

Supporting Information for

Reactive Ligand Influence on Initiation in Phenylene Catalyst-Transfer Polymerization

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I. Materials

iPrMgCl (2M in THF) was purchased in 100 mL quantities from Aldrich. Bis(cyclooctadiene)nickel (Ni(cod)₂) and 1,2-bis(diphenylphosphino)ethane (dppe) were purchased from Strem. All other reagent grade materials and solvents were purchased from Aldrich, Acros, EMD, or Fisher and used without further purification unless otherwise noted. THF was dried and deoxygenated using an Innovative Technology (IT) solvent purification system composed of activated alumina, copper catalyst, and molecular sieves. *N*-Bromosuccinimide (NBS) was recrystallized from hot water and dried over P₂O₅. Flash chromatography was performed on SiliCycle silica gel (40–63 μm) and thin layer chromatography was performed on Merck TLC plates pre-coated with silica gel 60 F254. Compounds **S2**,¹ and **2b–2f**² were prepared from modified literature procedures.

II. General Experimental

NMR Spectroscopy: Unless otherwise noted, ¹H, ¹³C, ¹⁹F and ³¹P NMR spectra for all compounds were acquired at rt in CD₂Cl₂ or CDCl₃ on a Varian vnmrs 700 operating at 700, 176, 660, and 283 MHz and Varian vnmrs 500 operating at 500, 126, 470, and 202 MHz, respectively. For ¹H and ¹³C spectra in deuterated solvents, the chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane (TMS) and referenced with residual solvent. ¹⁹F NMR spectra were reported relative to CFCl₃ and ³¹P NMR spectra were relative to H₃PO₄. For ¹H, ¹⁹F and ³¹P NMR spectra in non-deuterated THF, the chemical shift data are reported in units of δ (ppm) and referenced with the THF peak at 3.58 ppm in the ¹H NMR spectrum which is then applied to all nuclei. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m), broad resonance (br), and apparent triplet (at).

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

IR Spectroscopy: Samples were recorded using a Mettler Toledo ReactIR iC10 fitted with a Mercury Cadmium Telluride (MCT) detector, and AgX probe (9.5 mm x 1.5 mm) with a SiComp tip. The spectra were processed using icIR 4.0 software and raw absorbances were exported into Microsoft Excel or Sigma Plot 10 or 13 for analysis.

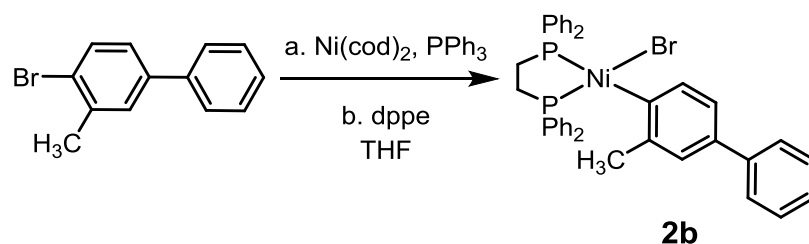
MALDI-TOF MS: MALDI-TOF mass spectra were recorded using a Bruker AutoFlex Speed in linear or reflectron mode at masses between 5000 and 15000. The matrix *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB), was prepared at a concentration of 0.1M in CHCl₃. The matrix sinapic acid was prepared as a saturated solution in a mixture of 30/70 (v/v) MeCN/0.1% TFA in H₂O. The instrument was calibrated with a mixture of peptides in the sinapic acid matrix or with a sample of polyphenylene with H/Br endgroups. The polymer sample was dissolved in THF or CH₂Cl₂ to obtain a approx.1 mg/mL solution. A 2.5 μL aliquot of polymer solution was mixed with 2.5 μL of the DCTB or sinapic acid matrix solution. This mixture (1 μL) was placed on the target plate and then air-dried. The data was analyzed using flexAnalysis and the percentages refer to the relative area ratios for each DP.

Gel-Permeation Chromatography: Polymer molecular weights were determined by comparison with polystyrene standards (Varian, EasiCal PS-2 MW 580-377,400) on a Waters 1515 HPLC instrument equipped with Waters Styragel® (7.8 x 300 mm) THF HR 0.5, THF HR 1, and THF HR 4 type columns in sequence and analyzed with Waters 2487 dual absorbance detector (254 nm) or on a Malvern Viscotek GPCMax VE2001 equipped with two Viscotek LT-5000L 8 mm (ID) x 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.

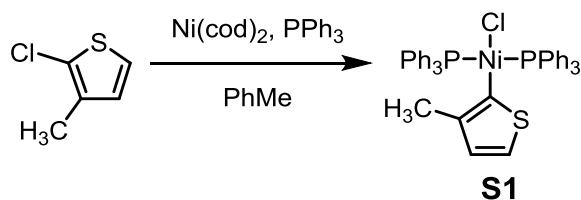
Titrations of the Grignard Reagents: An accurately weighed sample of salicylaldehyde phenylhydrazone³ (typically between 290–310 mg) was dissolved in 5.00 mL of THF. A 0.50 mL aliquot of this solution was stirred at rt while ArMgCl was added dropwise using a 500 µL syringe. The initial solution is yellow and turns bright orange at the end-point.

Statistical Analysis: Reported quantitative data represents the average of 2–3 experiments and the error bars represent standard deviation.

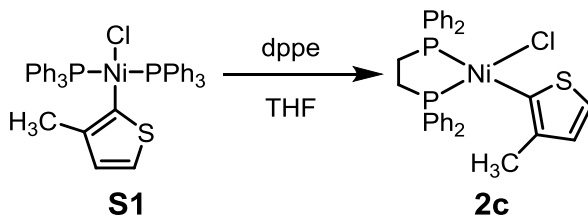
III. Synthetic Procedures



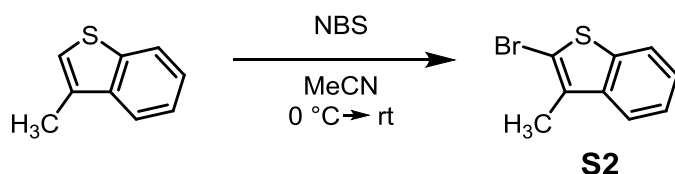
[1,2-bis(diphenylphosphino)ethane](2-methylbiphenyl)nickel(II) bromide (2d). In a glovebox, a 20 mL vial was equipped with a stir bar. Sequentially, Ni(cod)₂ (83.5 mg, 0.310 mmol, 1.00 equiv), PPh₃ (161 mg, 0.615 mmol, 2.00 equiv) and THF (2 mL) were added. The solution was stirred for 5 min and 4-bromo-3-methylbiphenyl (86 mg, 0.35 mmol, 1.1 equiv) and THF (2 mL) were added. The solution was stirred at rt for 2 h. To the deep red solution, dppe (134 mg, 0.335 mmol, 1.10 equiv) and THF (2 mL) were added. The solution was stirred for another 2 h. The orange solution was concentrated in vacuo until approx. 1 mL of solution was left. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL). The resulting solid was recrystallized from approx. 1/3 (v/v) THF/hexanes (approx. 20 mL), to give 106 mg of **2d** as an orange solid (50% yield). Elemental Analysis: Calcd for C₃₉H₃₅BrNiP₂, C, 66.51; H, 5.01; found C, 66.57; H, 5.16.



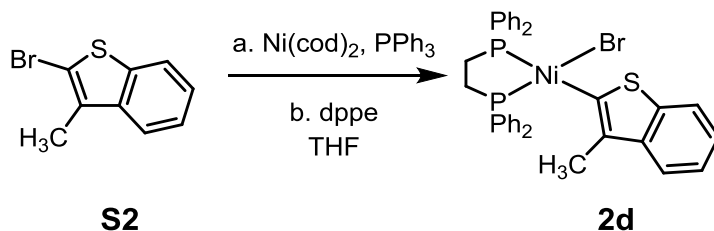
[Bis(triphenylphosphine)](3-methylthiophene)nickel(II) chloride (S1). A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, Ni(cod)₂ (139 mg, 0.506 mmol, 1.00 equiv), PPh₃ (262 mg, 1.00 mmol, 1.98 equiv), toluene (4 mL), and 2-chloro-3-methylthiophene (82 μL, 0.75 mmol, 1.5 equiv) were added. The solution was stirred at rt for 30 min and turned from dark red homogeneous solution to orange heterogeneous mixture. The reaction was removed from the glovebox. Addition of hexanes (30 mL) led to an orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was recrystallized from 1/3 (v/v) THF/hexanes (approx. 20 mL), to give 299 mg of **S1** as an orange solid (84% yield). Elemental analysis: Calcd for C₄₁H₃₅ClNiP₂S, C, 68.79; H, 4.93; Found C, 68.49; H, 4.88.



[1,2-bis(diphenylphosphino)ethane](3-methylthiophene)nickel(II) chloride (2c). In a glovebox, a 20 mL vial was equipped with a stir bar. Sequentially, **S1** (144 mg, 0.200 mmol, 1.00 equiv), dppe (89 mg, 0.22 mmol, 1.1 equiv), and THF (4 mL) were added. The solution was stirred at rt for 1 h. The heterogeneous orange solution was concentrated in vacuo until approx. 1 mL of solution remained. Addition of hexanes (18 mL) led to an orange precipitate. The solid was collected by vacuum filtration and washed with hexanes (20 mL). The resulting solid was recrystallized from 1/3 (v/v) THF/hexanes (approx. 20 mL), to give 78 mg of **2c** as an orange solid (66% yield). The product is air-sensitive and prone to decomposition.

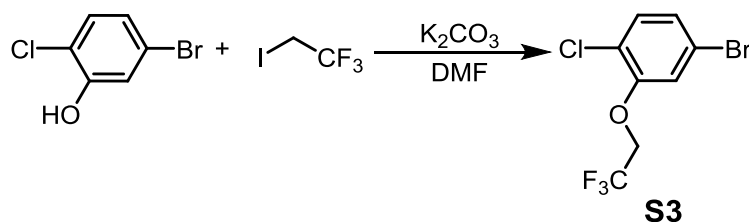


2-bromo-3-methylbenzo[b]thiophene (S2). A 10 mL round-bottom flask was equipped with a stir bar and cooled to 0 °C with an ice-water bath. Sequentially, 3-methylbenzothiophene (402 μL , 3.00 mmol, 1.00 equiv), MeCN (3.5 mL), and NBS (561 mg, 3.15 mmol, 1.05 equiv) were added. The ice-water bath was removed after 5 min and the solution was stirred at rt for 30 min. The reaction was quenched with water (15 mL) and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were dried over MgSO_4 , filtered, and concentrated in vacuo. The resulting oil was purified via silica gel chromatography, using 100% hexanes as the eluent, to give 618 mg of **S2** as a clear liquid (91% yield). HRMS (EI): $[\text{M}^+]$ Calcd for $\text{C}_9\text{H}_7\text{BrS}$, 225.9452; found, 225.9450.

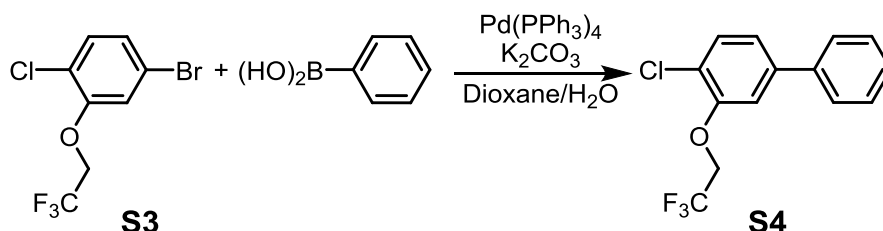


[1,2-bis(diphenylphosphino)ethane](3-methylbenzo[b]thiophene)nickel(II) bromide (2d). A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $\text{Ni}(\text{cod})_2$ (82 mg, 0.30 mmol, 1.0 equiv), PPh_3 (158 mg, 0.602 mmol, 2.00 equiv) and THF (3 mL) were added. The solution was stirred for 5 min and **S2** (1.04 mL, 0.460 mmol, 1.5 equiv) and THF (1 mL) were added. The

solution was stirred at rt for 1.5 h. To the deep red solution, dppe (2.0 mL, 0.17M in THF, 0.33 mmol, 1.1 equiv) were added. The solution was stirred for another 2 h. The orange solution was concentrated in vacuo until approx. 1 mL of solution was left. Addition of hexanes (18 mL) led to a yellow precipitate. The solid was filtered and washed with hexanes (5 mL). The resulting solid was recrystallized from approx. 1/3 (v/v) THF/hexanes (approx. 20 mL), to give 133 mg of **2d** as a dark orange solid (65% yield). Elemental Analysis: Calcd for C₃₅H₃₁BrNiP₂S, C, 61.44; H, 4.57; Found C, 61.33; H, 4.68.

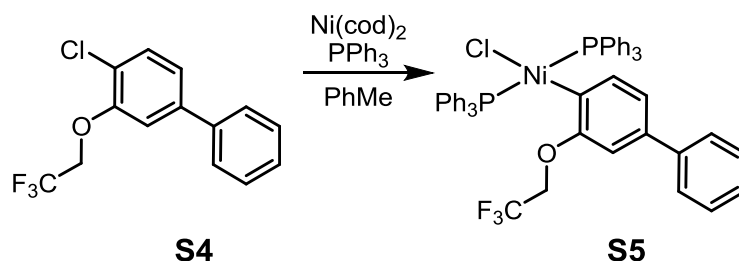


4-bromo-1-chloro-2-(2,2,2-trifluoroethoxy)benzene (S3). A 250 mL bomb flask was equipped with a stir bar. Sequentially, 5-bromo-2-chlorophenol (3.41 g, 16.4 mmol, 1.00 equiv), K₂CO₃ (6.80 g, 49.2 mmol, 3.00 equiv), DMF (35 mL), and 2-iodo-1,1,1-trifluoroethane (6.5 mL, 65 mmol, 4.0 equiv) were added. The mixture was stirred for 6 d at 65 °C. The mixture was poured into water (70 mL) and extracted with CH₂Cl₂ (3 x 50 mL). The organic layers were combined, washed with brine (25 mL), dried over MgSO₄, and concentrated in vacuo. The resulting oil was purified by silica gel chromatography using 5:95 (v/v) CH₂Cl₂/hexanes as the eluent to give 2.26 g of **S3** as a colorless oil (48% yield). HRMS (EI): [M⁺] Calcd for C₈H₅BrClF₃O, 287.9164; found, 287.9170.

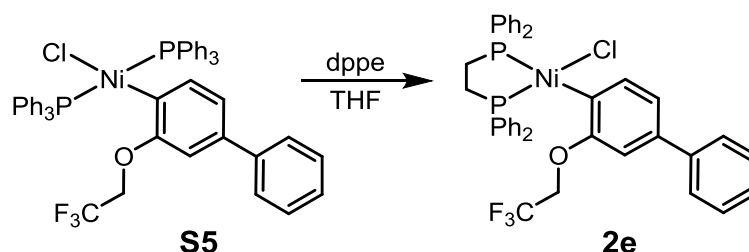


4-chloro-3-(2,2,2-trifluoroethoxy)-1,1'-biphenyl (S4). In a glovebox under a N₂ atmosphere, a 25 mL Schlenk flask was equipped with a stir bar and charged with Pd(PPh₃)₄ (139 mg, 0.120 mmol, 0.030 equiv). The flask was sealed with a septum, removed from the glovebox and charged with phenyl boronic acid (740 mg, 6.00 mmol, 1.50 equiv) and K₂CO₃ (1.66 g, 12.0 mmol, 3.00 equiv). A solution of 1,4-dioxane and water (9:1) was sparged with N₂ for 30 min, and 8 mL was added to the Schlenk flask. Then, **S3** (1.18 g, 4.07 mmol, 1.00 equiv) was dissolved in the dioxane/water solution (5.0 mL) and added to the reaction mixture. The reaction mixture was heated to 90 °C overnight. The reaction was quenched with satd. aq. NaHCO₃ (30 mL) and extracted with EtOAc (3 x 30 mL). The organic layers were combined and washed with brine (25 mL), dried over MgSO₄, and concentrated in vacuo. The product was purified by silica gel chromatography using 5/95 (v/v) EtOAc/hexanes to give 866 mg of **S4** as a colorless oil, which

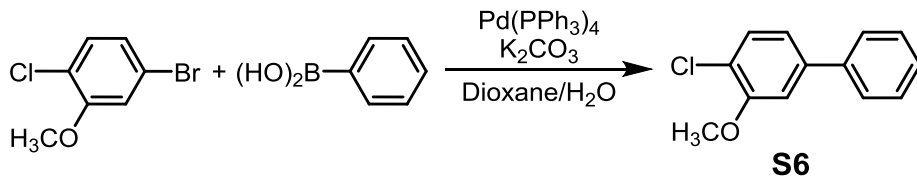
slowly crystallized into a white solid (76% yield). HRMS (EI): [M⁺] Calcd for C₁₄H₁₀ClF₃O, 286.0372; found, 286.0383.



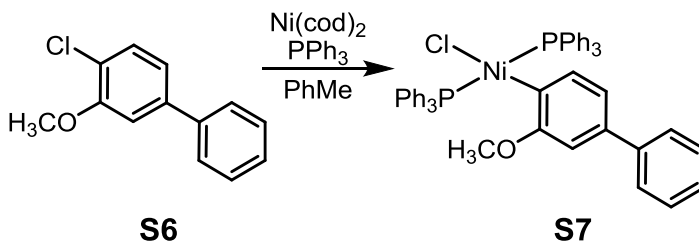
[Bis(triphenylphosphine)](3-(2,2,2-trifluoroethoxy)-1,1'-biphenyl)nickel(II) chloride (S5). In a glovebox, Ni(cod)₂ (68.8 mg, 0.250 mmol, 1.00 equiv) and triphenylphosphine (131 mg, 0.490 mmol, 2.00 equiv) and **S4** (94.6 mg, 0.330 mmol, 1.30 equiv) were dissolved in toluene (2.5 mL) in a 20 mL vial. The reaction mixture was stirred at rt for 2.5 h, then concentrated until approx. 0.5 mL toluene remained. Hexanes (approx. 15 mL) was added, and the yellow precipitate was isolated by vacuum filtration, giving 149 mg of a yellow powder (68% crude yield) which was carried on without further purification.



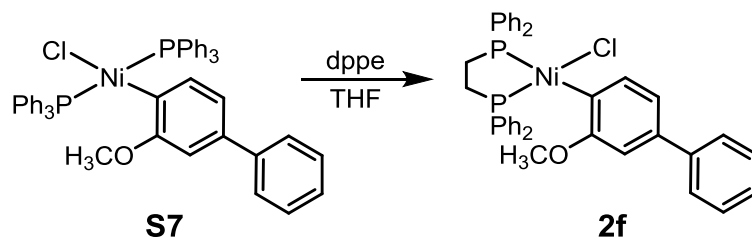
[1,2-bis(diphenylphosphino)ethane](3-(2,2,2-trifluoroethoxy)-1,1'-biphenyl)nickel(II) chloride (2e). In a glovebox, **S5** (149 mg, 0.170 mmol, 1.00 equiv) and dppe (76.5 mg, 0.187 mmol, 1.10 equiv) were dissolved in THF (2.5 mL) in a 20 mL vial. The solution was stirred at rt for 1 h, then concentrated until approx. 0.5 mL THF remained. Hexanes (approx. 15 mL) was added, and the yellow precipitate was isolated by vacuum filtration. The product was recrystallized from approx. 1/3 (v/v) THF/hexanes (approx. 20 mL), giving 100 mg of a yellow powder (79% yield.) Elemental Analysis: Calcd for C₄₀H₃₄ClF₃NiOP₂, C, 64.59; H, 4.61; Found C, 64.37; H, 4.65.



4-chloro-3-methoxy-1,1'-biphenyl (S6). A 25 mL Schlenk flask was equipped with a stir bar in the glovebox and charged with Pd(PPh₃)₄ (104 mg, 0.0900 mmol, 0.0600 equiv). The Schlenk flask was then removed from the glovebox and charged with phenylboronic acid (274 mg, 2.30 mmol, 1.50 equiv) and K₂CO₃ (622 mg, 4.50 mmol, 3.00 equiv). A solution of 1,4-dioxane and water (9:1) was sparged with N₂ for 30 min, and 7 mL were added to the Schlenk flask. Then, 4-bromo-1-chloro-2-methoxybenzene (332 mg, 1.50 mmol, 1.00 equiv) was dissolved in the dioxane/water solution (5 mL) and added to the reaction mixture. The reaction mixture was heated to 90 °C for 6 h. The reaction was quenched with saturated NH₄Cl (35 mL), extracted with EtOAc (3 x 35 mL), washed with brine (35 mL), dried over MgSO₄, and concentrated in vacuo. The product was purified by silica gel chromatography using 10/90 (v/v) toluene/hexanes to give 232 mg of a colorless oil (71% yield). HRMS (EI): [M⁺] Calcd for C₁₃H₁₁ClO, 218.0498; found, 286.0500.



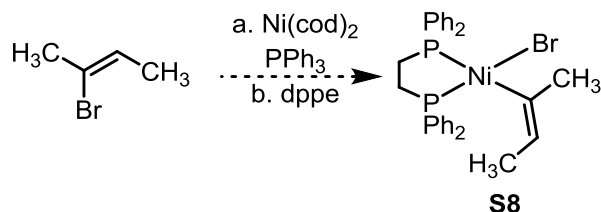
[Bis(triphenylphosphine)](3-methoxy-1,1'-biphenyl)nickel(II) chloride (S7). In the glovebox, Ni(cod)₂ (138 mg, 0.502 mmol, 1.0 equiv), and triphenyl phosphine (Ph₃P) (262 mg, 1.00 mmol, 2.0 equiv) were dissolved in THF (3 mL) in a 20 mL vial with stirring. In a separate 4 mL vial, 1-chloro-2-methoxy-4-phenylbenzene (142 mg, 0.650 mmol, 1.3 equiv) was dissolved in THF (2 mL). This solution was then added to the vial containing the Ni/Ph₃P and stirred at rt for 4 h, during which time a yellow precipitate formed. The solvent was removed under vacuum until approx. 0.5 mL remained. Hexanes (approx. 15 mL) were then added, and the yellow precipitate was collected by vacuum filtration, giving 157 mg of **S7** as a yellow powder (79% crude yield). The product was used immediately without further purification.



[1,2-bis(diphenylphosphino)ethane](3-methoxy-1,1'-biphenyl)nickel(II) chloride (2f). In a glovebox, in a 20 mL vial, **S7** (157 mg, 0.196 mmol, 1.0 equiv) and dppe (94 mg, 0.24 mmol, 1.2 equiv) were dissolved in THF (2.5 mL) in a 20 mL vial. The reaction mixture was stirred at rt for 1 h. (Note: a yellow precipitate was observed after 5 min.) After 1 h, hexanes (approx. 15 mL) was added, and the solution was cooled in a freezer at -30 °C overnight. The product was collected by vacuum filtration, giving 100 mg of **2f** as a yellow powder (59% yield). Elemental Analysis: Calcd for C₃₉H₃₅ClNiOP₂, C, 69.31; H, 5.22; Found C, 67.96; H, 5.22.

IV. Attempted Synthesis of [1,2-bis(diphenylphosphino)ethane](2-butenyl)nickel(II) Chloride

Precatalyst synthetic procedure:



[1,2-bis(diphenylphosphino)ethane](2-butenyl)nickel(II) chloride (S8). In a glovebox, Ni(cod)₂ (37.1 mg, 0.125 mmol) and PPh₃ (76.2 mg, 0.250 mmol) were dissolved in THF (1.0 mL). In a separate vial, Z-2-bromo-2-butene (24 μ L, 0.24 mmol) was dissolved in THF (0.2 mL), and the vial was sealed with a septum. The Ni solution (0.80 mL, containing 0.10 mmol Ni(cod)₂ and 0.20 mmol PPh₃) was transferred to a J. Young NMR tube which was sealed with a septum and removed from the glovebox along with the vial containing Z-2-bromo-2-butene. The alkene solution (0.10 mL, 0.12 mmol, 1.2 equiv relative to Ni(cod)₂) was added to the NMR tube, and a ³¹P NMR spectrum was immediately acquired, showing Ni(PPh₃)₂(cod) and a singlet at 20 ppm. A second ³¹P NMR spectrum was acquired 5 min later, showing formation of several other peaks, as well as Ni(PPh₃)₂(cod). After 1 hr, another ³¹P NMR spectrum was acquired, showing complete consumption of Ni(PPh₃)₂(cod). Then, a solution of dppe in THF (0.20 mL, 0.57M, 1.1 equiv) was added and a final ³¹P NMR spectrum was acquired, showing primarily Ni(dppe)₂. The product was analyzed by GCMS, showing a peak with m/z = 110, the mass of 3,4-dimethylhexa-2,4-diene (the expected organic product from a ligand disproportionation reaction followed by reductive elimination).

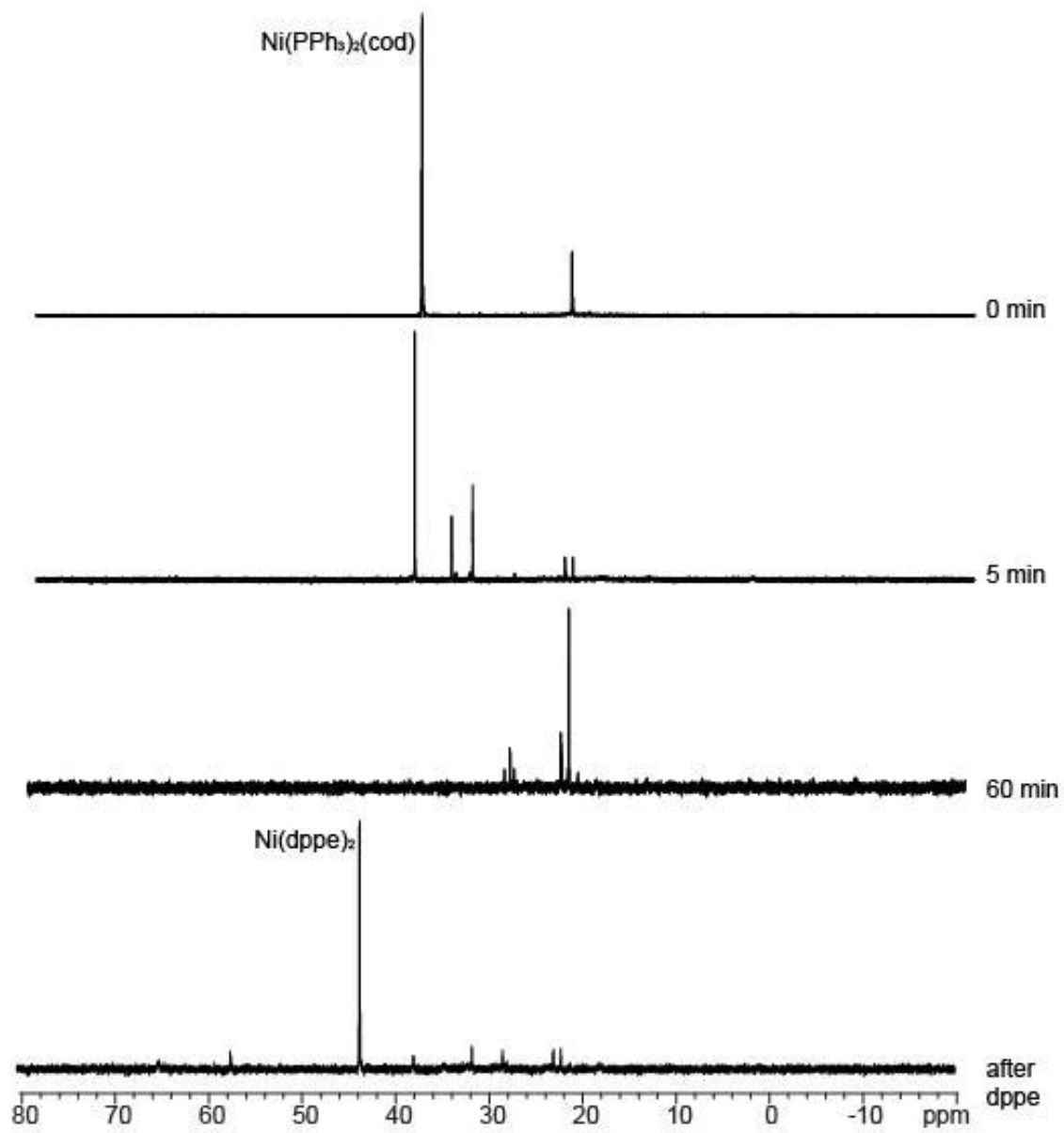
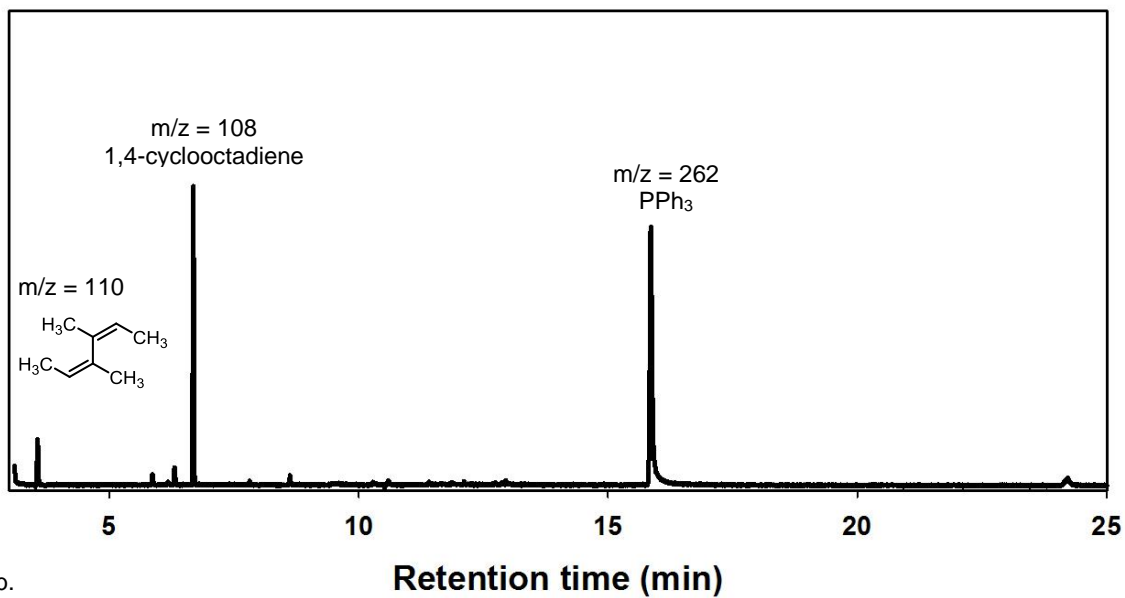


Figure S1. ^{31}P NMR spectra acquired during the attempted synthesis of **S8**

a.



b.

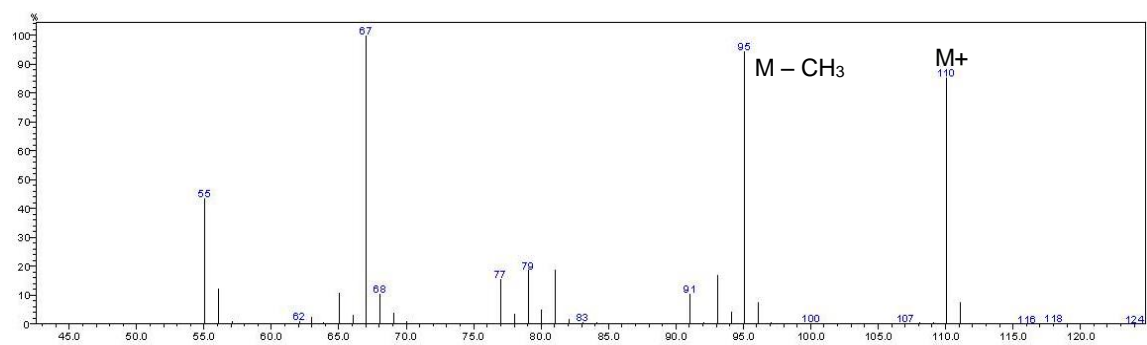


Figure S2. Gas chromatogram (a) for the attempted synthesis of **S8** and mass spectrum (b) for peak at 3.4 min

IV. NMR Spectra

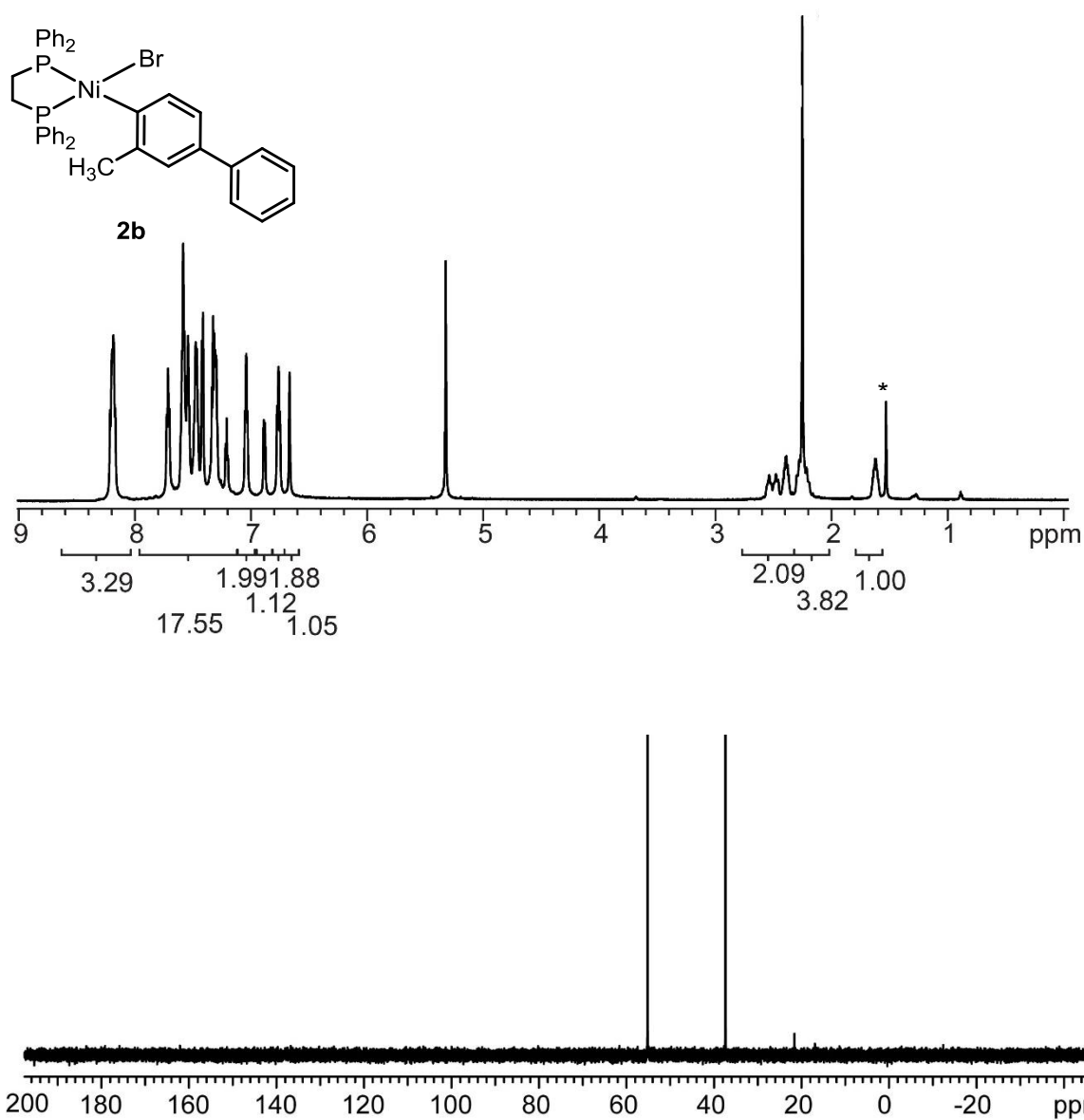


Figure S3. ¹H and ³¹P NMR spectra of **2b** ¹H NMR (700 MHz, CD₂Cl₂) δ 8.21–8.17 (m, 4H), 7.71–7.21 (m, 18 H), 7.04 (at, *J* = 6.3 Hz, 2H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.76 (at, *J* = 9.8 Hz, 2H), 6.68 (s, 1H), 2.51 (dt, *J* = 40.6, 13.3 Hz, 1H), 2.41–2.37 (m, 1H), 2.28–2.22 (m, 1H), 2.25 (s, 3H), 1.63–1.62 (m, 1H). *denotes residual H₂O

³¹P NMR (283 MHz, CD₂Cl₂) δ 55.16 (d, *J* = 19.0 Hz), 37.4 (d, *J* = 20.1 Hz).

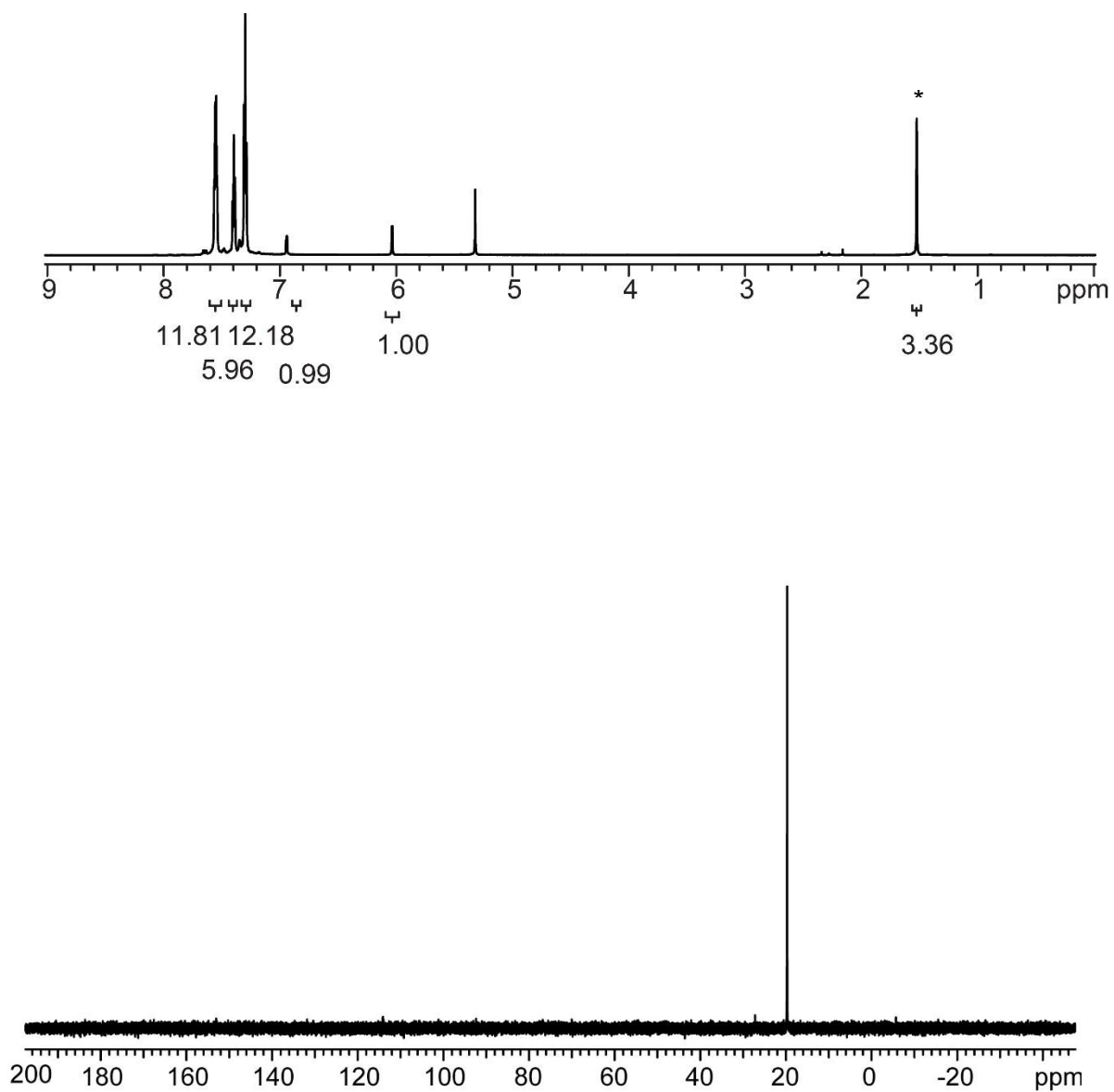
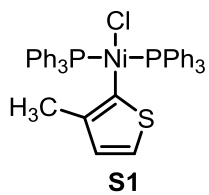


Figure S4. ^1H and ^{31}P NMR spectra of **S1**. ^1H NMR (700 MHz, CD_2Cl_2) δ 7.55 (dd, $J = 6.6$ Hz, 5.5 Hz, 12H), 7.40 (t, $J = 7.4$ Hz, 6H), 7.30 (at, $J = 7.4$ Hz, 12H), 6.94 (d, $J = 4.2$ Hz, 1H), 6.04 (d, $J = 4.2$ Hz, 1H), 1.52 (s, 3H). *denotes residual H_2O
 ^{31}P NMR (283 MHz, CD_2Cl_2) δ 19.69.

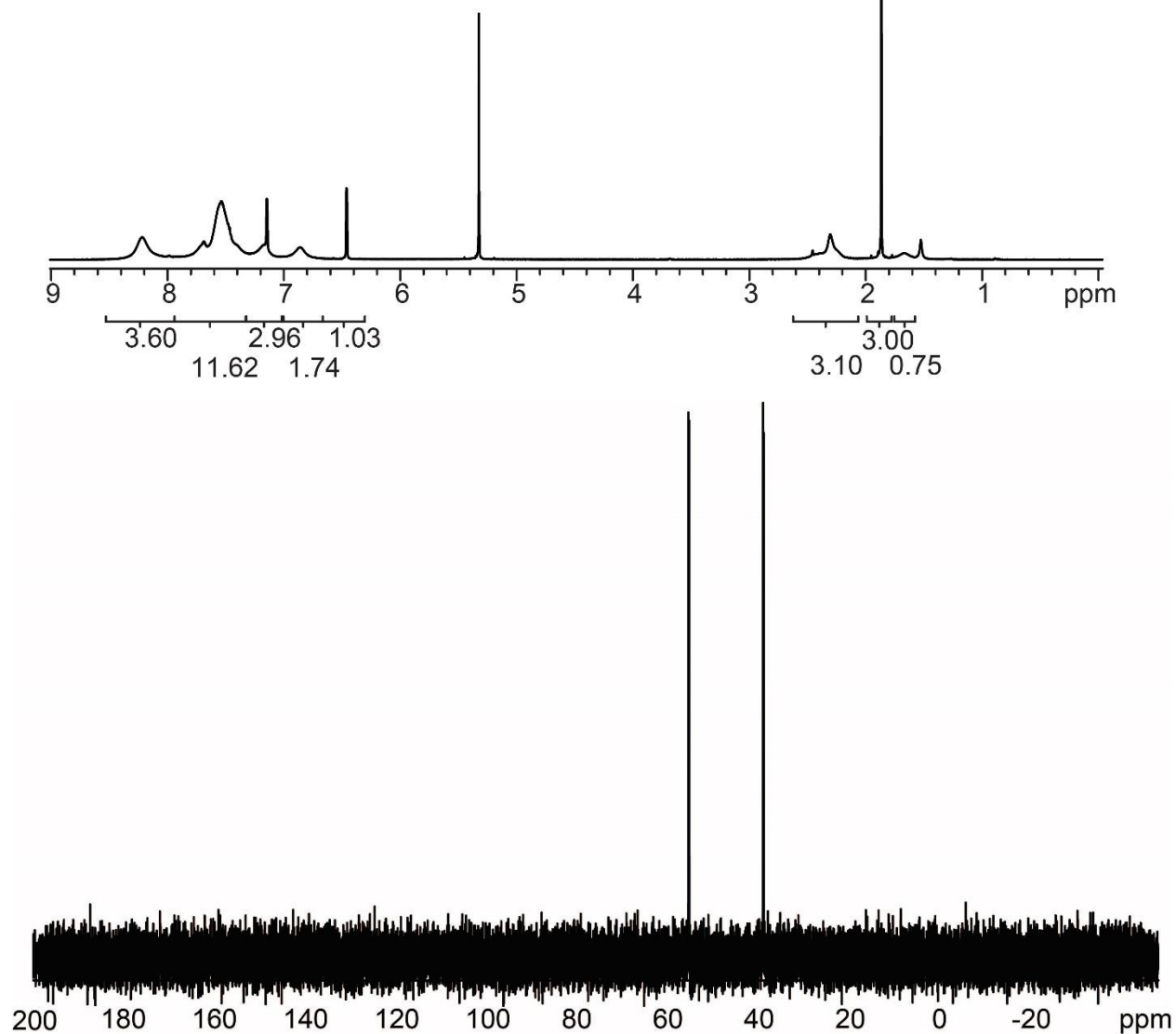
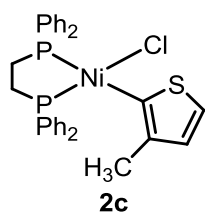


Figure S5. ^1H and ^{31}P NMR spectra of **2c**. ^1H NMR (500 MHz, C_6D_6) δ 8.05 (bs, 4H), 7.69–7.47 (m, 12 H), 7.15–7.14 (m, 3H), 7.20–6.96 (m, 3H), 6.89 (bs, 2H), 6.46 (s, 1H), 3.60–3.56 (m, 1H), 2.33 (s, 3H), 1.73 (bs, 2H), 1.44–1.41 (m, 1H).

^{31}P NMR (202 MHz, C_6D_6) δ 54.59 (d, $J = 33.5$ Hz), 38.20 (d, $J = 33.5$ Hz). This compound is unstable and prone to decomposition.

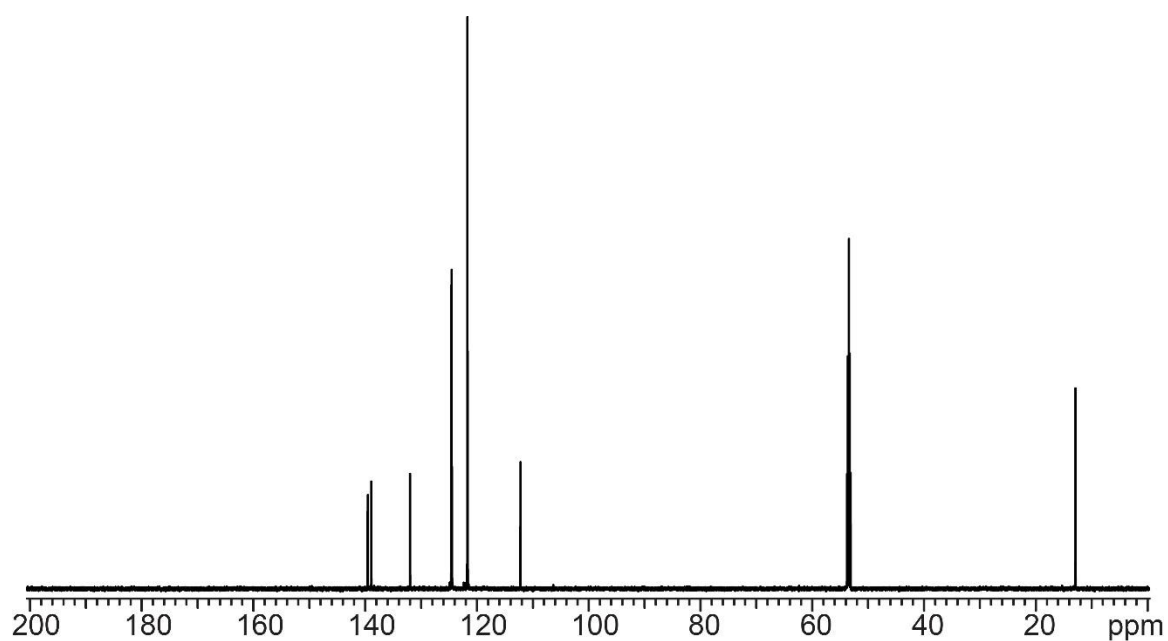
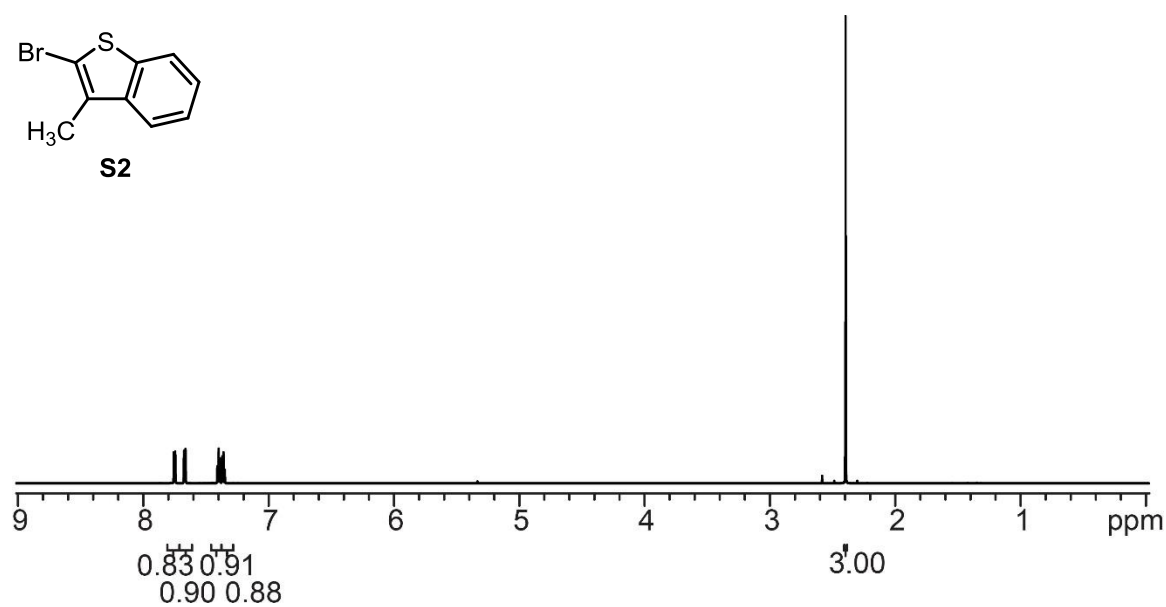
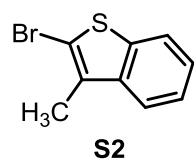


Figure S6. ^1H and ^{13}C NMR spectra of **S2**. ^1H NMR (700 MHz, CD_2Cl_2) δ 7.75 (dd, $J = 7.5$ Hz, 0.85 Hz, 1H), 7.66 (dd, $J = 7.5$ Hz, 0.51 Hz, 1H), 7.39 (at, $J = 7.7$ Hz, 1H), 7.36 (at, $J = 7.7$ Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (176 MHz, CD_2Cl_2) δ 139.53, 138.89, 131.97, 124.57, 124.49, 121.68 (2 C), 112.20, 12.86.

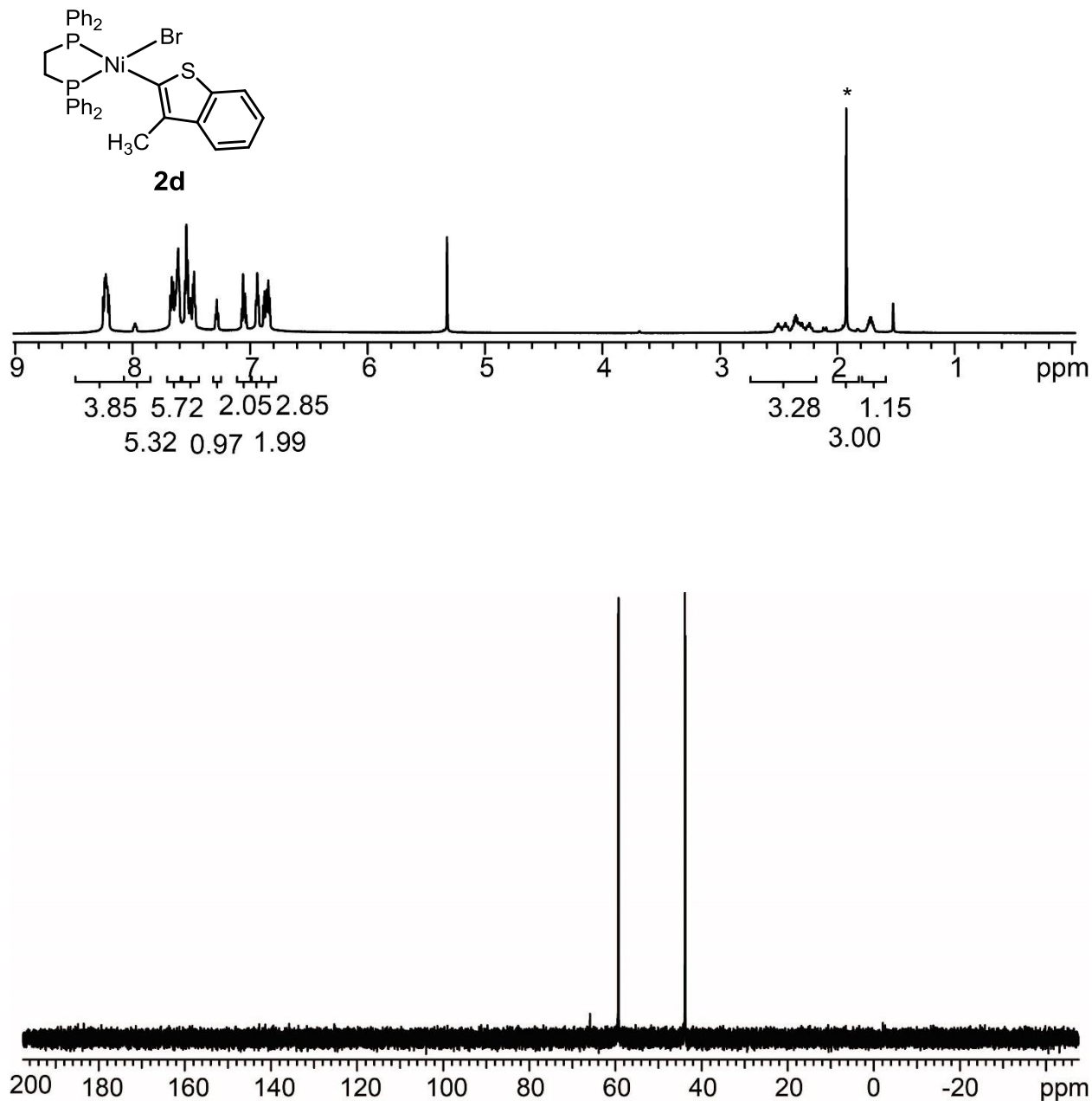


Figure S7. ¹H and ³¹P NMR spectra of **2d**. ¹H NMR (700 MHz, CD₂Cl₂) δ 8.25–8.20 (m, 4H), 7.68–7.61 (m, 5H), 7.55–7.46 (m, 6H), 7.28 (at, *J* = 7.3 Hz, 1H), 7.07–7.03 (m, 2H), 6.94 (at, *J* = 7.7 Hz, 2H), 6.89–6.83 (m, 3H), 2.47 (td, *J* = 42.7, 11.2 Hz, 1H), 2.38–2.22 (m, 2H), 1.92 (s, 3H), 1.74–1.69 (m, 1H). *denotes residual H₂O
³¹P NMR (283 MHz, CD₂Cl₂) δ 59.32 (d, *J* = 35.9 Hz), 43.82 (d, *J* = 35.9 Hz).

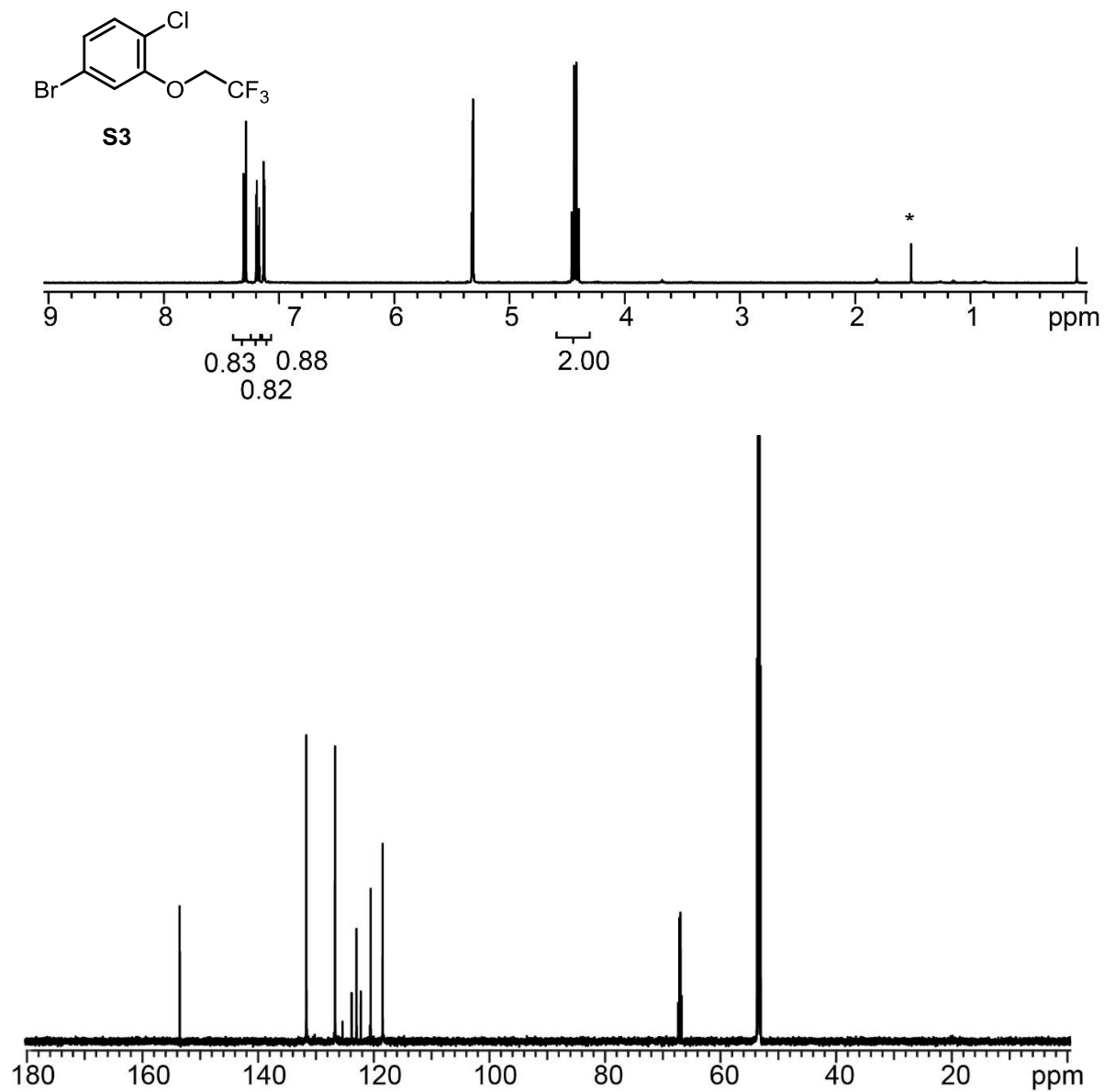
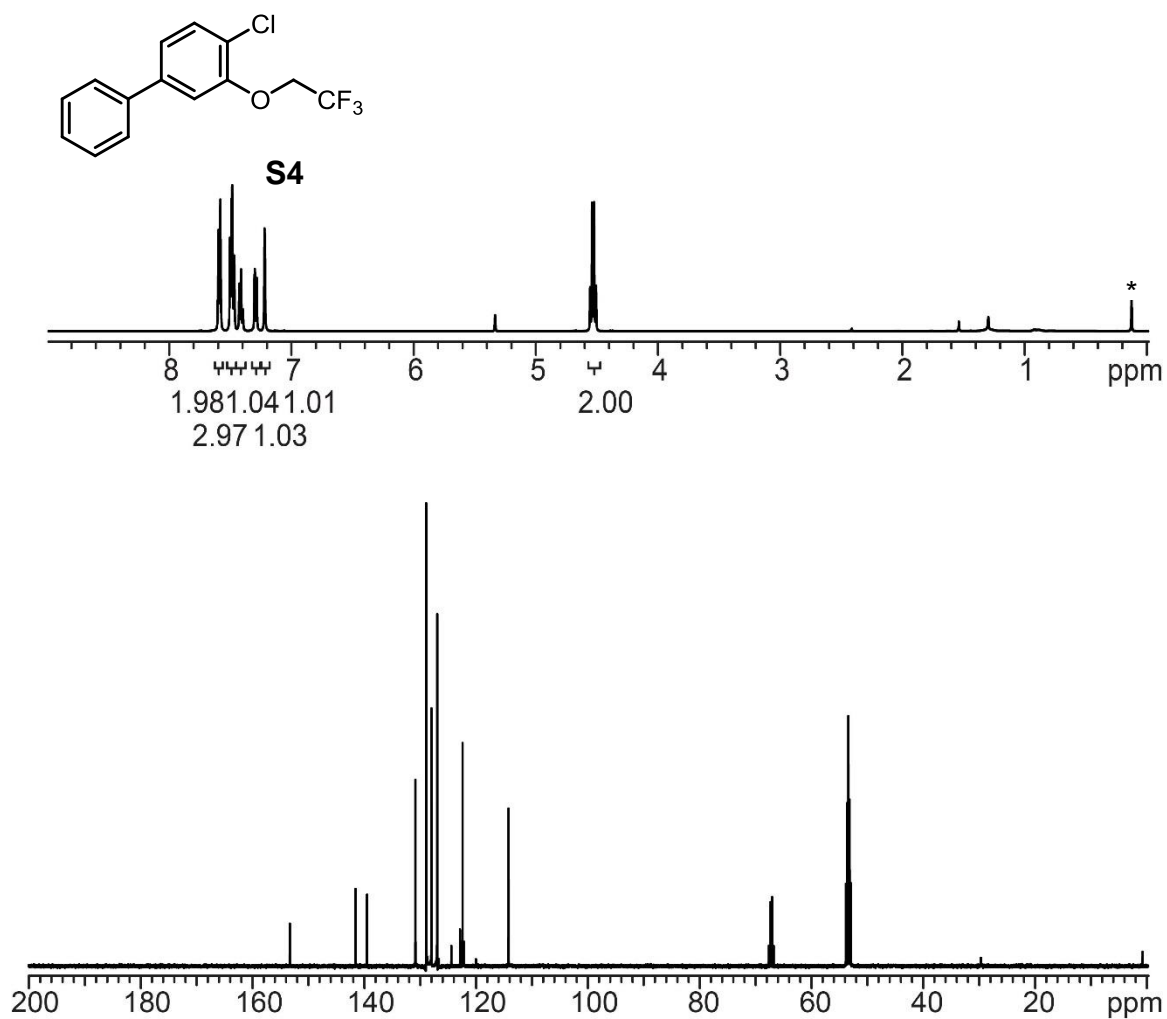


Figure S8. ^1H and ^{13}C NMR spectra of **S3**. ^1H NMR (400 MHz, CD_2Cl_2) δ 7.30 (d, $J = 8.4$ Hz, 1H), 7.19 (dd, $J = 8.4$ Hz, 2.1 Hz, 1 H), 7.13 (d, $J = 2.1$ Hz, 1 H), 4.43 (q, $J_{\text{H-F}} = 8.0$ Hz) *denotes residual H_2O

^{13}C NMR (176 MHz, CD_2Cl_2) δ 153.56, 131.66, 126.87, 123.02 (q, $J_{\text{C-F}} = 278.6$ Hz), 122.97, 120.51, 118.45, 67.04 (q, $J_{\text{C-F}} = 72.3$ Hz)



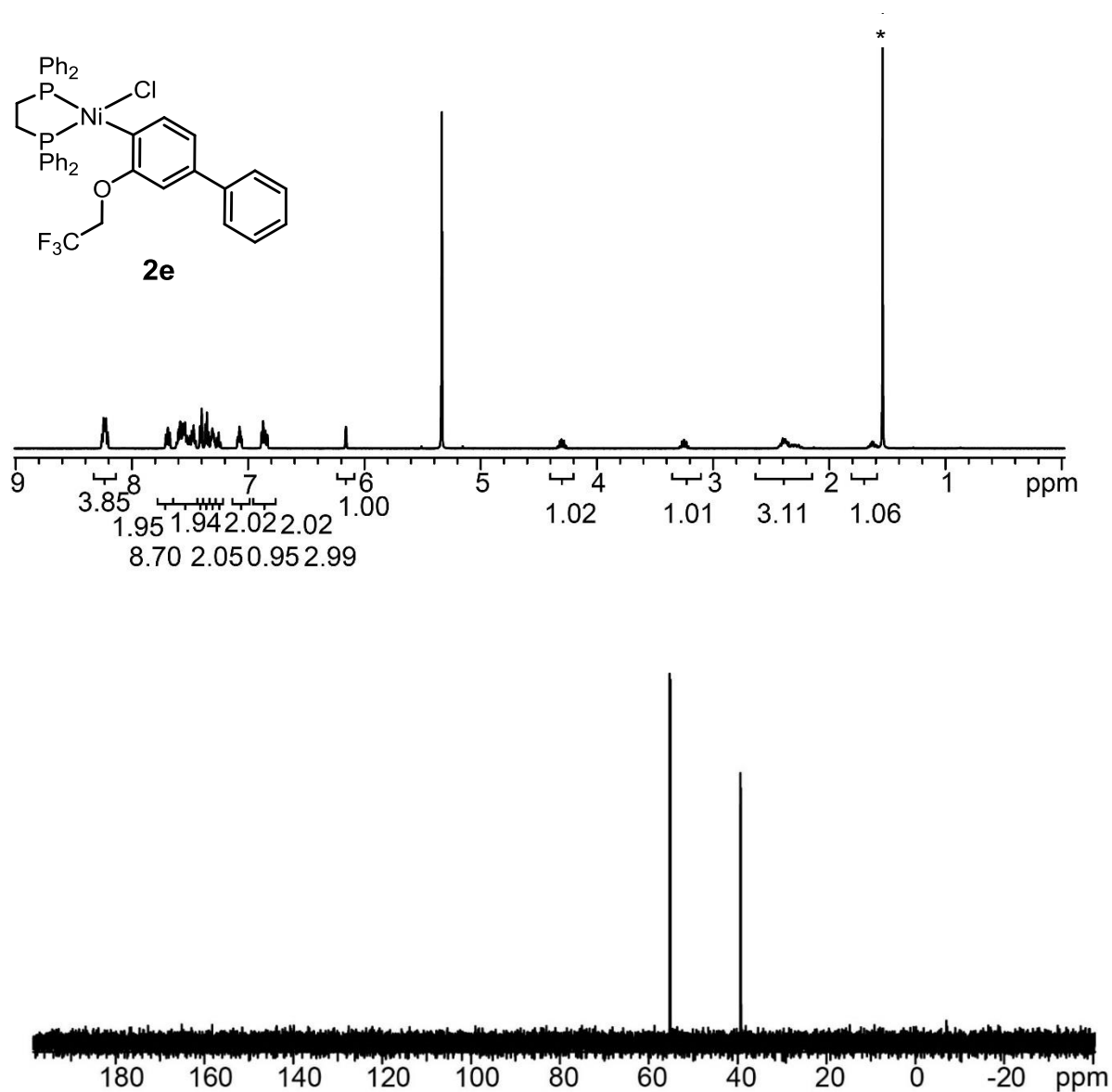


Figure S10. ^1H and ^{31}P NMR spectra of **2e**. ^1H NMR (500 MHz, CD_2Cl_2) δ 8.23 (m, 4H) 7.69 (dd, $J = 9.8, 1.7$ Hz, 2H), 7.60–7.47 (m, 9H), 7.41 (d, $J = 7.5$ Hz, 2H), 7.35 (at, $J = 7.5$ Hz, 2H), 7.32–7.29 (m, 2H), 7.27–7.24 (m, 2H), 7.09–7.06 (m, 2H), 6.88–6.83 (m, 3H), 6.16 (s, 1 H), 4–3.4–4.26 (m, 1H), 3.28–3.21 (m, 1H) 2.43–2.24 (m, 3H), 1.66–1.59 (m, 1H). *denotes residual H_2O
 ^{31}P NMR (202 MHz, CD_2Cl_2) δ 55.20 (d, $J = 30.3$ Hz), 39.31 (d, $J = 28.9$ Hz).

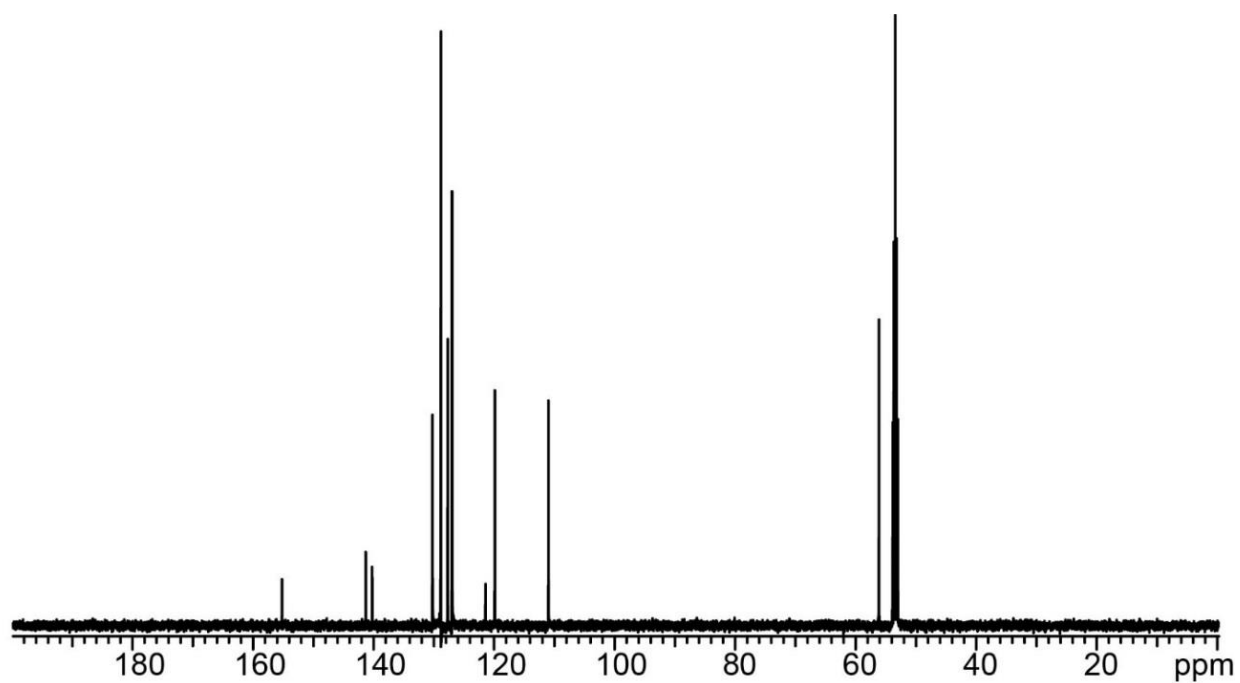
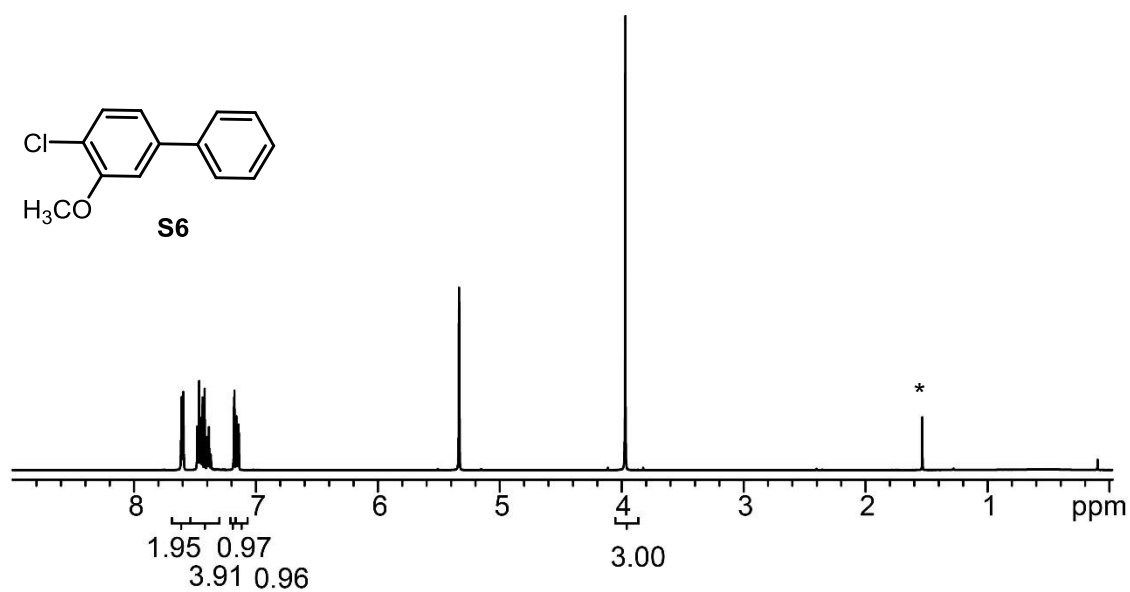


Figure S11. ^1H and ^{13}C NMR spectra of **S6** ^1H NMR (500 MHz, CD_2Cl_2) δ 7.61–7.59 (m, 2H), 7.48–7.37 (m, 4H), 7.18 (d, J = 2.0 Hz, 2H), 7.15 (dd, J = 8.1 Hz, 2.0 Hz, 1H), 3.97 (s, 3H), *denotes residual H_2O . *denotes residual H_2O
 ^{13}C NMR (176 MHz, CD_2Cl_2) 155.18, 141.28, 140.23, 130.23, 126.82, 128.79, 127.70, 126.97, 121.41, 119.86, 110.98, 56.11.

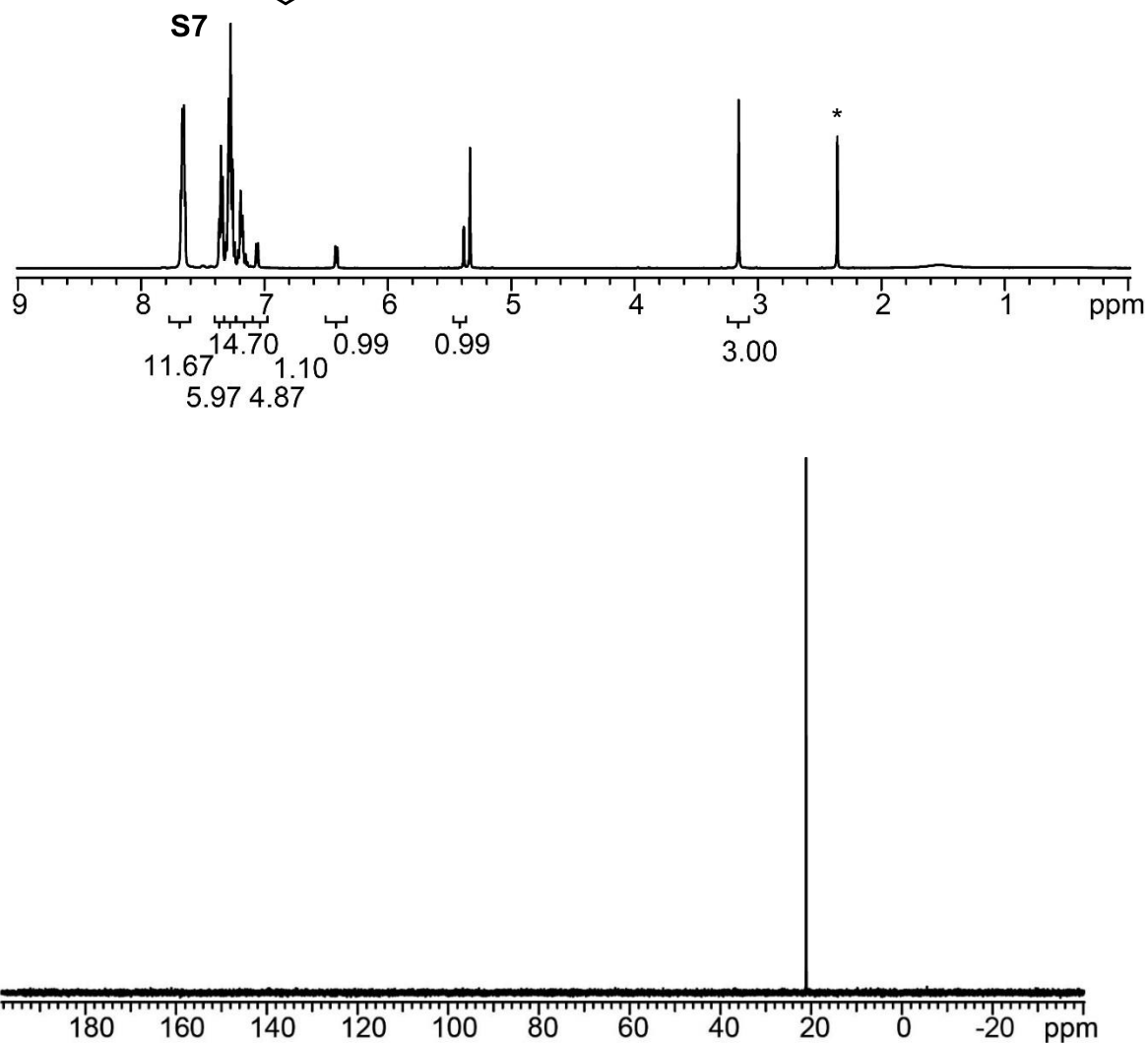
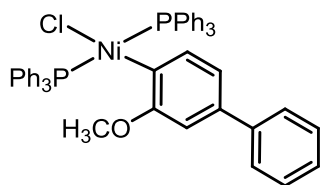


Figure S12. ^1H and ^{31}P NMR spectra of **S7**. ^1H NMR (500 MHz, CD_2Cl_2) δ 7.66 (dd, $J = 12.0, 5.1$, 12H) 7.35 (at, $J = 7.2$, 6 H) 7.31–7.24 (m, 15 H), 7.21–7.15 (m, 5H), 7.06 (d, $J = 7.5$ Hz, 1H), 6.41 (d, $J = 7.5$ Hz, 1H), 5.38 (s, 1H), 3.12 (s, 3H) * denotes residual toluene
 ^{31}P NMR (202 MHz, CD_2Cl_2) δ 21.08.

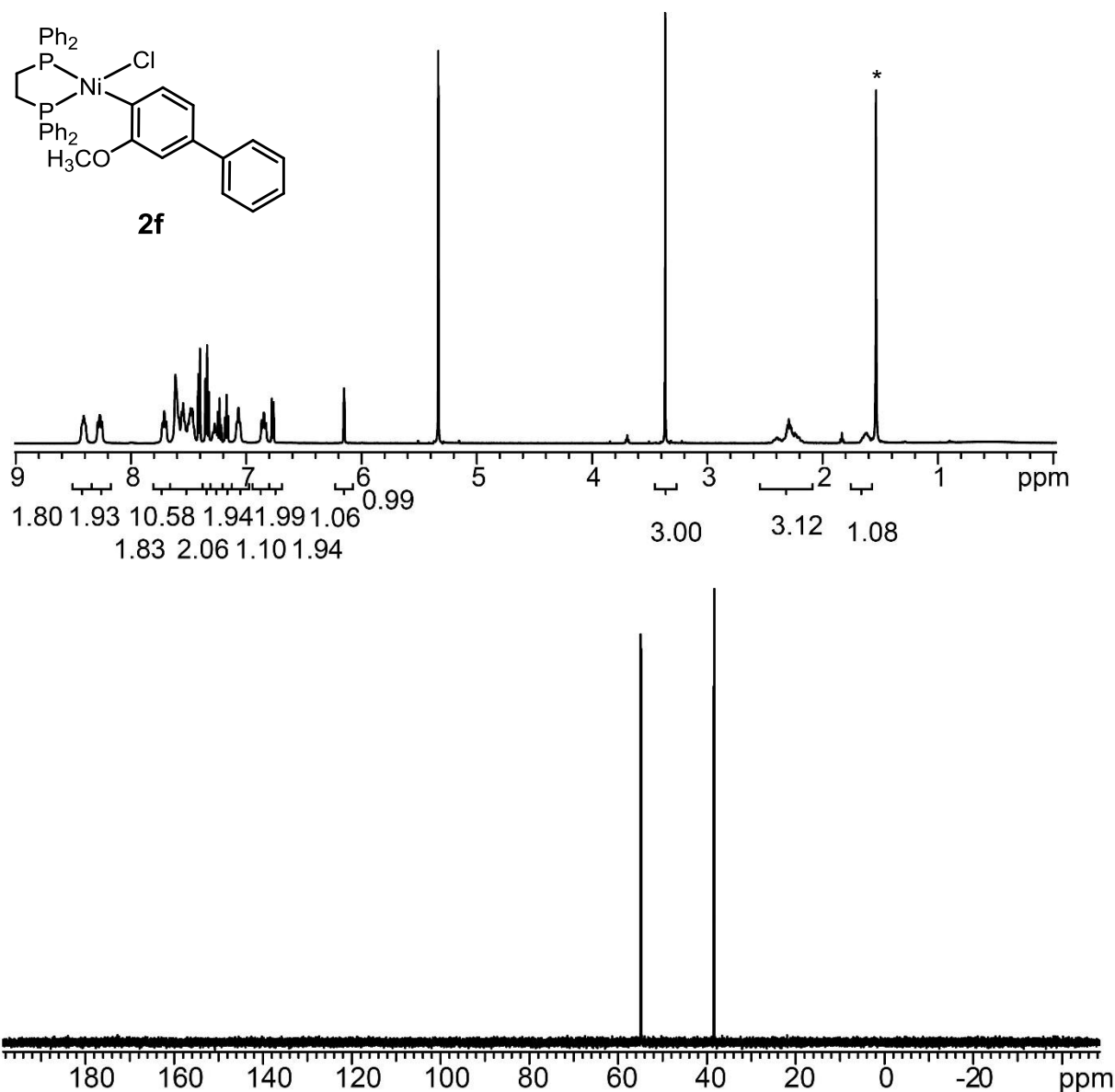


Figure S13. ^1H and ^{31}P NMR spectra of **2f**. ^1H NMR (500 MHz, CD_2Cl_2) δ 8.41 (br, 2H) 8.27 (at, $J = 9.0$ Hz, 2H), 7.71 (at, $J = 8.5$ Hz, 2H), 7.61–7.40 (m, 11H), 7.34 (at, $J = 7.5$ Hz, 2H), 7.27–7.22 (m, 2H), 7.17 (at, $J = 7.0$ Hz, 2H), 7.07 (at, $J = 6.6$, 2 H) 6.85 (at, $J = 9.1$ Hz, 2H), 6.77 (dt, $J = 6.1$ Hz, 1.5 Hz, 1H), 6.15 (at, $J = 2.1$ Hz, 1 H), 3.37 (s, 3H), 2.39–2.21 (m, 3H), 1.63–1.62 (m, 1H). *denotes residual H_2O

^{31}P NMR (202 MHz, CD_2Cl_2) δ 59.85 (d, $J = 27.5$ Hz), 38.37 (d, $J = 27.5$ Hz).

VI. Initiation Rate Studies

Representative Procedure for Performing React IR Propagation Rate Studies:

The IR probe was inserted through an O-ring sealed 14/20 ground glass adapter (custom-made) into an oven-dried 50 mL 2-neck flask equipped with a stir bar. The other neck was fitted with a three-way flow control adapter with a septum for injections/aliquot sampling and an N₂ line. The oven-dried flask was cooled under vacuum. The flask was then filled with N₂ and evacuated again for a total of three cycles. The flask was charged with a solution of precatalyst **2f** (3.0 mL, 0.005M in THF, 1.00 equiv) and cooled to 0 °C over 20 min. After recording a background spectrum, monomer (0.42 mL, 0.35M in THF, 10 equiv) was added by syringe and the reaction was stirred at 0 °C until monomer consumption stalled for 10 min. Then, THF (3.8 mL) and a second portion of monomer solution (2.8 mL, 0.35M in THF, 65 equiv) were injected and spectra were recorded every 15 s over the entire reaction. To account for mixing and temperature equilibration, spectra recorded in the first 60 s of the reaction were not analyzed. The propagation rate constant (k_p) was calculated by plotting [monomer] versus time over the first 10% conversion of monomer (the second addition). When PPh₃ was included, 2 equiv relative to precatalyst was added in the precatalyst stock solution.

Table S1. Table of k_p values

k_p without PPh ₃ (s ⁻¹ x 10 ⁻³)	k_p with PPh ₃ (s ⁻¹ x 10 ⁻³)
10.9	6.7
8.9	8.4
12.0	9.0
11.4	6.7
7.28	6.66
Average = 10 ± 2	Average = 7.5 ± 1

Representative Procedure for Performing React IR Initiation Rate Studies:

The IR probe was inserted through an O-ring sealed 14/20 ground glass adapter (custom-made) into an oven-dried 50 mL 2-neck flask equipped with a stir bar. The other neck was fitted with a three-way flow control adapter with a septum for injections/aliquot sampling and an N₂ line. The oven-dried flask was cooled under vacuum. The flask was then filled with N₂ and evacuated again for a total of three cycles. The flask was charged with THF (6.7 mL) and cooled to 0 °C for 15 min. After recording a background spectrum, monomer (2.3 mL, 0.44M in THF, 1.0 equiv) was added by syringe and allowed to equilibrate at 0 °C for at least 5 min before proceeding. The catalyst solution (1.0 mL, 0.015M, 0.015 equiv) was then injected and spectra were recorded every 15 s over the entire reaction. To account for mixing and temperature equilibration, spectra recorded in the first 60 s of the reaction were not analyzed.

Representative Procedure for k_{obs} Calculation:

The absorbance was converted to concentration using the appropriate calibration curves. The initial rate was obtained from 10% conversion and converted to the observed rate constant (k_{obs}) using equation S1:

$$initial\ rate = -\frac{d[monomer]}{dt} = k_{obs} [Ni]_{total} \quad (S1)$$

Derivation and Representative Procedure for k_i Calculation:

The observed rate constant (k_{obs}) is a weighted average of rate constant of initiation (k_i) and propagation (k_p) during the beginning of polymerization.

$$k_{obs} = k_i \frac{[Ni]_i}{[Ni]_{total}} + k_p \frac{[Ni]_p}{[Ni]_{total}}$$

The concentration of nickel precatalyst undergoing initiation ($[Ni]_i$) is determined by an exponential decay dependent on k_i , time, and the initial concentration of nickel ($[Ni]_{i(0)}$):

$$[Ni]_i = [Ni]_{i(0)} e^{-k_i t}$$

Assuming that all precatalyst undergoes initiation, $[Ni]_{i(0)} = [Ni]_{total}$, so we rearranged the exponential decay as follows:

$$\frac{[Ni]_i}{[Ni]_{total}} = e^{-k_i t}$$

We assume all nickel species in solution are undergoing initiation or propagation; therefore,

$$[Ni]_{total} = [Ni]_i + [Ni]_p$$

By dividing each side by $[Ni]_{total}$, we reach

$$\frac{[Ni]_{total}}{[Ni]_{total}} = \frac{[Ni]_i}{[Ni]_{total}} + \frac{[Ni]_p}{[Ni]_{total}}$$

and by rearranging and plugging in the exponential decay equation, we derive:

$$\frac{[Ni]_p}{[Ni]_{total}} = 1 - \frac{[Ni]_i}{[Ni]_{total}} = 1 - e^{-k_i t}$$

By substituting the new definitions for k_i and k_p into the equation defining k_{obs} , we arrive at equation 2:

$$k_{obs} = k_i(e^{-k_i t}) + k_p(1 - e^{-k_i t}) \quad (1)$$

The solve function of Mathematica was utilized to calculate k_i for each catalyst, using reaction time for 10% monomer conversion, and k_{obs} obtained from the initiation study. The propagation rate constant (k_p) was measured experimentally as described in the previous section.

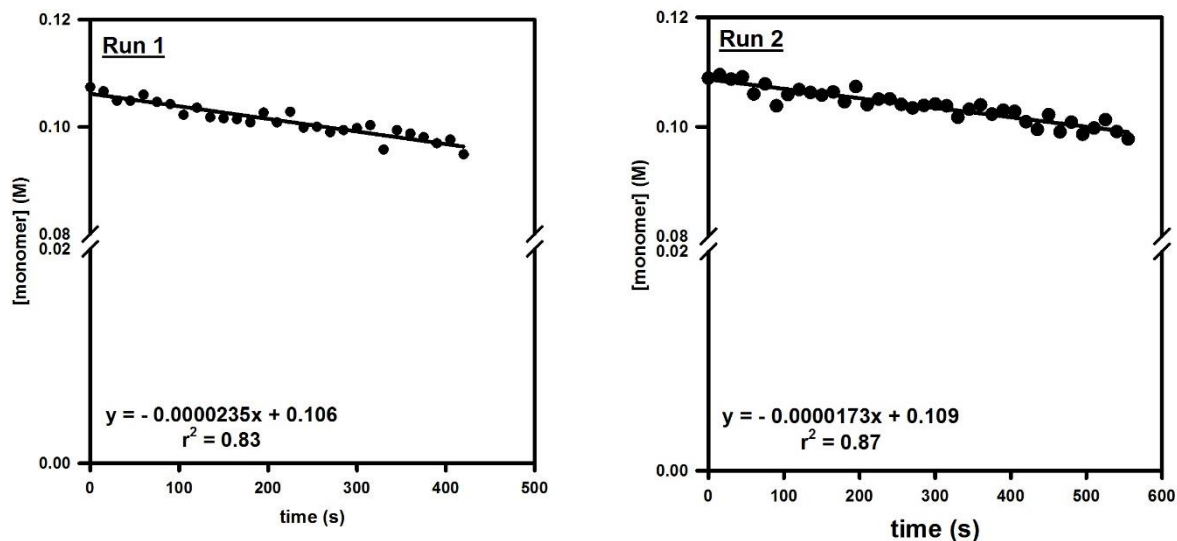


Figure S14. Plot of [monomer] versus for the polymerization of **monomer 1** catalyzed by **2b**. (temp = 0 °C, [**2b**] = 0.0015 M, [**monomer**] = 0.11M (Run 1), 0.11M (Run 2)). The initiation rate constant k_i was not calculated for run 1 because equation 1 fails when $k_{obs} > k_p$.

Table S2. Table of data for the plots in **Figure S14**.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_i ($10^{-3} \times \text{s}^{-1}$)
1	23.5	15.7	420	n/a
2	17.3	11.5	555	3.1
average	20 ± 4	13 ± 3		

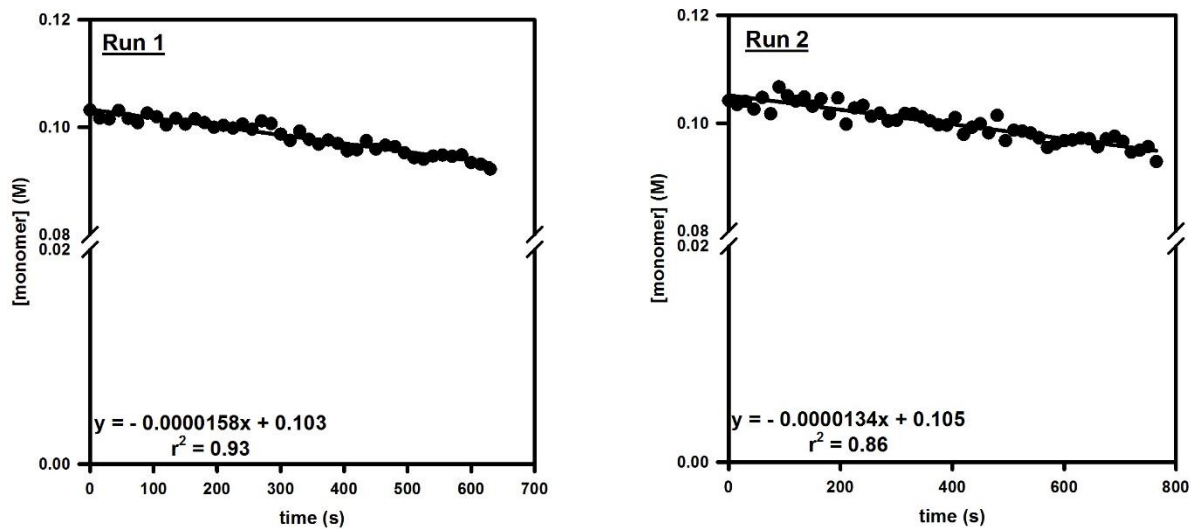


Figure S15. Plot of [monomer] versus time the polymerization catalyzed by **2c**. (temp = 0 °C, [2c] = 0.0015M, [monomer] = 0.10M (Run 1), 0.11M (Run 2)).

Table S3. Table of data for the plots in **Figure S15**.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_i ($10^{-3} \times \text{s}^{-1}$)
1	15.8	10.5	630	2.35
2	13.4	8.93	735	1.39
average	14 ± 2	9 ± 1		1.9 ± 0.6

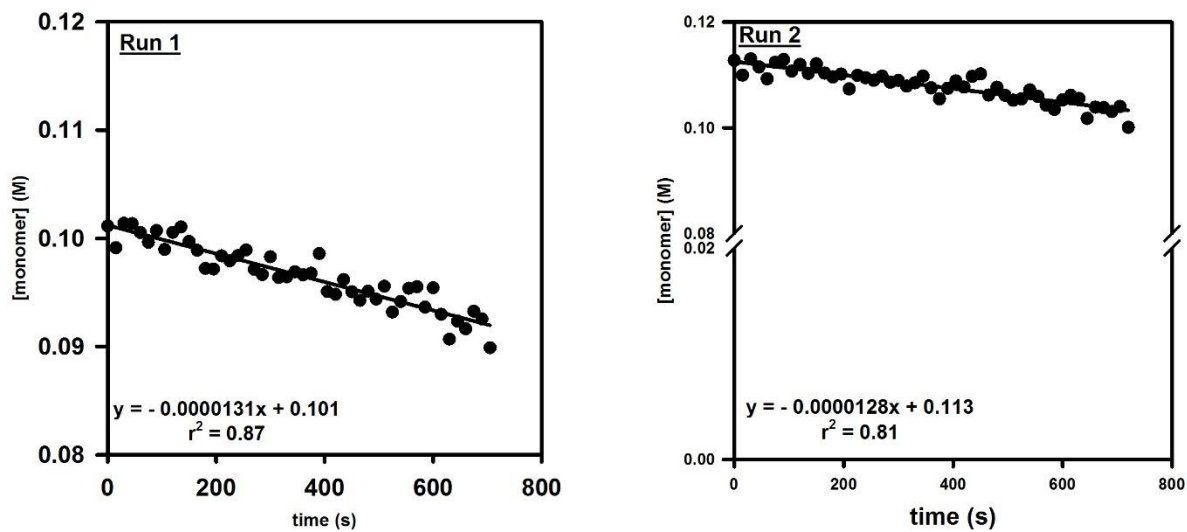


Figure S16. Plots of [monomer] versus time for the polymerization catalyzed by **2d**. (temp = 0 °C, [2d] = 0.0015M, [monomer] = 0.10M (Run 1), 0.10M (Run 2)). *Due to low solubility of precatalyst **2d**, a more dilute catalyst solution (2.0 mL, 0.0075M, 0.015 equiv) was used.

Table S4. Table of data for the plots in **Figure S16**.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_f ($10^{-3} \times \text{s}^{-1}$)
1	13.1	8.56	705	1.38
2	12.8	8.74	720	1.41
average	13.0 ± 0.2	8.7 ± 0.1		1.40 ± 0.02

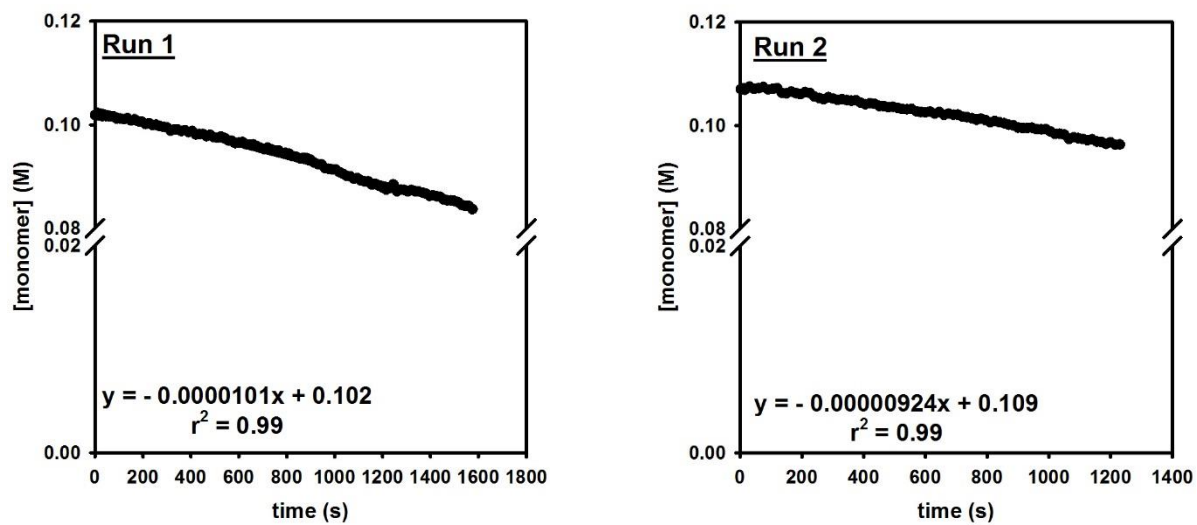


Figure S17. Plot of [monomer] versus time for the polymerization catalyzed by **2e**. (temp = 0 °C, [2e] = 0.0015M, [monomer] = 0.10M (Run 1), 0.11M (Run 2)).

Table S5. Table of data for the plot in **Figure S17**.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_i ($10^{-3} \times \text{s}^{-1}$)
1	10.08	7.95	990	0.656
2	9.24	6.16	1260	0.616
average	9.7 ± 0.6	7 ± 1		0.64 ± 0.03

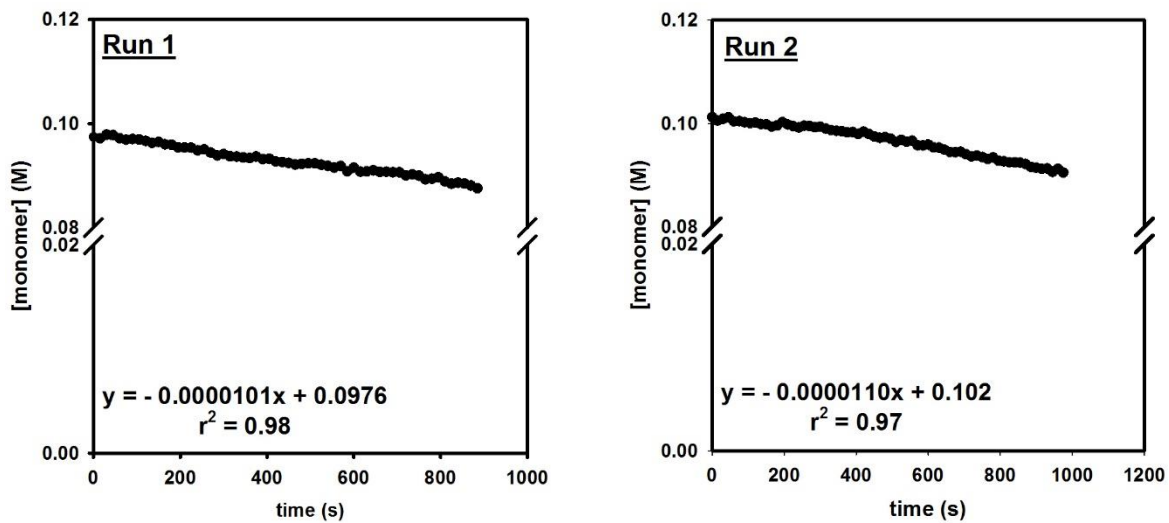


Figure S18. Plot of [monomer] versus time for the polymerization catalyzed by **2e** with PPh_3 . (temp = 0 °C, $[\mathbf{2e}] = 0.0015\text{M}$, $[\text{PPh}_3] = 0.0030$ [monomer] = 0.096M (Run 1), 0.11M (Run 2)).

Table S6. Table of data for the plot in **Figure S18**.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_i ($10^{-3} \times \text{s}^{-1}$)
1	10.1	7.18	885	1.28
2	11.0	7.35	975	1.00
average	10.6 ± 0.7	7.3 ± 0.1		1.1 ± 0.1

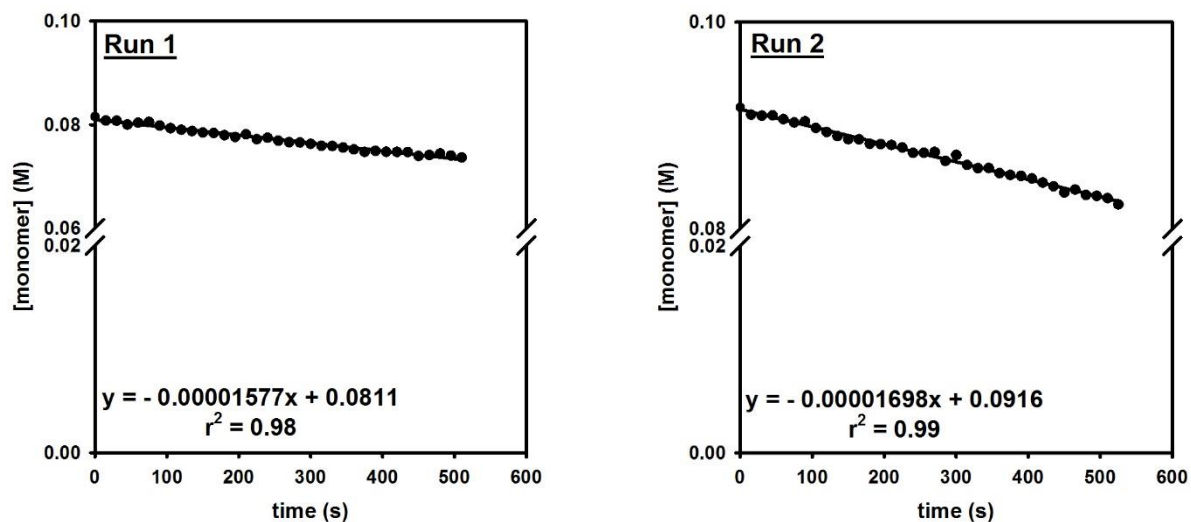


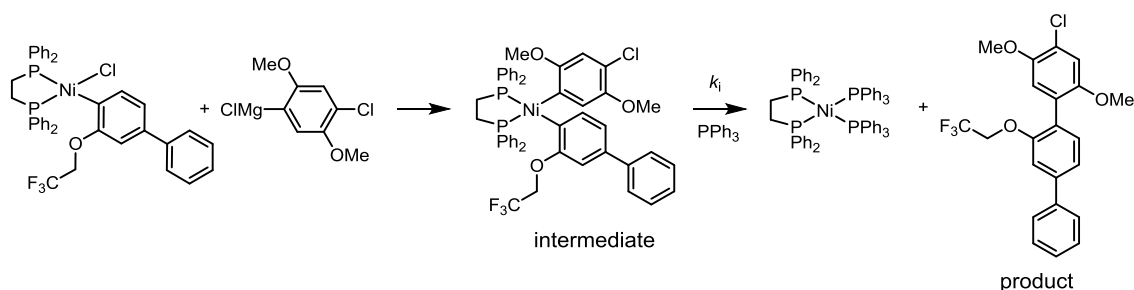
Figure S19. Plot of [monomer] versus time for the polymerization catalyzed by **2f**. (temp = 0 °C, [2f] = 0.0015M, [monomer] = 0.08M (Run 1), 0.09M (Run 2)). *Due to low solubility of precatalyst **2f**, a more dilute catalyst solution (3.0 mL, 0.005M, 0.015 equiv) was used.

Table S6. Table of data for the plot in **Figure S19**. The initiation rate constant k_i was not calculated because equation 1 fails when $k_{obs} > k_p$.

Run	Initial rate ($10^{-6} \times \text{M s}^{-1}$)	k_{obs} ($10^{-3} \times \text{s}^{-1}$)	Time at 10% conversion (s)	Calculated k_i ($10^{-3} \times \text{s}^{-1}$)
1	15.77	10.5	570	n/a
2	16.98	11.3	465	n/a
average	16.4 ± 0.9	10.9 ± 0.6		n/a

Representative Procedure for Performing ^{19}F NMR Spectroscopy Studies

In a glovebox under an N_2 atmosphere a stock solution of precatalyst **2e** (19.8 mg, 0.0265 mmol) and PPh_3 (15.1 mg, 0.0557 mmol) was prepared in THF (1 mL). To this stock solution, α,α,α -trifluoromethyltoluene (26 μL , 1.0M in THF) was added as an internal standard. A J. Young NMR tube was charged with this solution (0.8 mL), sealed with a septum, and cooled to 0 $^\circ\text{C}$ in the spectrometer for approx. 45 min. A solution of (4-chloro-2,5-dimethoxyphenyl)magnesium chloride (0.2 mL, 0.2M in THF, 2.0 equiv) was added, and the tube was inverted once to mix. The final solution contained 0.02 mmol precatalyst, 0.04 mmol PPh_3 , 0.02 mmol α,α,α -trifluoromethyltoluene, and 0.04 mmol (4-chloro-2,5-dimethoxyphenyl)magnesium chloride. All ^{19}F NMR spectra were acquired with acquisition time = 1.5 s, relaxation time = 3 s, scan size = 4.



Scheme 1. Initiation of precatalyst **2e**

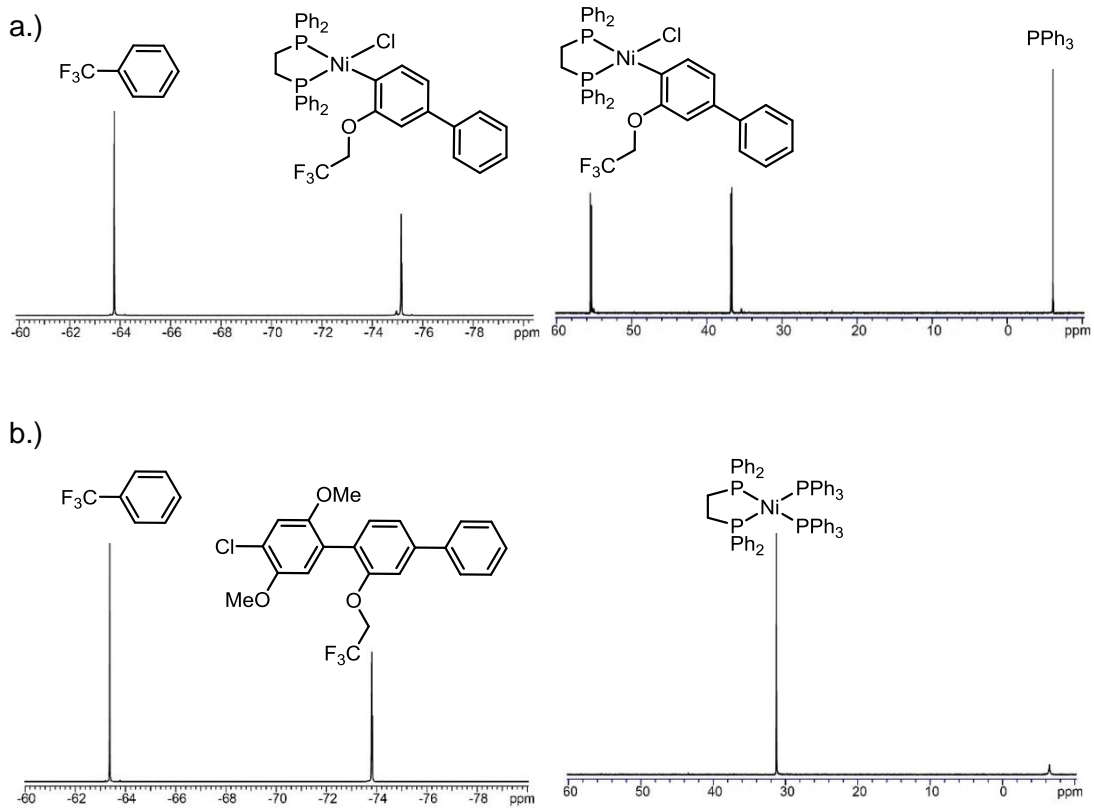
^{19}F NMR spectra **^{31}P NMR spectra**

Figure S20. (a) ^{19}F and ^{31}P NMR spectra at the beginning and (b) end of the reaction in Scheme 1.

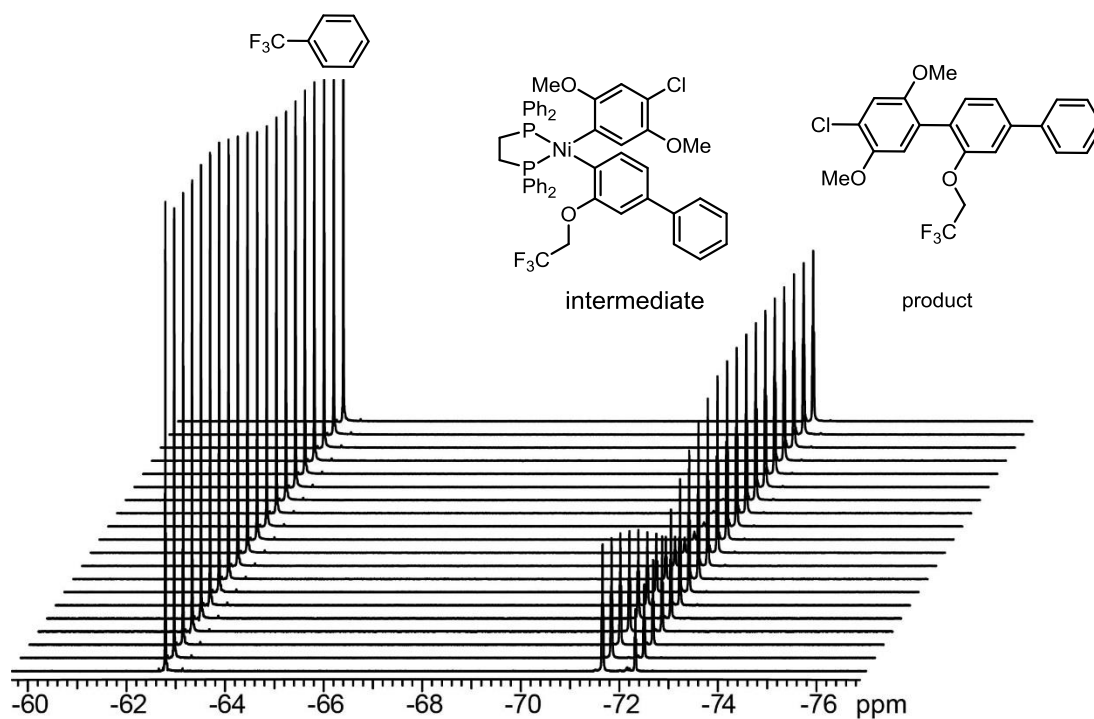


Figure S21. Representative ^{19}F NMR spectral array for precatalyst **2e**. Concentrations were calculated relative to an internal standard, α,α,α -trifluoromethyltoluene.

Procedure for Calculating Concentrations from Integrals

The internal standard concentration was used to calculate the ratio of integration:concentration, which was then used to calculate concentrations of the intermediate and product peaks from the integrals.

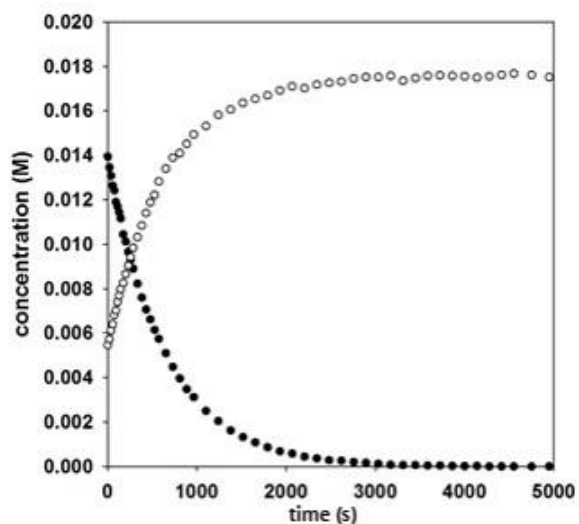


Figure S22. Plot of concentration of intermediate (\bullet) and product (\circ) versus time for the data in Figure S21.

Procedure for Calculating Rate Constants in Igor Pro

Initiation rate constants were calculated using Igor Pro v.6.22A, following the procedure in “Fitting to Differential equations in Igor Pro” provided by the Collum group⁴ and using Collum Kinetic 5000 as the master procedure file. The data was fit to the following equations:

$$\frac{d[\textit{intermediate}]}{dt} = -k_i \times [\textit{intermediate}] \quad (2)$$

$$\frac{d[\textit{product}]}{dt} = k_i \times [\textit{intermediate}] \quad (3)$$

Table S7. Initiation rate constants for **2e**

Run	k_i ($10^{-3} \times \text{s}^{-1}$)
1	1.310
2	1.307
average	1.309 ± 0.002

VII. Polymerization

Representative Procedure for M_n and \bar{D} versus Conversion Studies Utilizing *in situ* React IR Spectroscopy:

The IR probe was inserted through an O-ring-sealed 14/20 ground-glass adapter (custom-made) into an oven-dried 50 mL 2-neck flask equipped with a stir bar. The other neck was fitted with a three-way flow-control adapter with a septum for injections/aliquot sampling and an N₂ line. The oven-dried flask was cooled under vacuum, then filled with N₂. The flask was re-evacuated and filled for two additional cycles. The flask was charged with THF (6.7 mL) and cooled to 0 °C for 15 min. After recording a background spectrum, monomer **1** (2.3 mL, 0.44 M in THF, 1.0 equiv) was added by syringe and equilibrated at 0 °C for at least 5 min. Then the precatalyst solution (1.0 mL, 0.015 M, 0.015 equiv) was injected and spectra were recorded every 15 s. To account for mixing and temperature equilibration, spectra recorded in the first 60 s were not analyzed. Aliquots (approx. 0.5 mL) were taken via syringe and immediately quenched with aq. HCl (approx. 1 mL, 12 M). The resulting solution was then extracted with CH₂Cl₂ (2 x 1.5 mL) (with mild heating if polymer had precipitated), dried over MgSO₄, filtered, and then concentrated. At approximately 80% conversion, the polymerization was poured into aq. HCl (20 mL, 12 M), extracted with CH₂Cl₂ (3 x 25 mL), washed with H₂O (1 x 25 mL), brine (1 x 25 mL), dried over MgSO₄, filtered, and concentrated. The samples (both aliquots and the final reaction mixture) were each dissolved in THF (with heating), and passed through a 0.2 μm poly(tetrafluoroethylene) filter for analysis by gel permeation chromatography (GPC). The monomer conversion versus time data was calculated from the IR spectra using a calibration curve.

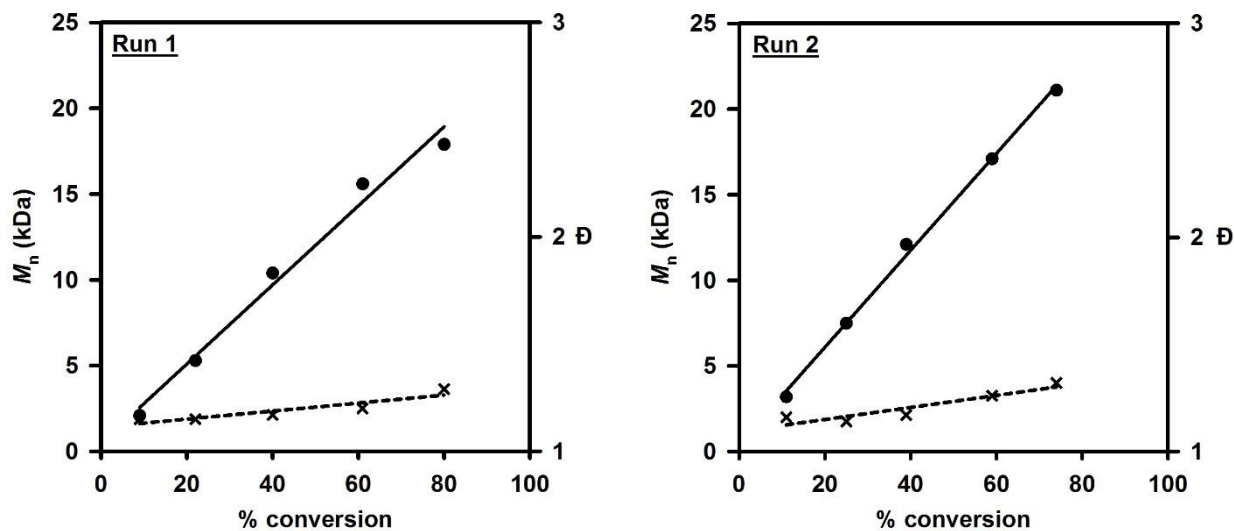


Figure S23. Plot of M_n (●) and \bar{D} (x) versus conversion for **2b** (temp = 0 °C, $[2b] = 0.0015M$, $[monomer] = 0.11M$ (Run 1), $0.11M$ (Run 2)).

Table S8. Data for the plot in **Figure S23**, Run 1.

% Conversion	M_n (kDa)	\bar{D}
9	2.1	1.15
22	5.3	1.15
40	10.4	1.17
61	15.6	1.20
80	17.9	1.29

Table S9. Data for the plot in **Figure S23**, Run 2.

% Conversion	M_n (kDa)	\bar{D}
11	3.2	1.16
25	7.5	1.14
39	12.1	1.17
59	17.1	1.26
74	21.1	1.32

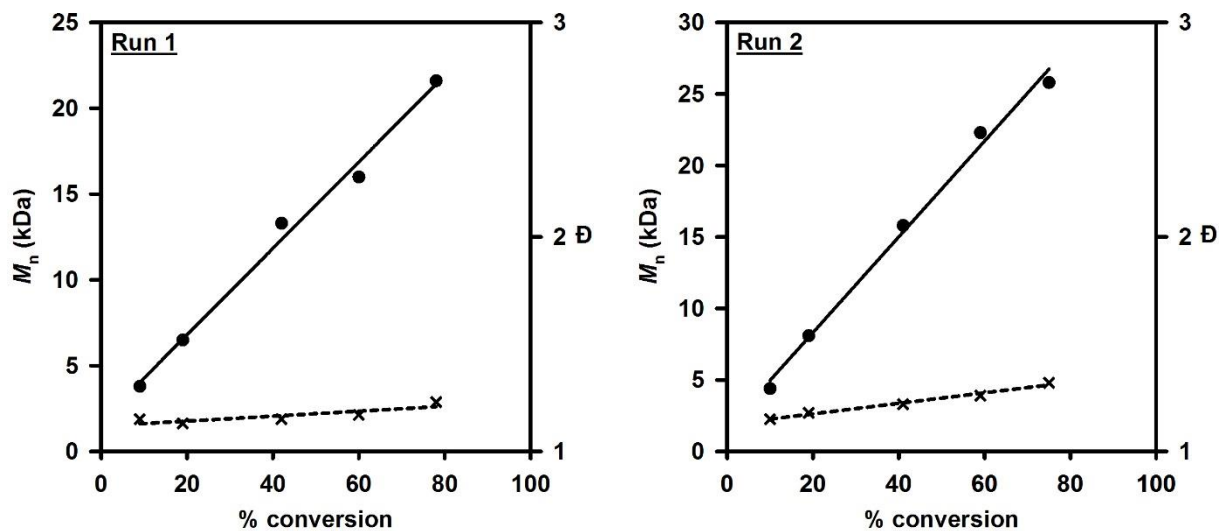


Figure S24. Plot of M_n (●) and \bar{D} (x) versus conversion for **2c** (temp = 0 °C, [2c] = 0.0015M, [monomer] = 0.10M (Run 1), 0.10M (Run 2)).

Table S10. Data for the plot in **Figure S24**, Run 1.

% Conversion	M_n (kDa)	\bar{D}
9	3.8	1.15
19	6.5	1.13
42	13.3	1.15
60	16.0	1.17
78	21.6	1.23

Table S11. Data for the plot in **Figure S24**, Run 2.

% Conversion	M_n (kDa)	\bar{D}
10	4.4	1.15
19	8.1	1.18
41	15.8	1.22
59	22.3	1.26
75	25.8	1.32

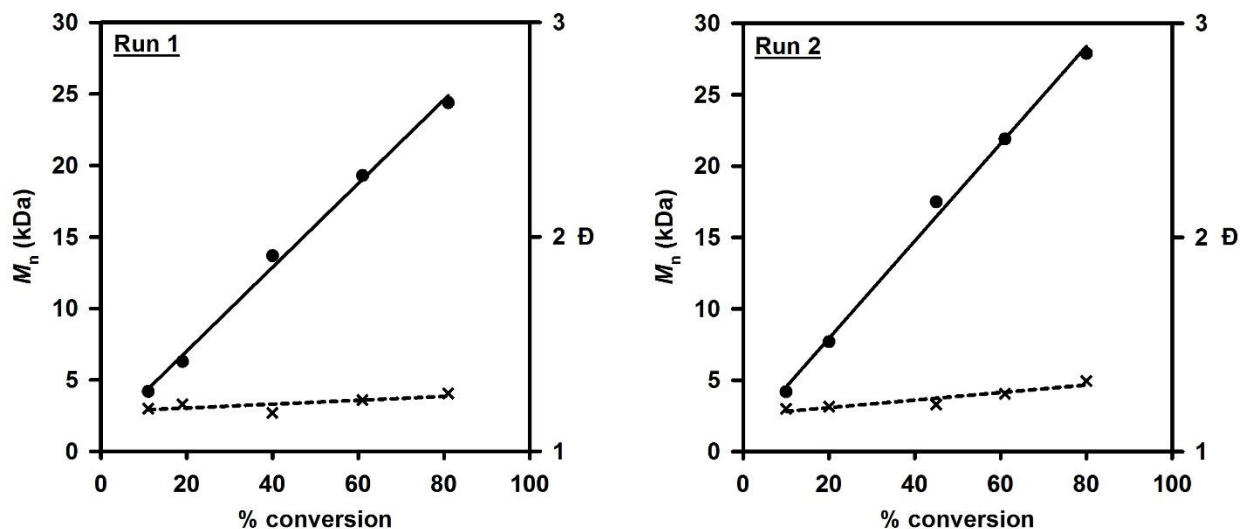


Figure S25. Plot of M_n (●) and \bar{D} (x) versus conversion for **2d** (temp = 0 °C, [**2d**] = 0.0015M, [monomer] = 0.10M (Run 1), 0.11M (Run 2)). *Due to low solubility of precatalyst **2d**, a dilute precatalyst solution (2.0 mL, 0.0075M, 0.015 equiv) was used.

Table S12. Data for the plot in **Figure S25**, Run 1.

% Conversion	M_n (kDa)	\bar{D}
11	4.2	1.20
19	6.3	1.22
40	13.7	1.18
61	19.3	1.24
81	24.4	1.27

Table S13. Data for the plot in **Figure S25**, Run 2.

% Conversion	M_n (kDa)	\bar{D}
10	4.2	1.20
20	7.7	1.21
45	17.5	1.22
61	21.9	1.27
80	27.9	1.33

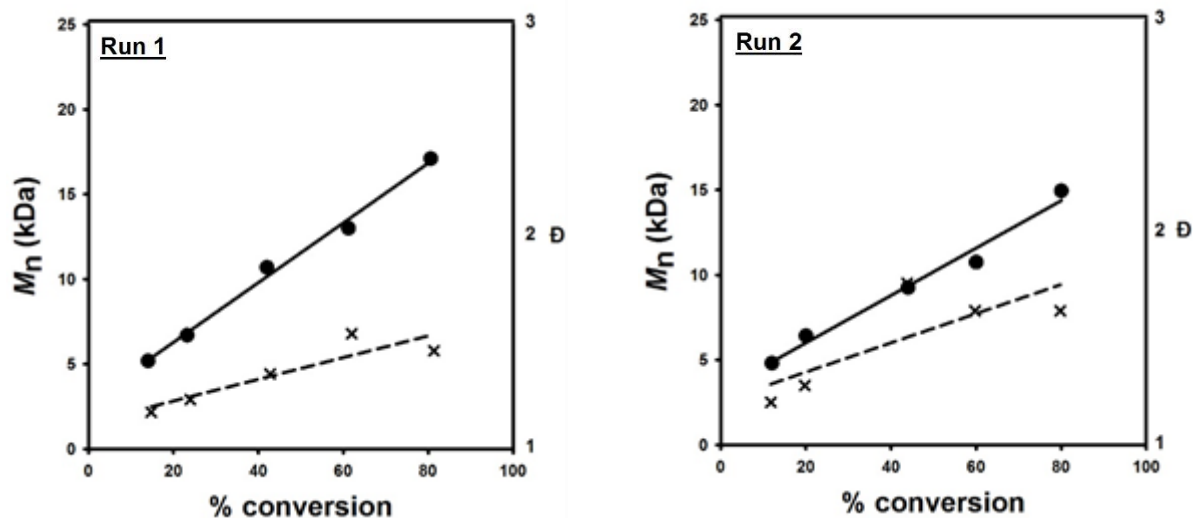


Figure S26. Plot of M_n (●) and \bar{D} (x) versus conversion for **2e** (temp = 0 °C, $[2e] = 0.0015M$, $[monomer] = 0.10M$ (Run 1), $0.11M$ (Run 2)).

Table S14. Data for the plot in **Figure S26**, Run 1.

% Conversion	M_n (kDa)	\bar{D}
14	5.2	1.16
23	6.7	1.22
42	10.7	1.34
61	13.0	1.53
81	17.1	1.45

Table S15. Data for the plot in **Figure S26**, Run 2.

% Conversion	M_n (kDa)	\bar{D}
12	4.8	1.19
20	6.4	1.27
44	9.3	1.55
60	10.8	1.75
80	15.0	1.62

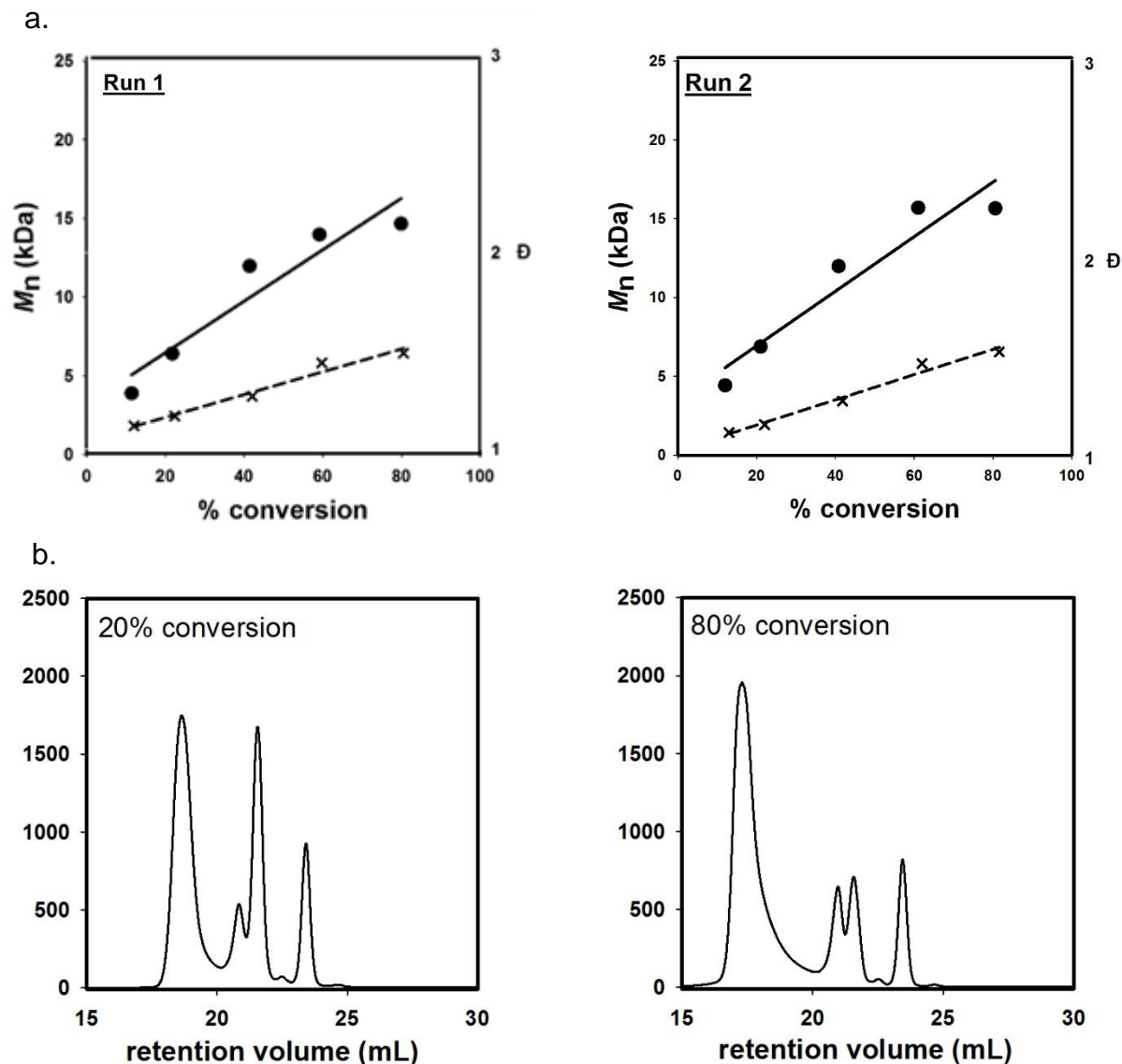


Figure S27. a.) Plot of M_n (●) and \bar{D} (x) versus conversion for **2f** (temp = 0 °C, $[2f] = 0.0015M$, $[monomer] = 0.082M$ (Run 1), $0.90M$ (Run 2)). *Due to low solubility of precatalyst **2f**, a dilute catalyst solution (3.0 mL, 0.005M, 0.015 equiv) was used. b.) GPC curves of aliquots removed at 20 and 80% monomer conversion during Run 1.

Table S16. Data for the plot in **Figure S27a**, Run 1.

% Conversion	M_n (kDa)	\bar{D}
11	3.9	1.12
22	6.4	1.17
41	12.0	1.27
59	14.0	1.44
80	14.7	1.49

Table S17. Data for the plot in **Figure S27b**, Run 2.

% Conversion	M_n (kDa)	\bar{D}
12	4.4	1.13
21	6.9	1.17
41	12.0	1.29
61	15.7	1.48
81	15.6	1.54

VIII. MALDI-TOF-MS Analysis

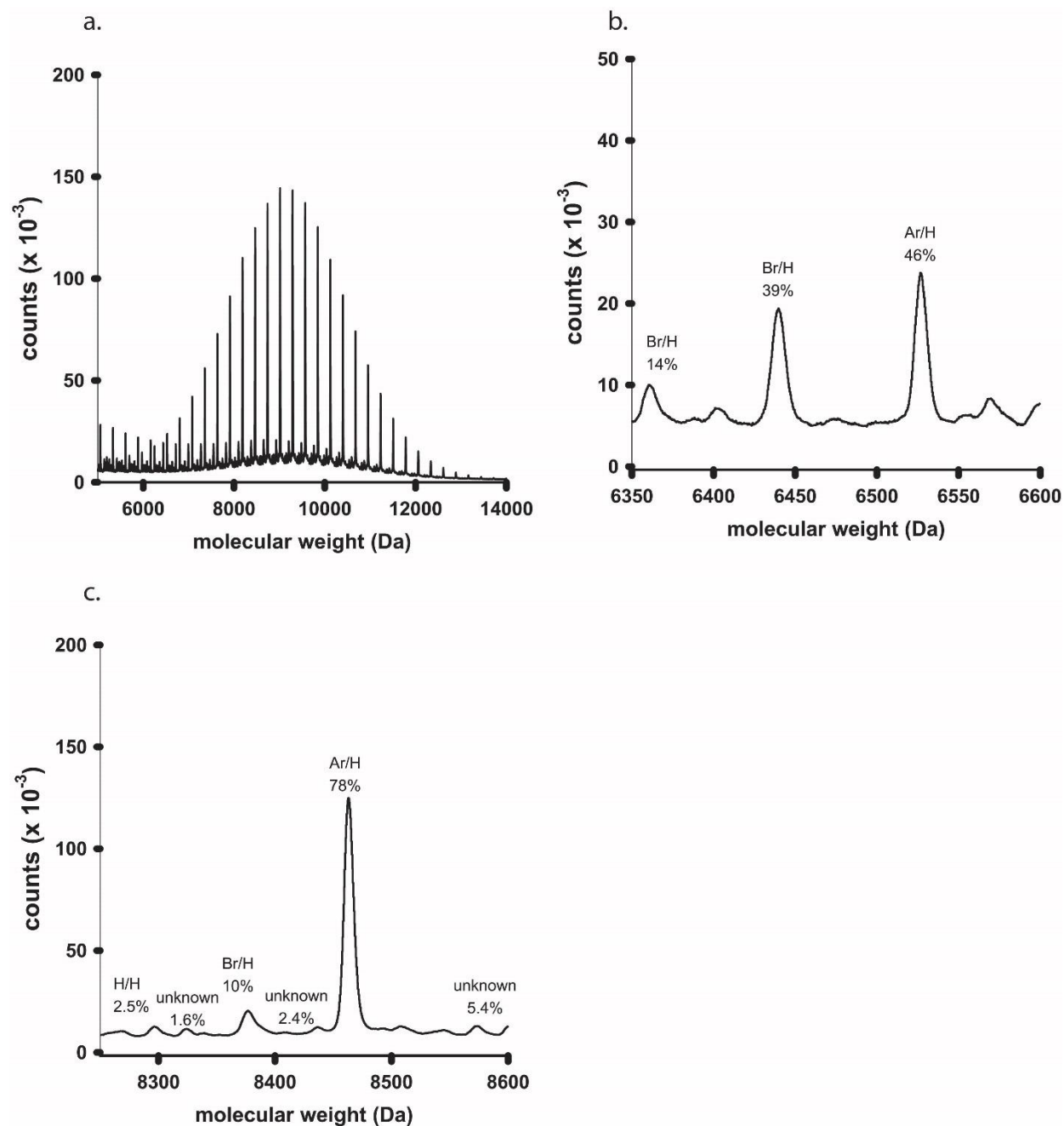


Figure S28. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with precatalyst **2b**, b., MALDI-TOF MS spectrum at 23 repeat units, and c., MALDI-TOF MS spectrum at 30 repeat units. The polymer sample analyzed was from an aliquot was taken at 20% conversion for the polymer described in **Figure S23**. Lower molecular weight polymers had a higher percentage of Br/H terminated polymers.

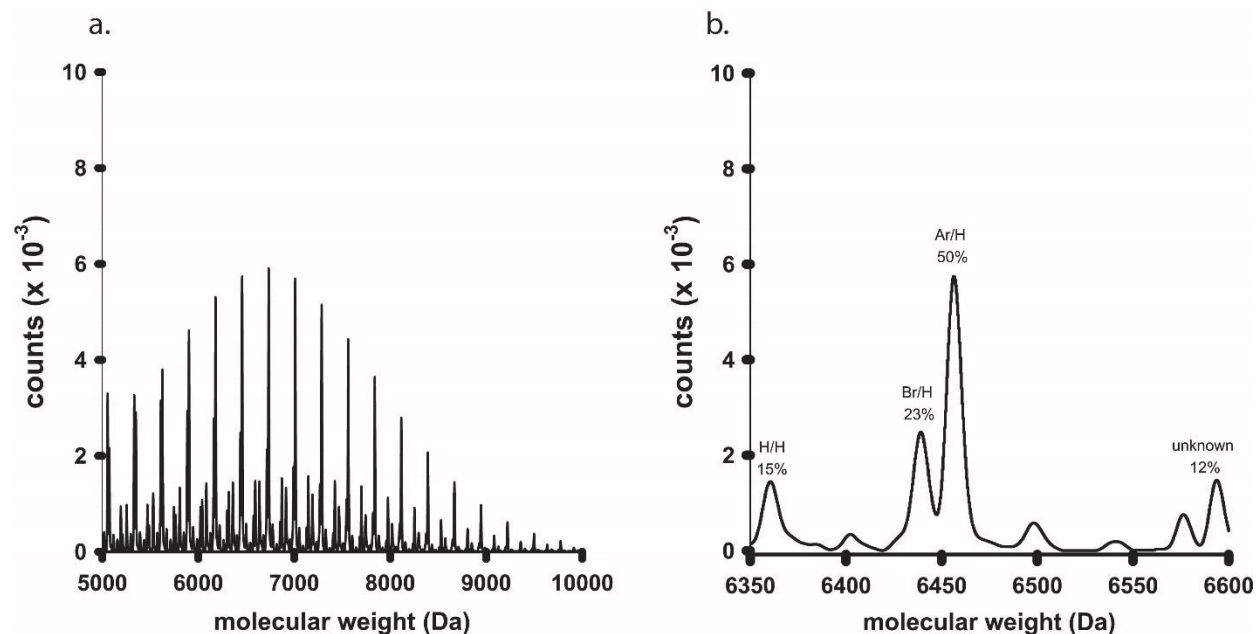


Figure S29. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with precatalyst **2c**, and b., MALDI-TOF MS spectrum at 23 repeat units. The polymer sample analyzed was from an aliquot was taken at 20% conversion for the polymer described in **Figure S24**.

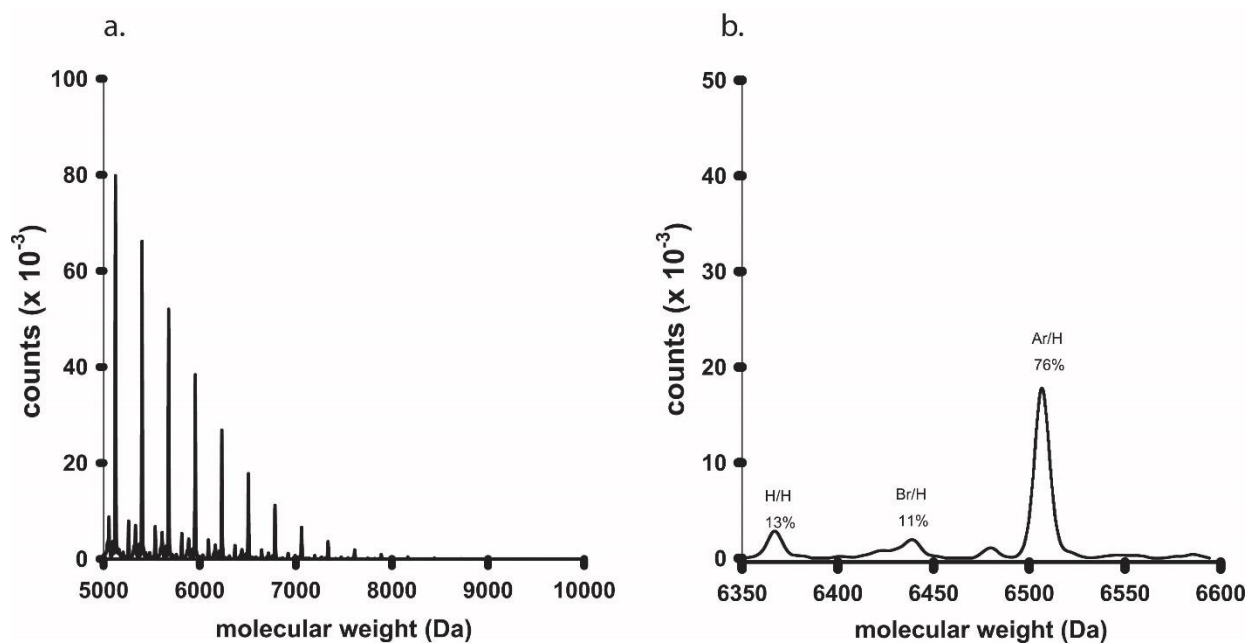
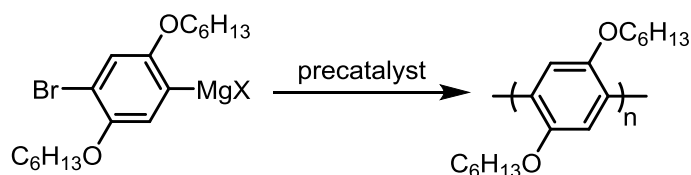


Figure S30. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with precatalyst **2d**, and b., MALDI-TOF MS spectrum at 23 repeat units. The polymer sample analyzed was from an aliquot was taken at 20% conversion for the polymer described in **Figure S25**.

Representative Procedure for Preparation of Polymers to Compare End-group Fidelity with Three dppe-Based Precatalysts:



In a glovebox, a precatalyst stock solution was made by combining **2f** (11.2 mg, 0.0165 mmol) with THF (3.3 mL) in a 4 mL vial. (Note: For Ni(dppe)Cl₂, a pre-initiation protocol was followed wherein monomer **1** (0.23 mL, 5 equiv) was added to the precatalyst and stirred until homogeneous). The precatalyst solution (3.0 mL, 0.015 mmol, 1 equiv) and THF (3.8 mL) were combined in a 50 mL Schlenk tube, sealed with a Teflon stopper, and then removed from the glovebox and put under N₂ pressure. The solution was cooled to 0 °C for 20 min. Then monomer solution (3.2 mL, 1.0 mmol, 66 equiv) was added. After 30 min, an aliquot was removed by syringe, then quenched with aq. HCl (approx. 1.0 mL, 12 M), extracted with CH₂Cl₂ (2 x 1 mL), dried over MgSO₄, filtered, concentrated, and then analyzed by MALDI-TOF MS analysis (SI). After 4 h, the polymerization was poured in aq. HCl (20 mL, 12 M), extracted with CH₂Cl₂ (3 x 25 mL), washed with water (1 x 25 mL), brine (1 x 25 mL), dried over MgSO₄, filtered, and concentrated. Both the aliquot and the bulk polymerization were analyzed by GPC.

Precatalyst	M_n (kDa)	\bar{D}
2f	16.1	1.45
Ni(dppe)(tol)Br	18.4	1.54
Ni(dppe)Cl ₂	23.0	1.41

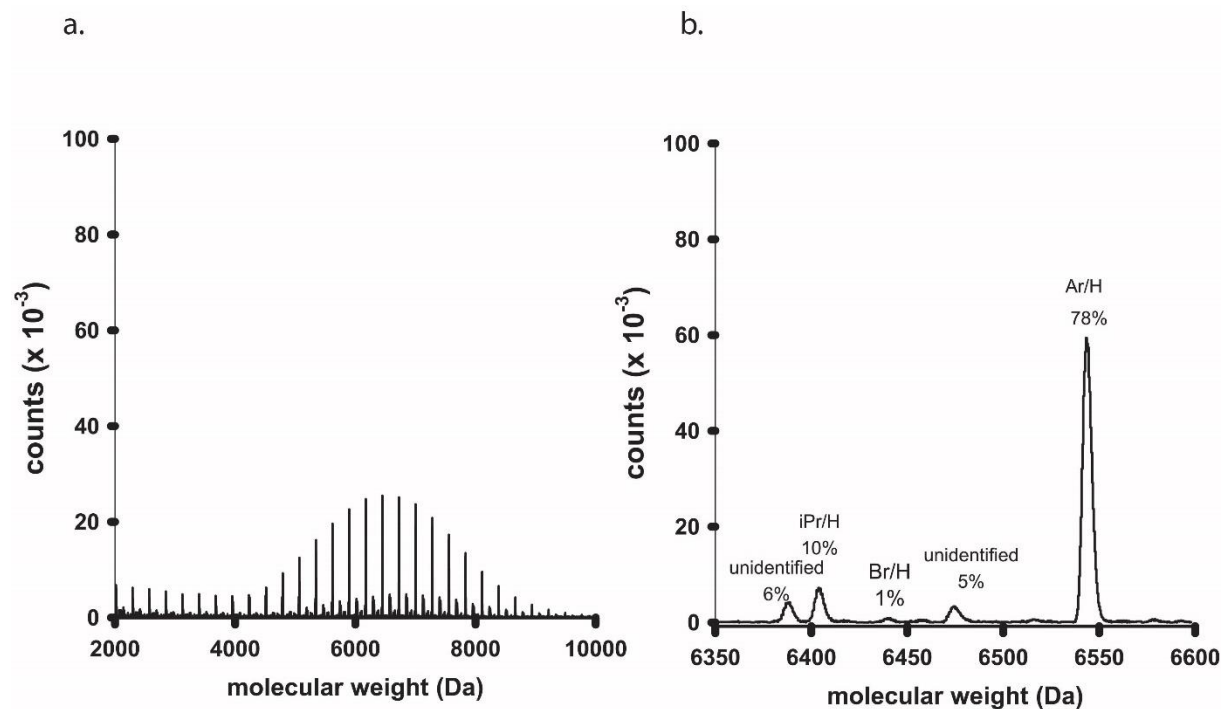


Figure S31. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with precatalyst **2f**, and b., MALDI-TOF MS spectrum at 23 repeat units.

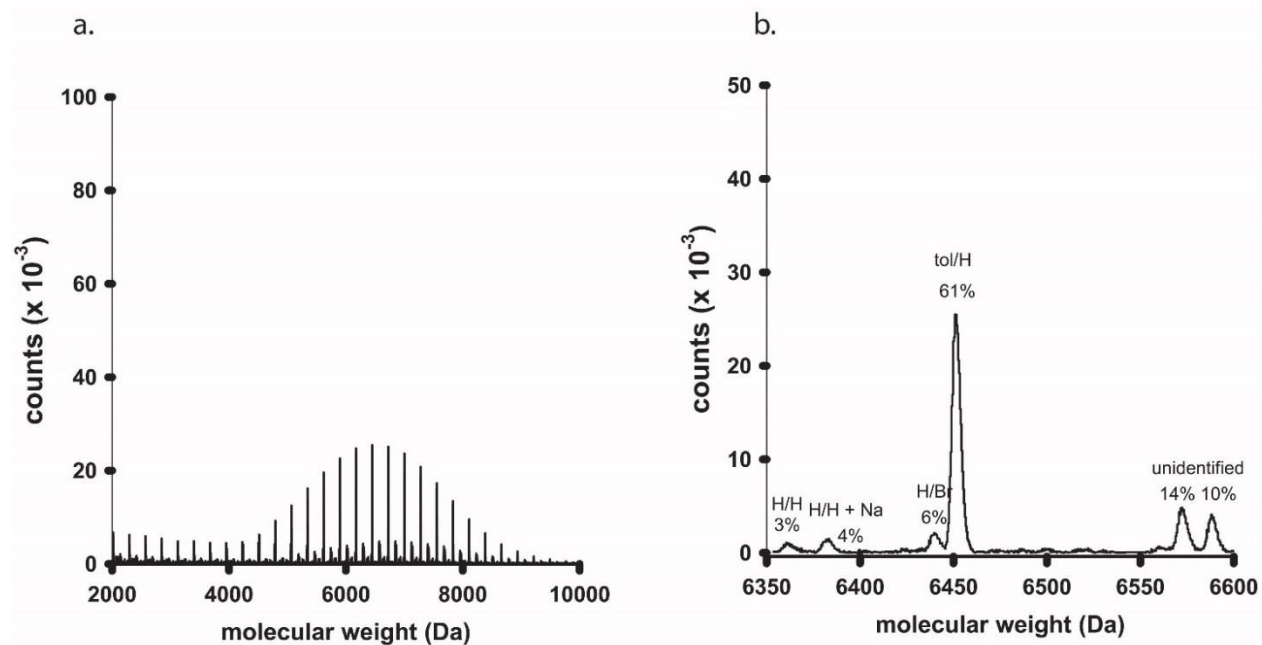


Figure S32. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with Ni(dppe)tolBr, and b., MALDI-TOF MS spectrum at 23 repeat units.

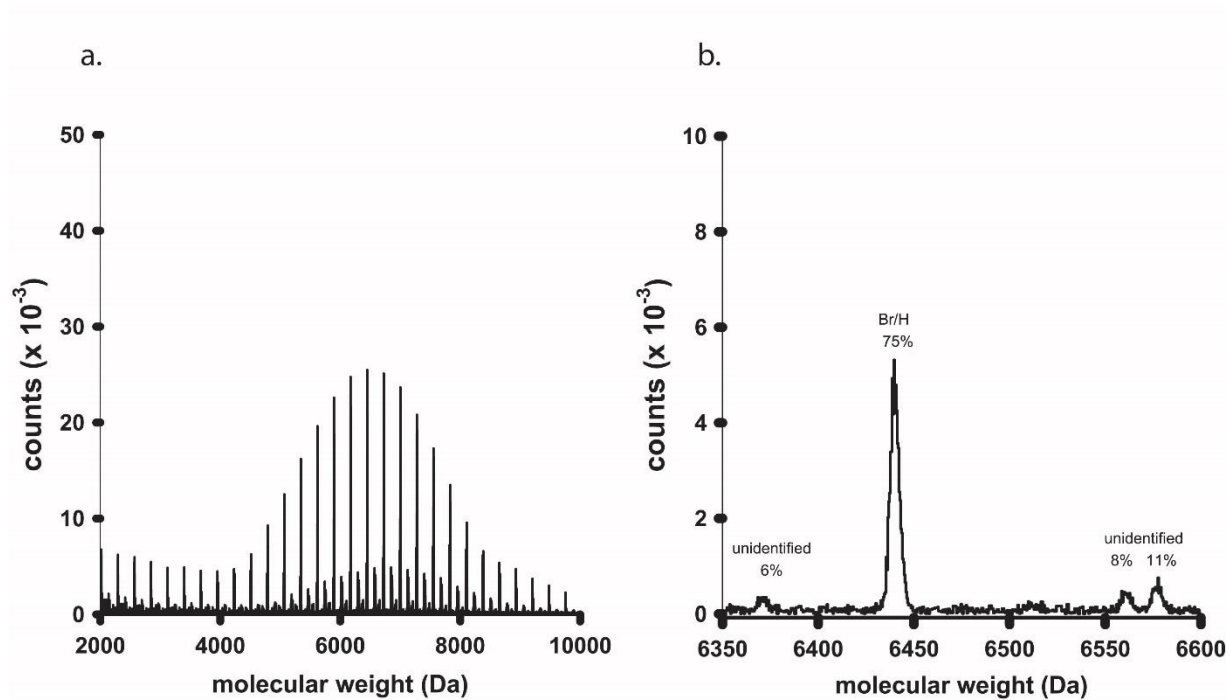
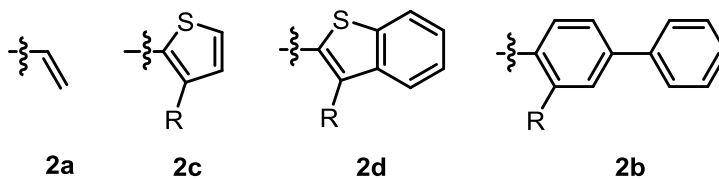
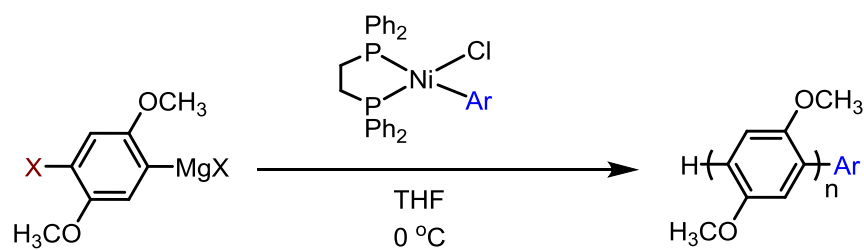


Figure S33. a. Full MALDI-TOF MS spectrum of polyphenylene initiated with Ni(dppe)Cl₂, and b., MALDI-TOF MS spectrum at 23 repeat units.

X. Computational Data

Computations were performed with the BP86 DFT functional⁵ paired with the 6-311+G(d) basis set⁶ was used for all non-metal atoms and the SDB-cc-pVTZ basis set with the small core, fully relativistic effective core potential⁷ was used for Ni. All computations were performed using Gaussian09.



Ar	X	R	E(Reactant)	G(Reactant)	E(TS)	G(TS)	Δq
1	Br	--	- 4971.905404	- 4971.387898	- 4971.894311	- 4971.377567	--
2	Br	CH ₃	- 5485.725328	- 5485.169361	-5485.70677	- 5485.151145	--
3	Br	CH ₃	- 5639.408931	- 5638.810395	- 5639.389398	- 5638.791431	--
4	Br	CH ₃	- 5396.017061	- 5395.356236	-5395.99755	- 5395.338129	0.244
5	Br	OCH ₃	- 5471.255943	- 5470.591858	- 5471.238104	- 5470.575208	0.247
5	Br	OCH ₂ CH ₃	- 5510.578995	- 5509.889101	- 5510.561344	- 5509.872064	0.249
5	Br	OCH ₂ CF ₃	- 5808.410915	-5807.74857	- 5808.391911	- 5807.728671	0.259
1	Cl	CH ₃	- 2857.765163	- 2857.245191	- 2857.754257	- 2857.234281	--
2	Cl	CH ₃	- 3371.584513	-3371.02894	- 3371.567536	- 3371.011248	--
3	Cl	CH ₃	- 3525.268913	-3524.66836	- 3525.249288	- 3524.647572	--
4	Cl	CH ₃	- 3281.876847	- 3281.214682	- 3281.856381	- 3281.193542	--

Table S18. Absolute electronic energies (E) and free energies (G), in hartrees, for reactants and transition states (TS), along with the corresponding change in NPA charges for select species (Δq).

Optimized Cartesian Coordinates for lowest-lying conformer of each reactant and transition state

X = Cl

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Ar = ethene reactant

Ni	-0.3717520	-0.1247440	-0.5619730
P	-2.4608960	-0.0748170	0.1254800
P	0.2323010	0.3811650	1.5149420
C	-2.5068100	0.5446130	1.9059270
C	-3.1925730	-1.7686380	0.2903650
C	-3.7765050	0.8914110	-0.7373430
C	1.4240490	-0.3381900	-1.2175490
C	-1.2473440	0.0423040	2.6259580
C	0.4778840	2.2060570	1.7538110
C	1.6730190	-0.3502320	2.4046390
H	-3.4284160	0.2168710	2.4140570
H	-2.5091560	1.6467730	1.8854750
C	-4.5212590	-1.9644210	0.7186240
C	-2.3794570	-2.8863900	0.0257790
C	-4.4473260	0.3135970	-1.8351490
C	-4.0511780	2.2331850	-0.4050310
C	2.0413440	-1.6008350	-1.0999080
C	2.1809610	0.6996370	-1.7891900
H	-1.1305090	0.5169470	3.6147330
H	-1.3039120	-1.0500770	2.7731220
C	1.0092270	2.7448780	2.9419830
C	0.0813180	3.0776250	0.7217190
C	2.9603680	-0.1415270	1.8654430
C	1.5389180	-1.1276460	3.5715300
C	-5.0271820	-3.2598110	0.8806390
H	-5.1699860	-1.1025530	0.9092550
C	-2.8907760	-4.1828730	0.1903130
H	-1.3484300	-2.7328730	-0.3125970
C	-5.3929770	1.0512150	-2.5583800
H	-4.2304320	-0.7181880	-2.1235280
C	-4.9969560	2.9690080	-1.1321220
H	-3.5302030	2.7215540	0.4239340
C	3.3660720	-1.8090780	-1.5181980
O	1.2616950	-2.6118190	-0.5406790
C	3.5145380	0.5260060	-2.2157570
H	1.7121390	1.6783040	-1.9230120

C	1.1299470	4.1318260	3.0963200
H	1.3450510	2.0777500	3.7429940
C	0.2001080	4.4662950	0.8789870
H	-0.3119800	2.6545960	-0.2106130
C	4.0862370	-0.6899220	2.4909300
H	3.0814240	0.4443630	0.9492770
C	2.6697110	-1.6782270	4.1924100
H	0.5535270	-1.3096960	4.0102860
C	-4.2116310	-4.3713210	0.6168110
H	-6.0623390	-3.4032490	1.2080190
H	-2.2552580	-5.0485170	-0.0234420
C	-5.6736580	2.3788790	-2.2080740
H	-5.9074490	0.5856080	-3.4052990
H	-5.2046240	4.0075280	-0.8537550
C	4.0941740	-0.7462360	-2.0656220
H	3.8592700	-2.7796450	-1.4314920
C	1.8645280	-3.8950440	-0.3915330
O	4.2959720	1.5118420	-2.7730380
C	0.7238830	4.9944300	2.0665810
H	1.5490890	4.5414890	4.0213990
H	-0.1082580	5.1350430	0.0685050
C	3.9449750	-1.4582610	3.6557200
H	5.0775500	-0.5207260	2.0589560
H	2.5502530	-2.2776780	5.1011560
H	-4.6101230	-5.3838390	0.7399690
H	-6.4130320	2.9538040	-2.7750870
Cl	5.7589100	-1.0211260	-2.5788870
H	2.7534630	-3.8546100	0.2645080
H	1.1032190	-4.5351670	0.0757900
H	2.1518080	-4.3271580	-1.3682840
C	3.6943420	2.7879450	-2.9801380
H	0.8239580	6.0779870	2.1885050
H	4.8272830	-1.8873640	4.1418160
H	2.8222900	2.7209080	-3.6554420
H	4.4721380	3.4060700	-3.4486310
H	3.3836070	3.2521470	-2.0260830
C	-0.8560620	-0.5171180	-2.3664630
C	-1.3775200	0.3173020	-3.2864080
H	-0.6284160	-1.5485890	-2.6850140
H	-1.5716080	-0.0097950	-4.3193350
H	-1.6250740	1.3658620	-3.0761580

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Ar = ethene TS

C	2.1169210	0.5624360	-1.9239610
C	3.2365090	-1.9632100	-1.5444210
C	1.2585590	-0.4967710	-1.5229080
H	3.7090880	-2.9357440	-1.3926880
Ni	-0.3754280	-0.1237090	-0.5450910
P	-2.4853280	0.0037950	0.1005390
P	0.2458910	0.4994290	1.4850680
C	-2.4994380	0.8066420	1.8074300
C	-3.2675380	-1.6442170	0.4558170
C	-3.8113760	0.8979190	-0.8241600
C	-1.2673620	0.3306590	2.5934140
C	1.6169340	-0.2795430	2.4457780
C	0.6157050	2.3158180	1.6347200
H	-2.4479130	1.8991970	1.6568170
H	-3.4318700	0.5814610	2.3520510
C	-4.6425190	-1.7854410	0.7283100
C	-2.4392800	-2.7825940	0.4858490
C	-4.6241940	1.9039420	-0.2636530
C	-3.9800700	0.5668550	-2.1861820
H	-1.3694270	-0.7391210	2.8473050
H	-1.1510370	0.8966180	3.5331800
C	2.8882960	-0.3321190	1.8344280
C	1.4504680	-0.8568910	3.7202430
C	1.3091890	2.8670630	2.7298180
C	0.1527030	3.1734550	0.6171030
C	-5.1771720	-3.0430460	1.0359950
H	-5.3018010	-0.9117940	0.6836880
C	-2.9767730	-4.0394070	0.8015880
H	-1.3740830	-2.6773650	0.2472310
C	-5.5918630	2.5543450	-1.0432640
H	-4.5155280	2.1848420	0.7881850
C	-4.9519390	1.2135250	-2.9589520
H	-3.3303790	-0.1851660	-2.6432590
C	3.9678810	-0.9333820	2.4917770
H	3.0324640	0.0948180	0.8364200
C	2.5327180	-1.4666680	4.3720960
H	0.4767130	-0.8326520	4.2185840
C	1.5259190	4.2493040	2.8078690
H	1.6932680	2.2118400	3.5186270
C	0.3617760	4.5573950	0.7012590
H	-0.3682300	2.7432930	-0.2471350
C	-4.3442880	-4.1715830	1.0771240
H	-6.2486600	-3.1440730	1.2394480

H	-2.3263320	-4.9202400	0.8239130
C	-5.7612080	2.2082070	-2.3906450
H	-6.2185620	3.3311530	-0.5921500
H	-5.0711950	0.9452050	-4.0139230
C	3.7935380	-1.5028700	3.7620880
H	4.9472900	-0.9628670	2.0037550
H	2.3880750	-1.9099420	5.3632120
C	1.0499720	5.0971870	1.7966320
H	2.0718410	4.6661370	3.6609980
H	-0.0067560	5.2136190	-0.0943840
H	-4.7642610	-5.1542270	1.3163440
H	-6.5185690	2.7154320	-2.9973090
H	4.6380060	-1.9768120	4.2731860
H	1.2215080	6.1768160	1.8601030
C	-0.3789970	-0.6407240	-2.4039810
H	1.6703810	1.5429110	-2.1069780
C	-0.6524470	0.1483990	-3.4807690
C	3.4901640	0.3944540	-2.1318620
O	4.3569410	1.3910640	-2.5096810
C	3.8031160	2.6821250	-2.7594350
H	3.0642280	2.6524890	-3.5806830
H	4.6518740	3.3130440	-3.0551450
H	3.3300350	3.1034130	-1.8539870
C	1.8639770	-1.7687930	-1.3247240
O	1.0236030	-2.7837920	-0.8907440
C	1.5683050	-4.1004310	-0.8089330
H	2.3574730	-4.1672750	-0.0379920
H	0.7324380	-4.7545250	-0.5258580
H	1.9757350	-4.4314410	-1.7816500
C	4.0430420	-0.8931460	-1.9418370
Cl	5.7612030	-1.1596530	-2.2076730
H	-0.5655960	-1.7190640	-2.5157120
H	-0.4573730	1.2267790	-3.4993600
H	-1.0495000	-0.2787060	-4.4104750

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Ar = methylthiophene reactant

Ni	-0.3036000	0.2435010	0.0096120
P	-2.3225430	-0.6819770	0.1177340
P	0.5323460	-1.7788600	0.3760100
C	-2.1279970	-2.4206820	0.8085460
C	-3.0185050	-1.0304530	-1.5642490
C	-3.7433400	0.0521720	1.0306460
C	1.4410530	1.0147700	-0.2223310

C	-0.8621150	-3.0279020	0.1872730
C	1.0280430	-2.0460710	2.1443360
C	1.9484040	-2.4900070	-0.5670430
H	-3.0181920	-3.0372040	0.6004270
H	-2.0112470	-2.3433780	1.9031860
C	-4.3458830	-1.4702100	-1.7359880
C	-2.1797400	-0.9013160	-2.6872170
C	-4.2399010	1.2980550	0.5900770
C	-4.3201570	-0.5550190	2.1633360
C	1.9943360	1.0350590	-1.5191400
C	2.2140850	1.5470940	0.8236130
H	-0.5989500	-3.9926060	0.6517480
H	-1.0201540	-3.1963250	-0.8916740
C	1.8070220	-3.1506670	2.5417330
C	0.5612880	-1.1489030	3.1231280
C	3.2172420	-1.8896580	-0.4213860
C	1.8057560	-3.5823170	-1.4447200
C	-4.8234860	-1.7865190	-3.0137630
H	-5.0135160	-1.5499880	-0.8714020
C	-2.6624410	-1.2225100	-3.9646630
H	-1.1552530	-0.5333320	-2.5581340
C	-5.2996630	1.9117530	1.2683270
H	-3.7954410	1.7896880	-0.2801450
C	-5.3796090	0.0667730	2.8399930
H	-3.9545210	-1.5197650	2.5271990
C	3.2713690	1.5680870	-1.7566890
O	1.2075630	0.4862030	-2.5261250
C	3.5040520	2.0824140	0.6186260
H	1.7992520	1.5563890	1.8348650
C	2.1048040	-3.3543420	3.8952360
H	2.1938940	-3.8463320	1.7899940
C	0.8558660	-1.3570310	4.4782250
H	-0.0284800	-0.2786510	2.8136070
C	4.3176920	-2.3822520	-1.1328530
H	3.3445750	-1.0325430	0.2464000
C	2.9110850	-4.0707490	-2.1562720
H	0.8348490	-4.0669220	-1.5811490
C	-3.9812150	-1.6652590	-4.1295470
H	-5.8583170	-2.1217190	-3.1402960
H	-2.0083910	-1.1140230	-4.8359930
C	-5.8716080	1.3001500	2.3934320
H	-5.6745250	2.8780170	0.9163000
H	-5.8218170	-0.4187070	3.7163340

C	4.0175330	2.0825390	-0.6900840
H	3.7133100	1.5947260	-2.7549930
C	1.6873680	0.5979080	-3.8646370
O	4.3019020	2.6082910	1.6079320
C	1.6283880	-2.4599470	4.8655890
H	2.7158420	-4.2127910	4.1932810
H	0.4872940	-0.6515940	5.2301820
C	4.1688450	-3.4736410	-2.0006190
H	5.2944890	-1.9040210	-1.0104830
H	2.7854950	-4.9236060	-2.8315950
H	-4.3579460	-1.9080020	-5.1286600
H	-6.6989890	1.7849520	2.9219610
Cl	5.6229360	2.7398220	-1.0045920
H	2.6319720	0.0414080	-4.0080150
H	0.9106690	0.1554320	-4.5034340
H	1.8346020	1.6545820	-4.1527810
C	3.7667730	2.6569080	2.9285180
H	1.8652560	-2.6205590	5.9224170
H	5.0314510	-3.8564090	-2.5558280
H	2.8488710	3.2706090	2.9718070
H	4.5469940	3.1247040	3.5439850
H	3.5502200	1.6454500	3.3185460
C	-0.9881350	2.0237450	-0.1858140
C	-1.3297210	2.9718270	0.7738920
S	-1.3005770	2.6809650	-1.7900390
C	-1.8426990	4.1951190	0.2136300
C	-1.8997310	4.1968120	-1.1590660
H	-2.1591450	5.0475040	0.8245540
H	-2.2420860	4.9851540	-1.8298470
C	-1.1785860	2.7710060	2.2625720
H	-0.3473160	3.3700430	2.6790850
H	-2.0917590	3.0614880	2.8117860
H	-0.9744440	1.7140670	2.4978090

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Ar = methylthiophene TS

C	-2.0746310	-1.6003900	0.9866470
C	-3.1522640	-1.8308650	-1.5767460
C	-1.1993950	-1.4114320	-0.1244420
H	-3.6067350	-1.9032290	-2.5670780
Ni	0.3285170	-0.2120080	0.0069950
P	2.3678330	0.6754150	0.0632310
P	-0.5158030	1.8341670	0.1299900
C	2.1591860	2.4842570	0.5462510

C	3.1729690	0.8356250	-1.6032530
C	3.7401980	0.0637940	1.1350800
C	0.9057460	3.0376250	-0.1524640
C	-1.8873130	2.4516530	-0.9393310
C	-1.0729020	2.3268930	1.8339780
H	2.0276270	2.5205630	1.6419530
H	3.0521740	3.0787510	0.2896930
C	4.5287450	1.1861770	-1.7557800
C	2.3810880	0.6342360	-2.7499200
C	4.4362770	0.8691780	2.0588670
C	4.0659220	-1.3068730	1.0426360
H	1.0782390	3.0957870	-1.2414610
H	0.6584150	4.0497440	0.2095120
C	-3.1079180	1.7430440	-0.8987440
C	-1.7647510	3.5459000	-1.8183810
C	-1.9600450	3.3960100	2.0660050
C	-0.5516870	1.6219420	2.9368310
C	5.0792050	1.3419580	-3.0343880
H	5.1606970	1.3254810	-0.8721150
C	2.9331520	0.7988510	-4.0286460
H	1.3338840	0.3324470	-2.6332400
C	5.4420860	0.3187960	2.8670050
H	4.2042350	1.9345270	2.1531340
C	5.0774700	-1.8489610	1.8438950
H	3.5195590	-1.9541760	0.3488060
C	-4.1836250	2.1355270	-1.7035960
H	-3.2183790	0.8792910	-0.2349250
C	-2.8419490	3.9297310	-2.6306950
H	-0.8311430	4.1134640	-1.8737100
C	-2.3103540	3.7549580	3.3745370
H	-2.3870100	3.9432570	1.2194710
C	-0.8944850	1.9882230	4.2460410
H	0.1230870	0.7763500	2.7586690
C	4.2814650	1.1519690	-4.1729490
H	6.1359310	1.6088420	-3.1428660
H	2.3102800	0.6397800	-4.9152020
C	5.7677730	-1.0397620	2.7588750
H	5.9754820	0.9576100	3.5791240
H	5.3216770	-2.9128210	1.7572520
C	-4.0543240	3.2295390	-2.5722950
H	-5.1240440	1.5774360	-1.6548490
H	-2.7324370	4.7851530	-3.3059090
C	-1.7761040	3.0554350	4.4667350

H	-3.0052060	4.5848350	3.5418250
H	-0.4781730	1.4341640	5.0940630
H	4.7142890	1.2720540	-5.1716630
H	6.5546880	-1.4681370	3.3883060
H	-4.8954890	3.5332560	-3.2040490
H	-2.0514870	3.3387500	5.4879410
H	-1.6701820	-1.4877660	1.9915230
C	-3.4353300	-1.9088180	0.8442360
O	-4.3096640	-2.0829790	1.8904980
C	-3.7945030	-1.9424350	3.2129950
H	-3.0094600	-2.6911110	3.4234660
H	-4.6492850	-2.1155720	3.8803800
H	-3.3922560	-0.9279460	3.3867210
C	-1.8060140	-1.4939010	-1.4166830
O	-0.9720720	-1.2037430	-2.4808740
C	-1.4285910	-1.5373970	-3.7935740
H	-2.2741800	-0.8963500	-4.1011960
H	-0.5767080	-1.3575340	-4.4628710
H	-1.7246260	-2.5994110	-3.8546860
C	-3.9650980	-2.0439290	-0.4557760
Cl	-5.6586180	-2.4602940	-0.6838490
C	0.4763590	-2.1376810	0.0027140
C	1.7926900	-4.2404570	-0.6317170
C	1.5848640	-4.1143060	0.7234590
H	2.2981400	-5.0424170	-1.1705430
H	1.9432590	-4.8475350	1.4535920
C	0.8605890	-2.9434950	1.1002260
C	0.5527880	-2.6544880	2.5468870
H	-0.4053780	-3.1097040	2.8639530
H	1.3359480	-3.0694010	3.2027730
H	0.4918970	-1.5737440	2.7519360
S	1.0875270	-2.9056390	-1.4981600

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Ar = methylbenzothiophene reactant

Ni	-0.1011150	-0.1793170	-0.0492820
P	-1.6962240	-1.7388940	0.0781410
P	1.3238790	-1.7454780	0.6232950
C	-0.9834890	-3.2299350	0.9765840
C	-2.0742150	-2.4579910	-1.5891630
C	-3.3645250	-1.4883220	0.8191570
C	1.3142620	1.0804740	-0.3865410
C	0.4685200	-3.4157710	0.5159230
C	1.6108020	-1.5906000	2.4498460

C	3.0202850	-2.0289730	-0.0400070
H	-1.5874550	-4.1329270	0.7880190
H	-1.0106940	-3.0163240	2.0587850
C	-3.1789160	-3.3093700	-1.7897040
C	-1.2069480	-2.1841470	-2.6637660
C	-4.2020070	-0.5085130	0.2456670
C	-3.8202490	-2.2082120	1.9401090
C	2.0227280	0.9780460	-1.6021390
C	1.7125290	2.0837170	0.5134120
H	0.9940620	-4.1737920	1.1201350
H	0.4902830	-3.7392800	-0.5388110
C	2.5866280	-2.3619180	3.1120870
C	0.7980930	-0.7192190	3.1990270
C	3.9898550	-1.0216300	0.1501250
C	3.3739170	-3.1938260	-0.7485230
C	-3.4069700	-3.8843970	-3.0460730
H	-3.8727380	-3.5100870	-0.9666040
C	-1.4390020	-2.7648910	-3.9196950
H	-0.3599370	-1.5041470	-2.5161260
C	-5.4728700	-0.2664680	0.7779470
H	-3.8496320	0.0773020	-0.6087480
C	-5.0938110	-1.9587030	2.4726450
H	-3.1917540	-2.9708190	2.4089210
C	3.0900820	1.8415900	-1.8975490
O	1.6092170	-0.0279400	-2.4749050
C	2.7854110	2.9606550	0.2502530
H	1.1545010	2.2036390	1.4453920
C	2.7389990	-2.2657810	4.5009360
H	3.2407200	-3.0278800	2.5394250
C	0.9502330	-0.6274680	4.5901590
H	0.0493390	-0.1053900	2.6847310
C	5.2878680	-1.1872120	-0.3480790
H	3.7292950	-0.1047460	0.6871590
C	4.6747800	-3.3538280	-1.2473940
H	2.6425020	-3.9899190	-0.9151570
C	-2.5362350	-3.6143640	-4.1125910
H	-4.2718030	-4.5393990	-3.1951530
H	-0.7664090	-2.5418680	-4.7544800
C	-5.9225180	-0.9906150	1.8918790
H	-6.1081910	0.5020010	0.3269220
H	-5.4364190	-2.5264890	3.3440990
C	3.4675220	2.8202810	-0.9717420
H	3.6459600	1.7784330	-2.8353220

C	2.3770410	-0.2185490	-3.6628010
O	3.2134980	3.9506050	1.1006680
C	1.9201750	-1.4000960	5.2421240
H	3.5039410	-2.8646650	5.0062380
H	0.3131950	0.0551050	5.1618220
C	5.6346980	-2.3530620	-1.0458010
H	6.0282470	-0.3962180	-0.1933730
H	4.9373250	-4.2677440	-1.7906120
H	-2.7195850	-4.0601120	-5.0957740
H	-6.9155100	-0.7957360	2.3098630
Cl	4.8147030	3.8897460	-1.3555870
H	3.4319970	-0.4488920	-3.4289230
H	1.9271180	-1.0771760	-4.1804090
H	2.3309670	0.6657140	-4.3247660
C	2.4717450	4.1488090	2.3048320
H	2.0438960	-1.3245320	6.3274270
H	6.6508610	-2.4803180	-1.4331160
H	1.4150030	4.3900810	2.0942070
H	2.9503190	5.0011840	2.8053420
H	2.5219160	3.2623200	2.9630510
C	-1.3009440	1.2836910	-0.2456380
C	-1.8525620	2.0011970	-1.2888990
C	-2.7407070	3.0659470	-0.8562130
C	-2.8462500	3.1682770	0.5614010
C	-3.6500240	4.1344520	1.1815340
H	-3.7148830	4.1947070	2.2730080
C	-4.3692140	5.0250700	0.3743190
H	-5.0013290	5.7882460	0.8402970
C	-4.2813320	4.9453700	-1.0310910
H	-4.8477640	5.6509170	-1.6484050
C	-3.4783370	3.9798810	-1.6446680
H	-3.4169680	3.9312970	-2.7374460
C	-1.5581120	1.7524400	-2.7459040
H	-2.4523610	1.4124190	-3.3017560
H	-1.2042660	2.6733900	-3.2447650
H	-0.7748390	0.9904070	-2.8625350
S	-1.8509890	1.9252850	1.3230470

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Ar = methylbenzothiophene TS

C	1.7130620	2.1621420	0.3978690
C	2.7598110	1.7954530	-2.1586740
C	0.9926470	1.3237910	-0.5003510
H	3.2144220	1.6458430	-3.1399680

Ni	-0.1160020	-0.2313600	-0.0418000
P	-1.7943680	-1.6860310	0.0793600
P	1.2505680	-1.7776570	0.7638960
C	-1.1687340	-3.1065880	1.1498840
C	-2.1932810	-2.5841290	-1.4987180
C	-3.4589520	-1.2891710	0.7678900
C	0.2943310	-3.3999120	0.7794440
C	2.8880950	-2.2032320	0.0243150
C	1.6513630	-1.5619890	2.5655420
H	-1.2387000	-2.7805880	2.2025190
H	-1.7937680	-4.0073730	1.0290150
C	-3.3793480	-3.3250370	-1.6676550
C	-1.2464930	-2.5561240	-2.5412350
C	-4.0922690	-2.0416880	1.7762660
C	-4.1058310	-0.1429840	0.2609400
H	0.3448070	-3.8224340	-0.2393880
H	0.7451010	-4.1281010	1.4744420
C	3.8131540	-1.1509300	-0.1479550
C	3.2404790	-3.4969980	-0.4083470
C	2.7241880	-2.2332840	3.1846760
C	0.8267680	-0.7258950	3.3433680
C	-3.6083040	-4.0329880	-2.8549500
H	-4.1337870	-3.3377330	-0.8741570
C	-1.4731910	-3.2765290	-3.7230690
H	-0.3397160	-1.9523900	-2.4226890
C	-5.3524840	-1.6602990	2.2603390
H	-3.6103040	-2.9316860	2.1920700
C	-5.3669590	0.2297000	0.7398000
H	-3.6116580	0.4678000	-0.5019200
C	5.0649890	-1.3933780	-0.7253320
H	3.5513540	-0.1360000	0.1690140
C	4.4927100	-3.7343860	-0.9945770
H	2.5452530	-4.3329570	-0.2868030
C	2.9597080	-2.0767420	4.5569250
H	3.3863490	-2.8712330	2.5901640
C	1.0588390	-0.5778330	4.7183080
H	0.0047020	-0.1823440	2.8633140
C	-2.6537470	-4.0149070	-3.8825220
H	-4.5374520	-4.5994010	-2.9790920
H	-0.7292170	-3.2549600	-4.5267140
C	-5.9934250	-0.5280580	1.7403450
H	-5.8338940	-2.2532630	3.0453740
H	-5.8528280	1.1253560	0.3404870

C	5.4082530	-2.6854160	-1.1511100
H	5.7710920	-0.5660820	-0.8485170
H	4.7533420	-4.7459240	-1.3239570
C	2.1259650	-1.2521970	5.3270170
H	3.8005980	-2.5984050	5.0262770
H	0.4089300	0.0738490	5.3116170
H	-2.8340930	-4.5699550	-4.8090140
H	-6.9766290	-0.2312820	2.1200250
H	6.3862660	-2.8728620	-1.6063280
H	2.3131260	-1.1307490	6.3990410
H	1.2869700	2.3330530	1.3876460
C	2.8968470	2.8232250	0.0491630
O	3.6039620	3.6489700	0.8868540
C	3.0619090	3.8884620	2.1868180
H	2.0603560	4.3501990	2.1275000
H	3.7591950	4.5857060	2.6697850
H	3.0037570	2.9575700	2.7791100
C	1.5840390	1.1292690	-1.7887390
O	0.9816300	0.1782320	-2.5981380
C	1.4624010	0.0531600	-3.9375020
H	2.5020960	-0.3194650	-3.9612050
H	0.8042880	-0.6774700	-4.4268770
H	1.4024910	1.0153990	-4.4780930
C	3.4069160	2.6446390	-1.2548440
Cl	4.8696420	3.4822180	-1.7536810
C	-0.8061710	1.5276310	-0.3392780
C	-1.5034480	2.2744180	-1.3035380
C	-2.4253980	3.2356110	-0.7403800
C	-2.4499590	3.2365810	0.6866050
C	-3.2877810	4.0822380	1.4233910
H	-3.2872560	4.0556030	2.5178980
C	-4.1234550	4.9692610	0.7311880
H	-4.7805660	5.6435380	1.2898760
C	-4.1147380	4.9978750	-0.6782490
H	-4.7692000	5.6975270	-1.2088850
C	-3.2803980	4.1486190	-1.4087930
H	-3.2908650	4.1927280	-2.5027050
S	-1.3347570	2.0279940	1.3179800
C	-1.2667600	2.1737610	-2.7838760
H	-2.0603840	2.6817100	-3.3532870
H	-0.3060770	2.6475180	-3.0686570
H	-1.2176860	1.1285810	-3.1225980

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Ar = methyl-parabiphenyl reactant

C	1.2693540	2.3603920	0.9342100
C	1.7747280	3.2627540	-1.6503070
C	0.9940070	1.4913620	-0.1375340
H	1.9819410	3.6483410	-2.6506930
Ni	0.3429140	-0.3102160	0.0603530
P	-0.4260640	-2.3894330	0.0457000
P	2.3937460	-1.1792280	0.1829450
C	0.9818530	-3.5388040	0.5333060
C	-0.7916230	-2.9727080	-1.6770000
C	-1.8834940	-2.9857400	1.0072440
C	2.2607550	-3.0280420	-0.1448480
C	3.8217550	-0.6142110	-0.8398850
C	3.0878130	-1.1613150	1.9052210
H	1.0933720	-3.4940430	1.6303050
H	0.7613770	-4.5821130	0.2524740
C	-1.4636240	-4.1870980	-1.9194230
C	-0.3317430	-2.2068060	-2.7651400
C	-1.7749550	-3.9174340	2.0588760
C	-3.1513960	-2.4493650	0.6951440
H	2.1869900	-3.1721310	-1.2363660
H	3.1552780	-3.5635850	0.2138980
C	4.2894210	0.7050440	-0.6584520
C	4.4406070	-1.4306930	-1.8065740
C	4.4501710	-1.4083440	2.1657470
C	2.2111620	-0.9462580	2.9852720
C	-1.6644560	-4.6323950	-3.2318990
H	-1.8447280	-4.7796980	-1.0810450
C	-0.5315150	-2.6600350	-4.0779050
H	0.1712170	-1.2507000	-2.5782810
C	-2.9116600	-4.3096340	2.7805320
H	-0.8058690	-4.3502550	2.3237220
C	-4.2828340	-2.8466440	1.4173630
H	-3.2528500	-1.7147040	-0.1090210
C	5.3594290	1.1874090	-1.4215610
H	3.8132770	1.3581660	0.0788600
C	5.5105110	-0.9418520	-2.5704020
H	4.1006060	-2.4569850	-1.9716680
C	4.9214010	-1.4468750	3.4843650
H	5.1478430	-1.5572240	1.3351970
C	2.6838750	-0.9904450	4.3049250
H	1.1554170	-0.7344230	2.7837090
C	-1.1962470	-3.8705840	-4.3131470

H	-2.1927890	-5.5746260	-3.4116730
H	-0.1743530	-2.0596260	-4.9211210
C	-4.1671320	-3.7764870	2.4607170
H	-2.8124680	-5.0373190	3.5928440
H	-5.2584890	-2.4189850	1.1662850
C	5.9735290	0.3663660	-2.3783190
H	5.7090290	2.2132820	-1.2690510
H	5.9845700	-1.5905900	-3.3145280
C	4.0395350	-1.2404100	4.5559140
H	5.9832100	-1.6340780	3.6760650
H	1.9923220	-0.8209100	5.1368480
H	-1.3570560	-4.2186540	-5.3388340
H	-5.0539160	-4.0829390	3.0250130
H	6.8102870	0.7462920	-2.9736080
H	4.4116250	-1.2683180	5.5852920
C	-1.4229900	0.4698530	0.0492190
C	-3.4551190	1.2418030	1.1709110
H	-3.8016430	1.5239260	-2.2071620
H	1.0789550	2.0180080	1.9544390
H	-4.0095520	1.3969410	2.1051910
C	-2.1520490	0.7180020	1.2429270
C	1.7906780	3.6599510	0.7558650
O	2.0801620	4.5362860	1.7753990
C	1.7673700	4.1271700	3.1051510
H	0.6888220	3.9166200	3.2210260
H	2.0439080	4.9756340	3.7454250
H	2.3498600	3.2372710	3.4065880
C	1.2627200	1.9729450	-1.4374470
O	1.0071780	1.0897770	-2.4854130
C	1.2507050	1.5590890	-3.8101500
H	2.3144210	1.8184890	-3.9620620
H	0.9852310	0.7292660	-4.4799510
H	0.6214490	2.4350560	-4.0531670
C	2.0375500	4.0958520	-0.5569250
Cl	2.6875470	5.7091270	-0.8427520
C	-4.0921640	1.5279840	-0.0537850
C	-3.3616190	1.2802530	-1.2331180
C	-2.0557070	0.7757870	-1.1746300
C	-5.4743530	2.0695900	-0.0957560
C	-6.3839940	1.6716120	-1.1010270
C	-5.9254200	3.0009410	0.8660490
C	-7.6873730	2.1810780	-1.1429680
H	-6.0687220	0.9333370	-1.8460440

C	-7.2297220	3.5082670	0.8279820
H	-5.2314190	3.3528640	1.6364510
C	-8.1190030	3.1015000	-0.1770310
H	-8.3738570	1.8498280	-1.9299220
H	-7.5497820	4.2367270	1.5810390
H	-9.1383780	3.5000640	-0.2087310
C	-1.5664750	0.4018460	2.6019600
H	-1.3133200	-0.6703150	2.6893060
H	-0.6389230	0.9710310	2.7845250
H	-2.2698340	0.6422740	3.4164340
H	-1.5104780	0.6331240	-2.1127040

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Ar = methyl-parabiphenyl TS

C	0.8962700	2.6707080	0.2739400
C	2.2749860	2.6273840	-2.1383540
C	0.7257720	1.5257720	-0.5556260
H	2.8540150	2.6258070	-3.0638150
Ni	0.3581610	-0.3419390	-0.0507600
P	-0.5331620	-2.3781220	0.0059000
P	2.2020210	-1.1321000	0.8687960
C	0.6403030	-3.4291180	1.0502090
C	-0.5405130	-3.3454630	-1.5840770
C	-2.1960880	-2.7488520	0.7255770
C	2.0900320	-3.0095560	0.7644760
C	3.9052530	-0.7359910	0.2726550
C	2.3444450	-0.8778080	2.7073460
H	0.3936850	-3.2392040	2.1095850
H	0.4944870	-4.5048030	0.8551620
C	-1.3845500	-4.4516270	-1.8023150
C	0.3724360	-2.9716050	-2.5900290
C	-2.4316410	-3.7757180	1.6623620
C	-3.2745580	-1.9349320	0.3219030
H	2.3725410	-3.2994060	-0.2628670
H	2.7911850	-3.4975950	1.4624570
C	4.2632810	0.6265170	0.1864190
C	4.8397060	-1.7107920	-0.1301660
C	3.5743870	-0.9464780	3.3908230
C	1.1678620	-0.6428770	3.4460530
C	-1.3088220	-5.1748850	-3.0005260
H	-2.1121520	-4.7432190	-1.0381700
C	0.4561500	-3.7066720	-3.7811050
H	1.0023670	-2.0887010	-2.4355620
C	-3.7183680	-3.9864330	2.1791080

H	-1.6148470	-4.4236720	1.9942520
C	-4.5596980	-2.1529310	0.8335490
H	-3.1055960	-1.1178430	-0.3865800
C	5.5303870	1.0010660	-0.2763030
H	3.5448340	1.3993260	0.4790670
C	6.1053180	-1.3319240	-0.6020190
H	4.5921680	-2.7749430	-0.0732000
C	3.6223540	-0.7891960	4.7826840
H	4.5010060	-1.1120710	2.8319960
C	1.2155340	-0.4975220	4.8394570
H	0.2095870	-0.5695360	2.9189350
C	-0.3849450	-4.8085270	-3.9897140
H	-1.9764250	-6.0279950	-3.1623840
H	1.1732200	-3.4127440	-4.5553390
C	-4.7850300	-3.1780400	1.7635200
H	-3.8859420	-4.7877560	2.9068310
H	-5.3840160	-1.5071560	0.5148840
C	6.4549090	0.0231780	-0.6725150
H	5.7910360	2.0625570	-0.3349630
H	6.8215290	-2.1016110	-0.9092130
C	2.4441070	-0.5683380	5.5105170
H	4.5861410	-0.8375260	5.3007470
H	0.2917540	-0.3192360	5.4000260
H	-0.3265700	-5.3760660	-4.9242960
H	-5.7889060	-3.3419260	2.1689170
H	7.4441030	0.3174260	-1.0383650
H	2.4847480	-0.4453650	6.5977810
C	-1.0376300	0.9682170	-0.4411410
C	-2.9427270	1.5965990	1.0151300
H	-3.8306750	1.7686860	-2.2622780
H	0.3164330	2.7196900	1.1973340
H	-3.3419360	1.7013870	2.0299900
C	-1.6163380	1.2150490	0.8431280
C	1.7009260	3.7650410	-0.0629640
O	1.8691830	4.8828550	0.7169630
C	1.1419730	4.9469360	1.9436760
H	0.0515670	4.9111180	1.7700320
H	1.4090720	5.9131320	2.3917830
H	1.4325420	4.1312770	2.6305390
C	1.4821640	1.5302280	-1.7701740
O	1.4734340	0.3538980	-2.5057620
C	2.0961820	0.3749910	-3.7912540
H	3.1882700	0.5196940	-3.7100950

H	1.8947930	-0.6069690	-4.2403740
H	1.6655850	1.1631480	-4.4357160
C	2.3786230	3.7405530	-1.3005640
Cl	3.3605620	5.1107720	-1.7984260
C	-3.7858190	1.8014790	-0.1010290
C	-3.2151110	1.5863840	-1.3731930
C	-1.8868670	1.1769980	-1.5768760
H	-0.9998350	1.0763570	1.7398020
C	-5.1985400	2.2174020	0.0560310
C	-6.1967710	1.7902330	-0.8509410
C	-5.6015440	3.0540280	1.1228800
C	-7.5318980	2.1808580	-0.6991730
H	-5.9244750	1.1214150	-1.6741290
C	-6.9373250	3.4415320	1.2779790
H	-4.8488950	3.4303250	1.8233390
C	-7.9121580	3.0080710	0.3678030
H	-8.2832910	1.8284740	-1.4142960
H	-7.2170980	4.0978380	2.1092900
H	-8.9567350	3.3134490	0.4871520
C	-1.4105560	1.0036600	-2.9965460
H	-0.6713160	1.7814580	-3.2641560
H	-0.9149790	0.0325420	-3.1480740
H	-2.2500150	1.0850940	-3.7052760

X = Br

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R = OMe reactant

C	1.4108450	1.8665120	0.8944370
C	2.3833920	2.5956060	-1.6146480
C	1.1387750	1.0247550	-0.1983060
H	2.7722140	2.9095420	-2.5853300
Ni	0.1709470	-0.6282970	-0.0527250
P	-0.9626520	-2.5302810	-0.1010300
P	1.9968890	-1.8381100	0.2858030
C	0.1661610	-3.9025940	0.5178460
C	-1.2976720	-3.0782360	-1.8410060
C	-2.5757280	-2.8195690	0.7466890
C	1.5733710	-3.6423880	-0.0380200
C	3.6179220	-1.5679790	-0.5516800
C	2.4537660	-1.8797040	2.0837480
H	0.1838380	-3.8537530	1.6200800
H	-0.2113780	-4.8958320	0.2230940
C	-2.1403120	-4.1709180	-2.1258310
C	-0.6493670	-2.4098730	-2.8970620
C	-2.7270850	-3.7303170	1.8105430
C	-3.6932280	-2.0670880	0.3259180
H	1.5808030	-3.7988760	-1.1303580
H	2.3204370	-4.3172800	0.4118860
C	4.2942330	-0.3518670	-0.3160850
C	4.1868020	-2.5058840	-1.4352800
C	3.6746780	-2.4232790	2.5294180
C	1.5258690	-1.3977340	3.0270370
C	-2.3238170	-4.5943170	-3.4480010
H	-2.6670310	-4.6832510	-1.3136790
C	-0.8344140	-2.8400280	-4.2197520
H	-0.0102320	-1.5462370	-2.6771000
C	-3.9719050	-3.8923980	2.4361250
H	-1.8791760	-4.3262950	2.1601330
C	-4.9338460	-2.2338520	0.9527700
H	-3.5917360	-1.3450040	-0.4897760
C	5.5178830	-0.0903850	-0.9438970
H	3.8605740	0.3943050	0.3564000
C	5.4116180	-2.2379700	-2.0638220
H	3.6849710	-3.4559640	-1.6398760

C	3.9584800	-2.4921800	3.8991790
H	4.4126930	-2.7800450	1.8032290
C	1.8129760	-1.4732280	4.3984290
H	0.5850030	-0.9545480	2.6785780
C	-1.6692580	-3.9304510	-4.4967740
H	-2.9846680	-5.4410890	-3.6614920
H	-0.3314390	-2.3146320	-5.0382950
C	-5.0778530	-3.1467150	2.0077320
H	-4.0750060	-4.6084340	3.2583540
H	-5.7902950	-1.6410500	0.6165010
C	6.0804910	-1.0317430	-1.8180330
H	6.0287940	0.8583070	-0.7519290
H	5.8438700	-2.9789900	-2.7445550
C	3.0268270	-2.0195580	4.8358860
H	4.9123870	-2.9109750	4.2367130
H	1.0883850	-1.0967010	5.1281500
H	-1.8173770	-4.2601060	-5.5304490
H	-6.0497000	-3.2750050	2.4955440
H	7.0375050	-0.8242610	-2.3078770
H	3.2517640	-2.0717040	5.9062940
C	-1.4019870	0.4653170	-0.1755570
C	-3.1461400	1.6618280	-1.4372480
H	-3.7820080	1.8622620	1.9014990
H	1.0090750	1.5953000	1.8739090
H	-3.5277160	2.0052670	-2.4049690
C	-1.9618390	0.9080870	-1.3867820
C	2.1657710	3.0533330	0.7732320
O	2.4645990	3.8982170	1.8168270
C	1.9460090	3.5660820	3.1027830
H	0.8414060	3.5384750	3.0995930
H	2.2890670	4.3664420	3.7722850
H	2.3355420	2.5957220	3.4610930
C	1.6354810	1.4169640	-1.4593060
O	1.3488370	0.5649230	-2.5244300
C	1.8319770	0.9431610	-3.8119250
H	2.9354070	1.0062750	-3.8314740
H	1.5061160	0.1529390	-4.5026250
H	1.4042530	1.9087200	-4.1395160
C	2.6476340	3.4002480	-0.4999000
Br	3.6821730	5.0038230	-0.7325670
C	-3.8115140	2.0274250	-0.2532320
C	-3.2542530	1.6100690	0.9776900
C	-2.0791570	0.8450400	1.0073080

H	-1.4534830	0.6704160	-2.3270970
C	-5.0583220	2.8343070	-0.2829120
C	-5.3127670	3.8270780	0.6895000
C	-6.0308740	2.6363900	-1.2885780
C	-6.4891620	4.5856960	0.6611310
H	-4.5599460	4.0280280	1.4589790
C	-7.2055590	3.3972270	-1.3211310
H	-5.8701170	1.8576560	-2.0415470
C	-7.4431890	4.3753570	-0.3446620
H	-6.6553920	5.3564260	1.4217270
H	-7.9453170	3.2183800	-2.1091420
H	-8.3620870	4.9702700	-0.3691630
O	-1.5097280	0.3917670	2.1960830
C	-2.1861190	0.7064120	3.4122770
H	-1.5917360	0.2498200	4.2161000
H	-2.2413250	1.7980700	3.5789740
H	-3.2063300	0.2827130	3.4323720

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R = OMe TS

C	1.2133790	2.0073120	0.8726020
C	2.3898680	2.4958400	-1.6030530
C	0.7455680	1.2501300	-0.2415010
H	2.8898460	2.6878790	-2.5538770
Ni	0.1522430	-0.6152170	-0.0519000
P	-1.1113890	-2.4196540	-0.0192860
P	1.9347550	-1.8812890	0.2342200
C	-0.0184980	-3.8355730	0.5755520
C	-1.6017930	-3.0233690	-1.7079950
C	-2.6792370	-2.6103250	0.9404020
C	1.3801460	-3.6619770	-0.0389560
C	3.5165200	-1.7384770	-0.7098270
C	2.5256070	-1.9546890	1.9962490
H	0.0449240	-3.7677360	1.6756840
H	-0.4511290	-4.8170820	0.3177800
C	-2.5314800	-4.0648850	-1.8973890
C	-0.9877400	-2.4374800	-2.8314800
C	-2.8569780	-3.5471310	1.9780760
C	-3.7322430	-1.7174370	0.6433430
H	1.3341660	-3.8316290	-1.1289010
H	2.0990350	-4.3806260	0.3896420
C	4.2136610	-0.5134560	-0.6246230
C	4.0270840	-2.7523460	-1.5449570
C	3.7556150	-2.5367620	2.3607120

C	1.6842380	-1.4415780	3.0025700
C	-2.8331000	-4.5183870	-3.1879200
H	-3.0325150	-4.5143350	-1.0332960
C	-1.2876290	-2.8974690	-4.1224010
H	-0.2825130	-1.6110770	-2.6837090
C	-4.0619890	-3.5967520	2.6949450
H	-2.0602080	-4.2522220	2.2328080
C	-4.9361260	-1.7750580	1.3550140
H	-3.6083710	-0.9712380	-0.1484250
C	5.3998560	-0.3179620	-1.3414050
H	3.8259460	0.2932230	0.0061690
C	5.2111850	-2.5497560	-2.2695390
H	3.5101760	-3.7125060	-1.6334920
C	4.1316640	-2.6124320	3.7081510
H	4.4290820	-2.9203040	1.5869290
C	2.0591680	-1.5268940	4.3516510
H	0.7391450	-0.9657360	2.7148280
C	-2.2092850	-3.9374480	-4.3025720
H	-3.5611080	-5.3251620	-3.3250260
H	-0.8067960	-2.4360150	-4.9915290
C	-5.1055080	-2.7151750	2.3831830
H	-4.1856730	-4.3344690	3.4951740
H	-5.7432290	-1.0782280	1.1068860
C	5.9027200	-1.3354190	-2.1667870
H	5.9292560	0.6365930	-1.2573800
H	5.5967880	-3.3496870	-2.9108350
C	3.2824620	-2.1115670	4.7064210
H	5.0929220	-3.0613930	3.9802430
H	1.3975580	-1.1290640	5.1287290
H	-2.4482080	-4.2917310	-5.3108500
H	-6.0471250	-2.7580490	2.9403610
H	6.8293420	-1.1805620	-2.7291820
H	3.5784650	-2.1716140	5.7590080
C	-1.0177310	0.9515690	-0.2315920
C	-2.9371410	1.8793800	-1.4988910
H	-3.5887060	2.0180510	1.8344040
H	0.7466330	1.8174790	1.8383360
H	-3.3631120	2.1360260	-2.4744910
C	-1.6766030	1.2857240	-1.4506690
C	2.2102740	2.9877180	0.7774580
O	2.6745890	3.7279320	1.8380520
C	2.0835290	3.4952590	3.1152640
H	1.0011530	3.7175430	3.1061650

H	2.5918320	4.1846670	3.8025800
H	2.2430800	2.4551690	3.4524370
C	1.4023320	1.5131420	-1.4898880
O	1.0330980	0.7124510	-2.5583170
C	1.6698000	0.9450010	-3.8164990
H	2.7584900	0.7717000	-3.7526020
H	1.2279690	0.2202780	-4.5135340
H	1.4774670	1.9686840	-4.1855630
C	2.7878220	3.2369020	-0.4819290
Br	4.1447480	4.5755640	-0.6785200
C	-3.6410690	2.1981360	-0.3196460
C	-3.0264730	1.8569600	0.9113350
C	-1.7756830	1.2425670	0.9569850
H	-1.1556640	1.0863140	-2.3879940
C	-4.9710100	2.8450550	-0.3510330
C	-5.3755930	3.7446150	0.6634320
C	-5.8882580	2.5855850	-1.3970710
C	-6.6363580	4.3514180	0.6363050
H	-4.6753370	3.9983930	1.4661450
C	-7.1470120	3.1952250	-1.4266830
H	-5.6177970	1.8734540	-2.1835370
C	-7.5313930	4.0811630	-0.4089200
H	-6.9167900	5.0520230	1.4304660
H	-7.8382940	2.9687140	-2.2457910
H	-8.5168030	4.5576700	-0.4320060
O	-1.2020890	0.8196380	2.1472400
C	-1.9347600	1.0318770	3.3563980
H	-1.3069410	0.6255760	4.1610060
H	-2.1130140	2.1067860	3.5409120
H	-2.8990150	0.4949180	3.3399850

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R = OEt reactant

C	1.4248340	1.8603660	0.8960440
C	2.3870390	2.6480200	-1.5993520
C	1.1566730	1.0391170	-0.2132060
H	2.7714410	2.9848390	-2.5640930
Ni	0.2002190	-0.6229590	-0.0962600
P	-0.9247590	-2.5286160	-0.1835070
P	2.0399020	-1.8343620	0.1739140
C	0.2192270	-3.9113860	0.3817000
C	-1.2745790	-3.0339350	-1.9338680
C	-2.5273740	-2.8493010	0.6720850
C	1.6137470	-3.6296320	-0.1955590

C	3.6324730	-1.5283490	-0.7054050
C	2.5623060	-1.9404650	1.9509000
H	0.2578210	-3.8902620	1.4843580
H	-0.1594720	-4.8986530	0.0688580
C	-2.1274300	-4.1134100	-2.2379260
C	-0.6249220	-2.3496080	-2.9789130
C	-2.6616240	-3.7844180	1.7169450
C	-3.6544900	-2.0966720	0.2780110
H	1.5972840	-3.7538320	-1.2918030
H	2.3726170	-4.3146490	0.2176250
C	4.3139950	-0.3204770	-0.4442070
C	4.1762230	-2.4310010	-1.6399380
C	3.8006910	-2.4957120	2.3292120
C	1.6684440	-1.5024130	2.9463600
C	-2.3202220	-4.5075460	-3.5678590
H	-2.6545840	-4.6385480	-1.4343520
C	-0.8189840	-2.7505980	-4.3094030
H	0.0221460	-1.4958520	-2.7445820
C	-3.8993290	-3.9701220	2.3501220
H	-1.8059010	-4.3818880	2.0444430
C	-4.8878070	-2.2868330	0.9125520
H	-3.5663840	-1.3570080	-0.5233810
C	5.5183000	-0.0325880	-1.0973990
H	3.8999320	0.3986050	0.2688680
C	5.3816100	-2.1367340	-2.2938240
H	3.6698910	-3.3739910	-1.8651520
C	4.1347010	-2.6196630	3.6835440
H	4.5125320	-2.8191090	1.5624740
C	2.0049540	-1.6337620	4.3020560
H	0.7140820	-1.0496860	2.6513380
C	-1.6644290	-3.8277530	-4.6055050
H	-2.9891290	-5.3441400	-3.7958840
H	-0.3148430	-2.2124480	-5.1188980
C	-5.0149010	-3.2238230	1.9484340
H	-3.9895500	-4.7055490	3.1566330
H	-5.7521570	-1.6943200	0.5965390
C	6.0560500	-0.9390610	-2.0225720
H	6.0335180	0.9093560	-0.8848100
H	5.7945540	-2.8507460	-3.0142520
C	3.2359640	-2.1912710	4.6721700
H	5.1018840	-3.0470680	3.9683900
H	1.3048130	-1.2926660	5.0715340
H	-1.8197450	-4.1344440	-5.6451720

H	-5.9813080	-3.3710850	2.4416810
H	6.9980880	-0.7111980	-2.5320060
H	3.4995650	-2.2868590	5.7306730
C	-1.3802150	0.4618440	-0.2264780
C	-3.1013960	1.6309520	-1.5470860
H	-3.8289150	1.8563970	1.7688830
H	1.0255970	1.5668990	1.8701400
H	-3.4595860	1.9614520	-2.5281600
C	-1.9118120	0.8903190	-1.4560330
C	2.1711260	3.0547760	0.7977880
O	2.4663750	3.8805400	1.8577390
C	1.9560460	3.5170010	3.1382000
H	0.8516620	3.4802150	3.1388780
H	2.2952110	4.3058240	3.8232400
H	2.3555720	2.5426410	3.4742070
C	1.6484510	1.4607960	-1.4668260
O	1.3675030	0.6282810	-2.5487450
C	1.8501940	1.0342910	-3.8279290
H	2.9532070	1.1043330	-3.8439340
H	1.5304000	0.2555230	-4.5343030
H	1.4169140	2.0032270	-4.1376810
C	2.6474670	3.4315020	-0.4688490
Br	3.6696420	5.0472650	-0.6703280
C	-3.8017190	1.9990890	-0.3846080
C	-3.2728120	1.5988950	0.8639040
C	-2.0907200	0.8446910	0.9365620
H	-1.3744850	0.6515130	-2.3795040
C	-5.0565400	2.7910530	-0.4542520
C	-5.3475500	3.7910170	0.5003560
C	-6.0005720	2.5706440	-1.4822320
C	-6.5318170	4.5349250	0.4335370
H	-4.6170630	4.0092130	1.2864970
C	-7.1830770	3.3166200	-1.5530830
H	-5.8112100	1.7858760	-2.2222000
C	-7.4572450	4.3022180	-0.5938520
H	-6.7266350	5.3117650	1.1810460
H	-7.9002840	3.1202970	-2.3576330
H	-8.3822590	4.8855840	-0.6482790
O	-1.5542460	0.4100400	2.1464680
C	-2.2781670	0.7303520	3.3447630
H	-2.3659010	1.8297650	3.4466060
H	-3.3021290	0.3148090	3.2835140
C	-1.5296700	0.1401210	4.5296350

H	-0.5154740	0.5631750	4.6094050
H	-2.0673210	0.3673720	5.4650160
H	-1.4488850	-0.9547750	4.4398810
100			
R = OEt TS			
C	1.1934680	2.0153300	0.8483630
C	2.4130530	2.5164930	-1.6041390
C	0.7576290	1.2514260	-0.2739340
H	2.9296200	2.7134550	-2.5450160
Ni	0.1774460	-0.6175990	-0.0882160
P	-1.0771900	-2.4291800	-0.0490840
P	1.9737310	-1.8820890	0.1263740
C	0.0373310	-3.8480780	0.4955870
C	-1.6005830	-3.0104900	-1.7362280
C	-2.6240780	-2.6478610	0.9380380
C	1.4143350	-3.6590370	-0.1614080
C	3.5153110	-1.7142990	-0.8794990
C	2.6488820	-1.9948480	1.8557400
H	0.1350110	-3.7939510	1.5939580
H	-0.3991660	-4.8280650	0.2385750
C	-2.5353720	-4.0482710	-1.9213000
C	-1.0063170	-2.4122600	-2.8639220
C	-2.7670880	-3.5899540	1.9763300
C	-3.6982650	-1.7737100	0.6612650
H	1.3306990	-3.8096390	-1.2517740
H	2.1498460	-4.3826770	0.2287050
C	4.2359030	-0.5054430	-0.7638320
C	3.9732280	-2.6916370	-1.7856520
C	3.8724440	-2.6285090	2.1498280
C	1.8836250	-1.4592950	2.9089910
C	-2.8617200	-4.4854400	-3.2114630
H	-3.0209450	-4.5077410	-1.0537070
C	-1.3313490	-2.8554310	-4.1546480
H	-0.2966750	-1.5891510	-2.7197880
C	-3.9588600	-3.6635340	2.7130780
H	-1.9536370	-4.2815040	2.2151860
C	-4.8885170	-1.8548740	1.3932200
H	-3.6020780	-1.0241270	-0.1311040
C	5.3941100	-0.2912660	-1.5200660
H	3.8893950	0.2734480	-0.0767720
C	5.1296030	-2.4704710	-2.5486440
H	3.4373080	-3.6385140	-1.9001790
C	4.3157040	-2.7326900	3.4744870

H	4.4888730	-3.0299520	1.3384060
C	2.3257500	-1.5713040	4.2355780
H	0.9436670	-0.9454860	2.6762950
C	-2.2581040	-3.8915790	-4.3304230
H	-3.5934080	-5.2895260	-3.3447570
H	-0.8663940	-2.3833320	-5.0266870
C	-5.0235230	-2.8005550	2.4214860
H	-4.0558310	-4.4061590	3.5125030
H	-5.7129340	-1.1734370	1.1594140
C	5.8454960	-1.2733200	-2.4151930
H	5.9428050	0.6497860	-1.4108830
H	5.4749200	-3.2432000	-3.2439920
C	3.5413810	-2.2076230	4.5202710
H	5.2711550	-3.2221200	3.6916660
H	1.7226180	-1.1534590	5.0487000
H	-2.5167210	-4.2327480	-5.3383720
H	-5.9550450	-2.8628330	2.9936080
H	6.7510360	-1.1045410	-3.0071460
H	3.8902500	-2.2890990	5.5550610
C	-1.0072630	0.9353590	-0.2955660
C	-2.8989850	1.8175050	-1.6365730
H	-3.6440060	2.0264880	1.6713990
H	0.7060490	1.8238780	1.8035780
H	-3.2997760	2.0487150	-2.6290710
C	-1.6346310	1.2385170	-1.5390300
C	2.1800900	3.0080370	0.7714210
O	2.6137930	3.7564120	1.8397340
C	2.0064990	3.5130530	3.1065550
H	0.9208410	3.7177560	3.0810750
H	2.4926740	4.2094110	3.8029110
H	2.1780320	2.4750110	3.4448300
C	1.4365380	1.5210950	-1.5092870
O	1.1019150	0.7127750	-2.5830570
C	1.7763760	0.9380850	-3.8228290
H	2.8635790	0.7741680	-3.7214370
H	1.3630240	0.2023300	-4.5257580
H	1.5872290	1.9561400	-4.2087960
C	2.7789320	3.2637210	-0.4762520
Br	4.1222770	4.6196460	-0.6476070
C	-3.6369400	2.1547560	-0.4842730
C	-3.0538930	1.8463560	0.7700180
C	-1.7994880	1.2420080	0.8674080
H	-1.0847880	1.0273720	-2.4568530

C	-4.9709230	2.7894230	-0.5654490
C	-5.4071800	3.7123450	0.4141980
C	-5.8598950	2.4939630	-1.6260810
C	-6.6716370	4.3075340	0.3399160
H	-4.7285850	3.9934800	1.2263750
C	-7.1223750	3.0917770	-1.7027510
H	-5.5642500	1.7633260	-2.3860680
C	-7.5385550	4.0014950	-0.7190450
H	-6.9770180	5.0269490	1.1076360
H	-7.7916240	2.8373550	-2.5319190
H	-8.5268590	4.4687380	-0.7790060
O	-1.2617960	0.8475180	2.0828420
C	-2.0432700	1.0700520	3.2720920
H	-2.2417850	2.1529460	3.3883210
H	-3.0153820	0.5530640	3.1716950
C	-1.2650680	0.5298510	4.4610660
H	-1.8404340	0.6912640	5.3875210
H	-0.2946390	1.0397380	4.5708740
H	-1.0850720	-0.5513900	4.3569080

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R = OCH₃CF₃ reactant

C	1.5100380	1.8234270	0.8051180
C	2.5663150	2.6645120	-1.6346270
C	1.2717710	1.0352260	-0.3344480
H	2.9879450	3.0214500	-2.5763030
Ni	0.2855210	-0.6146590	-0.2926960
P	-0.8439710	-2.5148660	-0.4372910
P	2.1094600	-1.8392060	0.0461710
C	0.2555620	-3.8930230	0.2152210
C	-1.0795000	-3.0347700	-2.2021940
C	-2.5026420	-2.8152780	0.3104760
C	1.6762410	-3.6365810	-0.3080340
C	3.7067660	-1.5456340	-0.8294530
C	2.6238330	-1.9258910	1.8245760
H	0.2439050	-3.8443330	1.3176140
H	-0.1188080	-4.8841530	-0.0905140
C	-1.9070590	-4.1204610	-2.5512470
C	-0.3664950	-2.3567530	-3.2094160
C	-2.7046360	-3.7046310	1.3834430
C	-3.6030930	-2.0899230	-0.1945340
H	1.7030090	-3.7853190	-1.4008160
H	2.4109830	-4.3188490	0.1502560
C	4.4132790	-0.3587560	-0.5400780

C	4.2304200	-2.4354220	-1.7872500
C	3.8659930	-2.4679160	2.2108600
C	1.7234220	-1.4891520	2.8135520
C	-2.0126860	-4.5262060	-3.8874050
H	-2.4825090	-4.6416510	-1.7788500
C	-0.4731630	-2.7693330	-4.5462400
H	0.2627280	-1.4996250	-2.9414120
C	-3.9828230	-3.8735150	1.9351260
H	-1.8695830	-4.2743290	1.8008940
C	-4.8775460	-2.2637460	0.3582820
H	-3.4626870	-1.3856990	-1.0201160
C	5.6217600	-0.0788200	-1.1889210
H	4.0170840	0.3491070	0.1939270
C	5.4406020	-2.1496850	-2.4360390
H	3.7055310	-3.3624250	-2.0347560
C	4.1958050	-2.5768540	3.5672990
H	4.5832340	-2.7921510	1.4496760
C	2.0554650	-1.6032580	4.1717140
H	0.7646700	-1.0526290	2.5136300
C	-1.2942130	-3.8522110	-4.8866830
H	-2.6619920	-5.3678460	-4.1506360
H	0.0809440	-2.2364870	-5.3260050
C	-5.0717720	-3.1563840	1.4228880
H	-4.1244790	-4.5702230	2.7678510
H	-5.7214760	-1.6948100	-0.0445960
C	6.1395750	-0.9728620	-2.1372430
H	6.1567770	0.8464530	-0.9532890
H	5.8380980	-2.8545380	-3.1739190
C	3.2904910	-2.1461060	4.5492050
H	5.1654610	-2.9939650	3.8589660
H	1.3490260	-1.2584850	4.9323630
H	-1.3809790	-4.1685740	-5.9313990
H	-6.0696350	-3.2908320	1.8530600
H	7.0856640	-0.7520870	-2.6422610
H	3.5522950	-2.2288130	5.6092320
C	-1.2756770	0.4803490	-0.5331430
C	-2.8684830	1.6693420	-1.9953630
H	-3.9036750	1.8689420	1.2356140
H	1.0825670	1.5080560	1.7601940
H	-3.1344270	2.0079860	-3.0026410
C	-1.6951910	0.9239670	-1.8023910
C	2.2726600	3.0114260	0.7642650
O	2.5425310	3.8034020	1.8545660

C	2.0005470	3.4026570	3.1123460
H	0.8964910	3.3795220	3.0893370
H	2.3346310	4.1637580	3.8301950
H	2.3803260	2.4126720	3.4226210
C	1.8126440	1.4818770	-1.5586810
O	1.5641160	0.6784510	-2.6703050
C	2.1004550	1.1086810	-3.9200770
H	3.2037890	1.1664440	-3.8916210
H	1.8002400	0.3503950	-4.6566500
H	1.6897690	2.0894920	-4.2232230
C	2.7946170	3.4159180	-0.4758760
Br	3.8390010	5.0248040	-0.5999710
C	-3.6745050	2.0310900	-0.9015020
C	-3.2635420	1.6165090	0.3856690
C	-2.0960070	0.8581310	0.5523760
H	-1.0759360	0.6922670	-2.6743490
C	-4.9158480	2.8270340	-1.0789550
C	-5.2858700	3.8258710	-0.1512440
C	-5.7659970	2.6103530	-2.1862590
C	-6.4579500	4.5729370	-0.3197980
H	-4.6257810	4.0424360	0.6954050
C	-6.9360100	3.3594520	-2.3583650
H	-5.5145340	1.8263440	-2.9082850
C	-7.2902910	4.3438770	-1.4245860
H	-6.7154360	5.3490880	0.4090440
H	-7.5807930	3.1664650	-3.2226660
H	-8.2056120	4.9295650	-1.5584180
O	-1.6765000	0.4072490	1.8149660
C	-2.5436020	0.6774000	2.8979790
H	-2.6766130	1.7629230	3.0679770
H	-3.5386030	0.2148870	2.7565760
C	-1.9377250	0.0952610	4.1671030
F	-2.7793540	0.3356840	5.2173210
F	-1.7457320	-1.2490480	4.0990530
F	-0.7338440	0.6575170	4.4781890

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R = OCH3CF3 TS

C	1.1845660	2.0611620	0.5979940
C	2.5615800	2.4396440	-1.7942510
C	0.8271920	1.2370350	-0.5094440
H	3.1384600	2.5899860	-2.7082260
Ni	0.2659830	-0.6342880	-0.2558780
P	-0.9825710	-2.4441010	-0.1452370

P	2.0697560	-1.8818620	0.0574260
C	0.1201230	-3.8161170	0.5236070
C	-1.4485960	-3.1355190	-1.8069530
C	-2.5610540	-2.5984520	0.8023300
C	1.5057910	-3.6718490	-0.1272700
C	3.6012220	-1.7691480	-0.9723840
C	2.7656380	-1.9027950	1.7806230
H	0.2013960	-3.6808360	1.6162400
H	-0.3126350	-4.8126830	0.3326060
C	-2.3703210	-4.1908900	-1.9549720
C	-0.8204820	-2.6072200	-2.9510850
C	-2.7157010	-3.4207910	1.9360060
C	-3.6463490	-1.7905250	0.3963540
H	1.4334670	-3.8935070	-1.2061550
H	2.2358800	-4.3690200	0.3168780
C	4.3560370	-0.5789490	-0.8843990
C	4.0208410	-2.7710540	-1.8699550
C	4.0021070	-2.5053570	2.0878150
C	2.0038050	-1.3336330	2.8178290
C	-2.6514880	-4.7123910	-3.2242120
H	-2.8805010	-4.5986050	-1.0757530
C	-1.0998880	-3.1347740	-4.2205850
H	-0.1190290	-1.7725690	-2.8370270
C	-3.9282220	-3.4426450	2.6410150
H	-1.8928830	-4.0547870	2.2789770
C	-4.8579180	-1.8210160	1.0972540
H	-3.5436540	-1.1348150	-0.4746140
C	5.5094190	-0.4069990	-1.6585890
H	4.0420550	0.2175840	-0.2020550
C	5.1727040	-2.5925470	-2.6509050
H	3.4593990	-3.7052650	-1.9632260
C	4.4619140	-2.5414710	3.4101810
H	4.6148200	-2.9360680	1.2888310
C	2.4619810	-1.3780530	4.1429090
H	1.0504870	-0.8509940	2.5785760
C	-2.0148910	-4.1868420	-4.3590250
H	-3.3731330	-5.5296080	-3.3290310
H	-0.6081110	-2.7167450	-5.1053780
C	-5.0033130	-2.6475370	2.2224940
H	-4.0317410	-4.0895690	3.5186350
H	-5.6913950	-1.1953090	0.7614860
C	5.9226380	-1.4137730	-2.5447800
H	6.0861140	0.5192710	-1.5686910

H	5.4882080	-3.3851380	-3.3379700
C	3.6914320	-1.9803750	4.4402390
H	5.4271500	-3.0064470	3.6376740
H	1.8589330	-0.9341030	4.9411290
H	-2.2381120	-4.5943930	-5.3506160
H	-5.9506750	-2.6697050	2.7709180
H	6.8254010	-1.2789830	-3.1495050
H	4.0538290	-2.0084600	5.4732070
C	-0.9173820	0.8865100	-0.6257400
C	-2.7312610	1.6350550	-2.1514470
H	-3.7238360	2.0278850	1.0687490
H	0.6407020	1.9189130	1.5311490
H	-3.0634830	1.7896490	-3.1833670
C	-1.4664540	1.0957880	-1.9275680
C	2.1747970	3.0522740	0.5343360
O	2.5396370	3.8562790	1.5846650
C	1.8604360	3.6727120	2.8271350
H	0.7792250	3.8758830	2.7301890
H	2.3085160	4.4019170	3.5150150
H	2.0083690	2.6528240	3.2225990
C	1.5832940	1.4449920	-1.7115130
O	1.3239850	0.5790320	-2.7595290
C	2.0683660	0.7506950	-3.9683170
H	3.1481730	0.5984990	-3.7967610
H	1.6990200	-0.0202710	-4.6577300
H	1.8968630	1.7482230	-4.4115750
C	2.8514090	3.2452010	-0.6852170
Br	4.1979920	4.5982660	-0.8405030
C	-3.5607700	2.0267840	-1.0816430
C	-3.0610760	1.8108660	0.2272320
C	-1.8050700	1.2498140	0.4466150
H	-0.8498880	0.8393090	-2.7891970
C	-4.8987770	2.6182950	-1.2962310
C	-5.4256190	3.5873660	-0.4100190
C	-5.7015750	2.2335400	-2.3963180
C	-6.6954010	4.1406420	-0.6100430
H	-4.8136440	3.9390890	0.4273300
C	-6.9689690	2.7898050	-2.5987770
H	-5.3354610	1.4658980	-3.0858370
C	-7.4762890	3.7456710	-1.7057900
H	-7.0720440	4.8969880	0.0871540
H	-7.5707890	2.4663260	-3.4550270
H	-8.4686040	4.1800820	-1.8641720

O	-1.3526850	0.9439090	1.7345860
C	-2.2725730	1.1304960	2.7956870
H	-2.5718960	2.1894870	2.9076100
H	-3.1777020	0.5105450	2.6595390
C	-1.6054240	0.7113770	4.0987480
F	-0.4987140	1.4578350	4.3810100
F	-1.2238510	-0.5918520	4.1075300
F	-2.4879170	0.8891210	5.1264720

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R = Me reactant

C	1.5388370	1.7893350	1.0800580
C	2.2498850	2.6981490	-1.4533470
C	1.1093000	1.0470300	-0.0350070
H	2.5412050	3.0789380	-2.4341400
Ni	0.1099540	-0.5951700	0.0703040
P	-1.0565830	-2.4773420	-0.0464390
P	1.9450490	-1.8599020	0.1704720
C	0.0868410	-3.9043920	0.3979880
C	-1.5009850	-2.8993140	-1.7973460
C	-2.6190910	-2.8125840	0.8753520
C	1.4528830	-3.6282740	-0.2453230
C	3.4740600	-1.5471570	-0.8140400
C	2.5980000	-2.0557880	1.8974410
H	0.1863100	-3.9319280	1.4967210
H	-0.3312770	-4.8693880	0.0664120
C	-2.4036080	-3.9372760	-2.1021230
C	-0.8715840	-2.1994770	-2.8444750
C	-2.7153250	-3.7919630	1.8840320
C	-3.7497610	-2.0211390	0.5787930
H	1.3699250	-3.7045000	-1.3430000
H	2.2171340	-4.3471100	0.0936150
C	4.1933960	-0.3581570	-0.5672540
C	3.9320480	-2.4264840	-1.8146560
C	3.8759400	-2.5881870	2.1587900
C	1.7651180	-1.7094360	2.9779750
C	-2.6656970	-4.2752850	-3.4356770
H	-2.9149310	-4.4734960	-1.2957380
C	-1.1342750	-2.5454210	-4.1785950
H	-0.1863660	-1.3765590	-2.6089000
C	-3.9190380	-3.9805710	2.5784310
H	-1.8562620	-4.4204950	2.1361870
C	-4.9492730	-2.2156770	1.2737210
H	-3.6900690	-1.2468540	-0.1916780

C	5.3499490	-0.0661040	-1.3000550
H	3.8462490	0.3433020	0.1972110
C	5.0896290	-2.1278990	-2.5480730
H	3.3961040	-3.3550960	-2.0303490
C	4.3057380	-2.7772000	3.4785530
H	4.5428330	-2.8429720	1.3286870
C	2.1952810	-1.9041490	4.2985540
H	0.7791050	-1.2767040	2.7761500
C	-2.0293940	-3.5813100	-4.4759230
H	-3.3730650	-5.0795220	-3.6638860
H	-0.6444220	-1.9965460	-4.9896690
C	-5.0379560	-3.1943130	2.2741970
H	-3.9798320	-4.7479410	3.3573150
H	-5.8159960	-1.5913030	1.0354400
C	5.8018610	-0.9491420	-2.2913440
H	5.8949020	0.8611220	-1.0972290
H	5.4355810	-2.8239790	-3.3194990
C	3.4660900	-2.4379750	4.5502530
H	5.3029940	-3.1865290	3.6713020
H	1.5386420	-1.6304730	5.1310200
H	-2.2381820	-3.8446000	-5.5180960
H	-5.9770250	-3.3418000	2.8174430
H	6.7064120	-0.7177490	-2.8632710
H	3.8062250	-2.5843050	5.5806580
C	-1.4659940	0.5201340	0.0802930
C	-3.3226550	1.6314640	1.2210330
H	-3.5556150	2.1160090	-2.1437430
H	1.2708570	1.4421080	2.0811740
H	-3.8493760	1.8545100	2.1575920
C	-2.1496870	0.8579940	1.2788370
C	2.3119650	2.9660620	0.9702830
O	2.7545320	3.7117200	2.0373640
C	2.3566120	3.2998610	3.3434970
H	1.2569360	3.3015190	3.4514320
H	2.7910040	4.0402130	4.0286420
H	2.7491570	2.2970060	3.5927500
C	1.4868230	1.5282020	-1.3079800
O	1.0735950	0.7672620	-2.4001200
C	1.4225060	1.2424470	-3.6990320
H	2.5183840	1.2901480	-3.8352800
H	1.0042930	0.5164940	-4.4102020
H	0.9845150	2.2376240	-3.8990960
C	2.6584020	3.4065290	-0.3173430

C	-3.8722850	2.0883060	0.0057880
C	-3.1871640	1.7500750	-1.1782930
C	-2.0073260	0.9954240	-1.1332750
C	-5.1196430	2.8939280	-0.0215020
C	-6.0740760	2.7271970	-1.0499150
C	-5.3930370	3.8541250	0.9781290
C	-7.2504580	3.4857910	-1.0778250
H	-5.8990690	1.9738510	-1.8253530
C	-6.5708560	4.6105480	0.9540490
H	-4.6553750	4.0285860	1.7683190
C	-7.5070940	4.4311310	-0.0743480
H	-7.9763670	3.3309500	-1.8836510
H	-6.7525960	5.3550000	1.7369550
H	-8.4271490	5.0244660	-0.0950640
C	-1.6584210	0.3775720	2.6270990
H	-1.6264570	-0.7261650	2.6723500
H	-0.6383470	0.7416720	2.8381050
H	-2.3107330	0.7224170	3.4465380
H	-1.4867730	0.7869000	-2.0730510
Br	3.7067700	5.0018560	-0.5391560

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R = Me TS

C	-1.1720230	2.0744470	-1.0589970
C	-2.3470630	2.5547570	1.4133320
C	-0.7151710	1.2943130	0.0433050
H	-2.8417800	2.7464180	2.3668560
Ni	-0.1277280	-0.5898430	-0.0379100
P	1.1540550	-2.3810000	0.1740670
P	-1.9076640	-1.8966270	-0.1897430
C	0.0568940	-3.8753710	-0.1663180
C	1.7308600	-2.7437210	1.9044680
C	2.6834120	-2.6915340	-0.8177480
C	-1.3417470	-3.5947470	0.4065910
C	-3.4756960	-1.5858240	0.7367780
C	-2.5317670	-2.3151090	-1.8945970
H	-0.0090620	-4.0059670	-1.2604240
H	0.4884390	-4.7969090	0.2592970
C	2.6739800	-3.7520320	2.1861600
C	1.1755270	-2.0057350	2.9664970
C	2.8325380	-3.7592260	-1.7255040
C	3.7338700	-1.7561040	-0.6901520
H	-1.2973310	-3.5579100	1.5092340
H	-2.0574910	-4.3828550	0.1177560

C	-4.1380530	-0.3623410	0.4980920
C	-4.0168160	-2.4753110	1.6866780
C	-3.8539770	-2.7356430	-2.1403390
C	-1.6319070	-2.2406000	-2.9768220
C	3.0462420	-4.0231350	3.5088700
H	3.1304930	-4.3187320	1.3675300
C	1.5478300	-2.2821990	4.2907610
H	0.4607010	-1.2061050	2.7427250
C	4.0058530	-3.8913530	-2.4834850
H	2.0392760	-4.5031510	-1.8452550
C	4.9056470	-1.8953340	-1.4423190
H	3.6312750	-0.9098260	-0.0030310
C	-5.3215380	-0.0480650	1.1771000
H	-3.7249030	0.3501090	-0.2233270
C	-5.1966450	-2.1530940	2.3737710
H	-3.5283090	-3.4320280	1.8934640
C	-4.2621050	-3.0763710	-3.4370920
H	-4.5720090	-2.7878540	-1.3160360
C	-2.0379360	-2.5930590	-4.2714010
H	-0.6070740	-1.8955310	-2.8025620
C	2.4817100	-3.2901810	4.5640030
H	3.7836810	-4.8057100	3.7172010
H	1.1151030	-1.7012500	5.1123240
C	5.0453630	-2.9626870	-2.3427190
H	4.1075150	-4.7292600	-3.1815870
H	5.7100050	-1.1615350	-1.3283900
C	-5.8544490	-0.9423140	2.1176500
H	-5.8225320	0.9039830	0.9748980
H	-5.6061470	-2.8573290	3.1059990
C	-3.3555580	-3.0098470	-4.5048970
H	-5.2950830	-3.3948470	-3.6136520
H	-1.3252280	-2.5310420	-5.1006780
H	2.7767610	-3.5009500	5.5973010
H	5.9610460	-3.0681390	-2.9336200
H	-6.7780510	-0.6944550	2.6509660
H	-3.6774770	-3.2761160	-5.5170000
C	1.0517000	0.9996020	0.0119030
C	3.0356830	1.7937230	-1.2012820
H	3.3861720	2.3967380	2.1335170
H	-0.6982310	1.9232540	-2.0280720
H	3.5831490	1.8639020	-2.1500670
C	1.7827890	1.1721700	-1.2154360
C	-2.1624510	3.0611540	-0.9611470

O	-2.6116250	3.8183810	-2.0153570
C	-2.0052440	3.6094730	-3.2899080
H	-0.9231200	3.8312910	-3.2646700
H	-2.5049470	4.3121350	-3.9698370
H	-2.1623440	2.5765160	-3.6502190
C	-1.3669560	1.5649700	1.2929950
O	-0.9976650	0.7641840	2.3636020
C	-1.6635310	0.9713450	3.6116350
H	-2.7497630	0.7976230	3.5181120
H	-1.2370770	0.2330290	4.3040720
H	-1.4808470	1.9873890	4.0060370
C	-2.7424180	3.3045330	0.2984440
C	3.6593550	2.2567760	-0.0215650
C	2.9577960	2.0471710	1.1876420
C	1.7030450	1.4463160	1.2004640
C	4.9880310	2.9076910	-0.0529800
C	5.9095130	2.7470880	1.0085070
C	5.3852100	3.7112590	-1.1473780
C	7.1670670	3.3596570	0.9768150
H	5.6442360	2.1098770	1.8585660
C	6.6444250	4.3208420	-1.1813230
H	4.6817270	3.8848000	-1.9682620
C	7.5443140	4.1495160	-0.1193840
H	7.8624400	3.2108510	1.8101460
H	6.9202270	4.9455920	-2.0379120
H	8.5284530	4.6286260	-0.1442800
H	1.1857600	1.3353730	2.1550790
C	1.2995030	0.5977400	-2.5343130
H	1.2326440	1.3638490	-3.3284810
H	2.0003450	-0.1756710	-2.8946980
H	0.3145800	0.1138210	-2.4348510
Br	-4.0863150	4.6541680	0.5026960

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Ar = ethene reactant

Ni	-0.6123520	-0.2230320	-0.4557080
P	-2.7639850	-0.1915200	-0.0035540
P	-0.2775100	0.7935790	1.4909990
C	-3.0487420	0.7899210	1.5819240
C	-3.4182050	-1.8618930	0.4575030
C	-4.0187790	0.4690350	-1.1862580
C	1.2535420	-0.4409320	-0.8686010
C	-1.8439560	0.5758730	2.5090330
C	-0.1896690	2.6397820	1.3135570

C	1.1028910	0.4269620	2.6580570
H	-3.9945020	0.4925620	2.0635300
H	-3.1305420	1.8563020	1.3154530
C	-4.7710860	-2.0600870	0.8008920
C	-2.5248790	-2.9478740	0.5131250
C	-4.5755010	-0.3858760	-2.1595900
C	-4.3468440	1.8394000	-1.2204530
C	1.9244570	-1.5767540	-0.3690810
C	2.0078900	0.4739000	-1.6232730
H	-1.8689720	1.2654460	3.3695640
H	-1.8410480	-0.4575900	2.8965510
C	0.1421410	3.4841790	2.3912600
C	-0.5006760	3.2101180	0.0646720
C	2.4238470	0.6303820	2.2053270
C	0.8955790	-0.0719230	3.9588170
C	-5.2217690	-3.3260610	1.1938650
H	-5.4805040	-1.2273150	0.7443980
C	-2.9809970	-4.2147840	0.9083410
H	-1.4740860	-2.7936630	0.2434370
C	-5.4654450	0.1137060	-3.1189030
H	-4.3139290	-1.4472500	-2.1655380
C	-5.2365310	2.3361990	-2.1825560
H	-3.9094470	2.5365730	-0.4993060
C	3.2963410	-1.7762400	-0.5980190
O	1.1462130	-2.4713720	0.3633500
C	3.3877030	0.3067290	-1.8695980
H	1.5013800	1.3423910	-2.0532580
C	0.1505680	4.8745840	2.2222820
H	0.4114780	3.0531700	3.3614370
C	-0.4937740	4.6027460	-0.1024510
H	-0.7377050	2.5489360	-0.7776470
C	3.5094660	0.3522540	3.0441430
H	2.6036780	0.9993870	1.1910400
C	1.9867210	-0.3532020	4.7940820
H	-0.1169470	-0.2441970	4.3353470
C	-4.3263630	-4.4056120	1.2483200
H	-6.2755740	-3.4726270	1.4532990
H	-2.2820200	-5.0568690	0.9433030
C	-5.8021170	1.4739670	-3.1316990
H	-5.8917010	-0.5651580	-3.8646960
H	-5.4873070	3.4021310	-2.1882950
C	4.0171540	-0.8322710	-1.3392340
H	3.8262040	-2.6504720	-0.2143910

C	1.8015010	-3.6138690	0.9092940
O	4.1630390	1.1800620	-2.5967080
C	-0.1690610	5.4359370	0.9763840
H	0.4148380	5.5231190	3.0642000
H	-0.7332230	5.0357830	-1.0793490
C	3.2947040	-0.1389990	4.3401420
H	4.5280360	0.5127220	2.6771700
H	1.8101440	-0.7375410	5.8043010
H	-4.6813000	-5.3959960	1.5521390
H	-6.4977480	1.8624320	-3.8826250
H	2.6087910	-3.3256930	1.6073410
H	1.0309620	-4.1696540	1.4616780
H	2.2190590	-4.2627200	0.1168630
C	3.5138100	2.3058750	-3.1839250
H	-0.1563720	6.5230750	0.8462100
H	4.1458460	-0.3577160	4.9932730
H	2.7235230	1.9955450	-3.8910140
H	4.3000320	2.8456500	-3.7288640
H	3.0779140	2.9714070	-2.4163140
C	-0.8762010	-1.0529870	-2.1554400
C	-1.3485320	-0.4928530	-3.2858190
H	-0.5508340	-2.1059070	-2.2072830
H	-1.4091720	-1.0573580	-4.2287950
H	-1.6848110	0.5503510	-3.3455310
Br	5.8947130	-1.1194500	-1.6388380

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Ar = ethene TS

C	1.9364370	0.4085910	-1.7467350
C	3.1528140	-1.9191670	-0.8088760
C	1.1037130	-0.6164480	-1.2219970
H	3.6572620	-2.8134770	-0.4382470
Ni	-0.6300570	-0.1857350	-0.4649260
P	-2.7949890	-0.0899450	-0.0304870
P	-0.2350940	0.8354470	1.4574620
C	-3.0113270	1.0074580	1.4878840
C	-3.5183390	-1.6958830	0.5627480
C	-4.0736780	0.5247610	-1.2136640
C	-1.8355810	0.7663320	2.4479190
C	1.0766770	0.3363180	2.6574310
C	0.0253660	2.6698860	1.2990160
H	-3.0018710	2.0553760	1.1405500
H	-3.9779510	0.8224490	1.9860000
C	-4.9034070	-1.8799240	0.7432120

C	-2.6375870	-2.7494050	0.8746130
C	-4.9813990	1.5639800	-0.9256640
C	-4.1018680	-0.0678480	-2.4947910
H	-1.9057500	-0.2447990	2.8860150
H	-1.8377170	1.4986110	3.2729680
C	2.4029010	0.2709890	2.1783400
C	0.8184720	-0.0223520	3.9953100
C	0.5822500	3.4541220	2.3280490
C	-0.3818620	3.2979730	0.1052390
C	-5.3973040	-3.0938640	1.2376430
H	-5.6009600	-1.0771390	0.4809010
C	-3.1351280	-3.9613210	1.3765320
H	-1.5617400	-2.6164220	0.7088300
C	-5.9043360	1.9914000	-1.8914540
H	-4.9823970	2.0450790	0.0569980
C	-5.0295470	0.3567560	-3.4533920
H	-3.3785450	-0.8496240	-2.7440590
C	3.4447600	-0.1270290	3.0240110
H	2.6204360	0.5284500	1.1365540
C	1.8638550	-0.4299870	4.8373490
H	-0.1992450	0.0167490	4.3949650
C	0.7198130	4.8393760	2.1675220
H	0.9223820	2.9783210	3.2537740
C	-0.2527130	4.6855030	-0.0502320
H	-0.7957350	2.6859800	-0.7055770
C	-4.5134900	-4.1352810	1.5590240
H	-6.4762800	-3.2298790	1.3680020
H	-2.4439830	-4.7758930	1.6178090
C	-5.9338500	1.3866310	-3.1552750
H	-6.6060340	2.7973270	-1.6510980
H	-5.0395830	-0.1134850	-4.4423030
C	3.1786000	-0.4794270	4.3557070
H	4.4674470	-0.1694440	2.6359980
H	1.6474050	-0.7042890	5.8754360
C	0.2996910	5.4581280	0.9806380
H	1.1599970	5.4383160	2.9719470
H	-0.5767880	5.1620520	-0.9815560
H	-4.9014870	-5.0841450	1.9441300
H	-6.6565090	1.7199830	-3.9073010
H	3.9940310	-0.7950860	5.0147710
H	0.4091570	6.5407090	0.8578560
C	-0.4348370	-1.0356380	-2.1864910
H	1.4559490	1.3050530	-2.1467210

C	-0.6495100	-0.4806680	-3.4122670
C	3.3304590	0.3020850	-1.8109320
O	4.1683320	1.2734830	-2.3022130
C	3.5682690	2.4559830	-2.8292740
H	2.9081320	2.2268160	-3.6853890
H	4.4039820	3.0812880	-3.1704990
H	2.9943420	2.9991130	-2.0568460
C	1.7572370	-1.7844500	-0.7388500
O	0.9372580	-2.7588080	-0.1884200
C	1.5427030	-3.9957550	0.1865780
H	2.2602110	-3.8626300	1.0166410
H	0.7209190	-4.6430340	0.5217590
H	2.0548660	-4.4720550	-0.6692940
C	3.9320760	-0.8860850	-1.3377460
H	-0.5543110	-2.1261050	-2.1048240
H	-0.5094340	0.5861930	-3.6206240
H	-0.9382200	-1.0988180	-4.2718600
Br	5.8364050	-1.0972950	-1.4220020

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Ar = methylbenzothiophene reactant

Ni	-0.3959630	-0.2595510	-0.0243600
P	-2.3437110	-1.3542530	-0.0699600
P	0.5372050	-2.1786780	0.5935810
C	-2.0911220	-3.0267220	0.7526140
C	-2.7981900	-1.8565630	-1.7966470
C	-3.9314330	-0.7199460	0.6170600
C	1.3122700	0.6055920	-0.2151990
C	-0.7126660	-3.5589050	0.3380850
C	0.7532090	-2.2077250	2.4361800
C	2.1367610	-2.8571720	-0.0224550
H	-2.8958330	-3.7292370	0.4794290
H	-2.1227060	-2.8735750	1.8449200
C	-4.0688190	-2.3861540	-2.0974810
C	-1.8332950	-1.7499580	-2.8161120
C	-4.4519340	0.4769720	0.0816080
C	-4.6238390	-1.3614770	1.6617930
C	2.0393210	0.3904480	-1.4051000
C	1.9016670	1.4205420	0.7657520
H	-0.4352930	-4.4605080	0.9090840
H	-0.7158460	-3.8174450	-0.7346170
C	1.4542970	-3.2464770	3.0805760
C	0.1583700	-1.1950280	3.2118830
C	3.3222200	-2.1528490	0.2766030

C	2.2152750	-4.0298870	-0.7986760
C	-4.3657400	-2.8105420	-3.3985470
H	-4.8342520	-2.4512780	-1.3170720
C	-2.1356890	-2.1783420	-4.1174820
H	-0.8519750	-1.3173270	-2.5894290
C	-5.6473800	1.0100260	0.5753210
H	-3.9093590	1.0004610	-0.7115310
C	-5.8201120	-0.8206150	2.1560260
H	-4.2422920	-2.2882110	2.0999590
C	3.3071520	0.9637890	-1.5976850
O	1.4329610	-0.4251850	-2.3596910
C	3.1762340	2.0050670	0.6066860
H	1.3404660	1.6297680	1.6799950
C	1.5502240	-3.2724050	4.4775100
H	1.9409860	-4.0289610	2.4888280
C	0.2527260	-1.2253320	4.6108270
H	-0.3733050	-0.3762960	2.7129610
C	4.5586090	-2.6234190	-0.1820740
H	3.2789380	-1.2333020	0.8677700
C	3.4558170	-4.4957320	-1.2577000
H	1.3129730	-4.5946040	-1.0503200
C	-3.3988930	-2.7086960	-4.4102190
H	-5.3578770	-3.2147510	-3.6253840
H	-1.3847410	-2.0850680	-4.9089110
C	-6.3348800	0.3630630	1.6127090
H	-6.0349280	1.9432360	0.1551730
H	-6.3494130	-1.3301910	2.9680200
C	3.8674810	1.7596800	-0.5924420
H	3.8769690	0.8079720	-2.5157160
C	2.1884340	-0.7357480	-3.5301610
O	3.7888420	2.8028670	1.5414940
C	0.9481780	-2.2633030	5.2446430
H	2.1021990	-4.0802670	4.9692450
H	-0.2128460	-0.4312330	5.2034260
C	4.6295980	-3.7957260	-0.9481980
H	5.4688350	-2.0647160	0.0568550
H	3.5021840	-5.4124550	-1.8549540
H	-3.6349370	-3.0352470	-5.4283550
H	-7.2676830	0.7849950	2.0007430
H	3.1372380	-1.2416490	-3.2762500
H	1.5633820	-1.4189080	-4.1218910
H	2.4018260	0.1683450	-4.1295260
C	3.0553110	3.1128230	2.7271920

H	1.0276610	-2.2843480	6.3364880
H	5.5979560	-4.1617120	-1.3047170
H	2.1078680	3.6295460	2.4936470
H	3.7058270	3.7823980	3.3055710
H	2.8425390	2.2054690	3.3212650
C	-1.1655700	1.4745160	-0.1669140
C	-1.4509590	2.3704350	-1.1785460
C	-2.0586200	3.6032510	-0.7086920
C	-2.2178940	3.6470870	0.7068990
C	-2.7816260	4.7515060	1.3600640
H	-2.8935570	4.7630990	2.4493270
C	-3.1983480	5.8440790	0.5889220
H	-3.6394130	6.7171730	1.0811770
C	-3.0508080	5.8260410	-0.8136240
H	-3.3790740	6.6894220	-1.4022900
C	-2.4881800	4.7220560	-1.4602160
H	-2.3767310	4.7227390	-2.5501160
C	-1.1452630	2.1381090	-2.6359260
H	-2.0625200	2.0778990	-3.2517350
H	-0.5353600	2.9607670	-3.0523550
H	-0.5813630	1.2048840	-2.7733650
S	-1.6236310	2.1452560	1.4190610
Br	5.6057230	2.5291670	-0.8740030

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Ar = methylbenzothiophene TS

C	1.9074590	1.5238330	0.7294160
C	3.0241100	1.0705540	-1.7835310
C	1.0717340	0.9571320	-0.2751650
H	3.4970250	0.8722350	-2.7471210
Ni	-0.4226500	-0.2907780	-0.0121950
P	-2.4163430	-1.2706980	-0.1095260
P	0.4468210	-2.1853510	0.7358620
C	-2.2517140	-2.8710010	0.8739780
C	-2.9062640	-1.9324590	-1.7764570
C	-3.9757130	-0.5066180	0.5125650
C	-0.8858640	-3.5049020	0.5635660
C	1.9747340	-2.9681110	0.0558490
C	0.7539270	-2.1986660	2.5684240
H	-2.3170890	-2.6083730	1.9444500
H	-3.0721580	-3.5713900	0.6436150
C	-4.2216300	-2.3432720	-2.0686840
C	-1.9089600	-2.0698700	-2.7615680
C	-4.8503730	-1.1344350	1.4208480

C	-4.2757530	0.7960290	0.0628170
H	-0.8667770	-3.8581910	-0.4823180
H	-0.6866280	-4.3686020	1.2199230
C	3.1481210	-2.1837260	0.0319810
C	2.0183020	-4.2741840	-0.4708610
C	1.5690160	-3.1658410	3.1889700
C	0.1171050	-1.2271320	3.3649120
C	-4.5302970	-2.8909270	-3.3208630
H	-5.0113660	-2.2220160	-1.3199350
C	-2.2189960	-2.6300480	-4.0095040
H	-0.8930850	-1.7202650	-2.5457170
C	-6.0073730	-0.4754230	1.8624410
H	-4.6387020	-2.1421480	1.7910830
C	-5.4353460	1.4472630	0.4985130
H	-3.5894660	1.3071610	-0.6205110
C	4.3378110	-2.7013630	-0.4932500
H	3.1302500	-1.1618080	0.4248540
C	3.2104020	-4.7865710	-1.0042050
H	1.1257070	-4.9066880	-0.4648580
C	1.7346410	-3.1645080	4.5802080
H	2.0871550	-3.9153570	2.5817910
C	0.2771650	-1.2330380	4.7579630
H	-0.4992480	-0.4576440	2.8856550
C	-3.5290150	-3.0404000	-4.2917300
H	-5.5578940	-3.1998670	-3.5402940
H	-1.4366460	-2.7393200	-4.7683110
C	-6.3040540	0.8131480	1.3990690
H	-6.6788330	-0.9740300	2.5696750
H	-5.6505790	2.4603720	0.1449410
C	4.3723680	-4.0038180	-1.0137330
H	5.2386410	-2.0796030	-0.5015670
H	3.2294080	-5.8045600	-1.4078810
C	1.0866870	-2.2010400	5.3676200
H	2.3758530	-3.9171540	5.0512570
H	-0.2250300	-0.4729460	5.3655400
H	-3.7720910	-3.4697030	-5.2692830
H	-7.2070250	1.3264870	1.7455430
H	5.3026800	-4.4059740	-1.4280290
H	1.2190430	-2.2015590	6.4545840
H	1.4626630	1.7331950	1.7035710
C	3.2419880	1.8847260	0.5057100
O	4.0618500	2.4474110	1.4515400
C	3.4978210	2.7237850	2.7348040

H	2.6496720	3.4272020	2.6597680
H	4.3071090	3.1858470	3.3154510
H	3.1657220	1.7983480	3.2387620
C	1.6944440	0.7020680	-1.5384810
O	0.9387070	-0.0103960	-2.4570530
C	1.4740910	-0.1656760	-3.7724770
H	2.3874680	-0.7869240	-3.7670500
H	0.6945770	-0.6726860	-4.3570500
H	1.6960110	0.8134660	-4.2347510
C	3.7896440	1.6680950	-0.7763450
C	-0.6227250	1.6025900	-0.2037190
C	-1.0339950	2.5627820	-1.1432650
C	-1.7265550	3.6895610	-0.5587680
C	-1.8607790	3.6052330	0.8595640
C	-2.5142100	4.5882390	1.6123740
H	-2.6051650	4.4923910	2.6991820
C	-3.0442700	5.7019690	0.9469200
H	-3.5523670	6.4848570	1.5191890
C	-2.9193270	5.8176640	-0.4525460
H	-3.3340390	6.6940610	-0.9617940
C	-2.2707010	4.8317230	-1.1996400
H	-2.1846780	4.9469680	-2.2850020
S	-1.1368030	2.1138770	1.4548120
C	-0.7155010	2.5000870	-2.6101680
H	-1.3120610	3.2271090	-3.1825490
H	0.3517110	2.7330750	-2.7981000
H	-0.9002940	1.4999960	-3.0286310
Br	5.5965440	2.1839340	-1.1535960

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Ar = methylthiophene reactant

Ni	0.5559230	-0.2120510	-0.0291960
P	2.6875800	0.4548180	-0.0649670
P	0.0442410	1.8485840	0.6166310
C	2.7921420	2.1398940	0.7654930
C	3.2318440	0.8617380	-1.7912570
C	4.1133030	-0.4961310	0.6135780
C	-1.2942020	-0.6988720	-0.2307850
C	1.5490600	2.9464810	0.3663030
C	-0.1492890	1.8966170	2.4615500
C	-1.3846390	2.8522560	0.0248010
H	3.7209450	2.6646830	0.4867660
H	2.8017790	1.9773810	1.8569040
C	4.5846610	1.1074510	-2.0990900

C	2.2597610	0.9740400	-2.8033330
C	4.3481480	-1.7903490	0.1033650
C	4.9564280	0.0059210	1.6236350
C	-1.9657010	-0.3222560	-1.4132600
C	-2.0373790	-1.3873010	0.7428890
H	1.4647520	3.8799970	0.9472010
H	1.5992390	3.2098700	-0.7040800
C	-0.6119520	3.0493080	3.1269990
C	0.2244220	0.7696790	3.2174220
C	-2.6881190	2.4031920	0.3250600
C	-1.2245150	4.0266440	-0.7362000
C	4.9573900	1.4692100	-3.3996420
H	5.3512790	0.9997290	-1.3245700
C	2.6387390	1.3386160	-4.1040890
H	1.2099380	0.7597500	-2.5713600
C	5.4159200	-2.5550080	0.5861280
H	3.6823370	-2.2045930	-0.6600150
C	6.0212090	-0.7678690	2.1086050
H	4.7957640	1.0039770	2.0413470
C	-3.3251570	-0.6195240	-1.6060100
O	-1.2077140	0.3625950	-2.3629430
C	-3.4055490	-1.6935820	0.5846360
H	-1.5282090	-1.7215300	1.6504160
C	-0.6908390	3.0731640	4.5250860
H	-0.9270350	3.9256240	2.5506800
C	0.1477950	0.7971070	4.6175010
H	0.5686890	-0.1339320	2.7006660
C	-3.8037140	3.1245290	-0.1172330
H	-2.8319860	1.4860670	0.9039790
C	-2.3450870	4.7442950	-1.1788710
H	-0.2266370	4.3967710	-0.9885250
C	3.9845600	1.5870170	-4.4037940
H	6.0118240	1.6520360	-3.6320560
H	1.8800320	1.4158400	-4.8898550
C	6.2547660	-2.0472810	1.5888620
H	5.5833490	-3.5591410	0.1841530
H	6.6697290	-0.3648850	2.8936020
C	-4.0349790	-1.2953410	-0.6073610
H	-3.8533410	-0.3378410	-2.5189780
C	-1.8881820	0.8389000	-3.5234370
O	-4.1667850	-2.3606520	1.5135130
C	-0.3095310	1.9481790	5.2723300
H	-1.0571590	3.9713170	5.0333360

H	0.4399560	-0.0861700	5.1946180
C	-3.6361340	4.2967910	-0.8682300
H	-4.8081060	2.7617470	0.1222330
H	-2.2049740	5.6591900	-1.7642120
H	4.2786080	1.8639050	-5.4215860
H	7.0861200	-2.6504610	1.9682430
H	-2.7114650	1.5256320	-3.2562430
H	-1.1385460	1.3870350	-4.1109580
H	-2.2863400	0.0070960	-4.1332920
C	-3.5101070	-2.8243460	2.6936450
H	-0.3754320	1.9686250	6.3651170
H	-4.5103140	4.8592550	-1.2121050
H	-2.6887640	-3.5220020	2.4525800
H	-4.2826960	-3.3514860	3.2693100
H	-3.1144070	-1.9851760	3.2942990
C	0.9518330	-2.0726590	-0.2097490
C	1.0321260	-2.9889840	-1.2514200
S	1.2548690	-2.8984650	1.3210650
C	1.3464090	-4.3257000	-0.8096500
C	1.4916300	-4.4507950	0.5502040
H	1.4443580	-5.1729470	-1.4970350
H	1.7152440	-5.3404150	1.1391790
C	0.7966700	-2.6537860	-2.7051420
H	1.7328910	-2.6653540	-3.2941660
H	0.1131370	-3.3818260	-3.1771490
H	0.3462330	-1.6563840	-2.8103120
Br	-5.8953810	-1.6875020	-0.8892700

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Ar = methylthipene TS

C	-2.0887530	-1.3254370	0.9658710
C	-3.0472420	-1.0973910	-1.6414630
C	-1.1384490	-1.1136930	-0.0732480
H	-3.4520870	-0.9794400	-2.6484450
Ni	0.5789900	-0.1845560	0.0398620
P	2.7327310	0.3646420	-0.1435220
P	0.1053920	1.9380230	0.4548100
C	2.8862220	2.1014900	0.5759270
C	3.3484760	0.6488650	-1.8750750
C	4.1128880	-0.5754460	0.6432920
C	1.6718990	2.9317920	0.1299420
C	-1.2344470	2.8892810	-0.3882270
C	-0.1997260	2.2975980	2.2525480
H	2.8992540	2.0014570	1.6755370

H	3.8277210	2.5852750	0.2656230
C	4.7192240	0.7129680	-2.1931350
C	2.3973610	0.8535590	-2.8941870
C	5.1210710	0.0187020	1.4278040
C	4.1264380	-1.9732180	0.4566920
H	1.7248410	3.1165650	-0.9573160
H	1.6447910	3.9084960	0.6416700
C	-2.5380960	2.3494880	-0.3440290
C	-1.0177800	4.0872050	-1.0978600
C	-0.8076700	3.4907780	2.6902670
C	0.2275910	1.3564390	3.2092980
C	5.1298330	0.9874250	-3.5045120
H	5.4696320	0.5354200	-1.4157790
C	2.8120200	1.1415570	-4.2026340
H	1.3312310	0.7690490	-2.6553370
C	6.1293400	-0.7677740	2.0042690
H	5.1301850	1.1000940	1.5949000
C	5.1405790	-2.7535210	1.0242700
H	3.3301250	-2.4529800	-0.1222960
C	-3.5989050	3.0020650	-0.9828790
H	-2.7240790	1.4120510	0.1904010
C	-2.0819900	4.7340460	-1.7436680
H	-0.0191060	4.5309790	-1.1488790
C	-0.9748450	3.7392990	4.0589690
H	-1.1639560	4.2233030	1.9585580
C	0.0671050	1.6108610	4.5788740
H	0.6793980	0.4157630	2.8736780
C	4.1777860	1.2080370	-4.5105840
H	6.1983320	1.0274160	-3.7419060
H	2.0658420	1.3066750	-4.9873620
C	6.1441250	-2.1538530	1.7991760
H	6.9064570	-0.2932280	2.6130050
H	5.1373120	-3.8375090	0.8713860
C	-3.3741840	4.1956300	-1.6851250
H	-4.6033000	2.5693970	-0.9368110
H	-1.8982420	5.6658380	-2.2892780
C	-0.5348210	2.8022690	5.0058240
H	-1.4545960	4.6674630	4.3874820
H	0.4053410	0.8710980	5.3120100
H	4.5008180	1.4243810	-5.5342400
H	6.9322860	-2.7667620	2.2488110
H	-4.2042890	4.7027170	-2.1878120
H	-0.6680640	2.9985350	6.0748370

H	-1.7122040	-1.4517030	1.9825900
C	-3.4653590	-1.4418660	0.7365630
O	-4.3995750	-1.6588760	1.7194620
C	-3.9263490	-1.8148400	3.0577600
H	-3.2410560	-2.6766960	3.1461220
H	-4.8230870	-1.9960700	3.6650870
H	-3.4175850	-0.9021000	3.4167840
C	-1.6743830	-0.9669030	-1.3915760
O	-0.7678700	-0.5980380	-2.3763080
C	-1.2320850	-0.5853860	-3.7264760
H	-1.9957250	0.1971100	-3.8859760
H	-0.3521490	-0.3649810	-4.3459550
H	-1.6454430	-1.5679700	-4.0193890
C	-3.9367680	-1.3431650	-0.5899090
C	0.3964180	-2.0905170	0.1768180
C	0.5985990	-3.2608330	-0.5851490
S	0.7785520	-2.4550020	1.8906340
C	1.0301050	-4.3780480	0.2014640
C	1.1665780	-4.1219870	1.5454070
H	1.2199490	-5.3639490	-0.2353290
H	1.4936660	-4.7912750	2.3409990
C	0.3132950	-3.4011350	-2.0553110
H	-0.7749160	-3.3560200	-2.2569080
H	0.7787000	-2.6007270	-2.6509390
H	0.6768120	-4.3712710	-2.4309860
Br	-5.8049790	-1.5502710	-0.9692950

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