N	-0.02868810	-1.22361639	1.38219388
N	-1.58378381	-0.64859480	-0.74044770
C	-1.31566684	-1.20676154	1.57329362
C	-2.18024923	-0.96324369	0.37543178
C	0.57070773	-0.35103994	-2.51427788
C	-2.20745230	-1.40874874	2.72436334
C	-3.57693684	-1.13379561	0.78994754
C	-3.53088433	-1.37298956	2.19541639
C	-4.68286206	-1.55682351	2.98547486
C	-2.03221299	-1.60969820	4.08381698
C	-3.18281072	-1.78104656	4.90050628
C	-4.46994721	-1.76200274	4.37963182
C	-4.80729781	-1.10451380	0.15339708
C	-5.93419346	-1.51635334	2.30295309
C	-5.98014161	-1.30206683	0.93205092
H	-4.89442397	-0.93838184	-0.91218238
H	-1.04787972	-1.63607510	4.53179326
H	-5.32309071	-1.90232308	5.03603799
H	-3.04390800	-1.93627655	5.96475916
H	-6.85455277	-1.65625135	2.86142930
H	-6.94179034	-1.27839114	0.43142658
C	0.87320714	-1.45332000	2.49022755
C	-2.34409862	-0.46250096	-1.95947326
C	1.42841296	-2.73051018	2.75221379
C	1.20721523	-0.34922016	3.28920428
C	2.38247254	-2.80437742	3.78342367
C	2.74643914	-1.70824160	4.58292205
C	2.13161436	-0.47252717	4.32795102
H	0.74142153	0.60684516	3.07825283
H	2.84238358	-3.76325025	3.99523699
H	2.37075041	0.39164415	4.94092950
C	-2.70672922	0.82154716	-2.42457950
C	-2.61716242	-1.61172293	-2.71770455
C	-3.28790497	0.88754762	-3.70353213
C	-3.23228845	-1.50584375	-3.96329920
C	-3.55876671	-0.24404939	-4.48676763
H	-3.54484559	1.85949984	-4.10714539
H	-3.43834075	-2.40323295	-4.53895104
H	-2.31761773	-2.58112468	-2.33304741
C	3.73237295	-1.87433766	5.71883229
H	4.46624928	-2.65813012	5.50291351
H	3.22083661	-2.16069735	6.64742723
H	4.27431060	-0.94494395	5.92356275
C	-4.17058336	-0.11078279	-5.86344001
H	-4.97556137	-0.83857098	-6.01584297
H	-3.42331432	-0.28766367	-6.64811329
H	-4.58471163	0.88920866	-6.02336879
C	1.03192711	-3.96042205	1.92169858
H	1.00503212	-3.58605514	0.89823081
C	-0.36792761	-4.55684100	2.20033207
C	2.10022831	-5.08067969	1.92437662
C	-2.42594328	2.08147094	-1.58842437
C	-3.40439156	2.33497523	-0.41389550
C	-2.24179664	3.36075227	-2.44214532
H	-3.17397357	3.70396340	-2.89989674
H	-1.50616309	3.19643666	-3.23733277
H	-1.87615720	4.17244936	-1.80574946
H	3.08498218	-4.68457520	1.65207596
H	1.82727546	-5.83825866	1.18341734
H	2.18022184	-5.58800567	2.89054505
C	-0.83102317	-4.91109470	3.49446095
C	-1.19858356	-4.84724077	1.08244321
C	-2.10870616	-5.47640201	3.64265460
C	-2.46490522	-5.41891334	1.27996553
C	-2.95037077	-5.72811833	2.55487001
C	-0.75607354	-4.59725969	-0.34819792
H	-3.07936787	-5.64081859	0.41087417
H	-2.44474405	-5.73959489	4.64229598
C	-0.01388158	-4.73739460	4.76160789
C	-4.33287397	-6.30877855	2.74919191
H	-4.65013864	-6.88819300	1.87584613
H	-5.07872241	-5.51673394	2.90359489
H	-4.37307993	-6.96673643	3.62380357
H	-1.51634875	-4.96412333	-1.04510257
H	0.18156977	-5.11085123	-0.59016479
H	-0.59007159	-3.53484294	-0.56168176
H	0.96099914	-5.23225889	4.70066799
H	-0.54522711	-5.17682451	5.61115866
H	0.17750724	-3.68602087	4.99850702
C	-4.81560558	2.40210954	-0.56827121
C	-5.62464461	2.64643725	0.55439369
C	-5.09978640	2.84515561	1.83453509
C	-3.70869522	2.82148664	1.96757541
C	-2.85908694	2.58070088	0.87665883
C	-5.53868758	2.24131501	-1.89274849
C	-6.00285246	3.07212102	3.02578844
H	-6.70136626	2.69472979	0.41443783
H	-3.26547036	3.00824034	2.94250857

C	-1.36536349	2.64194859	1.13421873
H	-1.44941892	1.89361558	-1.13227311
H	-5.47174540	1.22282823	-2.28844620
H	-5.14974741	2.90882825	-2.66766565
H	-6.59964719	2.47783089	-1.76774340
H	-0.87952097	3.43374265	0.55301943
H	-0.84529438	1.70874850	0.88976140
H	-1.17895557	2.85718444	2.19136871
H	-6.93000313	3.57643442	2.73378066
H	-5.51227301	3.68288734	3.79107852
H	-6.28481479	2.12091405	3.49849579
H	-0.02697383	0.52512153	-2.77099176
H	0.18653116	-1.24622952	-3.01275914
H	1.61302642	-0.18470855	-2.80746204
Cl	2.31822394	-2.45675406	-0.95037774
H	2.64634830	1.29875141	1.85428465
H	3.42861686	-1.77961953	-3.60447296
H	1.38475757	4.29582719	2.76794854
H	2.96759865	3.54866806	3.02988198
H	4.32934143	-2.23156643	1.66206496
H	3.36438947	-0.02518011	-5.30784643
C	2.37193507	1.85802745	0.96553496
C	2.35657722	4.09048179	2.30074170
Mg	3.45348778	-0.37030837	-0.88914680
C	4.32892129	-1.18371799	-3.75454251
C	4.36962493	-0.37072809	-5.04358905
H	5.53042091	0.00305469	3.10057679
C	5.23425574	-1.97126303	1.11013870
H	6.39879686	-2.28151302	2.92968661
H	4.76389212	-0.95152588	-5.88155028
C	2.18666583	1.21287197	-0.25094749
C	2.19878739	3.29081445	1.03445939
O	4.33645287	-0.13375908	-2.67646371
C	6.42685312	-1.67256541	2.02231872
O	4.95815040	-0.66340467	0.40990830
H	2.83019159	5.05778873	2.10779343
C	6.28713460	-0.16314846	2.32602741
H	5.42827459	-2.71507983	0.33728328
H	5.22012299	-1.80286343	-3.61552943
H	4.12914375	1.90267704	-3.13607529
C	5.81784504	0.41500666	0.99247418
C	5.28218641	0.82344443	-4.67800344
H	5.19413612	1.30652169	1.07457902
C	4.91037124	1.14515198	-3.22465383
H	5.12219535	1.68436423	-5.33220014
H	7.22602207	0.28642533	2.65990424
C	1.86746382	3.79970747	-0.19320418
H	7.37295896	-1.87476911	1.50828157
S	1.72855620	2.54745608	-1.47035023
H	6.33595489	0.53378183	-4.75379693
H	5.76660354	1.41363260	-2.60208944
H	6.64610862	0.59125257	0.29907082
Br	1.49884343	5.66855921	-0.60023575

TMprd -7806.6214+1.0822

Ni	0.27284715	-0.22256823	-0.21789397
N	-0.40921322	-0.84047743	1.71155297
N	-1.67685464	-0.53199288	-0.64527790
C	-1.69369024	-1.02966611	1.69845210
C	-2.39079528	-0.90507671	0.37603063
C	0.63290705	0.01389658	-2.11469955
C	-2.71309702	-1.36472671	2.70278748
C	-3.80374797	-1.23951686	0.58342006
C	-3.93707240	-1.48678579	1.98167471
C	-5.16231892	-1.82336404	2.59104718
C	-2.71901673	-1.56741507	4.07314362
C	-3.94807351	-1.89344881	4.70867881
C	-5.13603308	-2.02337497	4.00210001
C	-4.91918051	-1.35953918	-0.23044452
C	-6.29263313	-1.92936816	1.72951838
C	-6.16143130	-1.70842758	0.36490248
H	-4.86322591	-1.19802236	-1.29849950
H	-1.81741829	-1.48136567	4.66465619
H	-6.05283186	-2.27831651	4.52439457
H	-3.94949261	-2.04991626	5.78172933
H	-7.26067259	-2.18953028	2.14608610
H	-7.03297202	-1.80124066	-0.27360878
C	0.33510811	-0.94651066	2.94382672
C	-2.30422769	-0.38077335	-1.94214689
C	1.10490489	-2.09797814	3.22905350
C	0.34457503	0.16154323	3.80551854
C	1.94316676	-2.03332211	4.35753524
C	1.98622313	-0.93000140	5.22405580
C	1.15129620	0.16584039	4.94322292
H	-0.26061383	1.02693509	3.55694311
H	2.56512276	-2.89041489	4.58726883
H	1.14158921	1.02645794	5.60551857
C	-2.68796283	0.88974214	-2.42681324
C	-2.44935304	-1.53188300	-2.73067565
C	-3.19226166	0.93922097	-3.73869090
C	-2.97720272	-1.44375499	-4.01788791
C	-3.35008631	-0.19662203	-4.54695425
H	-3.47782990	1.90053531	-4.14920792
H	-3.08535889	-2.34323513	-4.61634428
H	-2.12878363	-2.48876524	-2.33153146
C	2.88487260	-0.92952609	6.44090940
H	3.51752430	-1.82156107	6.46945882
H	2.29926042	-0.90887622	7.36858873
H	3.54076939	-0.05056377	6.45797091
C	-3.89303133	-0.08266912	-5.95379864
H	-4.70208134	-0.80105456	-6.12971676
H	-3.11391334	-0.28733529	-6.69939691
H	-4.28433594	0.91955285	-6.15187083
C	1.03260354	-3.34699922	2.33634775
H	1.09307672	-2.96877719	1.31009095
C	-0.29162110	-4.14428045	2.43534228
C	2.24625459	-4.29505384	2.49605285
C	-2.48116768	2.16079494	-1.58560533
C	-3.43062803	2.35516663	-0.38020757
C	-2.41548013	3.45731774	-2.43214402
H	-3.38493129	3.72919145	-2.86033376
H	-1.69303846	3.36124355	-3.25099625
H	-2.10010175	4.28975861	-1.79522843
H	3.18830657	-3.75173370	2.36394899
H	2.20477805	-5.06823903	1.72469089
H	2.26209525	-4.79781005	3.46796794
C	-0.84298981	-4.59293300	3.66556816
C	-0.93716983	-4.52745352	1.22646958
C	-2.02369704	-5.35537529	3.65712255
C	-2.11352811	-5.29144270	1.27072632
C	-2.68562114	-5.70700407	2.47717640
C	-0.38004326	-4.17871221	-0.13957747
H	-2.58273622	-5.57988541	0.33350292
H	-2.42675649	-5.69503984	4.60777789

C	-0.22352240	-4.32705508	5.02585803
C	-3.97215183	-6.50099185	2.50440005
H	-4.05344786	-7.16363741	1.63599675
H	-4.84916381	-5.83899590	2.49048765
H	-4.04416498	-7.11719133	3.40666544
H	-1.00346213	-4.62067280	-0.92381572
H	0.64116067	-4.54363853	-0.28536981
H	-0.33996149	-3.09693511	-0.31564107
H	0.82217954	-4.64608812	5.08059830
H	-0.76898713	-4.88041719	5.79629877
H	-0.24549677	-3.26803400	5.30277966
C	-4.84500741	2.28162069	-0.47903067
C	-5.63083460	2.49652554	0.66537938
C	-5.07715824	2.80166950	1.91305528
C	-3.68556156	2.91809331	1.98767229
C	-2.85922952	2.71210202	0.87193958
C	-5.58488306	2.00803076	-1.77497231
C	-5.95044305	2.99958010	3.13146599
H	-6.71167304	2.43482514	0.56766344
H	-3.22603048	3.19555098	2.93310763
C	-1.36722114	2.91824089	1.05594302
H	-1.48117687	2.03580803	-1.15790387
H	-5.36841461	1.01691219	-2.18253358
H	-5.33315444	2.73275763	-2.55688893
H	-6.66445245	2.07338215	-1.60983096
H	-0.95852967	3.65948413	0.35875509
H	-0.79086681	1.99546088	0.90873617
H	-1.15878910	3.27940643	2.06806724
H	-6.91116979	3.45338508	2.86574828
H	-5.46540768	3.64494186	3.87117331
H	-6.16938274	2.04292374	3.62545416
H	-0.02011672	0.82494819	-2.44862795
H	0.30969261	-0.92818769	-2.57210022
H	1.65164548	0.25398020	-2.42787075
Cl	2.99445505	-3.13388668	-0.97462077
H	2.55287145	0.04647895	2.25972005
H	2.50626310	-1.48201779	-3.89332252
H	3.37737834	1.85681583	3.94560286
H	4.91779866	2.15005490	3.12416976
H	5.84771494	-2.70968846	-0.45991943
H	3.15852601	0.21752101	-5.49162676
C	2.56845866	0.83778641	1.52040198
C	3.85221066	2.41647912	3.13451127
Mg	3.26939659	-0.80934551	-0.86340298
C	3.56860347	-1.24440429	-3.93692010
C	3.98880259	-0.40858644	-5.14621690
H	7.00367143	-1.67336637	1.94684264
C	6.17052463	-1.70613441	-0.74443647
H	8.21767637	-2.13074955	-0.12132581
H	4.30710252	-1.03825726	-5.98133578
C	1.96086788	0.66053991	0.28134078
C	3.18513303	2.10782757	1.82015900
O	3.87270850	-0.36150368	-2.75151030
C	7.51086861	-1.29687565	-0.14156791
O	5.18540111	-0.73617823	-0.14376134
H	3.79002714	3.48238318	3.36954915
C	7.12714419	-0.81637989	1.27556711
H	6.09753795	-1.58989857	-1.82562750
H	4.15383784	-2.15719136	-3.81129409
H	3.98702175	1.69336297	-3.18071060
C	5.78859482	-0.09860466	1.06717751
C	5.13657357	0.47070683	-4.60016470
H	5.09009101	-0.23218006	1.89252852
C	4.65964016	0.83202927	-3.19348817
H	5.31342140	1.35959408	-5.21164874
H	7.87954496	-0.15327656	1.71085462
C	3.07533164	2.96987770	0.75873639
H	7.96494994	-0.48103977	-0.71571438
S	2.20605637	2.28120893	-0.64374617
H	6.07044863	-0.10142361	-4.55595180
H	5.45881329	0.97443189	-2.46445307
H	5.90255591	0.96566890	0.84732385
Br	3.74807214	4.79439836	0.67707466

Disolvated Grignard Monomer
-4290.7820+0.2572

C	1.71520580	0.42612446	1.34522030
C	2.76906281	-0.41040654	1.04719502
C	2.75095277	-1.14126867	-0.20819686
C	1.62378536	-0.85784060	-0.92445048
S	0.53201705	0.31376895	-0.09490816
Br	1.12525043	-1.57333269	-2.67808650
C	3.85561523	-2.07825892	-0.61744170
Mg	1.30402028	1.67169547	3.00344740
Cl	2.60908824	2.03761271	4.93400789
O	-0.45752206	1.05574014	3.81658628
C	-1.14774353	-0.19479491	3.38046406
C	-1.54520522	-0.86136058	4.69464980
H	-2.37218250	-1.56535192	4.56582218
H	-0.69297656	-1.40440204	5.11762371
C	-1.92275701	0.34108384	5.59232001
H	-1.85826576	0.10263469	6.65746845
H	-2.94817888	0.66359735	5.37907848
H	-0.43421974	-0.74787660	2.77013909
H	-2.01250087	0.09020164	2.77269204
C	-0.91583061	1.43166154	5.19403048
H	-0.01937597	1.45488736	5.81597190
H	-1.35436401	2.43025562	5.13284645
H	3.05282929	5.54276813	2.28646863
H	1.76519615	4.47496537	4.05683612
C	1.97935153	5.75982522	2.25617052
H	2.03975171	3.36811834	0.48837027
C	1.22328381	4.79399961	3.16577539
H	1.83275821	6.80326516	2.54946286
O	1.05130018	3.57333167	2.32276707
C	1.18629427	3.92963692	0.87290892
C	1.39850513	5.44993480	0.85628676
H	2.06988196	5.75418128	0.04846076
H	0.22559315	5.16171361	3.42938193
H	0.27949291	3.59898988	0.36451835
H	0.44475875	5.97175662	0.71623161
H	3.60278961	-0.52552980	1.73506237
H	3.64621290	-2.55404364	-1.57853264
H	3.99277979	-2.86911922	0.13077311
H	4.81065538	-1.54429425	-0.70365188

RE_{rct}(thiophene) -9806.4420+0.8846

Ni	0.0000000	0.0000000	0.0000000
N	0.7636585	0.5711337	1.8042440
N	1.9594601	-0.472494	-0.343243
C	2.0439536	0.3656571	1.8851398
C	2.7233414	-0.156584	0.6594216
C	3.0728407	0.5492453	2.9204131
C	4.1658237	-0.217865	0.9422611

C	4.3077923	0.1978717	2.2992162
C	5.5496617	0.2535021	2.9644200
C	3.0783900	0.9583912	4.2431687
C	4.3213681	1.0195235	4.9312697
C	5.5230195	0.6817018	4.3237840
C	5.2975484	-0.572614	0.2273410
C	6.6943916	-0.126509	2.2046687
C	6.5595931	-0.522294	0.8810358
H	5.2398219	-0.874115	-0.810079
H	2.1631796	1.2180923	4.7580167
H	6.4507572	0.7402143	4.8849583
H	4.3230094	1.3406710	5.9674445
H	7.6764817	-0.101214	2.6671019
H	7.4437708	-0.802921	0.3186726
C	0.0056804	1.0163812	2.9471206
C	2.5146224	-0.944137	-1.586959
C	-0.515537	2.3273964	3.0103218
C	-0.265837	0.0826312	3.9563981
C	-1.349082	2.6286777	4.0985735
C	-1.653678	1.7036239	5.1094461
C	-1.083534	0.4242774	5.0326909
H	0.1354692	-0.921412	3.8678028
H	-1.778781	3.6216232	4.1684492
H	-1.300027	-0.313806	5.7989310
C	2.3441114	-2.284781	-1.998196
C	3.1579219	-0.013007	-2.414342
C	2.7959158	-2.618799	-3.284142
C	3.6133303	-0.387218	-3.677517
C	3.4198740	-1.697511	-4.139443
H	2.6602583	-3.634449	-3.637829
H	4.0920565	0.3488361	-4.316281
H	3.2593879	1.0128054	-2.075732
C	-2.598721	2.0688290	6.2324420
H	-2.584439	3.1446664	6.4366347
H	-2.343051	1.5433340	7.1589885
H	-3.632101	1.7976471	5.9778978
C	3.8399812	-2.099343	-5.535503
H	4.7339588	-1.553900	-5.856958
H	3.0455220	-1.879921	-6.261347
H	4.0536498	-3.171502	-5.599652
C	-0.202028	3.3432793	1.9051518
H	-0.401586	2.7889705	0.9841061
C	1.2687718	3.8070098	1.8189511
C	-1.160623	4.5577802	1.8863381
C	1.6593540	-3.299813	-1.074627
C	2.4143124	-3.627352	0.2315279
C	1.2160672	-4.597164	-1.791490
H	2.0629055	-5.203822	-2.128859
H	0.5869661	-4.367319	-2.658408
H	0.6310228	-5.214574	-1.102098
H	-2.204343	4.2265718	1.8570025
H	-0.967961	5.1618097	0.9936646
H	-1.026257	5.2107662	2.7545852
C	2.0052124	4.2833548	2.9336970
C	1.8909539	3.8237837	0.5391367
C	3.3393010	4.6923815	2.7593394
C	3.2239713	4.2418111	0.4139539
C	3.9759926	4.6649246	1.5159499
H	3.6793643	4.2478420	-0.573773
H	3.8882587	5.0515790	3.6263329
C	3.7836112	-3.998412	0.2717731
C	4.3864137	-4.289966	1.5076437
C	3.6836497	-4.245067	2.7156177
C	2.3223194	-3.926339	2.6581831
C	1.6775647	-3.629969	1.4476585
C	4.3694032	-4.523715	4.0346931
H	5.4372401	-4.570060	1.5169682
H	1.7363719	-3.920960	3.5745286
H	0.7369978	-2.792143	-0.777726
C	-1.805096	0.4384905	0.3453398
C	1.4266524	4.4104607	4.3309493
C	1.1523136	3.4280709	-0.725392
C	4.6500347	-4.132529	-0.966691
C	0.1877135	-3.348452	1.4918903
C	-2.638494	1.4540189	-0.048075
C	-4.213325	0.3515001	1.2628424
C	-3.997101	1.4377768	0.4665279
H	-2.315883	2.2198341	-0.745638
C	-5.002169	2.5040919	0.1240528
S	-2.761702	-0.711620	1.4303223
Br	-5.862508	-0.126509	2.2046687
H	1.7915863	3.5706259	-1.602129
H	0.2470693	4.0271901	-0.882980
H	0.8365137	2.3764112	-0.717862
H	0.5030642	4.9986978	4.3461767
H	2.1437678	4.9136977	4.9875026
H	1.1874741	3.4415598	4.7794848
H	5.2249413	-5.196081	3.9079939
H	3.6831654	-4.983878	4.7541976
H	4.7476221	-3.598720	4.4921873
H	4.8291576	-3.173456	-1.462173
H	4.2004518	-4.791789	-1.716424
H	5.6231711	-4.557324	-0.699584
H	-0.383682	-4.040129	0.8611338
H	-0.059829	-2.334190	1.1524326
H	-0.190956	-3.453246	2.5131136
C	5.4245374	5.0734909	1.3625864
H	5.5828043	5.6569637	0.4483025
H	6.0818667	4.1949465	1.3034096
H	5.7616481	5.6777789	2.2113129
Br	-1.392040	-0.176799	-6.108631
S	-0.362312	0.5805206	-3.119984
C	-1.248553	-0.570091	-4.195271
C	-0.685968	-0.530280	-1.679616
C	-1.740342	-1.656920	-3.533259
C	-1.421443	-1.602089	-2.117400
C	-2.528718	-2.785869	-4.139752
H	-1.788563	-2.359272	-1.432612
H	-4.654623	3.4927717	0.4517430
H	-5.969233	2.3127511	0.5956514
H	-5.157865	2.5581561	-0.960908
H	-2.732496	-2.609686	-5.198580
H	-3.489051	-2.909041	-3.623762
H	-1.989174	-3.738416	-4.052943

RE_{ts}(thiophene) -9806.4046+0.8833

Ni	0.0000000	0.0000000	0.0000000
N	0.7264775	0.6226983	1.8026054
N	1.9538888	-0.482302	-0.293439
C	1.9951340	0.3702733	1.9307731
C	2.7000210	-0.158317	0.7200515
C	2.9995051	0.5245089	2.9954920
C	4.1352675	-0.222318	1.0344935
C	4.2479238	0.1740196	2.3999337

C	5.4737318	0.2098497	3.0950058
C	2.9759962	0.9108245	4.3249770
C	4.2027393	0.9508640	5.0440562
C	5.4170157	0.6158070	4.4605645
C	5.2798741	-0.577734	0.3414183
C	6.6337245	-0.167652	2.3565289
C	6.5272093	-0.543851	1.0245802
H	5.2428305	-0.871112	-0.699905
H	2.0506935	1.1687717	4.8236142
H	6.3311354	0.6590591	5.0451464
H	4.1812858	1.2534914	6.0857682
H	7.6047475	-0.157581	2.8425007
H	7.4224890	-0.824264	0.4796349
C	-0.089453	1.0846107	2.8902462
C	2.4903337	-0.938885	-1.544328
C	-0.610425	2.3980546	2.8912731
C	-0.458589	0.1662464	3.8844681
C	-1.528397	2.7226816	3.9016551
C	-1.930410	1.8119970	4.8912693
C	-1.367115	0.5269035	4.8785331
H	-0.059583	-0.841537	3.8425905
H	-1.951347	3.7207557	3.9226272
H	-1.657761	-0.200816	5.6303181
C	2.3150019	-2.279173	-1.958594
C	3.0864680	0.0027863	-2.396042

C 2.7151294 -2.603966 -3.263583
C 3.4867343 -0.360802 -3.681244
C 3.2863990 -1.670349 -4.142430
H 2.5766379 -3.620087 -3.615709
H 3.9296272 0.3830815 -4.336841
H 3.1934280 1.0271013 -2.055215
C -2.975042 2.1926611 5.9162834
H -3.035992 3.2785026 6.0442308
H -2.761960 1.7473720 6.8946743
H -3.968996 1.8409831 5.6079116
C 3.6404033 -2.057276 -5.561089
H 4.5099649 -1.498187 -5.923623
H 2.8070495 -1.843128 -6.244049
H 3.8645887 -3.126132 -5.644020
C -0.205212 3.3876313 1.7927987
H -0.364280 2.8238861 0.8676412
C 1.2793098 3.8130210 1.7883054
C -1.120887 4.6321211 1.7037298
C 1.6706104 -3.300102 -1.013122
C 2.4821288 -3.648174 0.2540818
C 1.1971708 -4.593902 -1.717284
H 2.0324980 -5.200379 -2.081980
H 0.5420501 -4.362341 -2.564342
H 0.6338700 -5.211388 -1.009900
H -2.172574 4.3384680 1.6136398
H -0.853631 5.2214314 0.8205632
H -1.016971 5.2873649 2.5745170
C 1.9636025 4.2690632 2.9438482
C 1.9717759 3.8142436 0.5456338
C 3.3128793 4.6524111 2.8427325
C 3.3168899 4.2067080 0.4933204
C 4.0152572 4.6151518 1.6355378
H 3.8262192 4.2019187 -0.467638
H 3.8222411 4.9977821 3.7391405
C 3.8521552 -4.016570 0.2260192
C 4.5071881 -4.338931 1.4270663
C 3.8571036 -4.325021 2.6646979
C 2.4952428 -4.004543 2.6745878
C 1.7992021 -3.679122 1.5010354
C 4.5996947 -4.636549 3.9451182
H 5.5576049 -4.616975 1.3842777
H 1.9520788 -4.018052 3.6165494
H 0.7650264 -2.791249 -0.666850
C -1.875258 0.2621225 -0.119855
C 1.3142402 4.3963458 4.3096850
C 1.2971858 3.4195419 -0.754331
C 4.6703697 -4.110627 -1.048931
C 0.3157638 -3.387038 1.6168210
C -2.690864 1.3805197 -0.273470
C -4.102212 0.2707281 1.2061410
C -3.928348 1.4050047 0.4607663
H -2.441624 2.1638939 -0.980442
C -4.894519 2.5573397 0.3744251
S -2.742921 -0.909730 1.0619622
Br -5.623282 -0.167652 2.3565289
H 1.9828655 3.5514600 -1.597087
H 0.4065414 4.0251695 -0.962344
H 0.9758298 2.3693042 -0.753419
H 0.4081561 5.0113554 4.2850630
H 2.0093412 4.8692906 5.0109687
H 1.0241327 3.4281775 4.7288048
H 5.4537348 -5.297908 3.7625501
H 3.9466955 -5.122247 4.6787401
H 4.9895581 -3.721596 4.4126282
H 4.8178351 -3.137238 -1.526929
H 4.2022525 -4.758232 -1.797905
H 5.6575015 -4.528822 -0.827150
H -0.288594 -4.037024 0.9724371
H 0.0740222 -2.351955 1.3428810
H -0.027405 -3.542069 2.6447537
C 5.4773367 4.9966440 1.5613979
H 5.6910953 5.5994098 0.6709999
H 6.1188932 4.1061566 1.5103284
H 5.7854215 5.5724297 2.4404427
Br -1.017048 -0.216928 -6.025929
S -0.620492 0.7043823 -2.942387
C -1.119013 -0.583281 -4.106438
C -1.056962 -0.435932 -1.519284
C -1.556166 -1.730854 -3.502726
C -1.519017 -1.629894 -2.067394
C -2.059441 -2.960966 -4.211084
H -1.913186 -2.419316 -1.437468
H -4.527665 3.4264962 0.9367832
H -5.874623 2.2904226 0.7774956
H -5.026687 2.8731800 -0.666779
H -2.008725 -2.847849 -5.296391
H -3.102253 -3.167543 -3.939305
H -1.469652 -3.843991 -3.934434

RE_{prd}(thiophene) -9806.4533+0.8878
Ni 0.0000000 0.0000000 0.0000000
N 0.8833681 0.8192247 1.6283524
N 1.6922963 -1.078909 -0.044274
C 2.0163433 0.2371630 1.9088629
C 2.5106133 -0.763750 0.9200174
C 3.0271206 0.3459844 2.9738087
C 3.8533122 -1.187021 1.3434352
C 4.0976466 -0.509831 2.5752217
C 5.2809457 -0.671085 3.3236255

C 3.1423572 1.0489298 4.1615788
C 4.3273506 0.8956327 4.9338560
C 5.3697539 0.0687178 4.5391088
C 4.8252086 -2.035197 0.8407508
C 6.2604083 -1.554788 2.7824373
C 6.0290141 -2.206573 1.5790541
H 4.6907190 -2.559051 -0.096890
H 2.3541243 1.7012423 4.5140207
H 6.2582314 -0.019921 5.1570867
H 4.4124027 1.4484383 5.8636466
H 7.1922704 -1.713680 3.3168076
H 6.7878481 -2.872920 1.1822427
C 0.2777918 1.7772330 2.5084605
C 2.0501094 -1.973247 -1.107007
C 0.2238316 3.1464233 2.1541769
C -0.327760 1.3184345 3.6883753
C -0.490243 4.0019562 3.0088857
C -1.108606 3.5626170 4.1906884
C -1.005426 2.2038182 4.5270113
H -0.284343 0.2608872 3.9264456
H -0.555558 5.0545901 2.7576964
H -1.466620 1.8338386 5.4383047
C 1.4612539 -3.257362 -1.202186
C 2.9211533 -1.509709 -2.105632
C 1.7472523 -4.009475 -2.351691
C 3.1987537 -2.296481 -3.224548
C 2.6005729 -3.556866 -3.371592
H 1.3025867 -4.992838 -2.457859
H 3.8671192 -1.921148 -3.993663
H 3.3506506 -0.518139 -2.009064
C -1.883134 4.5239858 5.0654226
H -1.569361 5.5593848 4.8980599
H -1.746911 4.2966633 6.1287840
H -2.960755 4.4714075 4.8585664
C 2.8455853 -4.399365 -4.604272
H 3.8008314 -4.148036 -5.077028
H 2.0590989 -4.243380 -5.355210
H 2.8572158 -5.468235 -4.364402
C 0.8955757 3.6410513 0.8670933
H 0.5278180 2.9532353 0.0987997
C 2.4369197 3.5352313 0.8378980
C 0.4405853 5.0524357 0.4257882
C 0.5308306 -3.766326 -0.094324
C 1.2063578 -4.036124 1.2699859
C -0.342227 -4.974472 -0.513159
H 0.2453214 -5.889905 -0.638728
H -0.875558 -4.774868 -1.449967
H -1.087392 -5.172711 0.2638131
H -0.650403 5.1045334 0.3408995
H 0.8656528 5.2792387 -0.556727
H 0.7774976 5.8340951 1.1145399
C 3.2734185 4.0209250 1.8755334
C 3.0468651 2.9875227 -0.323678
C 4.6677028 3.8866403 1.7604741
C 4.4438619 2.8764267 -0.395156
C 5.2764828 3.3027882 0.6454162
H 4.8868860 2.4503521 -1.292128
H 5.2915518 4.2589025 2.5695947
C 2.3839216 -4.813779 1.4172617
C 2.9193611 -5.021147 2.7004854
C 2.3288236 -4.499071 3.8542617
C 1.1417311 -3.773875 3.7005575
C 0.5693907 -3.541395 2.4415229
C 2.9480538 -4.705699 5.2184925
H 3.8234400 -5.617942 2.7939552
H 0.6366282 -3.384758 4.5816393
H -0.160247 -2.934582 0.0771039
C -2.835224 0.3876423 0.5568095
C 2.7492375 4.7122547 3.1203577
C 2.2355025 2.5152265 -1.514264
C 3.1120178 -5.470428 0.2591831
C -0.736794 -2.773180 2.3907176
C -3.196945 1.1922589 1.6051723
C -4.769874 -0.477251 1.9801120
C -4.294038 0.7249561 2.4206319
H -2.677071 2.1179079 1.8232129
C -4.815051 1.5013265 3.5987815
S -3.932064 -1.094607 0.5091070
Br -6.189414 -1.554788 2.7824373
H 2.8995100 2.2326666 -2.337536
H 1.5555955 3.2855827 -1.894663
H 1.6138003 1.6417735 -1.272067
H 2.1009165 5.5623141 2.8817751
H 3.5843647 5.0970421 3.7146391
H 2.1657514 4.0416502 3.7587060
H 3.6354166 -5.558340 5.2211449
H 2.1842509 -4.886628 5.9835283
H 3.5204168 -3.822598 5.5344812
H 3.5979782 -4.741949 -0.397624
H 2.4464239 -6.068168 -0.371861
H 3.8881782 -6.142145 0.6402201
H -1.530635 -3.326768 1.8758329
H -0.634991 -1.811146 1.8702759
H -1.095422 -2.565790 3.4037501
C 6.7769619 3.1252785 0.5727765
H 7.1436571 3.2207263 -0.455340
H 7.0762926 2.1316794 0.9343112
H 7.2979045 3.8666928 1.1882095
Br -0.911147 2.3987399 -4.510352
S -1.913600 2.2152098 -1.440269
C -1.253404 1.3374541 -2.892028
C -1.815836 0.5707895 -0.466878
C -1.034483 0.0099479 -2.736851
C -1.343744 -0.465121 -1.376756
C -0.578244 -0.942546 -3.806349
H -1.684814 -1.495344 -1.269164
H -3.990074 1.8308649 4.2405643
H -5.503481 0.9024013 4.1992568
H -5.352771 2.3995206 3.2674222
H -0.417237 -0.430599 -4.757651
H -1.332897 -1.724930 -3.965172
H 0.3530166 -1.442051 -3.519637

$RE_{rct}(CH_2TMS)$ -7090.0495+0.9531
Ni 0.0000000 0.0000000 0.0000000
N 0.8500081 0.3347312 1.8785230
N 1.7307413 0.9439045 -0.570812
C 1.9841814 0.9634993 1.8002879
C 2.4339986 1.3715441 0.4377293
C 2.9922622 1.4401697 2.7622501
C 3.6494593 2.1860156 0.5946950
C 3.9411239 2.1735921 1.9906650
C 5.0590390 2.8223653 2.5526115
C 3.1813094 1.3295915 4.1290500

C 4.3116717 1.9656935 4.7134000
C 5.2239615 2.6945628 3.9630576
C 4.4789222 2.8955590 -0.257579
C 5.9000757 3.5347736 1.6483296
C 5.6047183 3.5688380 0.2924032
H 4.2847846 2.9506952 -1.320673
H 2.4968877 0.7689769 4.7519049
H 6.0707164 3.1701905 4.4488274
H 4.4574772 1.8771427 5.7848222
H 6.7732327 4.0571036 2.0276638
H 6.2528617 4.1237631 -0.377626
C 0.3464553 -0.135091 3.1448637
C 2.1177762 1.2808218 -1.920455
C -0.702001 0.5386210 3.8129984
C 0.8747757 -1.328064 3.6559486
C -1.206758 -0.064530 4.9747857
C -0.705897 -1.268715 5.4959175
C 0.3580710 -1.888615 4.8253359
H 1.6733177 -1.824677 3.1147534
H -2.025859 0.4169281 5.4967795
H 0.7731548 -2.817521 5.2054430
C 2.8153795 0.3529471 -2.726694
C 1.7041533 2.5156516 -2.439295
C 3.0425591 0.7144917 -4.065479
C 1.9665376 2.8478306 -3.768291
C 2.6321100 1.9414167 -4.608601
H 3.5565602 0.0124178 -4.711580
H 1.6334688 3.8052622 -4.157882
H 1.1508047 3.1958561 -1.800559
C -1.320804 -1.886017 6.7330219
H -1.619740 -1.120202 7.4571069
H -0.623556 -2.568821 7.2299644
H -2.221222 -2.462719 6.4818303
C 2.8705323 2.2637946 -6.067188
H 3.0817161 3.3289985 -6.212099
H 1.9881169 2.0217336 -6.674646
H 3.7124828 1.6929708 -6.472200
C -1.289141 1.8352025 3.2406816
H -1.430056 1.6059611 2.1815827
C -0.377032 3.0801580 3.2944054
C -2.698316 2.1742191 3.7844611
C 3.2216270 -1.020701 -2.170958
C 4.3694678 -1.036419 -1.135673
C 3.4839943 -2.081783 -3.269407
H 4.3891777 -1.873189 -3.848475
H 2.6387988 -2.149619 -3.962825
H 3.6198050 -3.062577 -2.802562
H -3.377342 1.3251650 3.6580836
H -3.108697 3.0197694 3.2232277
H -2.683797 2.4619605 4.8406350
C 0.2626507 3.5310118 4.4775018
C -0.247142 3.8642683 2.1133405
C 1.0454814 4.6986239 4.4403560
C 0.5426435 5.0231031 2.1253547
C 1.2128742 5.4529343 3.2764191
H 0.6233675 5.6103579 1.2134785
H 1.5275699 5.0292891 5.3572256
C 5.6240749 -0.408944 -1.352305
C 6.6264280 -0.506909 -0.372265
C 6.4467201 -1.216618 0.8187119
C 5.2214295 -1.865706 1.0031326
C 4.1912467 -1.796865 0.0532843
C 7.5304086 -1.272341 1.8721059
H 7.5787657 -0.015317 -0.556537
H 5.0595526 -2.452538 1.9042580
H 2.3281390 -1.357489 -1.635621
C -1.579318 -0.813566 0.6584908
C 0.1345375 2.8350536 5.8201237
C -0.965541 3.5107076 0.8238019
C 5.9698855 0.3608231 -2.613013
C 2.9237343 -2.582556 0.3332579
C -1.760752 -2.001856 1.3243123
C -3.986120 -1.336886 1.4556732
C -3.100405 -2.321024 1.7873140
H -0.936305 -2.679244 1.5203090
C -3.410499 -3.583775 2.5439544
S -3.225869 0.0254964 0.5448270
Br -5.900168 -1.272341 1.8721059
H -0.790692 4.2845239 0.0690397
H -2.050222 3.4277776 0.9618729
H -0.630449 2.5529727 0.4025709
H -0.909552 2.7052763 6.1238378
H 0.6273749 3.4286392 6.5969650
H 0.5888310 1.8394993 5.8242165
H 8.5245878 -1.137662 1.4323285
H 7.5240451 -2.230395 2.4037168
H 7.3966285 -0.482640 2.6244204
H 5.3628353 1.2629366 -2.733376
H 5.8243739 -0.238637 -3.517759
H 7.0209092 0.6658901 -2.589555
H 2.7184210 -3.327889 -0.443798
H 2.0333381 -1.944762 0.3997155
H 3.0168773 -3.123229 1.2807875
C 2.0849514 6.6890052 3.2560388
H 1.6155546 7.5026712 2.6907412
H 3.0552298 6.4849889 2.7827043
H 2.2844847 7.0540498 4.2690295
H -3.163212 -4.469749 1.9451803
H -4.467830 -3.642446 2.8134107
H -2.818708 -3.638876 3.4670568
C -0.742357 -0.182702 -1.800046
H -1.647594 0.4414767 -1.795354
Si -1.175066 -1.878992 -2.546829
H 0.0002501 0.3158473 -2.434287
C -3.010720 -2.332469 -2.343712
C -0.137701 -3.329786 -1.873844
C -0.821870 -1.791302 -4.427616
H -3.282163 -2.454202 -1.290780
H -3.229664 -3.273127 -2.865556
H -3.657790 -1.554564 -2.765572
H -0.293035 -3.448383 -0.797004
H 0.9312519 -3.179083 -2.057707
H -0.430993 -4.266116 -2.365774
H -1.451426 -1.032348 -4.908240
H -1.024562 -2.753743 -4.914495
H 0.2248921 -1.525604 -4.624294

$RE_{ts}(CH_2TMS)$ -7090.0037+0.9502
Ni 0.0000000 0.0000000 0.0000000
N 0.6211584 0.4376569 1.8600919
N 1.7994591 0.8727237 -0.491797
C 1.8316808 0.9343363 1.8819569
C 2.4211397 1.3085722 0.5708014
C 2.7958274 1.3130847 2.9277124

C 3.6687399 2.0421780 0.8331194
C 3.8535729 1.9892692 2.2468191
C 4.9713294 2.5412496 2.9017180
C 2.8736826 1.1722706 4.3031837
C 3.9987051 1.7184128 4.9831919
C 5.0177342 2.3865641 4.3191996
C 4.6200620 2.6816173 0.0564220
C 5.9363716 3.1890302 2.0746446
C 5.7524209 3.2543903 0.7002533
H 4.5151950 2.7579655 -1.018584
H 2.1085450 0.6519722 4.8649016
H 5.8573471 2.7915350 4.8763101
H 4.0539930 1.6053983 6.0610815
H 6.8176501 3.6337923 2.5272960
H 6.4959436 3.7557134 0.0891789
C -0.035826 -0.005800 3.0581428
C 2.2043954 1.1942544 -1.826998
C -1.100660 0.7417808 3.6143219
C 0.3303325 -1.243838 3.6051071
C -1.773956 0.1811185 4.7091916
C -1.430156 -1.061823 5.2655567
C -0.355887 -1.765612 4.7031765
H 1.1395141 -1.800878 3.1448401
H -2.603625 0.7252053 5.1461783
H -0.065234 -2.729053 5.1121858
C 2.7292786 0.1911515 -2.678258
C 1.9459540 2.4825110 -2.322545
C 2.9446819 0.5337925 -4.022869
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