Electronic supplementary information (ESI):

The Role of Halogens in the Catalyst Transfer Polycondensation for π-Conjugated Polymers

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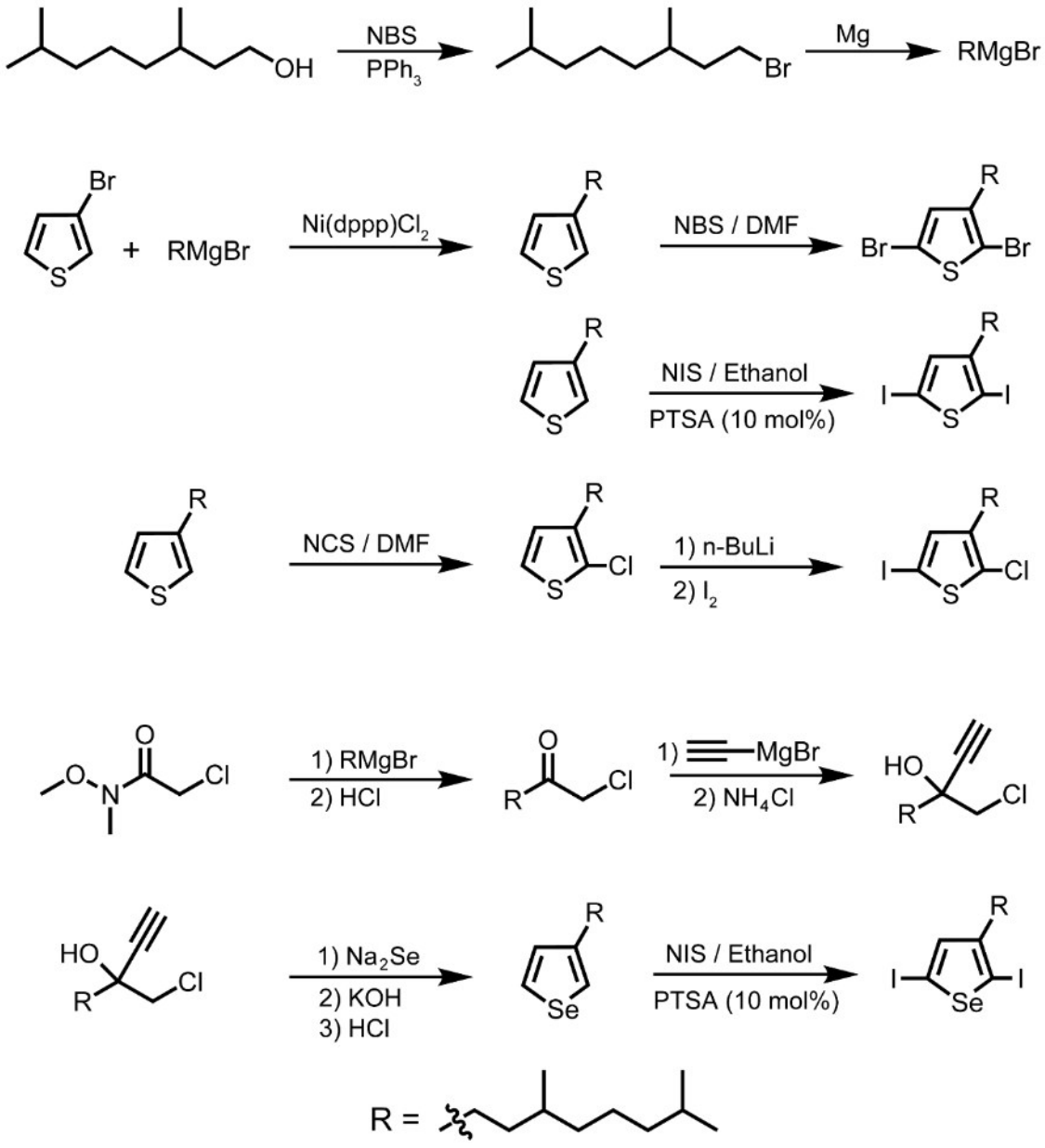
General Considerations. [**Caution**: the MSDS should be consulted before handling organoselenium compounds. Although the toxicity of these compounds is low, they should be handled with proper personal protective equipment.] Tetrahydrofuran (THF) and *N*,*N*-dimethylformamide (DMF) were purchased from Fisher Scientific, degassed, stored under argon, and dried over molecular sieves prior to use. Hexanes, 1,2,4-trichlorobenzene (spectrophotometric grade) and methanol were purchased from Fisher Scientific. Sodium thiosulfate diethyl ether and dichloromethane (DCM) were purchased from Caledon Laboratories. *N*-Iodosuccinimide (NIS) was purchased from Alfa Aesar. Anhydrous ethanol was purchased from Commercial Alcohols. *Trans*-2-[3-(4-*tert*-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) was purchased from Fluka Analytical. All other solvents and reagents were purchased from Sigma-Aldrich and used as received. Schlenk techniques were employed for experiments conducted under argon.

Instrumentation. Nuclear magnetic resonance (NMR) spectra were recorded on a Varian Mercury 400 spectrometer (400 MHz) and Agilent DD2-500 spectrometer (500 MHz). Masses were determined on a Waters GCT Premier TOF mass spectrometer (EI). Gas chromatography was conducted using a Perkin-Elmer Clarus gas chromatograph. Gel permeation chromatography (GPC) characterizations were carried out using a Viscotek HT-SEC module 350A (1,2,4-trichlorobenzene stabilized with butylated hydroxytoluene, 140 °C) with narrow weight distribution polystyrene standards using absorbance at 460 nm. MALDI spectra were obtained using a Bruker Microflex MALDI-TOF mass spectrometer from a matrix of DCTB (2500:1 matrix to polymer ratio) cast from chloroform.

Density functional theory calculations. Density functional theory calculations were carried out using the B3LYP hybrid functional in Gaussian 16.[1–3] Geometry optimizations and frequency calculations were performed using a split basis set consisting of LANL2DZ[4] for nickel, SVP[5] for chlorine, bromine, and iodine, and 6-31G(d)[6] for all other atoms. Transition states were optimized using the Berny algorithm, and verified by vibrational analysis. Grignard reagents were assumed to be solvated by two THF molecules, consistent with previous computational investigation of catalyst transfer polymerization.[7] Optimized geometries were used as the starting point for single point energy calculations, utilizing a split basis set of SDD[8] for nickel and iodine, TZVP[9] for chlorine and bromine, and 6-311+G(d,p)[10] for all other atoms. The energy of each structure was determined by adding the zero-point energy correction from frequency calculations to the SCF energy from single point energy calculations, and reported relative to the total energy of the starting geometry for the catalytic step. The side chains are replaced with methyl groups to reduce the calculation time.

Monomer Synthesis. 3-Alkylthiophene[11] and 3-alkylselenophene[12] were prepared according to literature procedures starting with 3,7-dimethyloctanol[13].



Scheme S1. Monomer synthesis

2-Chloro-5-iodo-3-(3,7-dimethyloctyl)thiophene[14]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.98 (s, 1H), 2.62-2.44 (m, 2H), 1.58-1.09 (m, 10H), 1.10 (d, *J* = 7.3 Hz, 3H), 0.89 (d, *J* = 8 Hz, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 141.78, 137.77, 127.68, 110.16, 39.43, 37.10, 36.83, 32.54, 28.12, 25.51, 24.79, 22.86, 22.78, 19.67. TOF MS (ESI+) $C_{14}H_{22}ClIS$ $[M]^+$ Expected: 384.01754 Found: 384.01702 Δ = -1.36 ppm.

2,5-Dibromo-3-(3,7-dimethyloctyl)thiophene[12]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.78 (s, 1H), 2.58-2.44 (m, 2H), 1.59-1.09 (m, 10H), 0.92 (d, *J* = 8Hz, 3H), 0.87 (d, *J* = 8Hz, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 143.34, 131.07, 110.48, 107.92, 39.44, 37.10, 36.86, 32.53, 28.13, 27.32, 24.80, 22.86, 22.78, 19.69. TOF MS (ESI+) $C_{14}H_{22}Br_2S$ $[M+H]^+$ Expected: 380.98872 Found: 380.98903 Δ = 0.82 ppm.

2,5-Diiodo-3-(3,7-dimethyloctyl)thiophene[15]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.90 (s, 1H), 2.58-2.44 (m, 2H), 1.58-1.10 (m, 10H), 0.93 (d, *J* = 8Hz, 3H), 0.88 (d, *J* = 8Hz, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 149.85, 137.90, 76.94, 75.95, 39.45, 37.25, 37.11, 32.57, 29.79, 28.14, 24.82, 22.89, 22.80, 19.77. TOF MS (ESI+) $C_{14}H_{22}I_2S$ $[M+H]^+$ Expected: 476.96098 Found: 476.96192 Δ = 1.96 ppm.

2,5-Diiodo-3-(3,7-dimethyloctyl)selenophene[15]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.17 (s, 1H), 2.56-2.41 (m, 2H), 1.58-1.10 (m, 10H), 0.94 (d, *J* = 4Hz, 3H), 0.88 (d, *J* = 4Hz, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 151.83, 141.37, 78.97, 78.08, 39.44, 37.14, 37.10, 32.61, 31.31, 28.14, 24.82, 22.89, 22.81, 19.79. TOF MS (ESI+) $C_{14}H_{22}I_2Se$ $[M+H]^+$ Expected: 524.90543 Found: 524.90544 Δ = 0.01 ppm.

2-Bromo-5-iodo-3-(2-ethylhexyl)tellurophene[16]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.76 (s, 1H), 2.49 (d, *J* = 7.3Hz, 2H), 1.59-1.53 (m, 1H), 1.33-1.20 (m, 8H), 0.94-0.83 (m, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 152.44, 149.05, 108.07, 64.44, 40.09, 36.43, 32.42, 28.74, 25.65, 23.05, 14.12, 10.84. TOF MS (ESI+) $C_{14}H_{22}I_2Se$ $[M+H]^+$ Expected: 498.87770 Found: 498.87858 Δ = 1.76 ppm.

General Procedure for Kinetics Studies. Isopropylmagnesium chloride (0.98 equiv) was added to a solution of 2,5-dibromo-3-(3,7-dimethyloctyl)thiophene (105 mg, 0.275 mmol) in THF ([M] = 0.1 M, internal standard: docosane). The mixture was stirred at r.t. for 60 mins. An aliquot was removed (t = 0 s) and quenched with dilute hydrochloric acid (HCl) and extracted with chloroform (CF) immediately after removal. A solution of containing Ni(*o*-tolyl)(dppe)Cl (2.5 mol %) was injected into the monomer solution as described above. Aliquots were removed during the polymerization (t = 10 s to t = 300 s) and all samples were quenched with dilute HCl and extracted with CF immediately after removal. Each aliquot was analyzed using gas chromatography. The molecular weight distribution was determined without purification by MALDI-TOF/MS.

General Procedure for *in situ* ^{31}P NMR studies. A higher concentration (0.2 M dihalogenated monomer) and low monomer to Ni(o-tolyl)(dppe)Cl catalyst ratio (around 10) were used to ensure sufficient signal. Isopropylmagnesium chloride (0.98 equiv) was added to a solution 2,5-dibromo-3-(3,7-dimethyloctyl)thiophene (117 mg, 0.305 mmol) in THF in glovebox filled with argon. The mixture was stirred at r.t. for 60 mins. 0.5 mL of the activated monomer solution was transferred into a NMR tube with a septum and cooled down to -20 °C. A solution of containing Ni(*o*-tolyl)(dppe)Cl (10 mol %) was injected into the monomer solution as described above. The spectra were recorded immediately after the addition (temperature setting: -15 °C). And then the sample was left at room temperature for 0.5 hour and another spectrum for post-polymerization mixtures was recorded with the same spectrometer settings. Finally, the polymerization was quenched with dilute HCl and extracted with CF immediately. The molecular weight distribution was determined without purification by MALDI-TOF/MS.

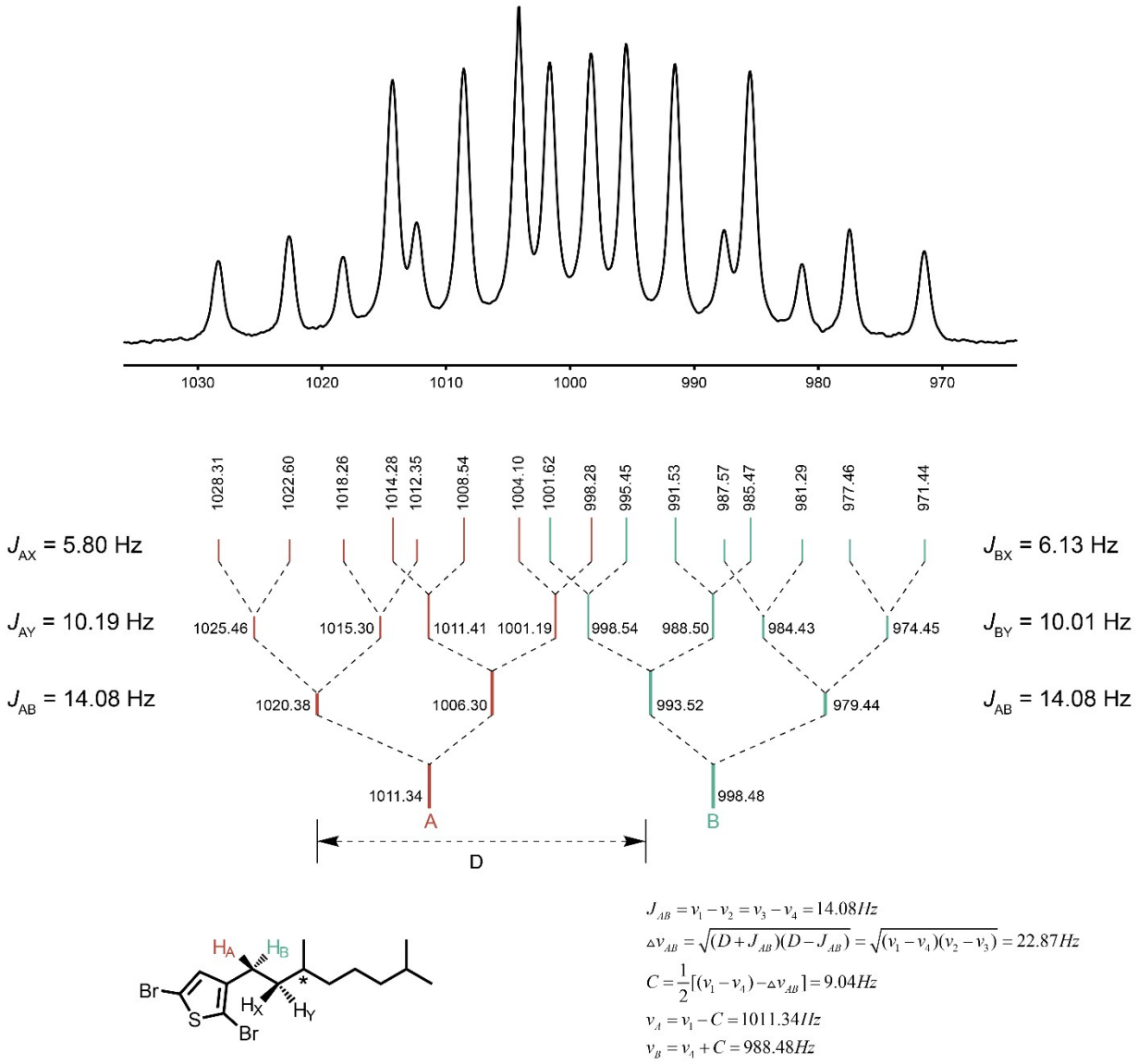


Fig. S1 ^{1}H NMR splitting pattern of the methylene protons in 2,5-dibromo-3-(3,7-dimethyloctyl)thiophene.

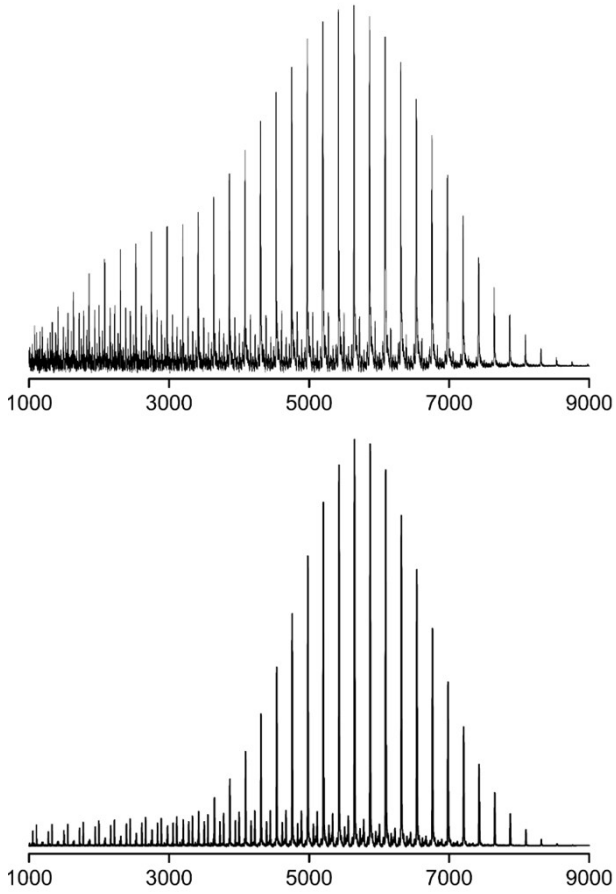


Fig. S2 MALDI-TOF/MS spectra of poly(3-(3,7-dimethyloctyl)thiophene) prepared by pre-initiation method (top) and external initiation (bottom).

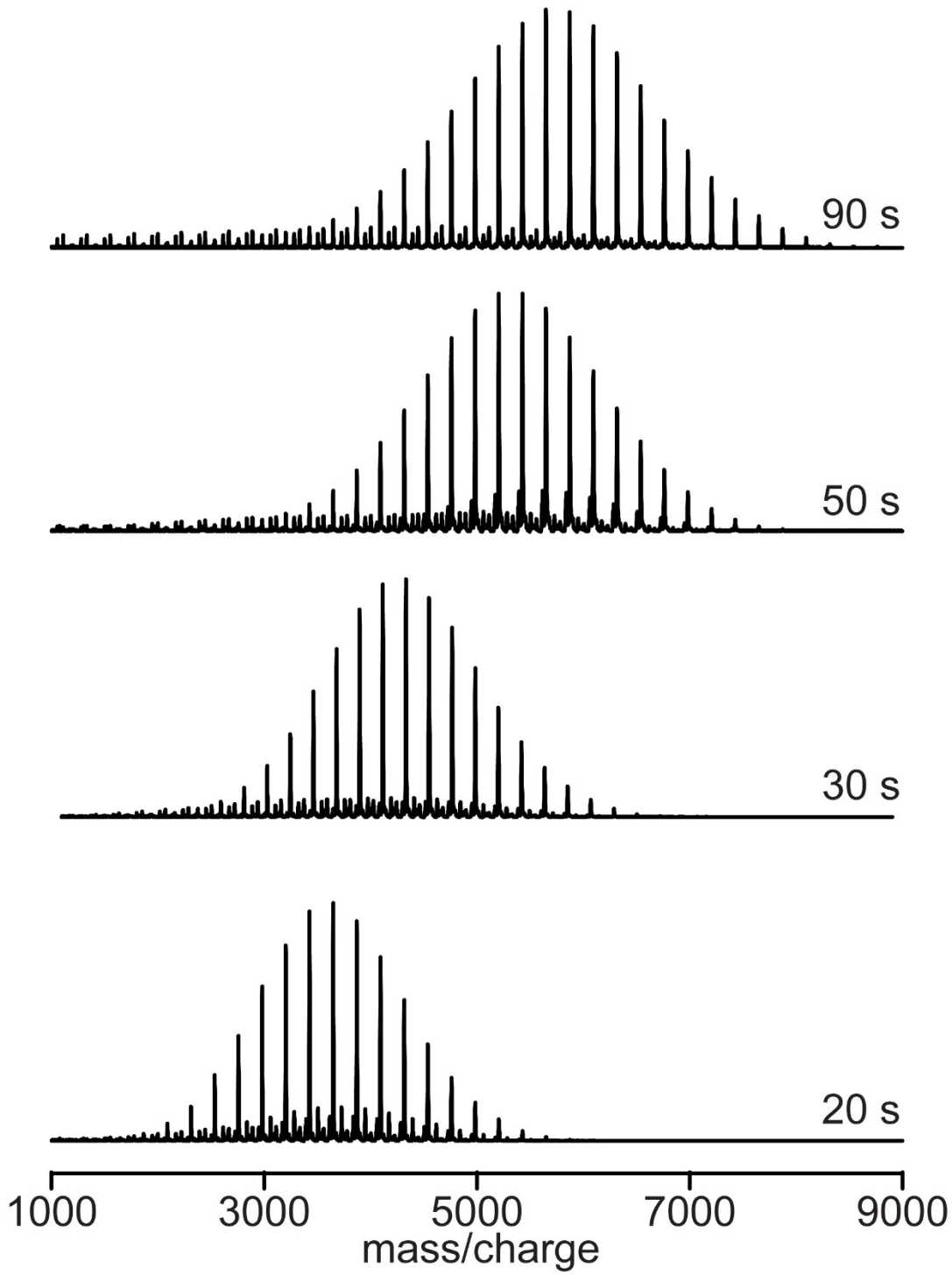


Fig. S3 MALDI-TOF/MS spectra of poly(3-(3,7-dimethyloctyl)thiophene from the polymerization of XMg-Th-**Br** (I/Br) to show **no serious broadening**.

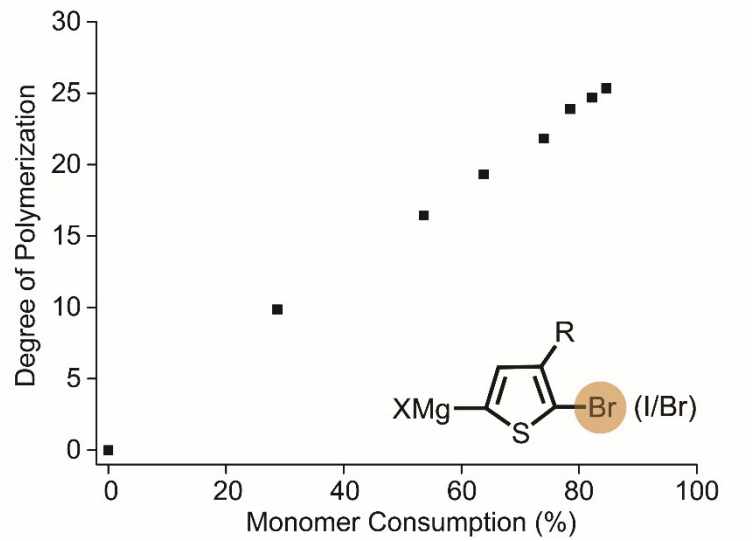


Fig. S4 Degree of polymerization versus monomer conversion for XMg-Th-**Br** (I/Br)**.**

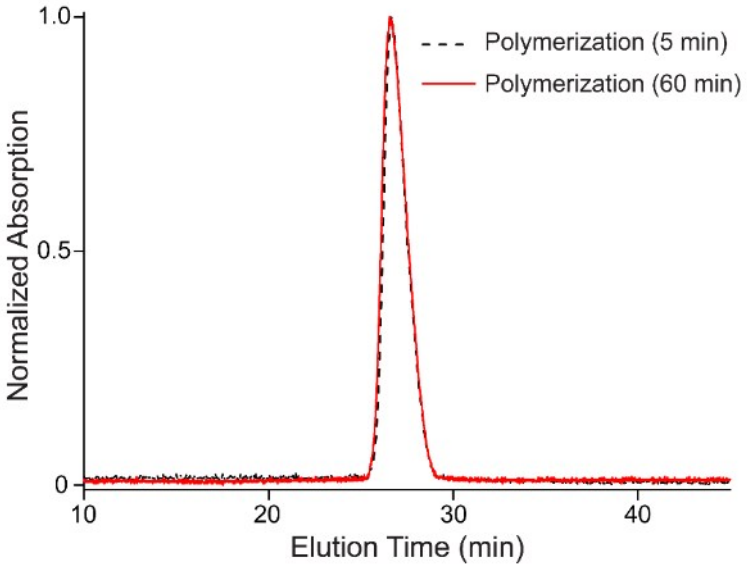


Fig. S5 Gel permeation Chromatography (GPC) curves of polymerization of XMg-Th-**Cl**. Aliquots were withdrew from the polymerization in 5 min and 60 min. This experiment shows that the polymerization of XMg-Th-**Cl** is complete in 5 min. No chain extension was observed after 5 min. M_n = 7.1 kDa, $Đ$ = 1.3. (For reference, M_n = 9.1 kDa, $Đ$ = 1.1 for XMg-Th-**Br**).

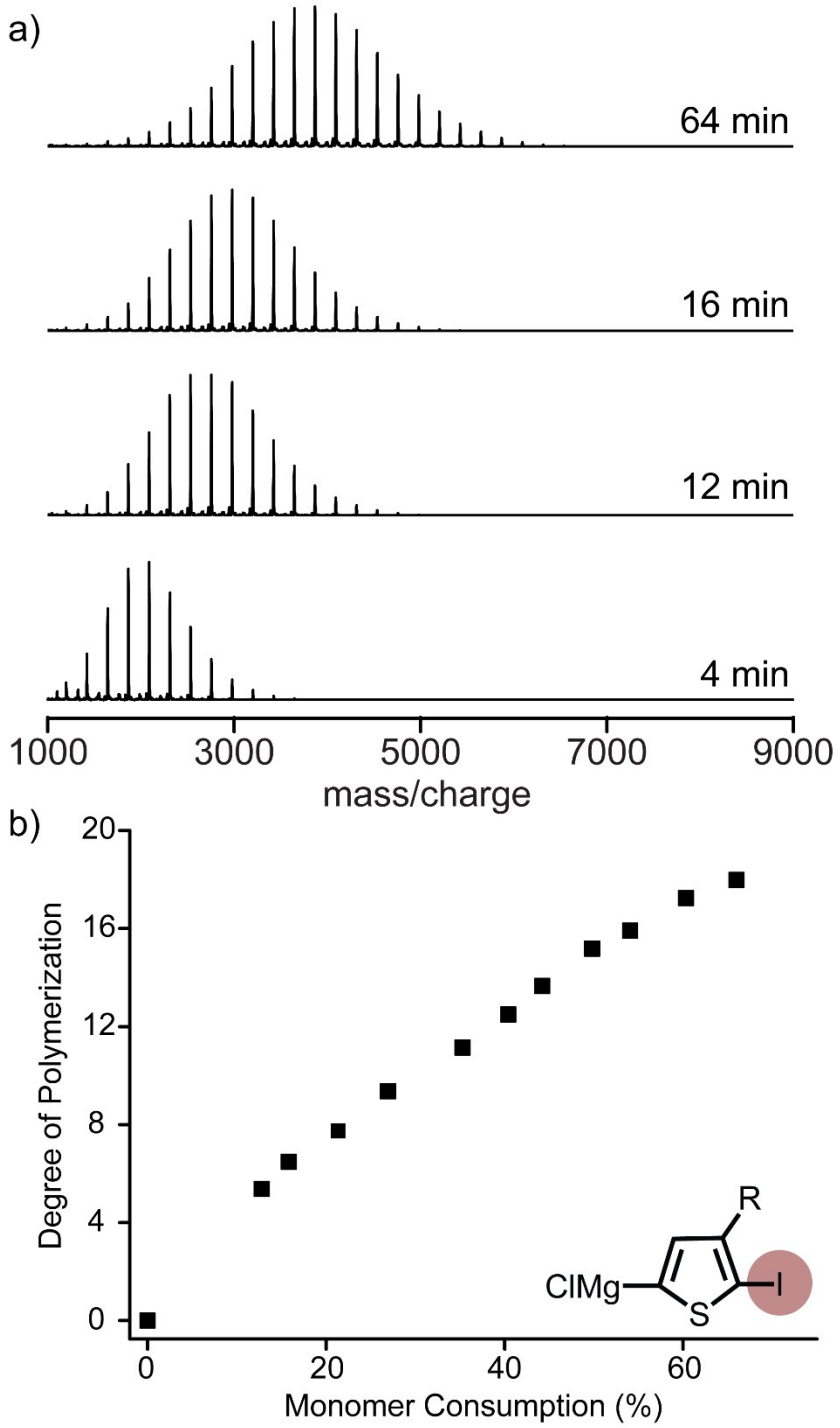


Fig. S6 a) MALDI-TOF/MS spectra of poly(3-(3,7-dimethyloctyl)thiophene from the polymerization of XMg-Th-**I** to show **no serious broadening**; b) Degree of polymerization versus monomer conversion for XMg-Th-**I**.

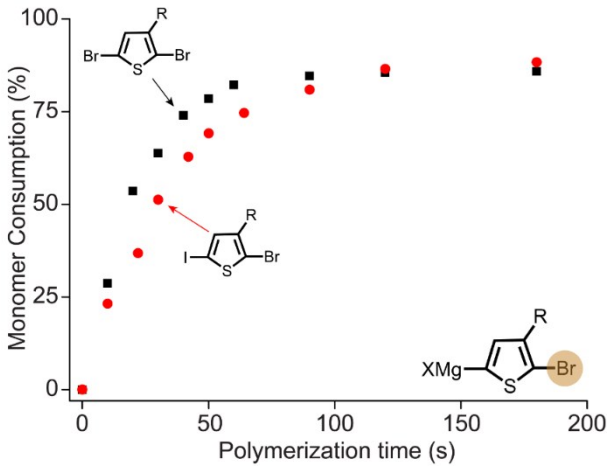


Fig. S7 Kinetic plots of monomer consumption during the polymerization of XMg-Th-**Br** (I/Br) and XMg-Th-**Br** (Br/Br).

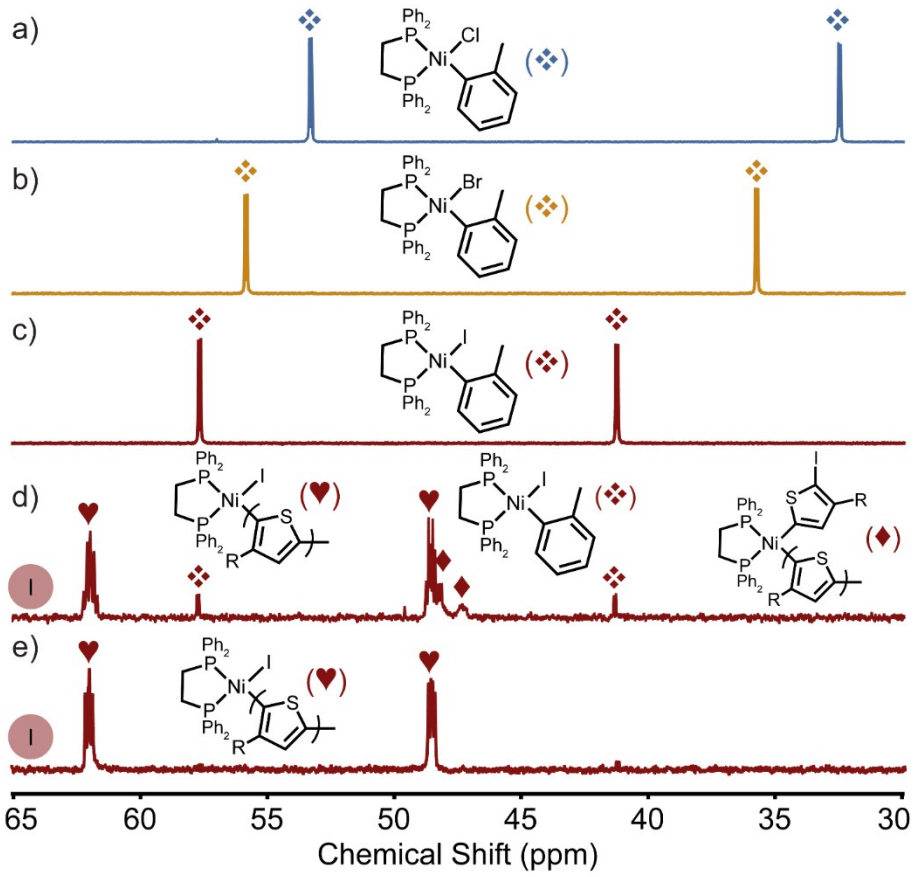


Fig. S8 ^{31}P NMR spectra for the a) Ni(*o*-tolyl)(dppe)**Cl** external initiator; b) Ni(*o*-tolyl)(dppe)**Br**; c) Ni(*o*-tolyl)(dppe)**I**; d) resting state during the polymerization of XMg-Th-**I** and the resting state after the polymerization of XMg-Th-**I**.

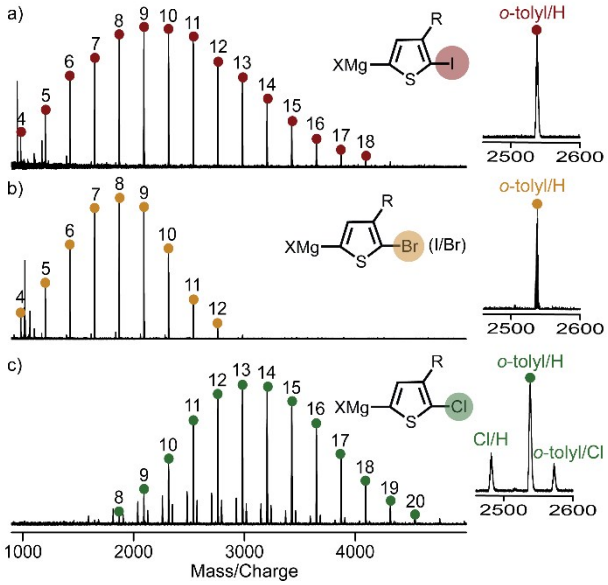


Fig. S9 MALDI-TOF/MS spectra of the polymers of a) XMg-Th-**I** (Found:2537.76; Prediction:2538.43), b) XMg-Th-**Br** (I/Br) (Found:2537.14; Prediction: 2538.43), and c) XMg-Th-**Cl** [Left peak: Found:2481.87; Prediction:2482.75; Middle peak: Found:2537.71; Prediction:2538.43; Right peak: Found: 2571.72; Prediction: 2572.87] (after *in situ* ^{31}P NMR studies).

[We used MALDI-TOF/MS to investigate the polymers that were prepared in this study (Fig. S9). When either brominated or iodinated monomers are polymerized, MALDI-TOF/MS spectra of the resulting polymers show only one distribution with *o*-tolyl and H end groups (Fig. S9a and S9b), whereas a mixture of polymers with different end-group compositions (*o*-tolyl/H, *o*-tolyl/Cl, Cl/H) are observed in the polymerization of XMg-Th-**Cl** (Fig. S9c). This is consistent with the observation of a chain-growth mechanism in the cases of XMg-Th-**Br** (I/Br) and XMg-Th-**I**. However, a strong carbon-chlorine bond suppresses OA in the polymerization of XMg-Th-**Cl**, leading to early chain termination and re-initiation. This is consistent with the observation of dissociated Ni(0)dppe complex in this polymerization. Considering the wide application of phosphine ligands, the combination of *in situ* ^{31}P NMR and MALDI-TOF/MS presents a general method to evaluate the degree of control in chain growth polymerizations.]

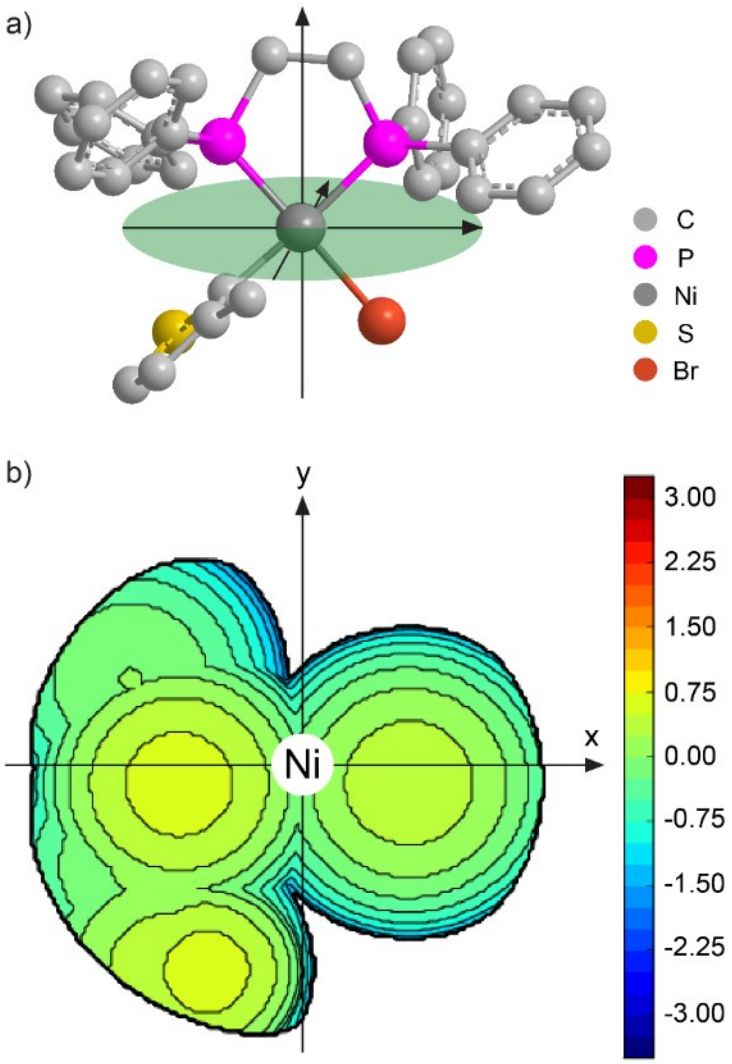


Fig. S10 Representative steric maps of optimized structure of Ni(II)-thienyl bromide complex **1**. Ni atom is placed at the center of the *xyz* coordinate system with *z*-axis bisecting the C-C bridge of the ligand. The side chain is replaced with methyl to reduce the calculation time. The percent buried volume ($\%V_{Bur}$, radius setting: 3.5 Å) of Ni centers occupied by the methylthiophene and halogen (in the southern hemisphere) increases from **Cl** (41.4%), to **Br** (42.4%) to **I** (43.4%).[17]

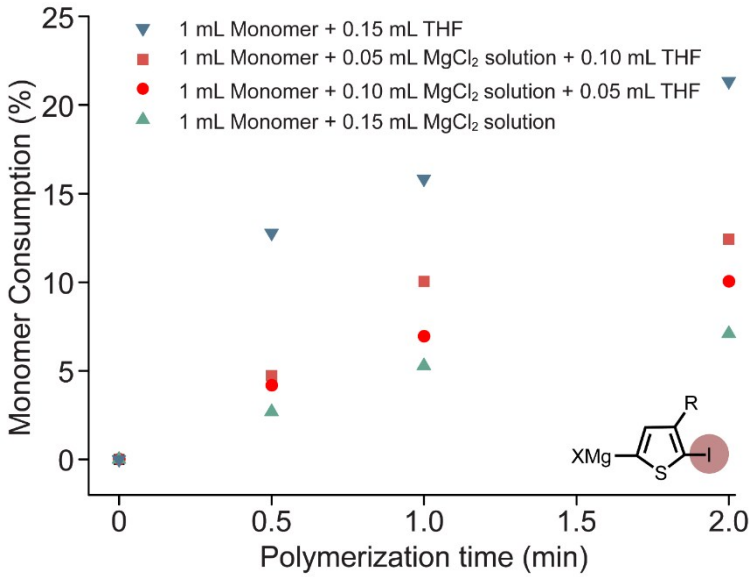


Fig. S11 Kinetic plots of monomer consumption during the polymerization of XMg-Th-**I** with different amount of saturated magnesium chloride solution. [M] = 0.1 M.

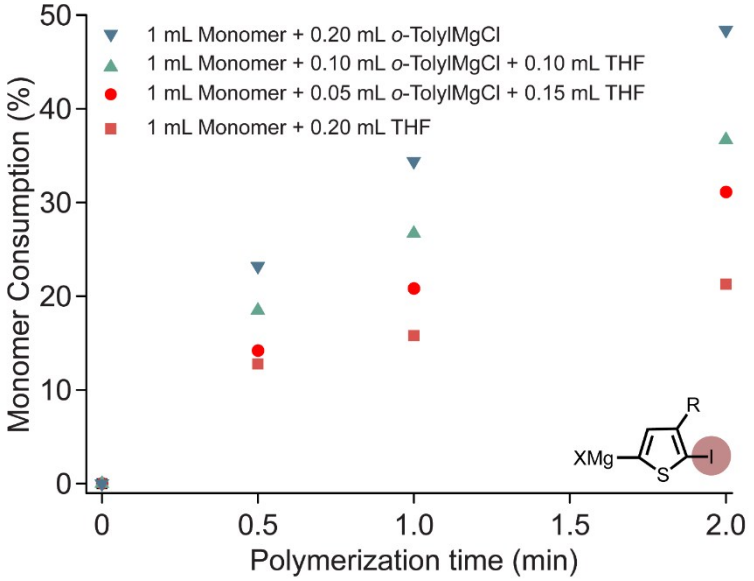


Fig. S12 Kinetic plots of monomer consumption during the polymerization of XMg-Th-**I** with different amount of *o*-TolylMgCl solution. [M] = 0.1 M, [*o*-TolylMgCl] = 1 M.

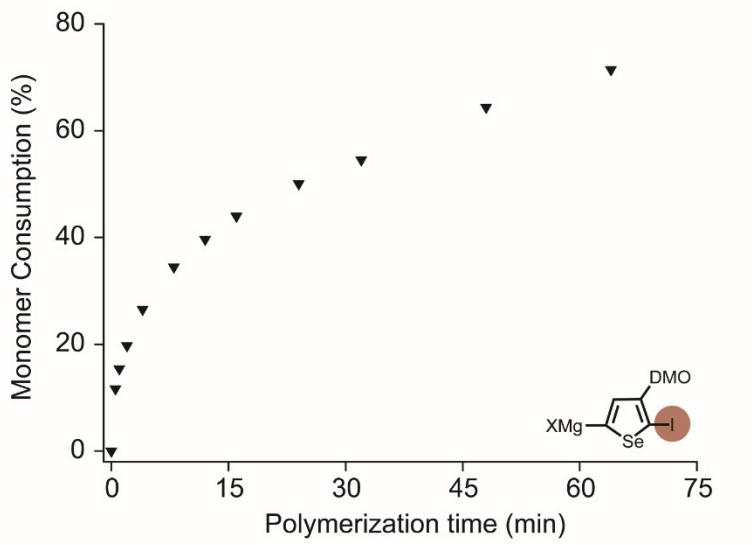


Fig. S13 Kinetic plots of monomer consumption during polymerization of XMg-Se-**I**. At 2.5% catalyst loading, 0.1 M monomer concentration. [Only the polymerizable monomers are considered in the monomer consumption calculation.]

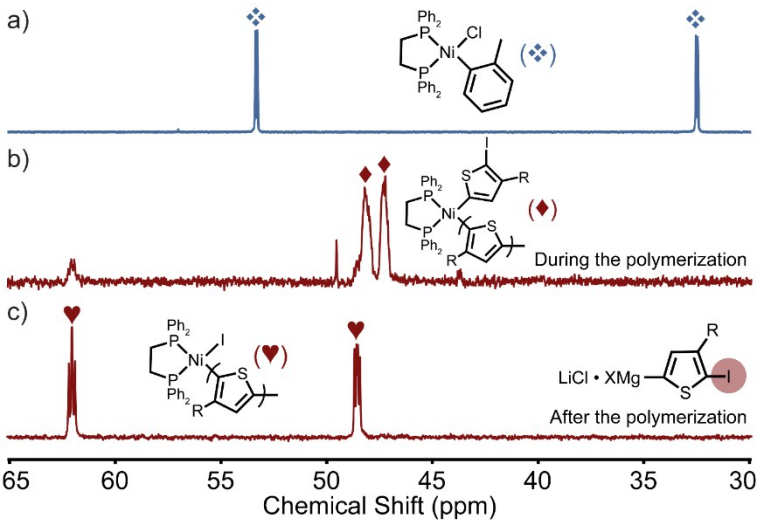
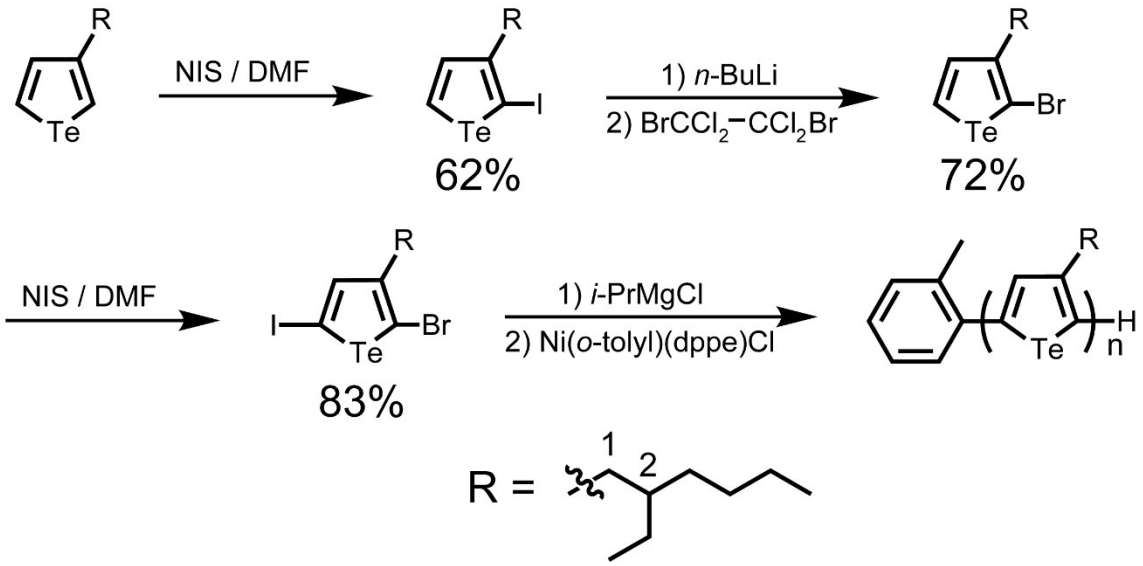


Fig. S14 ^{31}P NMR spectra for the a) Ni(*o*-tolyl)(dppe)**Cl** external initiator; b) resting state during the polymerization of XMg-Th-**I** with LiCl additive and c) the resting state after the polymerization of XMg-Th-**I** with LiCl additive.



Scheme S2 Monomer Synthesis 2-bromo-3-(2-ethylhexyl)-5-iodotellurophene

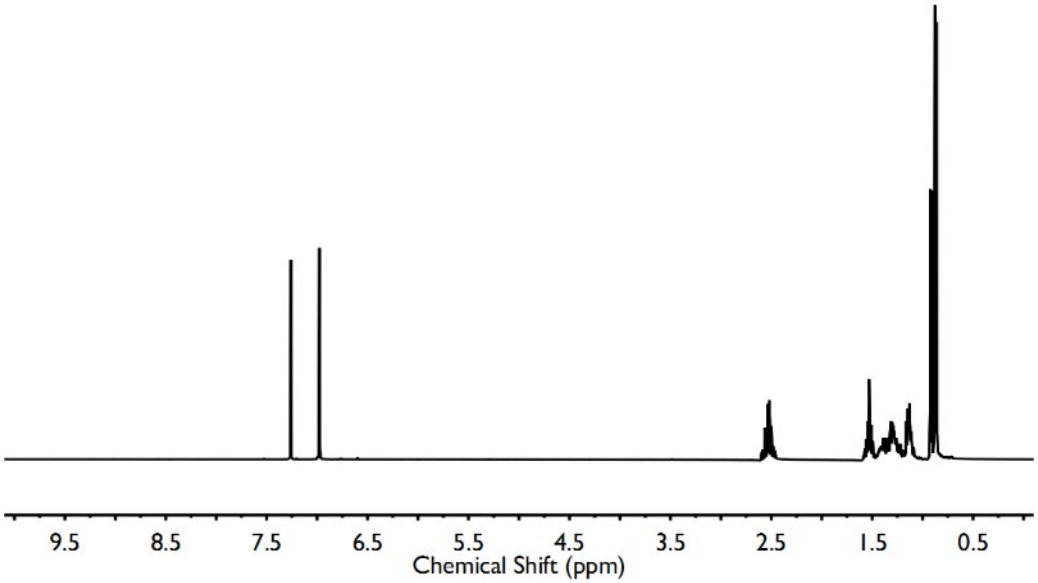


Fig. S15 ^{1}H NMR spectrum of 2-chloro-5-iodo-3-(3,7-dimethyloctyl)thiophene.

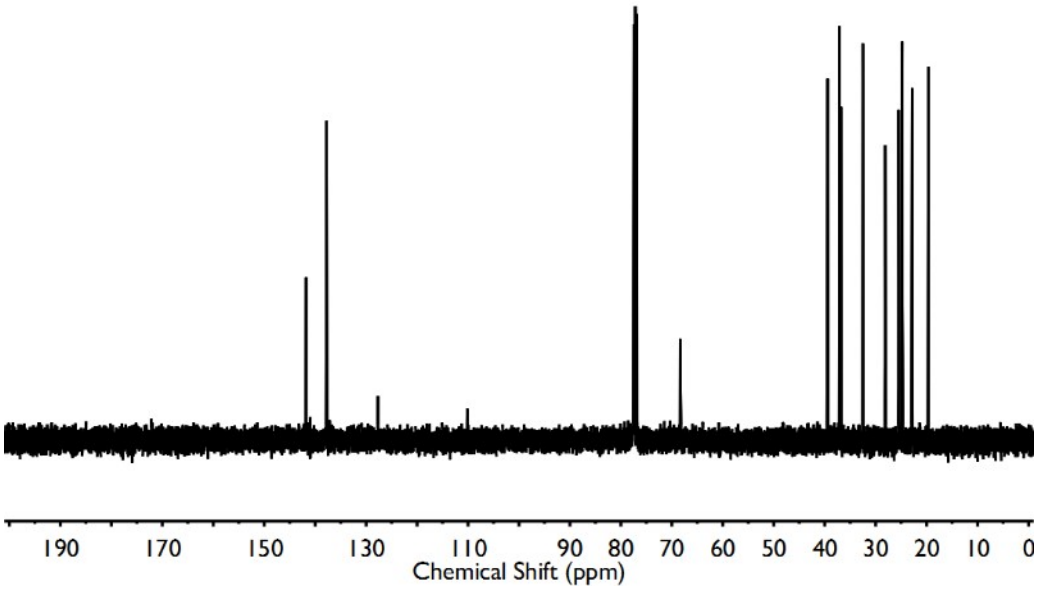


Fig. S16 ^{13}C NMR spectrum of 2-chloro-5-iodo-3-(3,7-dimethyloctyl)thiophene.

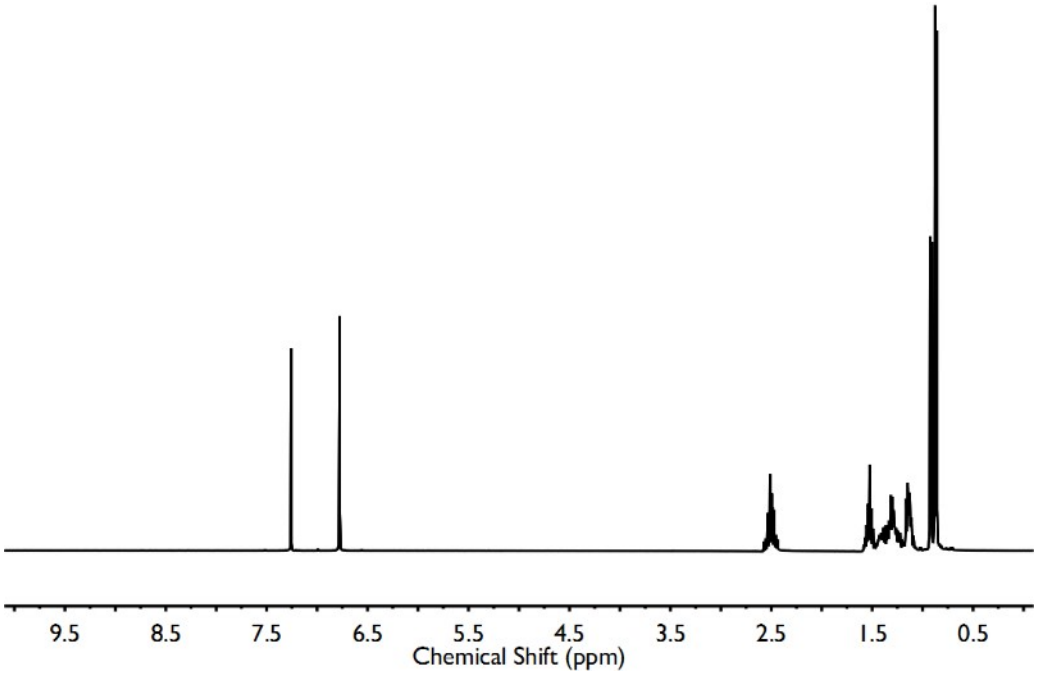


Fig. S17 ^{1}H NMR spectrum of 2,5-dibromo-3-(3,7-dimethyloctyl)thiophene.

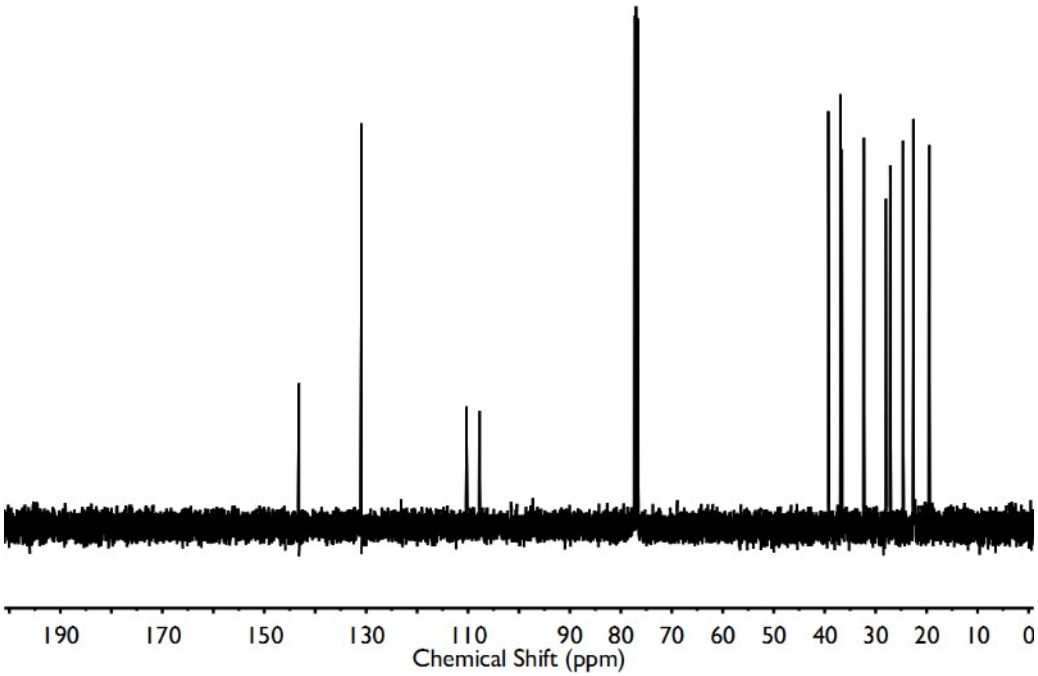


Fig. S18 ^{13}C NMR spectrum of 2,5-dibromo-3-(3,7-dimethyloctyl)thiophene.

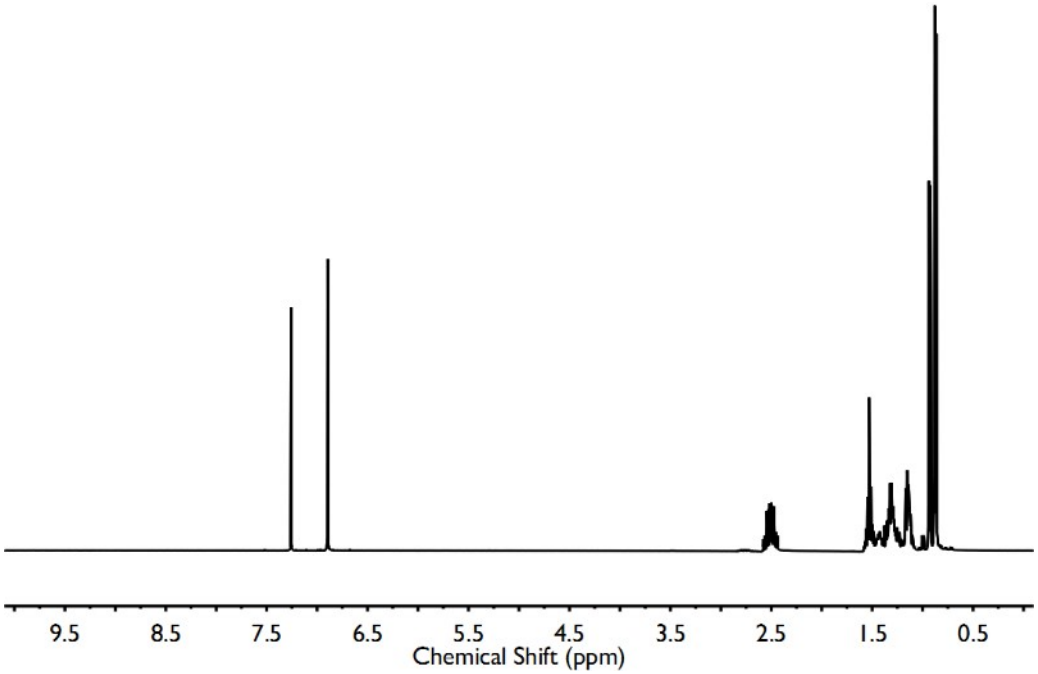


Fig. S19 ^{1}H NMR spectrum of 2,5-diiodo-3-(3,7-dimethyloctyl)thiophene.

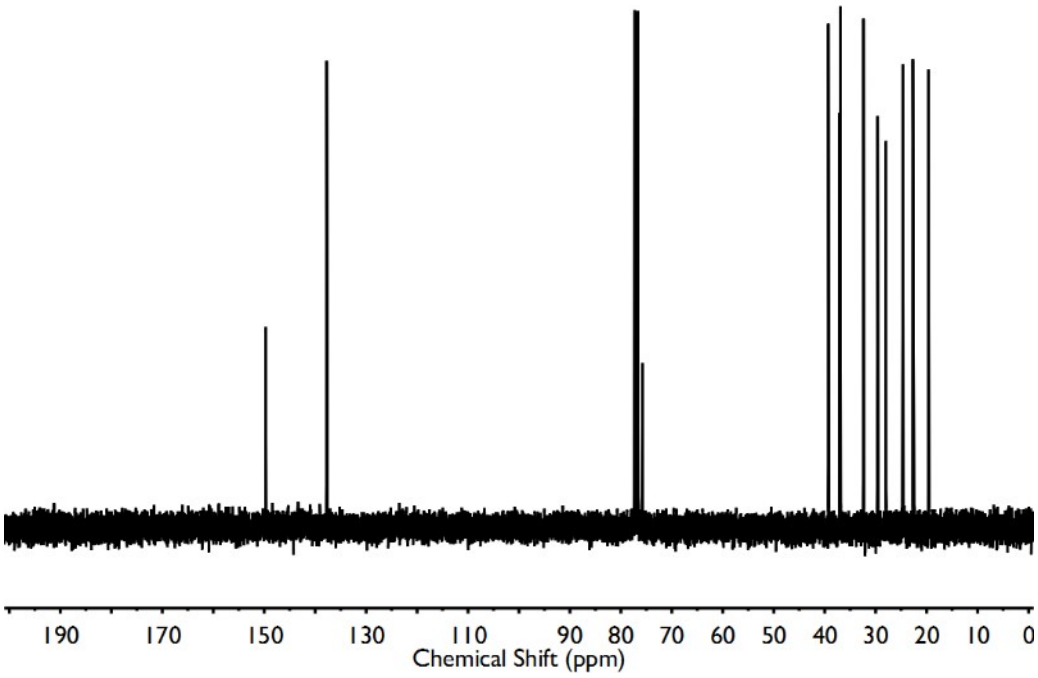


Fig. S20 ^{13}C NMR spectrum of 2,5-diiodo-3-(3,7-dimethyloctyl)thiophene.

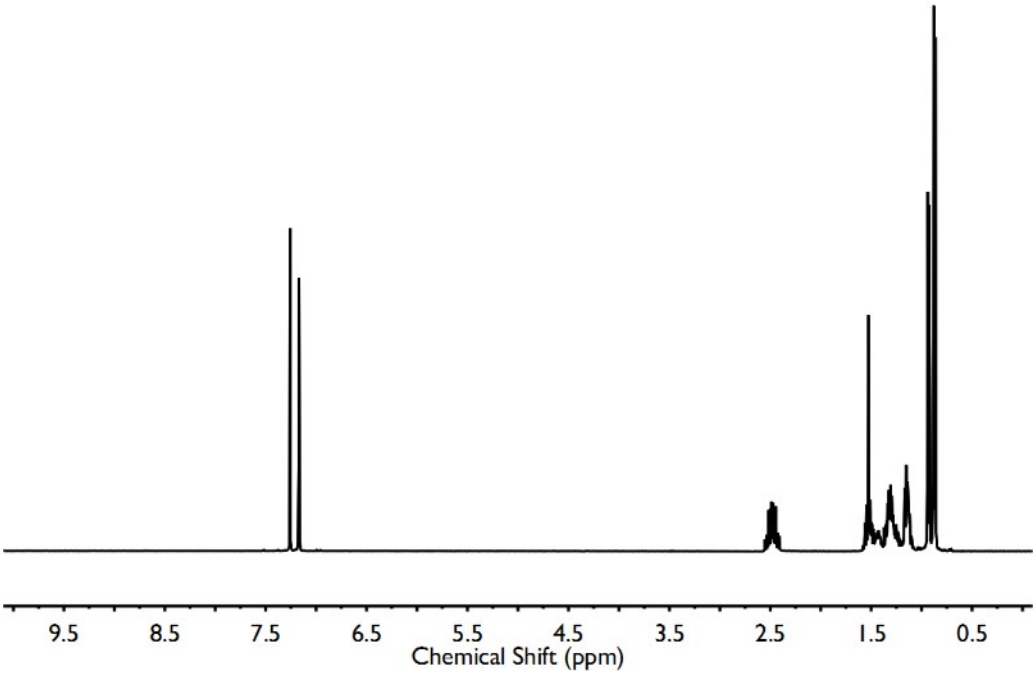


Fig. S21 ^{1}H NMR spectrum of 2,5-diiodo-3-(3,7-dimethyloctyl)selenophene.

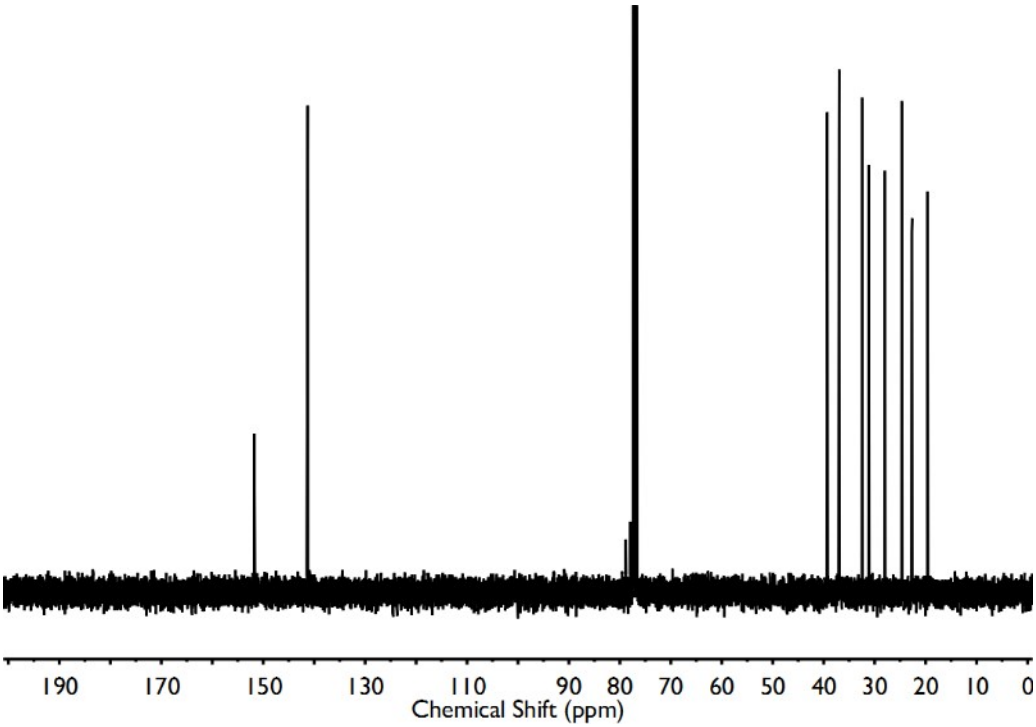


Fig. S22 ^{13}C NMR spectrum of 2,5-diiodo-3-(3,7-dimethyloctyl)selenophene.

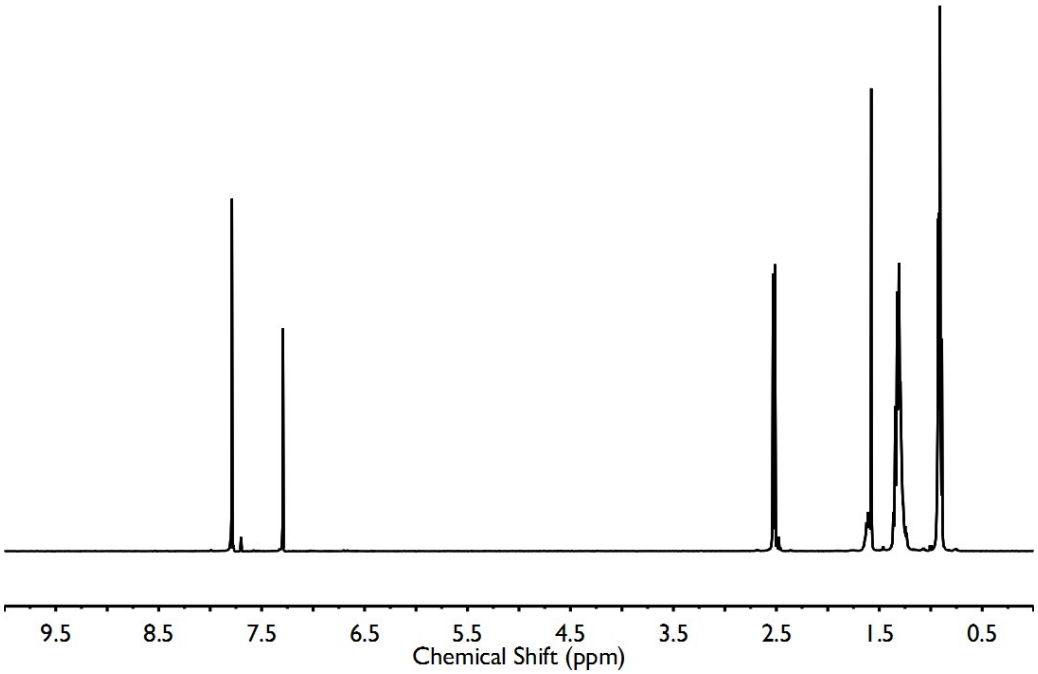


Fig. S23 ^{1}H NMR spectrum of 2-bromo-3-(2-ethylhexyl)-5-iodotellurophene.

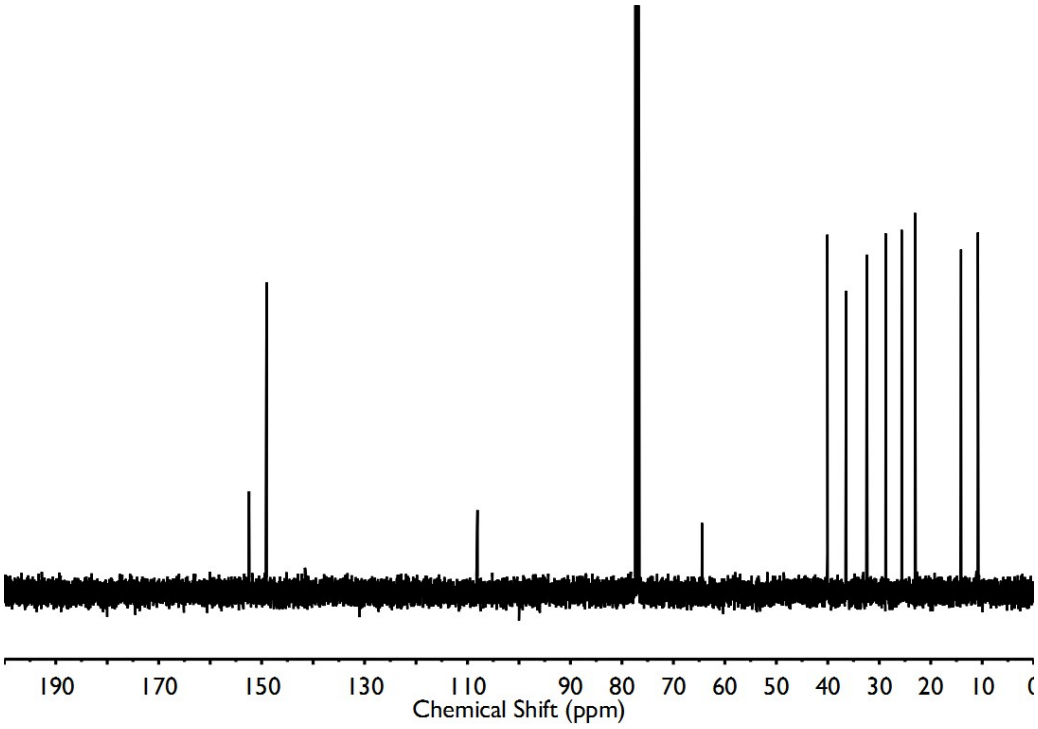
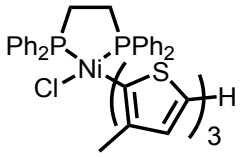


Fig. S24 ^{13}C NMR spectrum of 2-bromo-3-(2-ethylhexyl)-5-iodotellurophene.



Pre-Transmetalation – Chlorine

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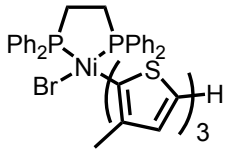
C	-0.65790	-1.70360	-0.66895
C	-2.06739	-1.56722	-0.85848
C	-2.51842	-0.26505	-0.92006
H	-2.73340	-2.41900	-0.96997
Ni	1.89358	-0.23104	-0.52763
P	1.79750	-0.03424	1.68495
P	4.19013	-0.13614	-0.34744
C	3.55156	0.15159	2.34311
H	3.74700	1.22947	2.34438
H	3.61566	-0.18687	3.38310
C	4.56024	-0.56282	1.43367
H	4.44638	-1.65172	1.49722
H	5.59302	-0.33800	1.72253
Cl	1.99046	-0.21572	-2.75899
C	5.27060	-1.28594	-1.28650
C	6.66965	-1.18649	-1.21571
C	4.68888	-2.31067	-2.04693
C	7.47444	-2.11024	-1.88118
H	7.13279	-0.37977	-0.65359
C	5.50018	-3.23416	-2.71033
H	3.60989	-2.35469	-2.14755
C	6.88962	-3.13815	-2.62616
H	8.55631	-2.02490	-1.82329
H	5.04196	-4.02138	-3.30265
H	7.51793	-3.85554	-3.14747
C	4.88932	1.54484	-0.61493
C	5.83846	2.13718	0.23295
C	4.42879	2.26315	-1.73329
C	6.32364	3.41951	-0.03354
H	6.20782	1.60967	1.10769
C	4.92300	3.54063	-1.99809
H	3.68362	1.81386	-2.38517
C	5.86892	4.12199	-1.15045
H	7.05642	3.86696	0.63278
H	4.56208	4.08382	-2.86722
H	6.24756	5.11944	-1.35699
C	1.00221	1.50177	2.29695
C	0.50525	1.61886	3.60355
C	0.98286	2.62103	1.45080
C	-0.00509	2.83756	4.05310
H	0.50567	0.75899	4.26658
C	0.47823	3.83912	1.90622
H	1.35197	2.53379	0.43228
C	-0.01808	3.94820	3.20672

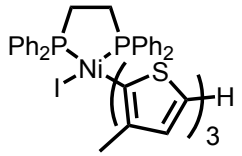
H	-0.39430	2.91760	5.06445
H	0.46149	4.69707	1.24013
H	-0.41939	4.89478	3.55835
C	1.05010	-1.40845	2.64198
C	1.84093	-2.38205	3.27158
C	-0.34972	-1.53274	2.68907
C	1.24742	-3.45232	3.94353
H	2.92452	-2.31936	3.24270
C	-0.93770	-2.60027	3.36724
H	-0.97872	-0.79874	2.19733
C	-0.14261	-3.56225	3.99443
H	1.87378	-4.19720	4.42671
H	-2.02059	-2.68040	3.39938
H	-0.60460	-4.39447	4.51842
S	-1.14262	0.81857	-0.72199
C	0.03139	-3.04534	-0.64985
H	1.03830	-2.96405	-0.22742
H	0.13539	-3.45349	-1.66406
H	-0.52583	-3.77890	-0.05358
C	-3.88701	0.20011	-1.03509
C	-4.41351	1.35233	-1.60101
S	-5.17221	-0.81427	-0.39331
C	-5.83463	1.38624	-1.53315
C	-6.42200	0.29349	-0.93110
H	-6.41885	2.19680	-1.95854
C	-7.83522	0.06353	-0.68993
C	-8.56283	-1.11223	-0.58962
S	-8.88506	1.46185	-0.48280
C	-9.95472	-0.86597	-0.36504
C	-10.28287	0.45786	-0.29358
H	-10.68326	-1.66590	-0.27482
H	-11.25835	0.90106	-0.14475
C	-8.00385	-2.50631	-0.72067
H	-7.21569	-2.56055	-1.47819
H	-7.57092	-2.86634	0.22219
H	-8.79489	-3.20912	-1.00371
C	-3.61103	2.44394	-2.26182
H	-3.22418	3.16669	-1.53129
H	-2.74919	2.04172	-2.80348
H	-4.23288	2.99935	-2.97225



Pre-Transmetalation – Bromine

C	-0.07181	-0.63366	-0.28435
C	-0.72611	-1.79995	0.06599
C	-2.13374	-1.74482	-0.16814
C	-2.58475	-0.55628	-0.70451
H	-2.79881	-2.57957	0.03744
Ni	1.82607	-0.36115	-0.29205
P	1.65564	0.65035	1.68809
P	4.11633	-0.17033	-0.08579
C	3.38708	1.06521	2.29821
H	3.59696	2.07066	1.91761
H	3.41120	1.12447	3.39183
C	4.41451	0.06978	1.74463
H	4.28103	-0.92393	2.18903
H	5.44130	0.37877	1.96994
Br	1.97537	-1.26529	-2.48304
C	5.23414	-1.56536	-0.50252
C	6.61951	-1.38586	-0.63644
C	4.68991	-2.85192	-0.63103
C	7.44916	-2.48062	-0.87954
H	7.05063	-0.39119	-0.56473
C	5.52491	-3.94498	-0.86875
H	3.61468	-2.98722	-0.57881
C	6.90317	-3.76163	-0.99194
H	8.52042	-2.33230	-0.98653
H	5.09401	-4.93685	-0.97336
H	7.55050	-4.61286	-1.18545
C	4.83075	1.31915	-0.89785
C	5.76166	2.16808	-0.27757
C	4.40393	1.61517	-2.20485
C	6.25953	3.28651	-0.94976
H	6.10769	1.96854	0.73233
C	4.91019	2.72974	-2.87420
H	3.67758	0.96750	-2.68929
C	5.83631	3.56809	-2.24956
H	6.97768	3.93559	-0.45577
H	4.57463	2.94413	-3.88518
H	6.22456	4.43845	-2.77170
C	0.85848	2.30292	1.66202
C	0.32699	2.89539	2.81730
C	0.87319	3.02908	0.46148
C	-0.18337	4.19337	2.76854
H	0.30067	2.34239	3.75138
C	0.36808	4.32867	0.41840
H	1.26953	2.57152	-0.44112
C	-0.16243	4.91139	1.57098

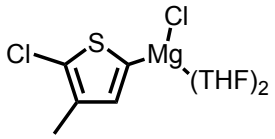
H	-0.59915	4.64203	3.66662
H	0.37794	4.87872	-0.51829
H	-0.56387	5.92048	1.53523
C	0.85846	-0.27402	3.05675
C	1.61555	-0.95327	4.02400
C	-0.54387	-0.36649	3.10082
C	0.98627	-1.70008	5.02169
H	2.70041	-0.91065	4.00889
C	-1.16776	-1.10844	4.10365
H	-1.14719	0.13990	2.35528
C	-0.40631	-1.77718	5.06467
H	1.58674	-2.21891	5.76391
H	-2.25224	-1.16654	4.12764
H	-0.89619	-2.35729	5.84190
S	-1.20972	0.52678	-0.90974
C	-0.03494	-3.04165	0.57188
H	0.89927	-2.79318	1.08715
H	0.21927	-3.71766	-0.25532
H	-0.66791	-3.59744	1.27434
C	-3.95247	-0.16724	-0.98758
C	-4.47571	0.70103	-1.93501
S	-5.24144	-0.88210	-0.02818
C	-5.89710	0.75526	-1.89081
C	-6.48806	-0.04587	-0.93663
H	-6.47878	1.35597	-2.58369
C	-7.90254	-0.17446	-0.63514
C	-8.63149	-1.23480	-0.11919
S	-8.95230	1.20295	-0.95333
C	-10.02423	-0.92527	-0.00544
C	-10.35171	0.33424	-0.41976
H	-10.75379	-1.63895	0.36498
H	-11.32755	0.80029	-0.44605
C	-8.07297	-2.58118	0.26599
H	-7.28082	-2.90491	-0.41638
H	-7.64548	-2.57522	1.27755
H	-8.86307	-3.33971	0.25217
C	-3.66957	1.48038	-2.94249
H	-3.28120	2.41646	-2.51990
H	-2.80849	0.90829	-3.30210
H	-4.28929	1.74477	-3.80613



Pre-Transmetalation – Iodine

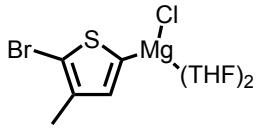
C	-0.13267	-0.62817	0.15789
C	-0.78577	-1.37689	1.12033
C	-2.19236	-1.47206	0.89715
C	-2.64630	-0.81469	-0.22812
H	-2.85504	-2.03570	1.54858
Ni	1.76259	-0.35719	0.03197
P	1.49563	1.62705	1.03685
P	4.04214	0.00200	0.15686
C	3.19506	2.36217	1.36722
H	3.43128	2.96705	0.48520
H	3.16684	3.04208	2.22559
C	4.23846	1.25175	1.53614
H	4.06923	0.68708	2.46100
H	5.25559	1.65443	1.59613
I	1.98645	-2.54465	-1.30921
C	5.20637	-1.32542	0.66187
C	6.57743	-1.26760	0.37239
C	4.70652	-2.39896	1.41481
C	7.43670	-2.26217	0.84168
H	6.97487	-0.45482	-0.22831
C	5.57046	-3.38624	1.88943
H	3.63989	-2.47520	1.60125
C	6.93556	-3.31953	1.60375
H	8.49668	-2.21252	0.60720
H	5.17254	-4.21624	2.46661
H	7.60586	-4.09481	1.96514
C	4.78273	0.80955	-1.32393
C	5.71780	1.85488	-1.24225
C	4.37828	0.35874	-2.59272
C	6.23826	2.43465	-2.40104
H	6.05050	2.22659	-0.27771
C	4.90635	0.93671	-3.74790
H	3.65525	-0.44887	-2.66885
C	5.83437	1.97589	-3.65597
H	6.95895	3.24406	-2.32060
H	4.58686	0.57388	-4.72097
H	6.24002	2.42776	-4.55714
C	0.70871	2.92874	0.01009
C	0.12193	4.07245	0.57212
C	0.78634	2.81159	-1.38603
C	-0.38040	5.08022	-0.25228
H	0.04636	4.17302	1.65059
C	0.28880	3.82404	-2.20660
H	1.22595	1.92206	-1.82944
C	-0.29679	4.95826	-1.64090

H	-0.83904	5.95960	0.19164
H	0.34783	3.71914	-3.28622
H	-0.69220	5.74289	-2.28019
C	0.62460	1.66195	2.65049
C	1.32832	1.69453	3.86478
C	-0.77892	1.58166	2.67886
C	0.64535	1.66142	5.08190
H	2.41298	1.74303	3.87568
C	-1.45670	1.55595	3.89767
H	-1.34211	1.54210	1.75275
C	-0.74838	1.59476	5.10058
H	1.20495	1.68939	6.01288
H	-2.54147	1.49897	3.90305
H	-1.28012	1.57061	6.04782
S	-1.27366	-0.04596	-1.02255
C	-0.08955	-2.09312	2.25062
H	0.74755	-1.50360	2.64221
H	0.31884	-3.05520	1.91388
H	-0.77567	-2.29176	3.08227
C	-4.01463	-0.66475	-0.68303
C	-4.53953	-0.50534	-1.95755
S	-5.30244	-0.69602	0.51445
C	-5.96108	-0.43868	-1.95137
C	-6.55062	-0.54194	-0.70910
H	-6.54391	-0.35067	-2.86341
C	-7.96490	-0.47595	-0.38723
C	-8.69151	-1.04562	0.64689
S	-9.01774	0.46303	-1.44091
C	-10.08498	-0.73011	0.56267
C	-10.41526	0.05865	-0.50226
H	-10.81300	-1.10072	1.27782
H	-11.39219	0.42197	-0.79168
C	-8.12989	-1.92176	1.73779
H	-7.33677	-2.57826	1.36639
H	-7.70272	-1.33226	2.56002
H	-8.91815	-2.55089	2.16512
C	-3.73479	-0.45077	-3.23098
H	-3.34705	0.55755	-3.42735
H	-2.87348	-1.12527	-3.19511
H	-4.35532	-0.73419	-4.08796



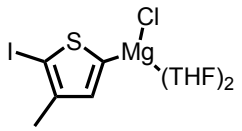
Thiophene Grignard – Chlorine

H	4.37141	0.79566	2.85928
Cl	-2.48462	-0.05921	2.31632
S	1.99613	-0.05329	-1.04293
Mg	-1.07785	-0.01592	0.50814
C	4.43570	-0.08091	2.20212
C	3.51449	-0.06271	-0.18376
C	3.33691	-0.07031	1.17535
C	1.93333	-0.06751	1.49289
C	1.04290	-0.05842	0.43685
H	1.59684	-0.07271	2.52828
H	4.36910	-0.96898	2.84340
H	5.42188	-0.07805	1.73019
H	-1.93464	4.15959	-2.08210
H	-3.64526	2.16912	-1.15442
H	-0.37817	2.33692	-1.98670
C	-1.52432	3.99736	-1.07887
C	-3.00443	2.31725	-0.27579
H	-3.51895	4.44385	-0.23920
O	-1.71893	1.68019	-0.53527
C	-0.75546	2.67274	-1.01763
C	-2.66183	3.78672	-0.06555
H	-0.88352	4.84951	-0.83545
H	-3.43562	1.81715	0.59297
H	0.07454	2.69368	-0.30706
H	-2.30637	3.94584	0.95870
Cl	5.02613	-0.06416	-1.04175
H	-3.75887	-1.58314	-1.40199
H	-3.56103	-1.66911	0.37333
H	-3.78931	-4.04342	0.06007
C	-3.18748	-2.03529	-0.58510
C	-3.13201	-3.57146	-0.67524
H	-3.44206	-3.91106	-1.66951
O	-1.80214	-1.57284	-0.69058
H	-1.42228	-3.94416	0.63283
C	-1.64543	-3.89755	-0.43869
C	-0.95139	-2.69312	-1.06059
H	-1.33753	-4.84159	-0.89758
H	-0.91430	-2.75818	-2.15554
H	0.04739	-2.47948	-0.67727



Thiophene Grignard – Bromine

H	3.65273	0.83315	3.22904
Cl	-3.12797	-0.05788	2.22736
S	1.56367	-0.04143	-0.82613
Mg	-1.60631	-0.01494	0.51547
C	3.77513	-0.04414	2.58124
C	3.02201	-0.03981	0.12855
C	2.75725	-0.04292	1.47416
C	1.33524	-0.04595	1.69850
C	0.51578	-0.04549	0.58648
H	0.93260	-0.04877	2.71005
H	3.66341	-0.93148	3.21722
H	4.79601	-0.03551	2.19022
H	-2.31140	4.15435	-2.13675
H	-4.06633	2.15054	-1.32871
H	-0.76349	2.33422	-1.94791
C	-1.96735	3.98989	-1.10929
C	-3.48855	2.30118	-0.40778
H	-4.01535	4.42505	-0.40312
O	-2.18481	1.67113	-0.57772
C	-1.19845	2.66778	-1.00247
C	-3.16832	3.77194	-0.17370
H	-1.34730	4.84352	-0.82146
H	-3.97619	1.79842	0.42901
H	-0.41201	2.69119	-0.24415
H	-2.88254	3.93108	0.87211
Br	4.72499	-0.03692	-0.70408
H	-4.14646	-1.59929	-1.55339
H	-4.06111	-1.69497	0.23020
H	-4.25898	-4.06848	-0.11479
C	-3.62531	-2.05337	-0.70463
C	-3.55485	-3.58837	-0.79975
H	-3.79287	-3.92336	-1.81523
O	-2.23869	-1.58263	-0.71960
H	-1.93709	-3.95653	0.62161
C	-2.08640	-3.90747	-0.46256
C	-1.35803	-2.69748	-1.03219
H	-1.74253	-4.84834	-0.90200
H	-1.24488	-2.75950	-2.12205
H	-0.38927	-2.47952	-0.58041

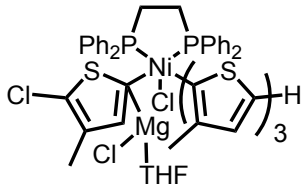


Thiophene Grignard – Iodine

H	3.03312	0.86221	3.45387
Cl	-3.66956	-0.05438	2.15968
S	1.14680	-0.04034	-0.68906
Mg	-2.08080	-0.01457	0.51022
C	3.19325	-0.01908	2.81988
C	2.56506	-0.03001	0.32487
C	2.23751	-0.02656	1.65854
C	0.80688	-0.03202	1.81973
C	0.03737	-0.03963	0.67259
H	0.36085	-0.03055	2.81294
H	3.04651	-0.90245	3.45422
H	4.23534	-0.01135	2.48916
H	-2.68341	4.15090	-2.17819
H	-4.46563	2.14510	-1.43783
H	-1.14928	2.32738	-1.93470
C	-2.37862	3.98509	-1.13865
C	-3.92530	2.29671	-0.49458
H	-4.45198	4.42053	-0.51131
O	-2.61567	1.66679	-0.61118
C	-1.61495	2.66216	-1.00439
C	-3.61436	3.76755	-0.24935
H	-1.76925	4.83796	-0.82679
H	-4.44602	1.79478	0.32252
H	-0.85413	2.68558	-0.22043
H	-3.36875	3.92712	0.80654
I	4.49566	-0.02695	-0.53016
H	-4.53543	-1.61686	-1.64455
H	-4.51285	-1.71056	0.14091
H	-4.68056	-4.08617	-0.20609
C	-4.04199	-2.06716	-0.77741
C	-3.95856	-3.60185	-0.86912
H	-4.16275	-3.93887	-1.89124
O	-2.65862	-1.58770	-0.74348
H	-2.38397	-3.96157	0.60223
C	-2.49933	-3.91172	-0.48604
C	-1.76132	-2.69603	-1.03053
H	-2.13548	-4.84958	-0.91568
H	-1.61393	-2.75522	-2.11646
H	-0.80849	-2.47294	-0.54841

THF

H	1.53490	-0.48300	1.16812
H	-0.79661	1.15527	1.31028
H	1.34447	1.76129	0.26322
C	1.16529	-0.43077	0.13206
H	1.94913	-0.82400	-0.52605
O	-0.00009	-1.25138	-0.00022
C	-0.73377	0.99675	0.22689
C	0.73401	0.99654	-0.22701
H	-1.94895	-0.82356	0.52688
C	-1.16544	-0.43057	-0.13178
H	-1.34406	1.76151	-0.26354
H	0.79692	1.15471	-1.31046
H	-1.53568	-0.48292	-1.16759

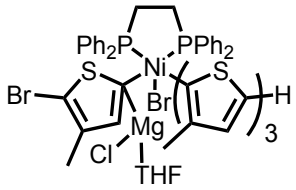


Transmetalation Transition State – Chlorine

Ni	-1.56339	0.37905	-0.23202
P	-1.46461	2.23899	1.03330
P	-3.91112	0.78338	-0.28288
C	-3.19979	2.91631	1.29296
C	-4.21774	1.77002	1.27171
C	-0.98384	1.88638	2.78019
C	-5.26101	-0.46159	-0.35614
C	-1.02223	0.57196	3.26256
C	-0.67969	2.93301	3.66851
C	-0.75125	0.30321	4.60690
C	-0.44184	1.34536	5.48027
C	-0.40854	2.66112	5.00882
H	-0.64224	3.95883	3.31400
H	-0.77329	-0.72443	4.95856
H	-0.16788	3.47746	5.68466
C	-5.29685	-1.33961	-1.45335
C	-6.23384	-0.58403	0.64957
C	-6.28058	-2.32437	-1.53474
C	-7.22214	-1.56675	0.55779
C	-7.24516	-2.43948	-0.53147
H	-6.27331	-3.01247	-2.37422
H	-7.97004	-1.65058	1.34189
H	-6.22655	0.07563	1.51174
C	0.35256	0.59692	-0.42660
Cl	-1.93333	-0.48293	-2.74541
C	1.02212	1.29719	-1.42719
C	2.90719	0.55002	-0.19973
C	2.44253	1.24373	-1.29917
C	0.38702	2.07899	-2.55116
S	1.52419	-0.06971	0.68755
H	-4.20560	-2.65083	3.97978
Cl	-2.78519	-4.33044	-2.13412
S	-0.33692	-2.62021	1.45981
Mg	-1.60186	-2.47217	-1.51435
C	-3.83838	-3.46269	3.33771
C	-1.36806	-3.31817	2.66688
C	-2.69237	-3.00896	2.47557
C	-2.83062	-2.18577	1.31265
C	-1.68268	-1.82404	0.61233
H	-3.81817	-1.89050	0.97908
H	-4.67923	-3.79522	2.71898
H	-3.54205	-4.29033	3.98792
H	3.18339	-2.94460	-2.33334
H	1.31122	-4.42122	-0.81769

H	1.43213	-1.27806	-2.43078
C	2.42714	-3.13786	-3.10261
C	0.83798	-4.35261	-1.80329
H	2.59112	-5.30521	-2.69840
O	0.35136	-2.98571	-1.96744
C	1.20816	-2.24203	-2.88873
C	1.83844	-4.54847	-2.93879
H	2.88759	-2.97377	-4.08144
H	-0.03020	-5.01286	-1.84496
H	0.64343	-2.08008	-3.81236
H	1.31930	-4.85815	-3.85311
H	-0.22512	1.13666	6.52452
H	-1.25645	-0.24130	2.58659
H	-4.54743	-1.26396	-2.23510
H	-8.00745	-3.21117	-0.59430
Cl	-0.70986	-4.27744	3.95750
H	3.10625	1.73297	-2.00715
H	-0.22300	1.43583	-3.19124
H	1.15617	2.55456	-3.16972
H	-0.25878	2.87820	-2.16867
C	-4.43041	2.00396	-1.57226
H	-4.07487	1.10670	2.13258
H	-3.22985	3.46777	2.23841
H	-3.43242	3.61696	0.48703
H	-5.23872	2.16570	1.30742
H	-0.66666	6.70944	-1.04701
H	1.74866	6.75757	-0.44968
C	-0.22162	5.88275	-0.49997
C	1.13239	5.90900	-0.16554
H	-2.06018	4.79262	-0.42641
C	-1.01517	4.79293	-0.13541
C	1.69283	4.83578	0.53045
C	-0.46474	3.71597	0.57801
H	2.74887	4.84002	0.78504
C	0.90408	3.74606	0.89636
H	1.35581	2.91661	1.43042
H	-3.12603	4.02895	-3.98492
H	-2.44489	2.30079	-2.34951
C	-3.87185	3.57647	-3.33692
C	-3.48170	2.60818	-2.40785
H	-5.51611	4.69642	-4.16928
C	-5.21241	3.94774	-3.44246
C	-6.16678	3.34444	-2.61884
C	-5.77977	2.37731	-1.69180
H	-7.21434	3.62099	-2.70360
H	-6.53350	1.90122	-1.07055
H	3.56336	-1.23777	2.68832
H	7.23029	-1.25770	-2.71744
H	4.79913	-0.28492	3.51864
H	8.76769	-1.07341	-3.57741
C	4.10429	-0.28291	2.67241
C	8.08897	-0.59422	-2.86406
H	6.86876	-0.53528	2.14033

C	4.85231	-0.07998	1.37964
C	6.26133	-0.24956	1.28695
C	4.28318	0.27942	0.16487
C	8.80622	-0.30649	-1.56973
C	6.80166	-0.03428	0.03639
S	5.51847	0.38758	-1.08461
H	10.87775	-0.44435	-2.33777
H	3.36291	0.50489	2.84433
H	7.71222	0.32188	-3.33786
C	8.20171	-0.06970	-0.34422
C	10.23379	-0.26892	-1.48162
C	10.70827	-0.00972	-0.22743
S	9.41475	0.21699	0.89970
H	11.73671	0.05951	0.10064

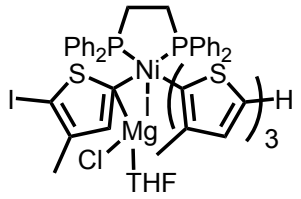


Transmetalation Transition State – Bromine

Ni	-1.48113	0.63740	-0.13608
P	-1.38104	2.00781	1.65867
P	-3.83848	1.02112	-0.04501
C	-3.11709	2.57381	2.10419
C	-4.13092	1.48347	1.74089
C	-0.91194	1.13476	3.21590
C	-5.19259	-0.14809	-0.47198
C	-1.03326	-0.25877	3.29402
C	-0.54337	1.85536	4.36559
C	-0.77963	-0.92433	4.49631
C	-0.40481	-0.20406	5.63006
C	-0.28936	1.18729	5.56276
H	-0.44429	2.93577	4.32667
H	-0.86548	-2.00651	4.53420
H	0.00173	1.75456	6.44286
C	-5.25762	-0.64740	-1.78458
C	-6.14338	-0.57689	0.46884
C	-6.24807	-1.56158	-2.14220
C	-7.13724	-1.48786	0.10291
C	-7.18948	-1.98352	-1.20099
H	-6.26737	-1.95494	-3.15388
H	-7.86773	-1.80995	0.84037
H	-6.11498	-0.21378	1.49126
C	0.43142	0.90540	-0.25624
Br	-1.82454	0.58047	-2.92686
C	1.11580	1.89290	-0.95961
C	2.98403	0.73952	-0.06570
C	2.53473	1.77439	-0.86146
C	0.49816	3.01970	-1.74997
S	1.58684	-0.11971	0.56380
H	-3.83812	-4.10959	3.11336
Cl	-2.57610	-3.44060	-3.29662
S	-0.28298	-2.76014	0.69486
Mg	-1.44130	-1.80201	-2.17442
C	-3.85721	-4.16025	2.01751
C	-1.35781	-3.79115	1.57730
C	-2.67852	-3.45116	1.40691
C	-2.77269	-2.32181	0.53375
C	-1.59726	-1.75939	0.03979
H	-3.74756	-1.95076	0.24291
H	-4.79465	-3.71423	1.67177
H	-3.86761	-5.22203	1.74542
H	3.36658	-2.00048	-2.78956
H	1.41671	-3.85325	-1.88150

H	1.57898	-0.37237	-2.64568
C	2.68910	-2.00145	-3.65093
C	1.03256	-3.52390	-2.85276
H	2.88771	-4.19870	-3.79299
O	0.53154	-2.16084	-2.68884
C	1.42628	-1.20358	-3.33460
C	2.13467	-3.41276	-3.90326
H	3.22818	-1.58980	-4.50938
H	0.18649	-4.14764	-3.14682
H	0.92953	-0.83699	-4.23893
H	1.70906	-3.48440	-4.91081
H	-0.20108	-0.72213	6.56337
H	-1.31660	-0.82391	2.41432
H	-4.52437	-0.33517	-2.52201
H	-7.95644	-2.70050	-1.48054
Br	-0.70993	-5.21059	2.65195
H	3.20882	2.46508	-1.36111
H	-0.01319	2.65042	-2.64432
H	1.26666	3.73520	-2.06265
H	-0.23676	3.57266	-1.15492
C	-4.38040	2.57722	-0.88764
H	-3.97995	0.58998	2.35763
H	-3.14981	2.81942	3.17077
H	-3.35160	3.48081	1.54123
H	-5.15268	1.84459	1.90163
H	-0.58268	6.91922	1.18994
H	1.85112	6.75108	1.68117
C	-0.13334	5.95382	1.40626
C	1.23074	5.85904	1.68134
H	-1.98663	4.91284	1.17533
C	-0.93224	4.80818	1.40677
C	1.79566	4.61073	1.95198
C	-0.37661	3.55016	1.68935
H	2.85885	4.52375	2.15714
C	1.00204	3.46472	1.95202
H	1.45736	2.50174	2.15848
H	-3.10590	5.29578	-2.50380
H	-2.39662	3.14768	-1.50113
C	-3.84571	4.64465	-2.04605
C	-3.44040	3.43704	-1.47167
H	-5.50978	5.93926	-2.49941
C	-5.19390	5.00326	-2.04655
C	-6.13954	4.14885	-1.47337
C	-5.73688	2.94333	-0.89944
H	-7.19261	4.41718	-1.47966
H	-6.48357	2.27951	-0.47251
H	3.58597	-1.95385	2.00207
H	7.32425	-0.06834	-3.04213
H	4.83739	-1.39515	3.11826
H	8.86901	0.41843	-3.75864
C	4.14835	-1.07086	2.33162
C	8.18412	0.59930	-2.92362
H	6.91507	-1.14505	1.76215

C	4.90939	-0.43073	1.19887
C	6.31799	-0.56961	1.06129
C	4.35417	0.34151	0.18662
C	8.89021	0.38156	-1.60965
C	6.87195	0.07041	-0.02771
S	5.60221	0.87402	-0.93514
H	10.96809	0.51016	-2.36170
H	3.42372	-0.38183	2.77896
H	7.81133	1.62713	-3.02479
C	8.27522	0.15916	-0.38650
C	10.31703	0.36652	-1.50501
C	10.78093	0.14132	-0.24036
S	9.47812	-0.04598	0.88323
H	11.80650	0.07301	0.09674

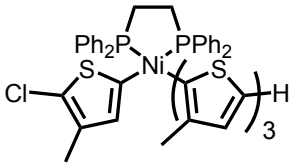


Transmetalation Transition State – Iodine

Ni	1.41956	-0.83741	0.01789
P	1.33972	-1.73087	2.10435
P	3.79819	-1.13254	0.20459
C	3.08332	-2.15951	2.65453
C	4.07661	-1.16066	2.05277
C	0.88277	-0.50991	3.41133
C	5.14363	-0.06383	-0.45675
C	1.09485	0.85590	3.17927
C	0.44532	-0.92817	4.68014
C	0.86264	1.79004	4.19204
C	0.41809	1.36862	5.44492
C	0.21227	0.00786	5.68723
H	0.27870	-1.98119	4.88295
H	1.01724	2.84581	3.98891
H	-0.13277	-0.32756	6.66169
C	5.26240	0.08922	-1.84945
C	6.04282	0.61578	0.38115
C	6.25553	0.90767	-2.38678
C	7.03814	1.43151	-0.16292
C	7.14517	1.58070	-1.54647
H	6.32232	1.02651	-3.46407
H	7.72795	1.94933	0.49825
H	5.97430	0.52283	1.46008
C	-0.48687	-1.15294	-0.02422
I	1.75200	-1.47257	-2.91390
C	-1.17884	-2.28999	-0.42994
C	-3.03666	-0.93288	0.13952
C	-2.59726	-2.14424	-0.35525
C	-0.56973	-3.58835	-0.89487
S	-1.63248	0.05747	0.50588
H	4.76232	3.81065	0.61649
Cl	2.14419	2.67653	-3.97388
S	0.20629	2.69046	0.19723
Mg	1.18063	1.20693	-2.51123
C	3.84736	4.37826	0.81135
C	1.32241	3.90298	0.72814
C	2.63221	3.54484	0.50436
C	2.67908	2.25160	-0.10765
C	1.48086	1.58229	-0.34848
H	3.63276	1.83621	-0.40880
H	3.87545	5.28181	0.19035
H	3.86143	4.70579	1.85773
H	-3.65663	1.04479	-2.91087
H	-1.78165	3.11001	-2.38853

H	-1.77562	-0.44816	-2.60713
C	-3.01519	0.94782	-3.79397
C	-1.41794	2.65615	-3.31639
H	-3.34408	3.08406	-4.25754
O	-0.83251	1.36079	-2.97318
C	-1.69748	0.27246	-3.42163
C	-2.55248	2.32931	-4.28373
H	-3.56323	0.38221	-4.55341
H	-0.62158	3.26930	-3.74201
H	-1.21768	-0.20475	-4.28236
H	-2.17184	2.26657	-5.30966
H	0.23012	2.09581	6.23025
H	1.42869	1.19072	2.20441
H	4.56736	-0.41680	-2.51271
H	7.91449	2.22191	-1.96760
I	0.65675	5.69968	1.61546
H	-3.27787	-2.94092	-0.64375
H	-0.20215	-3.51519	-1.92418
H	-1.30748	-4.39721	-0.84978
H	0.27762	-3.88261	-0.26802
C	4.39330	-2.82992	-0.23650
H	3.90100	-0.15287	2.44617
H	3.12239	-2.16171	3.74886
H	3.33194	-3.16453	2.30405
H	5.10444	-1.45151	2.29585
H	0.59885	-6.60246	2.94221
H	-1.84871	-6.34807	3.31351
C	0.13500	-5.62172	2.88177
C	-1.23662	-5.47864	3.08983
H	1.98503	-4.65036	2.43021
C	0.92324	-4.50479	2.59543
C	-1.81957	-4.21218	3.00547
C	0.34898	-3.22613	2.51678
H	-2.88829	-4.09004	3.15690
C	-1.03693	-3.09543	2.71652
H	-1.50681	-2.11980	2.64916
H	3.19930	-5.91604	-1.06245
H	2.42300	-3.60873	-0.62283
C	3.92094	-5.14395	-0.80961
C	3.47867	-3.84411	-0.55173
H	5.62786	-6.45237	-0.96906
C	5.28272	-5.44327	-0.76051
C	6.20311	-4.43796	-0.45331
C	5.76282	-3.14019	-0.19354
H	7.26607	-4.66191	-0.42234
H	6.48991	-2.36481	0.03040
H	-3.63448	2.17892	1.55404
H	-7.35865	-0.76047	-2.96658
H	-4.86917	1.85409	2.77581
H	-8.90719	-1.37691	-3.56528
C	-4.18502	1.37885	2.06523
C	-8.22700	-1.37517	-2.70717
H	-6.94997	1.35693	1.47654

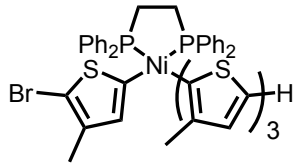
C	-4.95117	0.51241	1.09847
C	-6.35769	0.63281	0.92545
C	-4.40325	-0.47356	0.28839
C	-8.93402	-0.86240	-1.47852
C	-6.91630	-0.22922	0.00482
S	-5.65403	-1.23011	-0.69248
H	-11.01134	-1.13171	-2.19408
H	-3.44949	0.80226	2.63626
H	-7.86663	-2.40388	-2.57499
C	-8.31978	-0.38014	-0.33231
C	-10.36081	-0.80825	-1.38750
C	-10.82519	-0.30174	-0.20720
S	-9.52332	0.11649	0.85334
H	-11.85074	-0.14854	0.10082



Post-Transmetalation – Chlorine

C	-0.17496	0.27004	-0.46927
C	-0.79640	0.56375	-1.67173
C	-2.20310	0.77966	-1.54439
C	-2.69352	0.67848	-0.25883
H	-2.83723	1.03649	-2.38906
Ni	1.68065	-0.10232	-0.15412
P	1.29711	-2.35896	0.17792
P	3.92248	-0.62385	-0.08594
C	2.95468	-3.16638	0.51394
H	3.13432	-3.02035	1.58546
H	2.92324	-4.24846	0.34474
C	4.05997	-2.48293	-0.30007
H	3.93840	-2.68523	-1.37019
H	5.05164	-2.84956	-0.01446
C	5.03425	0.00444	-1.41003
C	6.14247	0.82090	-1.14728
C	4.71767	-0.30228	-2.74485
C	6.92844	1.30426	-2.19615
H	6.39324	1.08472	-0.12526
C	5.50638	0.17768	-3.78960
H	3.84226	-0.90507	-2.97525
C	6.61600	0.98200	-3.51709
H	7.78453	1.93652	-1.97670
H	5.24916	-0.06957	-4.81595
H	7.22815	1.36017	-4.33118
C	4.79424	-0.30135	1.50086
C	6.01305	-0.92195	1.82763
C	4.21352	0.58407	2.42217
C	6.62993	-0.66929	3.05232
H	6.49312	-1.59519	1.12259
C	4.83572	0.83707	3.64733
H	3.28527	1.08808	2.17236
C	6.04005	0.20930	3.96565
H	7.57135	-1.15591	3.29286
H	4.37628	1.52831	4.34829
H	6.52212	0.40513	4.91966
C	0.32589	-2.89076	1.64533
C	-0.44488	-4.06154	1.66485
C	0.42134	-2.11408	2.81099
C	-1.10625	-4.44820	2.83191
H	-0.53698	-4.66753	0.76884
C	-0.23339	-2.50739	3.97770
H	0.99762	-1.19217	2.80015
C	-1.00032	-3.67457	3.98908
H	-1.70590	-5.35443	2.83479

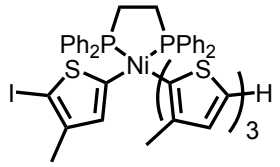
H	-0.15608	-1.89483	4.87169
H	-1.51890	-3.97642	4.89499
C	0.57497	-3.27018	-1.24548
C	1.29488	-4.22144	-1.98481
C	-0.73920	-2.95731	-1.64019
C	0.71644	-4.84943	-3.09055
H	2.31068	-4.48585	-1.70825
C	-1.31510	-3.59328	-2.73956
H	-1.30856	-2.21342	-1.09339
C	-0.58957	-4.53845	-3.46913
H	1.28859	-5.58400	-3.65099
H	-2.33248	-3.34363	-3.02738
H	-1.03990	-5.02831	-4.32816
S	-1.35638	0.27510	0.81636
C	-0.08833	0.64555	-3.00169
H	0.96394	0.90979	-2.86326
H	-0.54359	1.40600	-3.64790
H	-0.13003	-0.30929	-3.54524
C	-4.06806	0.79792	0.18466
C	-4.60314	1.20479	1.39892
S	-5.35073	0.39389	-0.94895
C	-6.02595	1.21064	1.38703
C	-6.60746	0.81927	0.19942
H	-6.61382	1.53538	2.24040
C	-8.02259	0.69382	-0.09917
C	-8.71564	0.80924	-1.29440
S	-9.12717	0.34008	1.22589
C	-10.12450	0.62818	-1.11909
C	-10.49924	0.37967	0.17049
H	-10.82997	0.69798	-1.94144
H	-11.49507	0.22121	0.56209
C	-8.10540	1.11389	-2.63898
H	-7.28230	1.83113	-2.56071
H	-7.70394	0.21323	-3.12237
H	-8.85907	1.53531	-3.31291
C	-3.80495	1.64055	2.60114
H	-3.45222	0.78398	3.19062
H	-2.92088	2.21814	2.31295
H	-4.41838	2.26201	3.26238
S	1.35208	2.84633	0.95924
C	2.12534	4.25142	0.26659
H	4.61847	4.62125	-1.86712
C	2.01511	1.78337	-0.27545
C	2.82518	3.95467	-0.87139
C	2.75017	2.54431	-1.15523
C	3.57855	4.93996	-1.72107
H	3.25460	2.12193	-2.01910
H	3.58692	5.93326	-1.26417
H	3.12660	5.03164	-2.71748
Cl	1.95259	5.81116	1.01546



Post-Transmetalation – Bromine

C	-0.25061	0.00542	-0.51017
C	-0.86908	0.21830	-1.73082
C	-2.26747	0.48934	-1.61756
C	-2.75359	0.51026	-0.32658
H	-2.89782	0.69575	-2.47872
Ni	1.59441	-0.40085	-0.17602
P	1.14062	-2.61125	0.33017
P	3.81915	-0.99139	-0.09189
C	2.77526	-3.44962	0.70176
H	2.97649	-3.23399	1.75752
H	2.70501	-4.53925	0.61060
C	3.89024	-2.86454	-0.17356
H	3.74545	-3.13797	-1.22482
H	4.87334	-3.24417	0.12446
C	4.92870	-0.49746	-1.47368
C	6.06815	0.29641	-1.28619
C	4.57898	-0.88685	-2.77835
C	6.85155	0.67686	-2.37849
H	6.34538	0.62285	-0.28940
C	5.36515	-0.50970	-3.86629
H	3.68011	-1.47390	-2.95201
C	6.50560	0.27304	-3.66830
H	7.73211	1.29286	-2.21745
H	5.08212	-0.81991	-4.86845
H	7.11591	0.57124	-4.51629
C	4.72623	-0.58478	1.45504
C	5.92603	-1.22496	1.81284
C	4.19332	0.38982	2.31308
C	6.57091	-0.90353	3.00660
H	6.36976	-1.96787	1.15562
C	4.84369	0.71164	3.50703
H	3.28046	0.90822	2.03749
C	6.02864	0.06423	3.85716
H	7.49715	-1.40620	3.27180
H	4.42140	1.47152	4.15853
H	6.53262	0.31365	4.78703
C	0.17659	-2.99207	1.84810
C	-0.61477	-4.14212	1.97764
C	0.29930	-2.11842	2.94011
C	-1.26924	-4.41294	3.18057
H	-0.72837	-4.82198	1.13887
C	-0.34905	-2.39585	4.14324
H	0.89145	-1.21189	2.84240
C	-1.13621	-3.54307	4.26440
H	-1.88487	-5.30403	3.26889

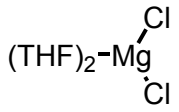
H	-0.25089	-1.70887	4.97920
H	-1.64964	-3.75482	5.19836
C	0.36108	-3.60205	-1.00681
C	1.03800	-4.62373	-1.69067
C	-0.95292	-3.28069	-1.39518
C	0.41750	-5.31229	-2.73588
H	2.05243	-4.89653	-1.41712
C	-1.57082	-3.97663	-2.43370
H	-1.48978	-2.48450	-0.89072
C	-0.88795	-4.99176	-3.10843
H	0.95646	-6.10115	-3.25381
H	-2.58742	-3.71920	-2.71732
H	-1.37094	-5.52856	-3.92037
S	-1.42357	0.15490	0.77444
C	-0.16640	0.16614	-3.06506
H	0.89872	0.38627	-2.94947
H	-0.58671	0.89895	-3.76474
H	-0.25957	-0.82296	-3.53615
C	-4.12090	0.71032	0.10998
C	-4.63536	1.22486	1.29194
S	-5.42262	0.26837	-0.98720
C	-6.05713	1.27977	1.28310
C	-6.65786	0.82196	0.12935
H	-6.62906	1.68728	2.11142
C	-8.07799	0.72394	-0.15563
C	-8.77297	0.77955	-1.35396
S	-9.18675	0.50048	1.19404
C	-10.18616	0.65868	-1.16242
C	-10.56222	0.51303	0.14243
H	-10.89326	0.69516	-1.98553
H	-11.56075	0.41597	0.54697
C	-8.15981	0.96991	-2.71811
H	-7.31007	1.65926	-2.69109
H	-7.79520	0.02429	-3.14107
H	-8.90121	1.37315	-3.41634
C	-3.81658	1.72018	2.45669
H	-3.48130	0.89672	3.10097
H	-2.92018	2.25352	2.12448
H	-4.40849	2.40111	3.07769
S	1.37959	2.62745	0.72526
C	2.18812	3.95287	-0.07277
H	4.63748	4.03762	-2.31514
C	1.98634	1.45873	-0.43909
C	2.86004	3.55435	-1.19737
C	2.73250	2.13078	-1.37989
C	3.63296	4.44025	-2.13455
H	3.20999	1.63237	-2.21822
H	3.73716	5.45294	-1.73565
H	3.13450	4.51400	-3.11018
Br	2.06528	5.71005	0.62852



Post-Transmetalation – Iodine

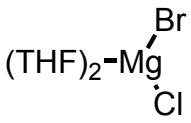
C	-0.33688	-0.23467	-0.53683
C	-0.95141	-0.04607	-1.76331
C	-2.33645	0.28951	-1.65709
C	-2.81456	0.38510	-0.36663
H	-2.96186	0.48697	-2.52394
Ni	1.49081	-0.70237	-0.18787
P	0.94795	-2.86972	0.40755
P	3.69017	-1.37784	-0.07215
C	2.54711	-3.75652	0.81841
H	2.75524	-3.50453	1.86475
H	2.43321	-4.84533	0.77305
C	3.68601	-3.25394	-0.07713
H	3.53192	-3.56522	-1.11645
H	4.65258	-3.65970	0.23991
C	4.82376	-0.98270	-1.46603
C	5.98470	-0.21459	-1.30451
C	4.47161	-1.41879	-2.75517
C	6.78634	0.09447	-2.40606
H	6.26457	0.14747	-0.32086
C	5.27590	-1.11290	-3.85224
H	3.55716	-1.98654	-2.91063
C	6.43747	-0.35565	-3.67967
H	7.68348	0.69115	-2.26502
H	4.99073	-1.45877	-4.84204
H	7.06202	-0.11304	-4.53498
C	4.60716	-0.94666	1.46212
C	5.78420	-1.61367	1.84564
C	4.10567	0.07475	2.28382
C	6.43720	-1.27237	3.02938
H	6.20403	-2.39327	1.21575
C	4.76417	0.41629	3.46782
H	3.21170	0.61406	1.98718
C	5.92600	-0.25784	3.84398
H	7.34566	-1.79598	3.31477
H	4.36663	1.21250	4.09087
H	6.43636	0.00710	4.76603
C	-0.03296	-3.15027	1.93649
C	-0.87967	-4.25481	2.10534
C	0.13269	-2.24564	2.99723
C	-1.54671	-4.45030	3.31599
H	-1.02623	-4.95777	1.29112
C	-0.52831	-2.44818	4.20833
H	0.76893	-1.37341	2.86890
C	-1.37108	-3.55025	4.36860
H	-2.20533	-5.30643	3.43469

H	-0.39624	-1.73784	5.01973
H	-1.89428	-3.70330	5.30857
C	0.13233	-3.88122	-0.89175
C	0.76927	-4.95624	-1.53082
C	-1.16642	-3.52304	-1.29877
C	0.12454	-5.66075	-2.55041
H	1.77092	-5.25864	-1.24173
C	-1.80891	-4.23485	-2.31131
H	-1.67192	-2.68588	-0.82948
C	-1.16570	-5.30306	-2.94159
H	0.63265	-6.49097	-3.03373
H	-2.81346	-3.94836	-2.60966
H	-1.66762	-5.85221	-3.73355
S	-1.49592	0.01853	0.74426
C	-0.25844	-0.18311	-3.09657
H	0.81920	-0.03025	-2.98941
H	-0.63205	0.55511	-3.81686
H	-0.41803	-1.17724	-3.53832
C	-4.16997	0.66153	0.06593
C	-4.65504	1.25710	1.22184
S	-5.49581	0.21465	-0.99978
C	-6.07367	1.36739	1.21769
C	-6.70020	0.87391	0.09271
H	-6.62320	1.84004	2.02633
C	-8.12518	0.81732	-0.17930
C	-8.82618	0.83869	-1.37519
S	-9.23184	0.70702	1.18595
C	-10.24156	0.78330	-1.17020
C	-10.61342	0.71949	0.14241
H	-10.95273	0.80526	-1.99031
H	-11.61198	0.68246	0.55670
C	-8.21607	0.93463	-2.75057
H	-7.33918	1.58952	-2.76339
H	-7.89289	-0.04524	-3.12667
H	-8.94589	1.33153	-3.46446
C	-3.80876	1.78068	2.35412
H	-3.51087	0.98166	3.04580
H	-2.88932	2.24971	1.98965
H	-4.36486	2.52481	2.93440
S	1.41250	2.36931	0.58094
C	2.27089	3.62626	-0.27440
H	4.68494	3.46213	-2.57273
C	1.95777	1.12609	-0.53223
C	2.91613	3.14704	-1.38546
C	2.72561	1.72408	-1.50527
C	3.72033	3.94529	-2.37405
H	3.17644	1.16996	-2.32319
H	3.91405	4.95947	-2.01373
H	3.19565	4.02724	-3.33527
I	2.21635	5.61605	0.42914



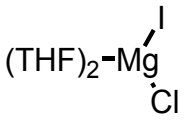
$MgCl_2(THF)_2$

Cl	0.01530	2.09984	-1.43594
Cl	-0.00844	-2.08986	-1.44765
Mg	0.00109	0.00253	-0.54963
H	4.60722	0.96316	1.35978
H	2.59450	-1.36733	1.98730
H	2.40582	1.37999	2.05595
C	3.89426	0.75320	0.55676
C	2.48536	-1.18194	0.91036
H	4.65348	-1.32875	0.65207
O	1.63627	-0.01830	0.73359
C	2.46462	1.15234	0.98518
C	3.80199	-0.76641	0.25815
H	4.21543	1.31154	-0.32632
H	1.97877	-2.02037	0.43136
H	2.02832	1.96892	0.40915
H	3.74608	-0.94549	-0.81998
H	-3.74840	0.92994	-0.82501
H	-2.03222	-1.96837	0.38616
H	-1.98596	2.01748	0.42611
H	-4.23628	-1.32177	-0.30853
C	-3.80631	0.75905	0.25441
C	-2.46404	-1.15840	0.97483
O	-1.63929	0.01595	0.72670
C	-2.49047	1.17783	0.90523
C	-3.89892	-0.75763	0.56477
H	-4.65833	1.32444	0.64276
H	-2.39394	-1.39730	2.04238
H	-2.59910	1.36277	1.98232
H	-4.59999	-0.95816	1.38063



$MgClBr(THF)_2$

Cl	0.05057	-1.73939	2.07528
Br	0.11827	2.31770	0.59135
Mg	0.01515	-0.12000	0.47433
H	4.54324	-1.92577	-0.85269
H	2.44083	-0.00204	-2.56622
H	2.33050	-2.44199	-1.52530
C	3.79726	-1.32221	-0.32747
C	2.40921	0.29085	-1.50859
H	4.59293	0.37714	-1.51557
O	1.56376	-0.65765	-0.80713
C	2.37603	-1.84726	-0.60465
C	3.77344	0.15018	-0.82764
H	4.02564	-1.36592	0.74061
H	1.94695	1.27296	-1.40381
H	1.92378	-2.39921	0.21945
H	3.83820	0.84403	0.01525
H	-3.92800	-0.71082	0.92874
H	-2.23374	1.42293	-0.88416
H	-2.07386	-2.23871	0.46849
H	-4.57624	0.88272	-0.77441
C	-3.89670	-1.10065	-0.09429
C	-2.49276	0.46009	-1.32720
O	-1.69155	-0.54558	-0.63051
C	-2.52711	-1.70676	-0.36882
C	-3.96552	0.04601	-1.12400
H	-4.70756	-1.82554	-0.21114
H	-2.19844	0.45816	-2.38173
H	-2.52973	-2.34365	-1.26346
H	-4.39637	-0.31001	-2.06568



$MgClI(THF)_2$

Cl	0.02822	1.73226	2.29468
I	-0.24998	-2.29219	0.27971
Mg	0.01785	0.36674	0.47166
H	-4.34140	2.66193	-0.68845
H	-2.28880	0.89687	-2.62572
H	-2.06870	3.11143	-1.18965
C	-3.66376	1.92467	-0.24820
C	-2.33192	0.43077	-1.63267
H	-4.51257	0.51428	-1.73924
O	-1.45970	1.18184	-0.74840
C	-2.19917	2.38102	-0.38171
C	-3.71604	0.55943	-0.99109
H	-3.93879	1.80553	0.80300
H	-1.94610	-0.58828	-1.67991
H	-1.75048	2.75703	0.53776
H	-3.87123	-0.25883	-0.28230
H	4.10821	0.69565	0.87915
H	2.33003	-1.05877	-1.04416
H	2.24667	2.29394	0.86039
H	4.66294	-0.47769	-1.18794
C	4.01544	1.28991	-0.03645
C	2.52336	-0.04601	-1.40240
O	1.76856	0.85876	-0.53294
C	2.64052	1.94019	-0.09304
C	3.99686	0.38427	-1.28215
H	4.82672	2.02343	-0.05532
H	2.13250	0.05355	-2.41961
H	2.59768	2.74592	-0.83757
H	4.30563	0.95035	-2.16767

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