Supporting Information

Gold-catalyzed C-H functionalization with aryl germanes

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General Information

Reagents and Solvents

Unless otherwise stated, all reagents and starting materials were commercially available and used as received. Solvents used in work up and purification were distilled prior to use. Anhydrous and degassed 1,4-dioxane was purchased from Sigma Aldrich. [(Ph_3P)Au][X] (X = OAc, OTs, BF_4) were synthesized according to literature reported procedures.[1]

Experimental Techniques

All reactions involving air- or moisture-sensitive reagents or intermediates were carried out in dried glassware under an argon atmosphere and were performed either in an argon-filled glovebox or by using standard *Schlenk* techniques unless otherwise stated.

Column chromatography was carried out using silica gel (35–70 mesh; 60 Å). Thin layer chromatography (TLC) was performed on Merck silica gel 60 F254 aluminum plates; detection either under UV light or by dipping into a solution of $KMnO_4$ (1.5 g) and $NaHCO_3$ (5.0 g) in H_2O (400 mL) followed by heating. Preparative HPLC was performed on a Gilson-Abimed HPLC (employing UV detector model 117) using a Merck LiChrosorb Si60 column (porosity 7 µm, 250 x 25 mm).

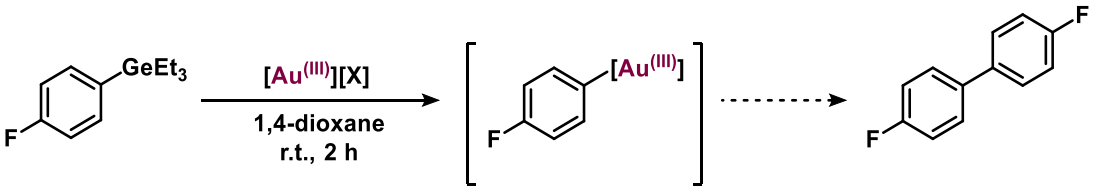
All ^1H, ^{13}C and ^{19}F NMR spectra were recorded at ambient temperature on a Varian V NMRS 600 or a Varian V NMRS 400 spectrometer. Chemical shifts (δ) are reported in parts per million (ppm) relative to $SiMe_4$ and referenced to either the residual solvent peak (for ^1H and ^{13}C NMR spectra) or internally by the instrument after locking and shimming to the deuterated solvent (for ^{19}F). Coupling constants (*J*) are given in Hertz (Hz).

High-resolution mass spectrometry (HRMS) was performed using a Thermo Scientific LTQ Orbitrap XL (ESI) or an Finnigan MAT95 (EI, 70 eV). IR spectra were recorded on a Spectrum 100 spectrometer with an UATR Diamond/KRS-5 crystal with attenuated total reflectance (ATR).

Low-resolution mass spectrometry and reaction monitoring were performed with an Agilent Technologies 5975 series MSD mass spectrometer under electron ionization (EI) mode coupled with an Agilent Technologies 7820A gas chromatograph employing an Agilent HP-5MS column (30 m × 0.25 mm inner diameter × 0.25 µm (5% phenyl)-methylpolysiloxane film) or an Agilent CP-Sil8-CB column (30 m × 0.25 mm inner diameter × 1.00 µm (5% phenyl)-methylpolysiloxane film). Operating with a constant He-flow of 1.2 mL min^{-1}, injector temperature 250 °C, detector-line temperature 280 °C.

Mechanistic Investigation

Stoichiometric Transmetalation Experiments with $Au^{(III)}$ Complexes



X = Br and OAc:

In a glovebox, $[Au^{(III)}X_3]$ (X = Br or OAc; 0.03 mmol, 1.0 equiv.) and triethyl(4-fluorophenyl)germane (8.0 mg, 0.03 mmol, 1.0 equiv.) were dissolved in 1,4-dioxane (0.3 mL) and stirred for 2 h at room temperature. The reaction was analyzed by GC-MS and ^{19}F NMR analysis. The results are shown in Table S1 and discussed below.

X = OCSA (camphorsulfonate):

In a glovebox, $[(Ph_3P)Au^{(I)}][Cl]$ (14.8 mg, 0.03 mmol, 1.0 equiv.) $PhI(OAc)_2$ (14.5 mg, 0.045 mmol, 1.5 equiv) and camphorsulfonic acid (10.4 mg, 0.045 mmol, 1.5 equiv.) were dissolved in 1,4-dioxane (0.3 mL) and stirred for 20 min to form $[Au(OCSA)_3]$ *in situ*. Triethyl(4-fluorophenyl)germane (dissolved in 1,4-dioxane; 8.0 mg, 0.03 mmol, 1.0 equiv.) was added and stirred for 2 h at room temperature. The reaction was analyzed by GC-MS and ^{19}F NMR analysis. The results are shown in Table S1 and discussed below.

Table S1: Stoichiometric Transmetalation with $Au^{(III)}$.

entry	[X]	consumption $ArGeEt_3$ [%][a]
1	Br	0
2	OAc	0
3	OCSA[b]	90

[a]Yields by ^{19}F NMR analysis using 1,4-difluorobenzene as internal standard [b]OCSA = camphorsulfonate.

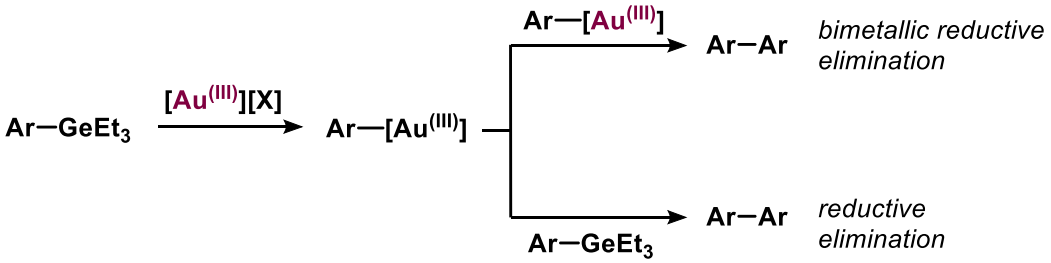
R = Br and OAc (entries 1 and 2):

No reaction after 12 h at room temperature or at 70 °C.

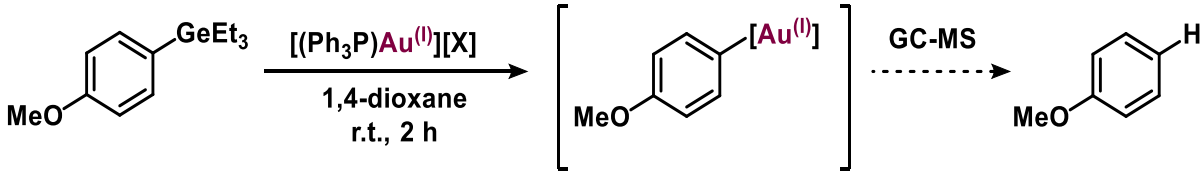
R = OCSA (entry 3):

After 2 h, ^1H NMR and GC-MS analysis revealed 90% consumption of triethyl(4-fluorophenyl)germane and formation of the homocoupling product 4,4'-difluoro-1,1'-biphenyl (45%; observed in GC-MS and *in-situ* ^{19}F NMR analysis using mesitylene or 1,4-

difluorobenzene as internal standard, respectively). This observation supports the formation of an Ar–Au$^{(III)}$ species which subsequently performs reductive elimination – bimetallic with second equivalent of [(Ar)Au$^{(III)}$] or after second transmetalation with aryl germane – to form the homocoupling product. Since the gold(III) center is non-ligated with stabilizing ligands and hence rather reactive, the reductive elimination occurs immediately after double transmetalation. It is hence not possible to isolate such highly reactive species. This observation is consistent with mechanistic investigations for aryl silanes.[2]



Stoichiometric Transmetalation Experiments with Au$^{(I)}$ Complexes



In a glovebox, [(Ph_3P)Au$^{(I)}$][X] (1.0 equiv.) and triethyl(4-methoxy)germane (8.0 mg, 0.03 mmol, 1.0 equiv.) were dissolved in 1,4-dioxane (0.3 mL) and stirred for 2 h at room temperature. The reaction was analyzed by GC-MS analysis. The results are shown in Table S2 and discussed below.

Table S2: Stoichiometric Transmetalation with Au$^{(I)}$.

entry	[X]	consumption $ArGeEt_3$ [%][a]	yield anisole [%][a]
1	Cl	0	0
2	OAc	0	0
3	OTf	100	96
4	BF_4	100	34

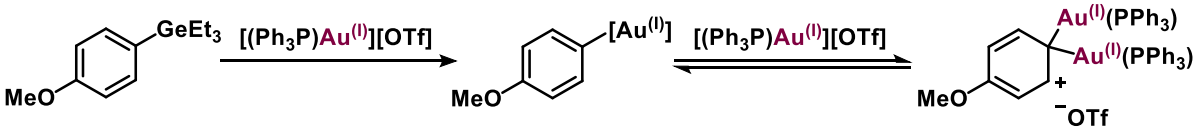
[a]Yields by calibrated gas chromatography using mesitylene as the internal standard.

Coordinating counterions (Cl, OAc; entries 1 and 2):

No reaction after 12 h at room temperature or at 70 °C.

Non-coordinating OTf counterion (entry 3):

After 2 h, ^{1}H NMR and GC-MS analysis revealed full consumption of triethyl(4-methoxy)germane and formation of new species. Calibrated GC-MS revealed quantitative formation of anisole. This observation supports the formation of a metal-organic species Ar–Au$^{(I)}$ which is quenched under injection conditions of the GC-MS to form anisole. It was not possible to isolate or characterize the corresponding [(Ar)Au$^{(I)}$] species by NMR analysis since the resulting signals in ^{1}H NMR were rather broad, indicating an equilibrium of different products. Nevertheless, electrospray ionization mass spectrometry (ESI-MS) unambiguously confirmed, that the observable species is in fact not [(Ph_3P)Au(Ar)] but a *gem*-diaurated [(Ph_3P)$_2$Au$_2$(Ar)][OTf]. Those species have been reported to occur as an overreaction of [(Ph_3P)Au(Ar)] with a further equivalent of [(Ph_3P)Au][X].[1a,3] This explanation is consistent with the experimental observations.

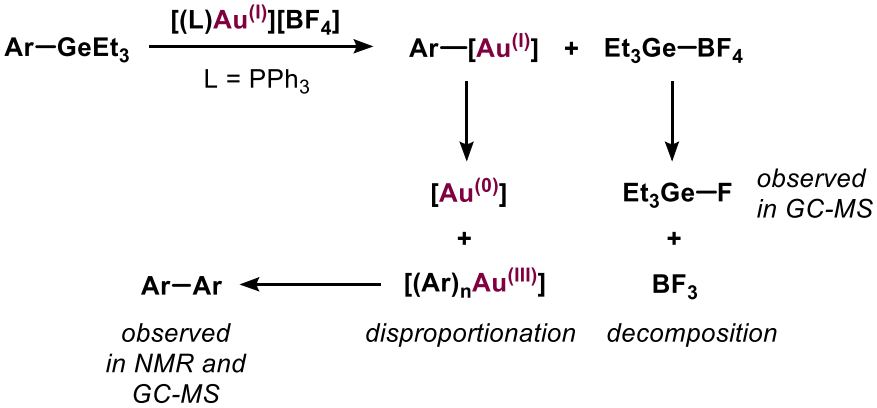


observed in ESI-MS

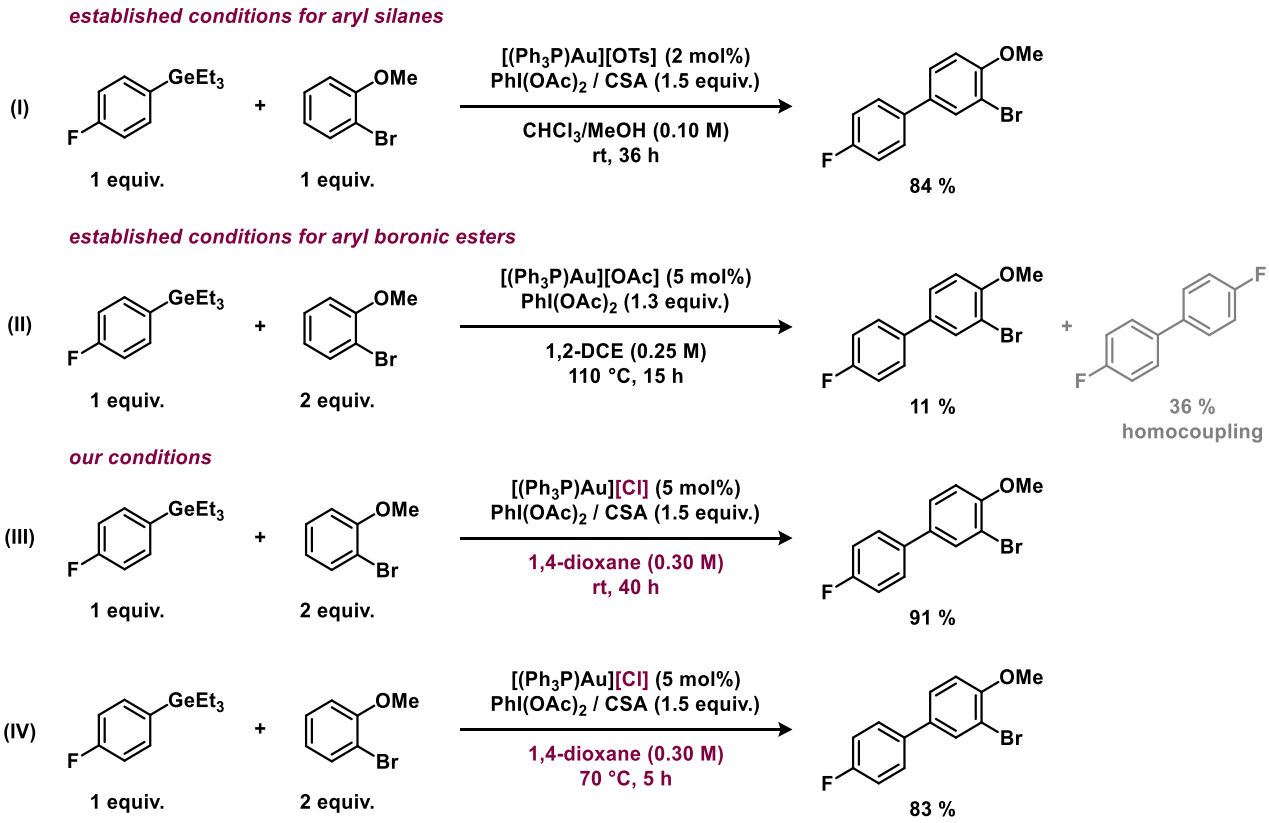
$C_{43}H_{37}Au_2OP_2OTf$:
calc. 1025.1645 $[M\text{-}OTf]^+$
found: 1025.1636

Non-coordinating BF_4 counterion (entry 4):

Reaction with [(Ph_3P)Au$^{(I)}$][BF_4] showed full consumption of triethyl(4-methoxy)germane and formation of anisole (34%) and 4,4'-dimethoxy-1,1'-biphenyl (GC-MS analysis). Again, the corresponding [(Ar)Au$^{(I)}$] complex was not observed. Instead the formation of [(Ph_3P)$_2$Au$_2$(Ar)]$^+$ was confirmed by ESI-MS. Additionally, the rather electrophilic nature of this non-coordinated gold complex is likely to results disproportionation to give gold(0) (black and golden precipitate observable) and an Au$^{(III)}$–aryl species. The Au$^{(III)}$–aryl species undergoes subsequent reductive elimination, explaining the formation of the homocoupling product. GC-MS analysis additionally confirmed the formation of Et_3GeF, a decomposition product of Et_3GeBF_4 after transmetalation.



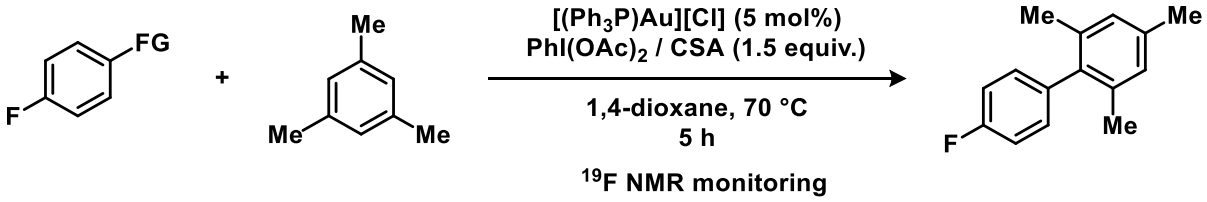
Reaction Development



2-Bromoanisole, $PhI(OAc)_2$ (48.3 mg, 0.15 mmol, 1.5 equiv.), $[(Ph_3P)Au][X]$ and triethyl(4-fluorophenyl)germane (25.6 mg, 0.10 mmol, 1.0 equiv.) [and for **II**, **III** and **IV** camphorsulfonic acid] were added to a reaction vial, dissolved in solvent and stirred under conditions as specified in the scheme above. The solvent was evaporated and subsequently analyzed by quantitative ^{19}F NMR analysis. Products were quantified *via* an internal standard (1,4-difluorobenzene, 1.0 equiv.).

Competition Experiments

Determination of Individual Reaction Rates



Mesitylene (55.9 µL, 040 mmol, 2.0 equiv.), $PhI(OAc)_2$ (96.6 mg, 0.30 mmol, 1.5 equiv.), CSA (69.7 mg, 0.30 mmol, 1.5 equiv.), [$(Ph_3P)AuCl$] (4.6 mg, 0.01 mmol, 5.0 mol%) and triethyl(4-fluorophenyl)germane (51.0 mg, 0.20 mmol, 1.0 equiv.) **or** (4-fluorophenyl)trimethylsilane (**FG** = **SiMe$_3$**; 33.7 mg 0.20 mmol, 1.0 equiv.) **or** 2-(4-fluorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**FG** = **Bpin**; 44.4 mg, 0.20 mmol, 1.0 equiv.) were added to a reaction vial, dissolved in 1,4-dioxane-d_8 (0.65 mL) and transferred to a NMR tube. The reaction was monitored at 70 °C (heated in the NMR spectrometer) *via* ^{19}F NMR analysis for 4 h (quantified with 1,4-difluorobenzene as the internal standard). The results are shown in Figure S1.

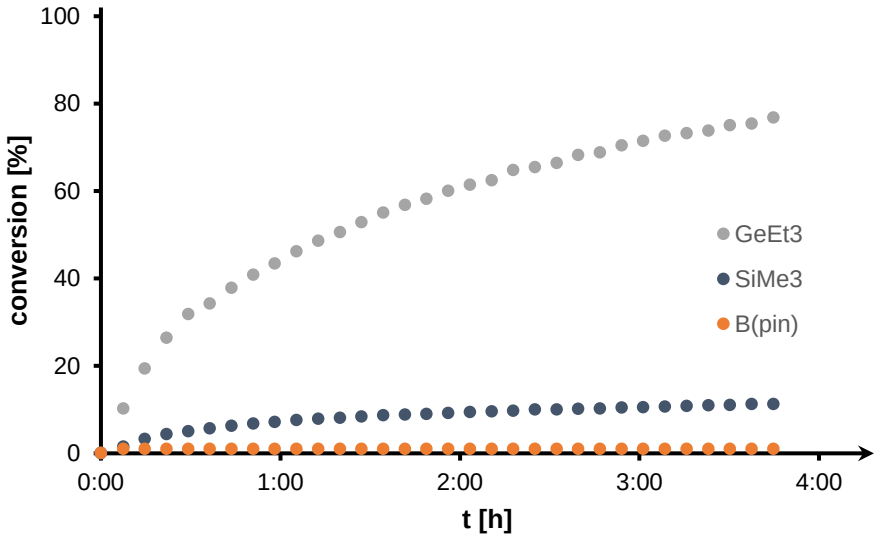
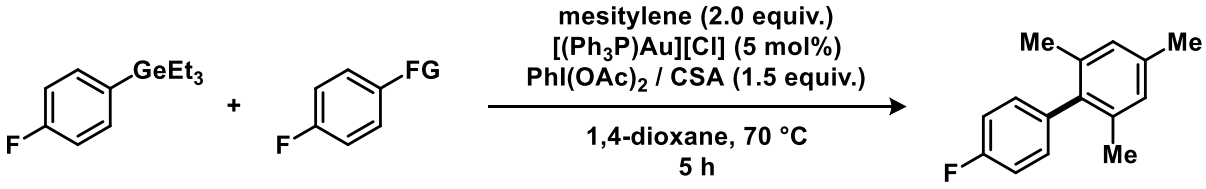


Figure S1: Individual reaction rates of C–H functionalization (formation of product [%] *versus* time [h]). Yields determined by quantitative ^{19}F NMR using 1,4-difluorobenzene as internal standard.

Intermolecular Competition Experiments



Mesitylene (55.9 µL, 040 mmol, 2.0 equiv.), $PhI(OAc)_2$ (96.6 mg, 0.30 mmol, 1.5 equiv.), CSA (69.7 mg, 0.30 mmol, 1.5 equiv.), $[(Ph_3P)AuCl]$ (4.6 mg, 0.01 mmol, 5.0 mol%), triethyl(4-fluorophenyl)germane (51.0 mg, 0.20 mmol, 1.0 equiv.) **and** (4-fluorophenyl)trimethylsilane (33.7 mg, 0.20 mmol, 1.0 equiv.) **or** 2-(4-fluorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (44.4 mg, 0.20 mmol, 1.0 equiv.) were added to a reaction vial, dissolved in 1,4-dioxane-d_8 (0.65 mL) and stirred for 12 h at 70 °C. The reaction mixture was quenched by dilution with dioxane-d_8 and subsequently analyzed by ^{19}F NMR analysis. Starting material and products were quantified *via* an internal standard (1,4-difluorobenzene, 1.0 equiv.). The results are shown in Table S3.

Table S3: Intermolecular competition of aryl germanes with aryl silane and aryl boronic ester.

entry	FG	consumption of $ArGeEt_3$[a]	consumption of $Ar[SiMe_3/B(pin)]$[a]	product yield[a]
1	$SiMe_3$	100%	0%	70%
2	B(pin)	100%	0%	46%[b]

[a]Yields determined by ^{19}F NMR using 1,4-difluorobenzene as internal standard. [b]Low product yield results from homocoupling of aryl germane.

Synthesis of Aryl Germanes

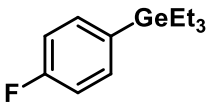
General Procedure 1 (GP 1)

Triethylgermanium chloride (1.05 equiv.) and the corresponding aryl iodide or aryl bromide (1.0 equiv.) were dissolved in anhydrous and degassed tetrahydrofuran (THF) (0.2 M) under an argon atmosphere. A solution of *i*PrMgCl (1.2 equiv.) was added slowly and the reaction solution was stirred for 3 h at room temperature. The reaction was quenched by addition of aqueous solution of NH_4Cl (sat.), the organic phase was separated and the aqueous phase was extracted with dichloromethane (DCM) (3x). The combined organic phases were dried with $MgSO_4$, filtered through Celite, the solvent was removed under reduced pressure and the crude product mixture was purified by silica gel column chromatography.

General Procedure 2 (GP 2)

Triethylgermanium chloride (1.0 equiv.) and the corresponding aryl Grignard reagent (1.1 equiv.) were dissolved in anhydrous and degassed THF (0.2 M) under argon and stirred for 3 h at room temperature. The reaction was quenched by addition of aqueous solution of NH_4Cl (sat.), the organic phase was separated and the aqueous phase was extracted with DCM (3x). The combined organic phases were dried with $MgSO_4$, filtered through Celite, the solvent was removed under reduced pressure and the crude product mixture was purified by silica gel column chromatography.

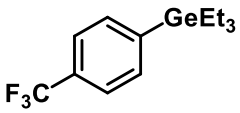
Triethyl(4-fluorophenyl)germane



Prepared according to GP 2 by using 4-fluorophenyl magnesium chloride. The title product was obtained after purification by column chromatography (pentane) as a colorless oil (732 mg, 2.87 mmol, 96%).

R_f = 0.85 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.43 – 7.36 (dd, *J* = 7.9 Hz, 2H), 7.09 – 7.01 (dd, *J* = 8.8 Hz, 2H), 1.05 (t, *J* = 7.5 Hz, 9H), 1.01 – 0.94 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 163.4 (d, *J* = 246.4 Hz), 135.7 (d, *J* = 6.9 Hz), 135.0 (d, *J* = 3.7 Hz), 115.1 (d, *J* = 19.1 Hz), 9.0, 4.4. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -113.75 – -113.84 (m). **HRMS** (EI) calculated for $C_{12}H_{19}F^{74}Ge$: 256.0683 $[M]^+$, found: 256.0673. **IR** (neat): ν/ cm^{-1} = 3029 (w), 2949 (s), 2875 (s), 2332 (w), 2162 (w), 2092 (w), 1890 (w), 1752 (w), 1636 (w), 1584 (s), 1495 (s), 1459 (m), 1380 (w), 1304 (w), 1226 (s), 1160 (s), 1082 (m), 1014 (s), 965 (m), 816 (s), 698 (s).

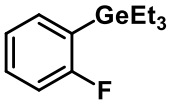
Triethyl(4-(trifluoromethyl)phenyl)germane



Prepared according to GP 1 by using 1-iodo-4-(trifluoromethyl)benzene. The title product was obtained after purification by column chromatography (pentane) as a colorless oil (815 mg, 2.67 mmol, 89%).

R_f = 0.93 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.57 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 1.08 – 0.99 (m, 15H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 145.3, 134.4, 130.4 (q, *J* = 32.0 Hz), 124.5 (q, *J* = 272.0 Hz), 124.4 (q, *J* = 3.7 Hz), 9.0, 4.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -62.83. **HRMS** (EI) calculated for $C_{13}H_{19}F_3{}^{74}Ge$: 306.0651 $[M]^+$, found: 306.0645. **IR** (neat): *ν*/ cm^{-1} = 2951 (s), 2876 (m), 2650 (w), 2326 (w), 2105 (w), 1999 (w). 1921 (w), 1604 (w), 1460 (w), 1389 (m), 1322 (s), 1230 (w), 1161 (s), 1126 (s), 1055 (m), 1014 (m), 961 (w), 823 (s), 693 (s).

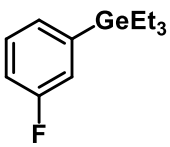
Triethyl(2-fluorophenyl)germane



Prepared according to GP 1 by using 1-fluoro-2-iodobenzene. The title product was obtained after purification by column chromatography (hexane) as a colorless liquid (668 mg, 2.61 mmol, 87%).

R_f = 0.84 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.38 – 7.29 (m, 2H), 7.15 – 7.09 (m, 1H), 7.03 – 6.96 (m, 1H), 1.09 – 1.02 (m, 15H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 166.9 (d, *J* = 238.4 Hz), 135.6 (d, *J* = 12.5 Hz), 130.5 (d, *J* = 7.9 Hz), 125.3 (d, *J* = 35.7 Hz), 123.9 (d, *J* = 2.9 Hz), 114.7 (d, *J* = 26.5 Hz), 9.0, 4.7. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -98.08 – -101.21 (m). **HRMS** (EI) calculated for $C_{12}H_{19}F^{74}Ge$: 256.0677 $[M]^+$, found: 256.0687. **IR** (neat): *ν*/ cm^{-1} = 3067 (w), 2949 (s), 2874 (s), 2014 (w), 1914 (w), 1596 (m), 1568 (m), 1435 (s), 1380 (m), 1254 (m), 1203 (s), 1110 (m), 1065 (m), 1015 (s), 968 (m), 855 (w), 816 (s), 755 (s), 701 (s).

Triethyl(3-fluorophenyl)germane

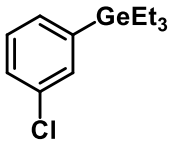


Prepared according to GP 1 by using 1-fluoro-3-iodobenzene. The title product was obtained after purification by column chromatography (hexane) as a colorless liquid (722 mg, 2.82 mmol, 94%).

R_f = 0.82 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.38 – 7.29 (m, 1H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.15 (dd, *J* = 8.6, 2.7 Hz, 1H), 7.07 – 6.97 (m, 1H), 1.15 – 0.95 (m, 15H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.8 (d, *J* = 249.0 Hz), 143.0 (d, *J* = 3.3 Hz), 129.6 (d, *J* = 3.1 Hz), 129.5 (d, *J* = 6.7 Hz), 120.4 (d, *J* = 18.0 Hz), 115.1 (d, *J* = 21.0 Hz), 9.0, 4.3. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -113.9 – -114.0 (m). **HRMS** (EI) calculated for $C_{12}H_{19}F^{74}Ge$: 256.0677 $[M]^+$, found:

256.0677. **IR** (neat): ν/ cm^{-1} = 3058 (w), 2948 (s), 2330 (w), 2082 (w), 1999 (w), 1924 (w), 1755 (w), 1576 (s), 1470 (s), 1412 (s), 1257 (m), 1211 (s), 1159 (w), 1095 (m), 1014 (s), 967 (s), 862 (s), 781 (s), 693 (s).

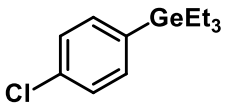
Triethyl(3-chlorophenyl)germane



Prepared according to GP 1 by using 1-chloro-3-iodobenzene. The title product was obtained after purification by column chromatography (hexane) as a colorless liquid (726 mg, 2.67 mmol, 89%).

R$_f$ = 0.85 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.42 (d, *J* = 2.2 Hz, 1H), 7.35 – 7.25 (m, 3H), 1.15 – 1.05 (m, 9H), 1.05 – 0.97 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 142.7, 134.4, 133.7, 132.0, 129.3, 128.3, 9.0, 4.3. **HRMS** (EI) calculated for $C_{12}H_{19}{}^{35}Cl^{74}Ge$: 272.0382 $[M]^+$, found: 272.0387. **IR** (neat): ν/ cm^{-1} = 3053 (w), 2948 (s), 2327 (m), 2090 (w), 1997 (w), 1924 (w), 1753 (w), 1558 (m), 1461 (s), 1385 (m), 1237 (w), 1170 (w), 1105 (s), 1014 (s), 966 (m), 881 (w), 774 (s), 694 (s).

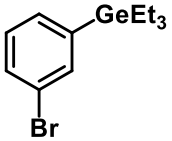
Triethyl(4-chlorophenyl)germane



Prepared according to GP 1 by using 1-chloro-4-iodobenzene. The title product was obtained after purification by column chromatography (pentane) as a colorless oil (797 mg, 2.94 mmol, 98%).

R$_f$ = 0.87 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.36 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 1.08 – 1.02 (m, 9H), 1.01 – 0.94 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 138.2, 135.4, 134.5, 128.2, 9.0, 4.3. **HRMS** (EI) calculated for $C_{12}H_{19}{}^{35}Cl^{74}Ge$: 272.0387 $[M]^+$, found: 272.0385. **IR** (neat): ν/ cm^{-1} = 3070 (w), 2949 (s), 2873 (s), 2332 (w), 2150 (w), 2091 (w), 2030 (w), 1900 (w) 1637 (w), 1572 (m), 1468 (s), 1428 (m), 1378 (m), 1304 (w), 1229 (w), 1075 (s), 1012 (s), 966 (m), 806 (s), 699 (s).

Triethyl(3-bromophenyl)germane

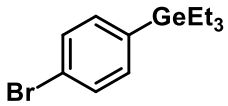


Prepared according to GP 1 by using 1-bromo-3-iodobenzene. The title product was obtained after purification by column chromatography (hexane) as a colorless liquid (910 mg, 2.88 mmol, 96%).

R$_f$ = 0.83 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.55 (d, *J* = 1.7 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.36 (d, *J* = 7.3 Hz, 1H), 7.25 – 7.18 (m, 1H), 1.14 – 1.04 (m, 9H), 1.04 – 0.97 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 143.2, 136.5, 132.4, 131.2, 129.7, 123.1, 9.0, 4.3. **HRMS** (EI)

calculated for $C_{12}H_{19}{}^{79}Br^{74}Ge$: 315.9876 $[M]^+$, found: 315.9891. **IR** (neat): ν/ cm^{-1} = 3053 (w), 2946 (s), 2337 (w), 2090 (w), 1759 (w), 1552 (w), 1460 (s), 1382 (m), 1235 (w), 1105 (m), 1064 (m), 1014 (s), 962 (w), 883 (w), 774 (s), 694 (s).

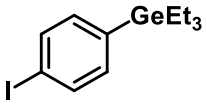
Triethyl(4-bromophenyl)germane



Prepared according to GP 1 by using 1-bromo-4-iodobenzene. The title product was obtained after purification by column chromatography (pentane) as a colorless oil (820 mg, 2.60 mmol, 87%).

R_f = 0.90 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.47 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 1.09 – 1.01 (m, 9H), 1.01 – 0.94 (m, 6H). **^{13}C NMR (**151 MHz, $CDCl_3$) δ/ ppm = 138.8, 135.7, 131.1, 123.0, 9.0, 4.3. **HRMS** (EI) calculated for $C_{12}H_{19}{}^{79}Br^{74}Ge$: 315.9882 $[M]^+$, found: 315.9867. **IR** (neat): ν/ cm^{-1} = 3068 (w), 2949 (s), 2872 (s), 2328 (w), 2113 (w), 1993 (w), 1900 (w), 1742 (w), 1633 (w), 1566 (m), 1464 (s), 1427 (m), 1374 (m), 1228 (w), 1061 (m), 1009 (s), 866 (m), 801 (s), 701 (s).

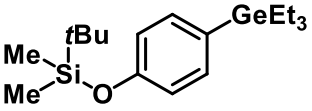
Triethyl(4-iodophenyl)germane



Prepared according to GP 1 by using 1,4-diiodobenzene (990 mg, 3.0 mmol, 1.00 equiv.). The title product was obtained after purification by column chromatography (pentane) as a colorless oil (963 mg, 2.65 mmol, 88%).

R_f = 0.90 (pentane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.67 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 1.09 – 1.01 (m, 9H), 1.01 – 0.93 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 139.4, 137.0, 135.9, 95.0, 9.0, 4.2. **HRMS** (EI) calculated for $C_{12}H_{19}{}^{74}Ge^{127}I$: 363.9738 $[M]^+$, found: 363.9744. **IR** (neat): ν/ cm^{-1} = 3060 (w), 2948 (s), 2872 (s), 2734 (w), 2329 (w), 2097 (w), 1900 (w), 1741 (w), 1631 (w), 1561 (m), 1463 (m), 1426 (m), 1372 (m), 1228 (w), 1051 (w), 1041 (s), 966 (m), 797 (s), 696 (s).

***tert*-Butyldimethyl(4-(triethylgermyl)phenoxy)silane**



Prepared according to GP 1 by using *tert*-butyl(4-iodophenoxy)dimethylsilane (1.00 g, 3.0 mmol, 1.00 equiv.). The title product was obtained after purification by column chromatography (hexane) as a colorless liquid (1.56 g, 4.23 mmol, 85%).

R_f = 0.65 (pentane). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.34 – 7.27 (m, 2H), 6.87 – 6.82 (m, 2H), 1.10 – 1.04 (m, 9H), 1.00 (s, 9H), 0.99 – 0.95 (m, 6H), 0.22 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ/ ppm = 155.9, 135.2, 131.1, 119.8, 25.8, 18.3, 9.1, 4.4, -4.2. **HRMS** (ESI) calculated for

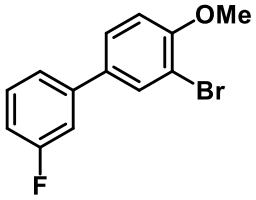
$C_{18}H_{34}{}^{74}GeOSi$: 391.1488 $[M+Na]^+$, found: 391.1487. **IR** (neat): ν/ cm^{-1} = 2946 (s), 2869 (s), 2328 (w), 2086 (w), 1587 (m), 1495 (m), 1465 (m), 1388 (w), 1258 (s), 1173 (m), 1088 (m), 1013 (m), 913 (s), 828 (s), 781 (s), 695 (m).

C–H Functionalization of Arenes

General Procedure 3 (GP 3)

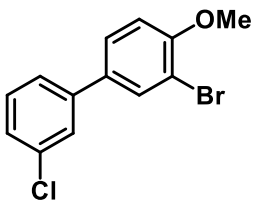
Aryl triethylgermane (1.0 equiv.), $PhI(OAc)_2$ (2.0 equiv.), CSA (1.5 equiv.) and $[(Ph_3P)AuCl]$ (5.0 mol%) were dissolved in 1,4-dioxane (0.33 M). Arene (2.0 equiv.) was added and the solution was stirred at 70 °C (reaction time specified for individual compounds). After completion of reaction, the composition was analyzed by ^1H or ^{19}F NMR to determine the yield. The reaction mixture was concentrated in *vacuo* and purified by silica gel column chromatography (eluent as specified for individual compounds).

3-Bromo-3'-fluoro-4-methoxy-1,1'-biphenyl



According to GP 3 the C–H functionalization was performed using triethyl(3-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (82%; >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a white crystalline solid (61.1 mg, 0.218 mmol, 73%). $\mathbf{R_f}$ = 0.31 (hexane/ toluene, 10:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.77 (d, *J* = 2.3 Hz, 1H), 7.48 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.43 – 7.32 (m, 1H), 7.34 – 7.26 (m, 1H), 7.26 – 7.17 (m, 1H), 7.07 – 6.97 (m, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ/ ppm = 163.3 (d, *J* = 245.7 Hz), 155.8, 141.8 (d, *J* = 7.6 Hz), 133.9(d, *J* = 1.9 Hz), 132.0 130.4 (d, *J* = 8.3 Hz), 127.2, 122.5 (d, *J* = 2.9 Hz), 114.1 (d, *J* = 21.2 Hz), 113.7 (d, *J* = 22.1 Hz), 112.3, 112.2, 56.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -112.83 – -112.97 (m). **HRMS** (EI) calculated for $C_{13}H_{10}OF^{79}Br$: 279.9893 $[M]^+$, found: 279.9887.

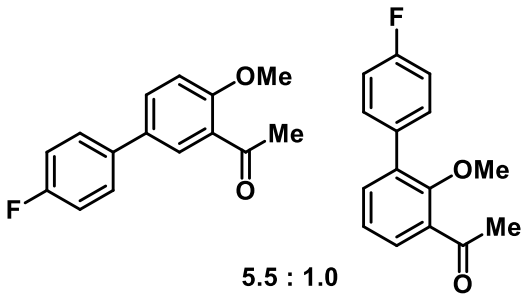
3-Bromo-3'-chloro-4-methoxy-1,1'-biphenyl



According to GP 3 the C–H functionalization was performed using triethyl(3-chlorophenyl)germane (81.6 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^1H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (86%; >95% regioselectivity). The title product was purified by column chromatography (hexane/toluene, 10:1) as a viscous liquid (68.1 mg, 0.230 mmol, 77%).

R_f = 0.30 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.76 – 7.75 (m, 1H), 7.51 – 7.49 (m, 1H), 7.46 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.40 – 7.38 (m, 1H), 7.4 – 7.3 (m, 1H), 7.31 – 7.28 (m, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 155.8, 141.3, 134.8, 133.7, 132.0, 130.2, 127.3, 127.2, 126.9, 125.0, 112.3, 112.2, 56.5. **HRMS** (EI) calculated for $C_{13}H_{10}O^{79}Br^{35}Cl$: 295.9598 $[M]^+$, found: 295.9600.

1-(4'-Fluoro-4-methoxy-[1,1'-biphenyl]-3-yl)ethan-1-one

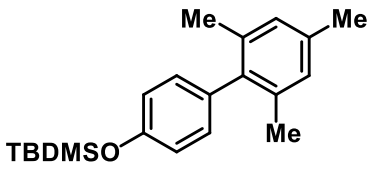


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 1-(2-methoxyphenyl)ethan-1-one (82.7 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (68%; 5.5:1 ratio of *para*:*ortho* isomer). The title product was purified by column chromatography (hexane/ EtOAc, 10:1) to give a mixture of both regioisomers as a viscous liquid (44.7 mg, 0.183 mmol, 61%).

Characterization data for 1-(4'-fluoro-4-methoxy-[1,1'-biphenyl]-3-yl)ethan-1-one:

R_f = 0.24 (hexane/ EtOAc, 10:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.93 (d, *J* = 2.5 Hz, 1H), 7.64 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.56 – 7.46 (m, 3H), 7.15 – 7.05 (m, 2H), 7.03 (d, *J* = 8.6 Hz, 1H), 3.95 (s, 3H), 2.65 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ/ ppm = 199.8, 162.4 (d, *J* = 246.2 Hz), 158.5, 136.1 (d, *J* = 3.3 Hz), 132.8, 132.0, 128.9, 128.5, 128.4 (d, *J* = 8.1 Hz), 115.8 (d, *J* = 21.2 Hz), 112.3, 55.8, 32.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -115.90 – -116.09 (m). **HRMS** (EI) calculated for $C_{15}H_{13}O_2F$: 267.0792 $[M+Na]^+$, found: 267.0793.

***tert*-Butyldimethyl((2',4',6'-trimethyl-[1,1'-biphenyl]-4-yl)oxy)silane**

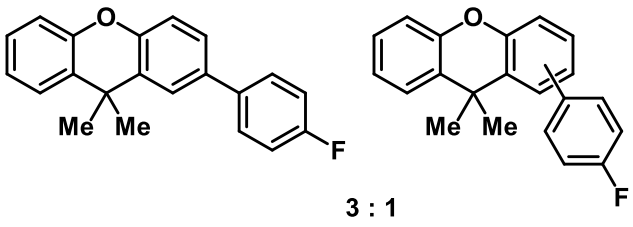


According to GP 3 the C–H functionalization was performed using *tert*-butyldimethyl(4-(triethylgermyl)phenoxy)-silane (110.4 mg, 0.300 mmol, 1.0 equiv.) and mesitylene (83.1 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{1}H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (88%). The reaction was quenched by addition of aqueous solution of NH_4Cl (sat.), the organic phase was separated and the aqueous phase was extracted with DCM (3x). The combined organic phases were dried with $MgSO_4$ and the solvent was removed

under reduced pressure. The title product was purified by column chromatography (hexane/ toluene, 10:1) as a viscous liquid (73.4 mg, 0.225 mmol, 75%).

R_f = 0.57 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 6.98 (d, *J* = 8.6 Hz, 2H), 6.94 (s, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 2.33 (s, 3H), 2.01 (s, 6H), 1.02 (s, 9H), 0.24 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 154.3, 139.0, 136.5, 136.5, 134.0, 130.4, 128.1, 120.0, 25.8, 21.2, 20.9, 18.4, -4.2. **HRMS** (EI) calculated for $C_{21}H_{30}OSi$: 326.2060 $[M]^+$, found: 326.2070.

2-(4-fluorophenyl)-9,9-dimethyl-9H-xanthene

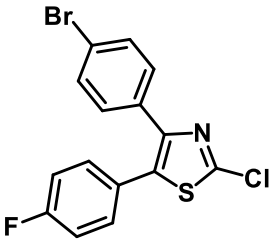


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 9,9-dimethyl-9H-xanthene (126.2 mg, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (66%; 3:1 ratio of isomers). The title product was purified by column chromatography (hexane/ toluene, 10:1) to give a mixture of both regioisomers as a colorless viscous liquid (53.9 mg, 0.177 mmol, 59%).

Characterization data for both isomers:

R_f = 0.46 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.64 – 7.58 (m, 1H), 7.59 (d, *J* = 2.2 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.50 – 7.43 (m, 2H), 7.40 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.24 – 7.08 (m, 8H), 6.99 (dd, *J* = 8.1, 1.3 Hz, 0.35H), 1.72 (s, 6H), 1.70 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 245.8 Hz), 162.3 (d, *J* = 246.0 Hz), 150.7, 150.4, 150.1, 147.7, 137.3 (d, *J* = 3.1 Hz), 135.4, 134.1 (d, *J* = 3.7 Hz), 131.5 (d, *J* = 7.7 Hz), 131.3, 130.5, 130.5, 129.9, 128.9, 128.8, 128.5 (d, *J* = 8.1 Hz), 127.6, 127.4, 126.3 (d, *J* = 5.6 Hz), 125.9, 125.4, 125.0, 123.4, 123.3, 123.1, 116.9, 116.5, 116.5, 115.7 (d, *J* = 21.5 Hz), 115.0 (d, *J* = 21.2 Hz), 34.6, 34.3, 32.7, 32.0. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -115.57 – -115.72 (m), -116.15 – -116.30 (m). **HRMS** (EI) calculated for $C_{21}H_{17}OF$: 304.1258 $[M]^+$, found: 304.1271.

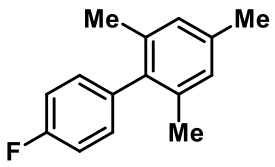
4-(4-Bromophenyl)-2-chloro-5-(4-fluorophenyl)thiazole



According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 4-(4-bromophenyl)-2-chlorothiazole (81.6 mg, 0.600 mmol, 2.0 equiv.). Reaction time: 16 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (80%). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a red viscous liquid (74.0 mg, 0.201 mmol, 67%).

$\mathbf{R_f}$ = 0.22 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.41 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 7.29 (dd, *J* = 8.7, 5.3 Hz, 2H), 7.09 – 7.03 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 163.1 (d, *J* = 250.3 Hz), 149.9, 147.7, 134.0, 132.4, 131.8, 131.6 (d, *J* = 8.4 Hz), 130.5, 126.6 (d, *J* = 3.5 Hz), 122.7, 116.5 (d, *J* = 21.9 Hz). **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -111.29 – -111.36 (m). **HRMS** (EI) calculated for $C_{15}H_8{}^{79}Br^{35}ClFNS$: 367.9306 $[M+H]^+$, found: 367.9305.

4'-Fluoro-2,4,6-trimethyl-1,1'-biphenyl

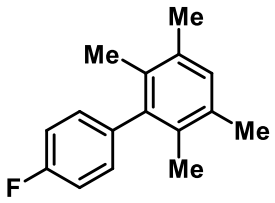


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and mesitylene (83.1 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 2 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (90%). The title product was purified by column chromatography (hexane) as a white solid (48.7 mg, 0.227 mmol, 76%).

$\mathbf{R_f}$ = 0.49 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.12 (d, *J* = 1.9 Hz, 2H), 7.11 (s, 2H), 6.96 (br s, 2H), 2.35 (s, 3H), 2.01 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 161.81 (d, *J* = 244.5 Hz), 138.1, 137.0 (d, *J* = 3.3 Hz), 136.9, 136.3, 130.9 (d, *J* = 8.0 Hz), 128.2, 115.5 (d, *J* = 21.1 Hz), 21.2, 20.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -116.50 (p, *J* = 7.3 Hz). **HRMS** (EI) calculated for $C_{15}H_{15}F$: 214.1152 $[M]^+$, found: 214.1147.

These data are in agreement with those reported previously in the literature.[4]

4'-Fluoro-2,3,5,6-tetramethyl-1,1'-biphenyl

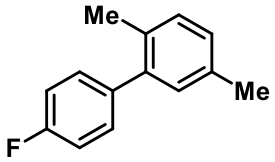


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 1,2,4,5-tetramethylbenzene (80.5 mg, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield of mono- and bis-arylated product was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (*monoarylated*: 61%; *bis-arylated*: 9%). The title product was purified by column chromatography (hexane) as a white solid (54%) in a mixture with inseparable starting material triethyl(4-fluorophenyl)germane (5%).

$\mathbf{R_f}$ = 0.52 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.15 – 7.04 (m, 4H), 7.01 (s, 1H), 2.27 (s, 6H), 1.88 (s, 6H) **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 161.7 (d, *J* = 244.6 Hz), 141.1, 138.3 (d, *J* = 3.3 Hz), 133.7, 132.3, 131.0 (d, *J* = 7.5 Hz), 130.7, 115.3 (d, *J* = 21.1 Hz), 20.4, 17.3. **^{19}F NMR** (564 MHz, CDCl3) δ/ ppm = -116.68 – -116.75 (m). **HRMS** (EI) calculated for $C_{16}H_{17}F$: 228.1308 $[M]^+$, found: 228.1305.

These data are in agreement with those reported previously in the literature.[4]

4'-Fluoro-2,5-dimethyl-1,1'-biphenyl



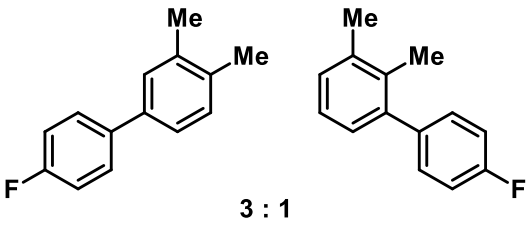
According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 1,4-dimethylbenzene (74.0 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 2 h.

The yield of mono- and bis-arylated product was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (*monoarylated*: 59%; *bis-arylated*: 15%). The title product (monarylated) was purified by column chromatography (hexane) followed by preparative HPLC (hexane/ EtOAc, 97:3) as a viscous liquid (27.5 mg, 0.138 mmol, 46%).

$\mathbf{R_f}$ = 0.48 (hexane). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.27 (dd, *J* = 8.7, 5.5 Hz, 2H), 7.16 (d, *J* = 7.7 Hz, 1H), 7.12 – 7.06 (m, 3H), 7.03 (d, *J* = 1.8 Hz, 1H), 2.35 (s, 3H), 2.21 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.0 (d, *J* = 245.1 Hz), 140.9, 138.1 (d, *J* = 3.4 Hz), 135.4, 132.3, 130.8 (d, *J* = 7.5 Hz), 130.7, 130.4, 128.2, 115.0 (d, *J* = 21.1 Hz), 21.1, 20.1. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -116.28 – -116.40 (m). **HRMS** (EI) calculated for $C_{14}H_{13}F$: 200.0995 $[M]^+$, found: 200.0992.

These data are in agreement with those reported previously in the literature.[4]

4'-Fluoro-3,4-dimethyl-1,1'-biphenyl



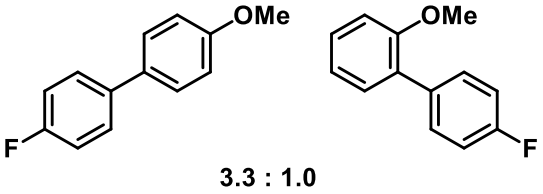
According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 1,2-dimethylbenzene (72.5 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (73%; 3:1 ratio of *meta*:*ortho* isomers). The title product was purified by column chromatography (hexane) to give a mixture of both regioisomers as a viscous liquid (35.1 mg, 0.175 mmol, 58%).

Characterization data for major regioisomer (4'-fluoro-3,4-dimethyl-1,1'-biphenyl):

R_f = 0.45 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.52 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.32 (d, *J* = 2.0 Hz, 1H), 7.28 (dd, *J* = 7.8, 2.0 Hz, 1H), 7.20 (d, *J* = 7.7 Hz, 1H), 7.13 – 7.07 (m, 2H), 2.33 (s, 3H), 2.30 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 245.5 Hz), 138.0, 137.5 (d, *J* = 3.0 Hz), 137.1, 135.9, 130.2, 128.6 (d, *J* = 7.9 Hz), 128.4, 124.5, 115.6 (d, *J* = 21.3 Hz), 20.1, 19.6. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -116.4 – -116.6 (m). **HRMS** (EI) calculated for $C_{14}H_{13}F$: 200.0995 $[M]^+$, found: 200.0991.

These data are in agreement with those reported previously in the literature.[4]

4-Fluoro-4'-methoxy-1,1'-biphenyl



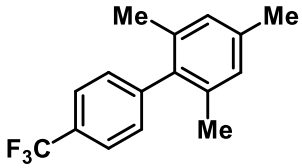
According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and methoxybezene (65.2 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (*monoarylated*: 63%; 3.3:1 ratio of *para*:*ortho* isomers; *bis-arylated*: 6%). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a white solid (33.3 mg, 0.165 mmol, 55%).

Characterization data for major regioisomer (4-fluoro-4'-methoxy-1,1'-biphenyl):

R_f = 0.42 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.52 – 7.45 (m, 4H), 7.15 – 7.08 (m, 2H), 6.98 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.2 (d, *J* = 245.7 Hz), 159.2, 137.1 (d, *J* = 3.3 Hz), 133.0, 128.3 (d, *J* = 7.5 Hz), 128.2, 115.7 (d, *J* = 21.4 Hz), 114.4, 55.5. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -116.72 – -116.79 (m). **HRMS** (EI) calculated for $C_{13}H_{11}O_1F$: 202.0788 $[M]^+$, found: 202.0786.

These data are in agreement with those reported previously in the literature.[4]

2,4,6-Trimethyl-4'-(trifluoromethyl)-1,1'-biphenyl



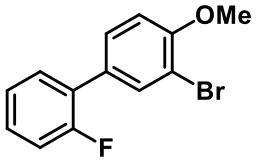
According to GP 3 the C–H functionalization was performed using triethyl(4-(trifluoromethyl)phenyl)germane (91.8 mg, 0.300 mmol, 1.0 equiv.) and mesitylene (83.1 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (87%). The title product was purified by column chromatography (hexane) as a white solid (63.4 mg, 0.240 mmol, 80%).

R_f = 0.67 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.70 (d, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 6.98 (s, 2H), 2.37 (s, 3H), 2.01 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 145.2, 137.8, 137.4, 135.8, 129.9, 129.0 (q, *J* = 32.2 Hz), 128.4, 125.5 (q, *J* = 3.8 Hz), 124.5 (q, *J* = 271.9 Hz), 21.2, 20.8. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -62.35. **HRMS** (EI) calculated for $C_{16}H_{15}F_3$: 264.1120 $[M]^+$, found: 264.1116.

These data are in agreement with those reported previously in the literature.[5]

Repeating the reaction under air yielded the desired product in 85% (determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard).

3'-Bromo-2-fluoro-4'-methoxy-1,1'-biphenyl

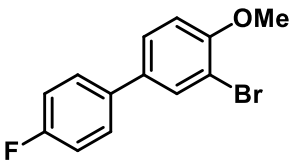


According to GP 3 the C–H functionalization was performed using triethyl(2-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (65%; >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a viscous liquid (49.0 mg, 0.173 mmol, 58%).

R_f = 0.34 (hexane/ toluene, 10:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.76 (dd, *J* = 2.3, 1.3 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.43 – 7.36 (m, 1H), 7.35 – 7.27 (m, 1H), 7.22 – 7.17 (m, 1H), 7.17 – 7.11 (m, 1H), 6.98 (d, *J* = 8.5 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ/ ppm = 159.8 (d, *J* = 247.5 Hz), 155.6, 133.8 (d, *J* = 2.9 Hz), 130.5 (d, *J* = 3.3 Hz), 129.7, 129.3 (d, *J* = 3.5 Hz), 129.1 (d, *J* = 8.2 Hz), 127.5 (d, *J* = 13.2 Hz), 124.6 (d, *J* = 3.5 Hz), 116.3 (d, *J* = 22.7 Hz), 111.9, 111.8, 56.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -118.07. **MS** (70 eV, EI): *m/z* (%): 282.9 (11), 282.0 (84), 280.9 (12) 280.0 (86) $[M]^+$, 266.9 (42), 264.9 (42), 238.9 (47), 236.9 (48), 186.0 (21), 171.0 (16), 170.0 (59), 169.0 (12), 158.0 (38), 157.0 (100), 138.0 (15), 133.0 (15), 132.0 (12), 131.0 (16), 120.0 (12), 107.0 (11), 75.0 (12), 74.0 (13), 63.0 (11), 62.0 (10).

These data are in agreement with those reported previously in the literature.[4]

3-Bromo-4'-fluoro-4-methoxy-1,1'-biphenyl

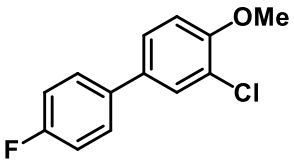


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 2 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (83%; >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a viscous liquid (64.1 mg, 0.229 mmol, 76%).

R_f = 0.31 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.73 (d, *J* = 2.3 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.43 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.13 – 7.08 (m, 2H), 6.95 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 246.1 Hz), 155.4, 135.7 (d, *J* = 3.0 Hz), 134.3, 131.9, 128.4 (d, *J* = 7.9 Hz), 127.0, 115.8 (d, *J* = 21.6 Hz), 112.2, 112.2, 56.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -115.64 – -115.76 (m). **HRMS** (EI) calculated for $C_{13}H_{10}OF^{79}Br$: 279.9893 $[M]^+$, found: 279.9891.

These data are in agreement with those reported previously in the literature.[4]

3-Chloro-4'-fluoro-4-methoxy-1,1'-biphenyl

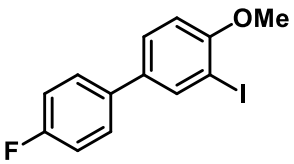


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 2-chloroanisole (76.2 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (85%; >95% regioselectivity). The title product was purified by column chromatography (hexane/toluene, 10:1) as a viscous liquid (55.1 mg, 0.233 mmol, 78%; >95% isomeric purity; ^{1}H and ^{19}F NMR analysis).

R_f = 0.35 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.56 (d, *J* = 2.3 Hz, 1H), 7.49 – 7.45 (m, 2H), 7.38 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.13 – 7.08 (m, 2H), 6.98 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 246.1 Hz), 154.5, 135.8 (d, *J* = 3.6 Hz), 133.8, 128.8, 128.4 (d, *J* = 8.1 Hz), 126.2, 122.9, 115.8 (d, *J* = 21.5 Hz), 112.4, 56.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -115.66 – -115.78 (m). **HRMS** (EI) calculated for $C_{13}H_{10}OF^{35}Cl$: 236.0399 $[M]^+$, found: 236.0399.

These data are in agreement with those reported previously in the literature.[4]

3-Iodo-4'-fluoro-4-methoxy-1,1'-biphenyl

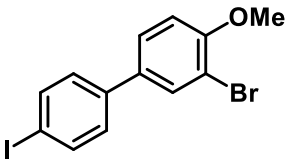


According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 2-iodoanisole (78.4 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (83%, >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a viscous liquid (73.8 mg, 0.225 mmol, 75%).

R_f = 0.31 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.96 (d, *J* = 2.3 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.16 – 7.07 (m, 2H), 6.87 (d, *J* = 8.5 Hz, 1H), 3.91 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 246.7 Hz), 157.6, 138.0, 135.5 (d, *J* = 3.6 Hz), 134.9, 128.4 (d, *J* = 8.1 Hz), 128.1, 115.8 (d, *J* = 21.5 Hz), 111.1, 86.5, 56.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ/ ppm = -115.70 – -115.81 (m). **HRMS** (EI) calculated for $C_{13}H_{10}OF^{127}I$: 327.9755 $[M]^+$, found: 327.9756.

These data are in agreement with those reported previously in the literature.[4]

3-Bromo-4'-iodo-4-methoxy-1,1'-biphenyl

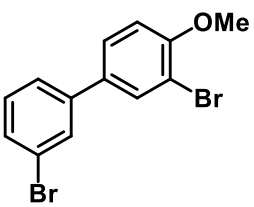


According to GP 3 the C–H functionalization was performed using triethyl(4-iodophenyl)germane (109.2 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{1}H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (87%; >95% regioselectivity). After analysis, the title product was purified by column chromatography (hexane/ toluene, 10:1) as a white solid (88.4 mg, 0.228 mmol, 76%).

R_f = 0.38 (hexane/ toluene, 10:1). **^{1}H NMR (**600 MHz, $CDCl_3$) δ/ ppm = 7.83 – 7.66 (m, 3H), 7.45 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.26 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 155.7, 139.1, 138.0, 134.0, 131.8, 128.7, 127.0, 112.3, 112.3, 93.0, 56.5. **HRMS** (EI) calculated for $C_{13}H_{10}O^{79}Br^{127}I$: 387.8954 $[M]^+$, found: 387.8960.

These data are in agreement with those reported previously in the literature.[4]

3,3'-Dibromo-4-methoxy-1,1'-biphenyl



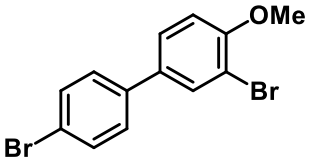
According to GP 3 the C–H functionalization was performed using triethyl(3-bromophenyl)germane (94.8 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{1}H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (90%; >95% regioselectivity). The title

product was purified by column chromatography (hexane/ toluene, 10:1) as a white solid (85.7 mg, 0.252 mmol, 84%).

R_f = 0.31 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.75 (d, *J* = 2.3 Hz, 1H), 7.66 (dd, *J* = 1.9, 1.9 Hz, 1H), 7.49 – 7.41 (m, 3H), 7.28 (dd, *J* = 1.9, 1.9 Hz, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 155.9, 141.7, 133.7, 132.0, 130.5, 130.3, 129.9, 127.2, 125.5, 123.1, 112.3, 112.2, 56.5. **HRMS** (EI) calculated for $C_{13}H_{10}O^{79}Br_2$: 339.9111 $[M]^+$, found: 339.9107.

These data are in agreement with those reported previously in the literature.[4]

3,4'-Dibromo-4-methoxy-1,1'-biphenyl

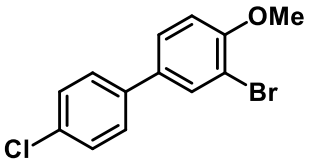


According to GP 3 the C–H functionalization was performed using triethyl(4-bromophenyl)germane (94.8 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{1}H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (90%; >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a viscous liquid (83.7 mg, 0.246 mmol, 82%).

R_f = 0.38/ (hexane/ toluene, 10:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ/ ppm = 7.75 (d, *J* = 2.3 Hz, 1H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.45 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ/ ppm = 155.7, 138.5, 134.0, 132.1, 131.8, 128.4, 127.0, 121.6, 112.3, 112.3, 56.5. **HRMS** (EI) calculated for $C_{13}H_{10}O^{79}Br_2$: 339.9093 $[M]^+$, found: 339.9094.

These data are in agreement with those reported previously in the literature.[4]

3-Bromo-4'-chloro-4-methoxy-1,1'-biphenyl



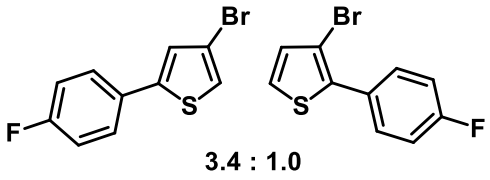
According to GP 3 the C–H functionalization was performed using triethyl(4-chlorophenyl)germane (81.6 mg, 0.300 mmol, 1.0 equiv.) and 2-bromoanisole (74.8 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 5 h. The yield was determined by quantitative ^{1}H NMR using 1,3,5-tris(trifluoromethyl)benzene as an internal standard (88%; >95% regioselectivity). The title product was purified by column chromatography (hexane/ toluene, 10:1) as a white solid (70.2 mg, 0.237 mmol, 79%).

R_f = 0.30 (hexane/ toluene, 10:1). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.75 (d, *J* = 2.3 Hz, 1H), 7.46 – 7.43 (m, 3H), 7.40 – 7.37 (m, 2H), 6.95 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (151 MHz,

$CDCl_3$) δ/ ppm = 155.6, 138.0, 133.9, 133.4, 131.8, 129.1, 128.1, 127.0, 112.2, 112.2, 56.5. **HRMS** (EI) calculated for $C_{13}H_{10}O^{79}Br^{35}Cl$: 295.9598 $[M]^+$, found: 295.9599.

These data are in agreement with those reported previously in the literature.[4]

4-Bromo-2-(4-fluorophenyl)thiophene & 3-bromo-2-(4-fluorophenyl)thiophene:



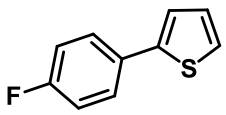
According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and 3-bromothiophene (56.2 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 16 h. The yield of mono- and bis-arylated product was determined by quantitative ^{19}F NMR using 1,4-difluorobenzene as an internal standard (*monoarylated*: 46%; 3.4:1 ratio of 5- and *2*-isomer; *bis-arylated*: 12%). The title product was purified by column chromatography (hexane/ toluene, 10:1) to give a mixture of both regioisomers as a viscous liquid (30.1 mg, 0.117 mmol, 39%).

Characterization data for 2- and 5-(4-fluorophenyl)-3-bromothiophene:

$\mathbf{R_f}$ = 0.55 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.65 – 7.57 (m, 2H), 7.56 – 7.49 (m, 0.65H), 7.28 (d, *J* = 5.3 Hz, 1H), 7.17 (d, *J* = 1.3 Hz, 0.28H), 7.15 – 7.07 (m, 3H), 7.05 (d, *J* = 5.3 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.7 (d, *J* = 248.2 Hz), 144.3, 137.1, 131.6, 130.9 (d, *J* = 8.5 Hz), 129.5 (d, *J* = 3.6 Hz), 128.9 (d, *J* = 3.7 Hz), 127.5 (d, *J* = 8.1 Hz), 125.7, 125.0, 121.9, 116.0 (d, *J* = 22.1 Hz), 115.6 (d, *J* = 22.0 Hz), 110.6, 107.8. **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -113.0 – -113.1 (m), -113.2 – -113.3 (m). **HRMS** (EI) calculated for $C_{10}H_6{}^{79}BrFS$: 255.9352 $[M]^+$, found: 255.9348.

These data are in agreement with those reported previously in the literature.[4]

2-(4-Fluorophenyl)thiophene



According to GP 3 the C–H functionalization was performed using triethyl(4-fluorophenyl)germane (76.8 mg, 0.300 mmol, 1.0 equiv.) and thiophene (48.1 µL, 0.600 mmol, 2.0 equiv.). Reaction time: 16 h. The yield of mono- and bis-arylated product was determined by quantitative ^{19}F NMR using fluorobenzene as an internal standard (*monoarylated*: 56%; *bis-arylated*: 16%). The title product was purified by column chromatography (hexane) followed by preparative HPLC (hexane/EtOAc, 97:3) to give a white solid (25.6 mg, 0.144 mmol, 48%).

Characterization data for mixture of 2-(4-fluorophenyl)thiophene:

R_f = 0.46 (hexane). **^{1}H NMR** (600 MHz, $CDCl_3$) δ/ ppm = 7.59 – 7.55 (m, 2H), 7.27 (dd, *J* = 5.1, 0.9 Hz, 1H), 7.24 (dd, *J* = 3.6, 1.1 Hz, 1H), 7.09 – 7.05 (m, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ/ ppm = 162.4 (d, *J* = 247.0 Hz), 143.4, 130.8 (d, *J* = 3.6 Hz), 128.2, 127.7 (d, *J* = 7.9 Hz), 124.9, 123.2, 116.0 (d, *J* = 21.6 Hz). **^{19}F NMR** (564 MHz, $CDCl_3$) δ/ ppm = -114.72 – -114.87 (m). **HRMS** (EI) calculated for $C_{10}H_7FS$: 178.0247 $[M]^+$, found: 178.0251.

These data are in agreement with those reported previously in the literature.[6]

Computational Details

General Details

All calculations were performed using the Gaussian software package (Gaussian16, revision A.03).[7] Structures were optimized with ωB97XD and 6-31G(d) basis set (LANL2DZ for Au). Single point energy calculations were performed on the optimized structures using M06L in combination with a 6-311++G(d,p) basis set (LANL2DZ for Au). The effect of solvation was accounted for using the CPCM solvation model for 1,4-dioxane. All stationary points were fully characterized *via* frequency calculations, at the same level of theory, as either ground states (zero imaginary frequencies) or transition states (one imaginary frequency). For transition states, IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by each transition state. Frequency calculations also provided zero-point energy (ZPE) and Gibbs free energy (ΔG) corrections in the gas-phase, computed at 298.15 K and 1 atm. Reported Gibbs free energies were determined by summing the SCF energy, zero-point energy and Gibbs free energy correction determined at the 1 M standard state (addition of 1.89 kcal mol^{-1} to every species). Images were created using the CYLview software.[8]

Distortion/Interaction Analysis

In order to gain insight into the factors that affect the reaction barrier for transmetalation on $Au^{(I)}$ and $Au^{(III)}$, the distortion/interaction model was used.[9] The transition state and preceding ground state structures were each divided into two fragments, Ph–Y (Y = $SiMe_3$, $GeMe_3$) and the active gold complex ($Au^{(I)}$ or $Au^{(III)}$). Single point energy calculations were performed on each fragment in the same geometry as the original optimized structures. The distortion energy ($\Delta E_{\text{Distortion}}$) is the energy difference between the distorted structure of the transition state and the distorted structure of the preceding ground-state or the isolated optimized fragments. The results are displayed in Table S4 and S5. Energies are reported in kcal mol^{-1}.

Table S4: Distortion/interaction energy analysis with $[Au(OMs)_3]$.

entry	Ph–Y	ΔE	ΔE_{Dist}(Ph–Y)	ΔE_{Dist}(Au)	ΔE_{Int}
1	Ph–$SiMe_3$	5.8	51.7	0.1	46.0
2	Ph–$GeMe_3$	1.6	28.3	3.5	30.2

Table S5: Distortion/interaction energy analysis with [(PPh_3)Au][OMs].

entry	Ph–Y	ΔE	ΔE_{Dist}(Ph–Y)	ΔE_{Dist}(Au)	ΔE_{Int}
1	$PhGeMe_3$	13.2	67.3	7.1	61.2

Bond Dissociation Energies

Bond strengths discussed in the main text were calculated using DFT. BDE is defined as the change in enthalpy (ΔH) for homolytic cleavage of the Ph–Y bond. The geometry of each radical containing fragment was optimized, and single point calculations were performed at the same level of theory as previously stated. Reported enthalpies were determined by summing the SCF energy, zero-point energy and enthalpy energy correction. The results are displayed in Table S6. Energies are reported in kcal mol^{-1}.

Table S6: Bond dissociation energies.

Entry	Ph–Y	ΔH (kcal mol^{-1})
1	$Ph–SiMe_3$	94.7
2	$Ph–GeMe_3$	85.2

Bond Activation with Au(III)

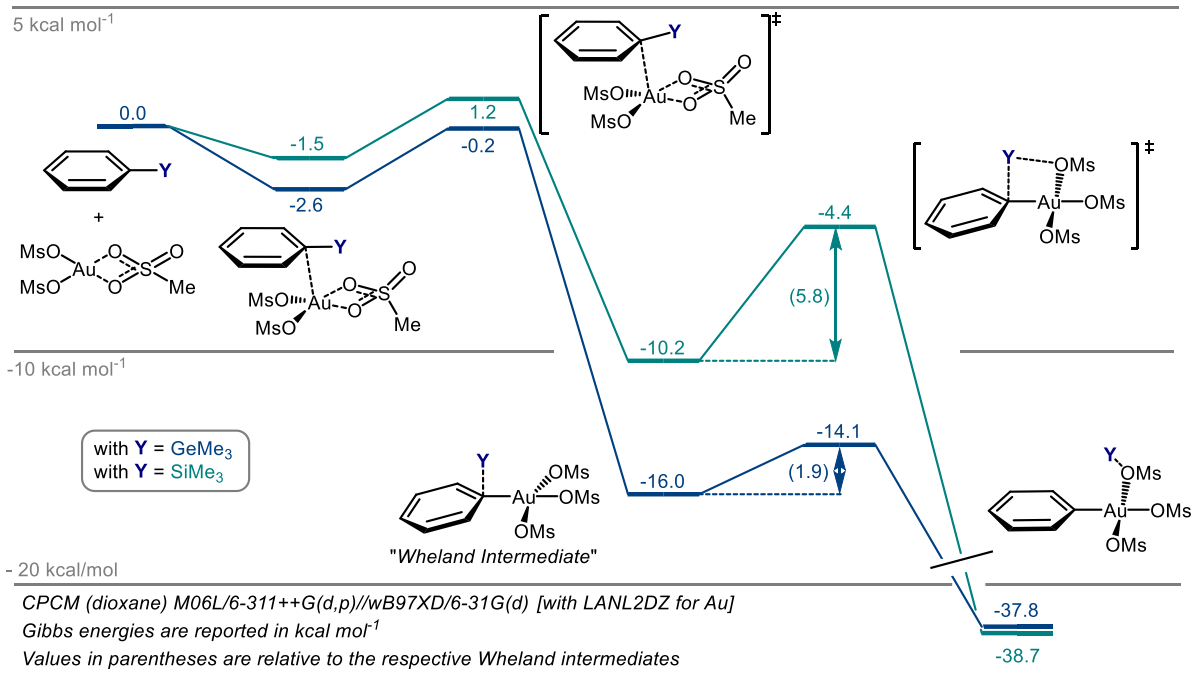


Figure S2: CPCM (1,4-dioxane) M06L/6-311++G(d,p)// ωB97XD/6-31G(d) [with LANL2DZ for Au]. Gibbs energies are reported in kcal mol-1. Values in parentheses are relative to Wheland complex

Bond Activation with Au(I)

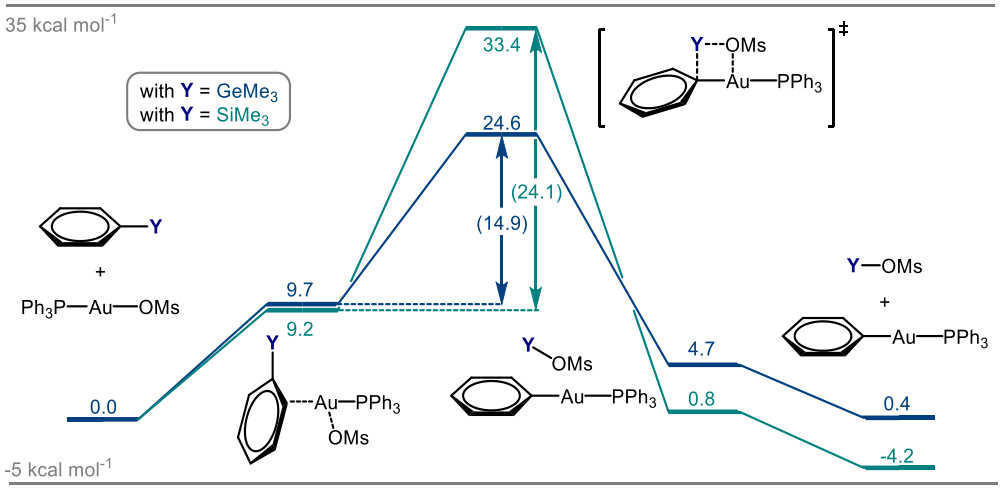
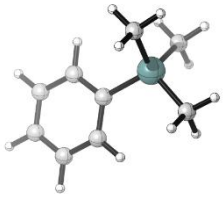


Figure S3: CPCM (1,4-dioxane) M06L/6-311++G(d,p)// ωB97XD/6-31G(d) [with LANL2DZ for Au]. Gibbs energies are reported in kcal mol-1. Values in parentheses are relative to precoordination complex

XYZ Coordinates and Energies of Optimized Structures

General Structures



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H	0.94598	2.16520	-0.00013
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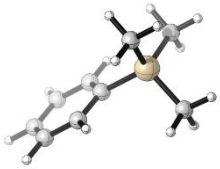
H	3.36131	-2.15769	0.00018
H	4.63122	-0.02348	0.00010
H	-2.93985	-1.02355	1.60408
H	-1.42748	-1.94860	1.64066
H	-1.53942	-0.40613	2.50504
H	-2.93953	-1.02358	-1.60455
H	-1.53838	-0.40710	-2.50503
H	-1.42752	-1.94922	-1.63988
H	-1.53243	2.38828	0.88739
H	-1.53252	2.38816	-0.88784
H	-2.97476	1.86764	-0.00010
C	2.85871	1.19924	-0.00003
C	1.46514	1.20946	-0.00006
C	0.72996	0.01971	-0.00001
C	1.44075	-1.18674	0.00007
C	2.83234	-1.20867	0.00011
C	3.54496	-0.01156	0.00006
C	-1.84844	-0.93882	1.60066
C	-1.84810	-0.93926	-1.60057
C	-1.88047	1.85035	-0.00017
Ge	-1.22389	0.00510	-0.00001

Zero-point correction= 0.203747 (Hartree/Particle)
Thermal correction to Energy= 0.216464
Thermal correction to Enthalpy= 0.217409
Thermal correction to Gibbs Free Energy= 0.163872
Sum of electronic and zero-point Energies= -2425.848786
Sum of electronic and thermal Energies= -2425.836068
Sum of electronic and thermal Enthalpies= -2425.835124
Sum of electronic and thermal Free Energies= -2425.888661
E(RM06L) = -2428.35884854



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H	-3.05728	-2.15598	-0.00034
H	-4.32684	-0.02227	-0.00016
H	3.16549	-0.95850	-1.55623
H	1.68186	-1.92391	-1.57510
H	1.74476	-0.38852	-2.45059
H	3.16536	-0.95880	1.55630
H	1.74455	-0.38902	2.45065
H	1.68173	-1.92422	1.57484
H	1.78380	2.32675	-0.88602
H	1.78373	2.32659	0.88660
H	3.21157	1.77601	0.00029
C	-2.55482	1.20077	0.00003
C	-1.16125	1.21208	0.00008
C	-0.42195	0.02189	-0.00002
C	-1.13656	-1.18610	-0.00017
C	-2.52776	-1.20728	-0.00022
C	-3.24057	-0.01005	-0.00012
C	2.07087	-0.89977	-1.53803
C	2.07074	-0.90007	1.53801
C	2.11547	1.77380	0.00025
Si	1.46321	0.00615	0.00006

Zero-point correction= 0.204755 (Hartree/Particle)
Thermal correction to Energy= 0.216891
Thermal correction to Enthalpy= 0.217835
Thermal correction to Gibbs Free Energy= 0.166453
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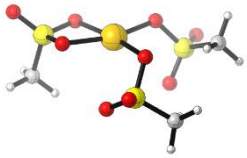
Sum of electronic and thermal Energies= -640.566780
Sum of electronic and thermal Enthalpies= -640.565836
Sum of electronic and thermal Free Energies= -640.617219
E(RM06L) = -640.965489233

Bond Activation with $Au^{(III)}$



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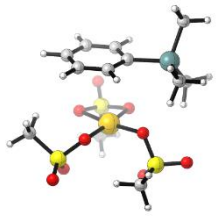
H	3.72359	-1.55201	-1.52718
H	3.17962	0.08592	-1.03498
H	4.49180	-0.74708	-0.12197
H	3.24607	2.56977	-0.01200
H	2.57782	3.26256	1.49604
H	2.68217	1.47440	1.31356
C	-3.11086	0.00904	1.91810
C	3.56689	-0.87301	-0.68817
C	2.52995	2.42420	0.79826
O	0.97225	1.16395	-0.89395
O	-1.91989	-1.52998	0.09704
O	-4.24811	-0.67369	-0.38525
O	-0.06316	2.07601	1.16400
O	-2.16105	0.75506	-0.43894
O	1.07999	-1.67228	-0.55417
O	2.08095	-0.67427	1.49049
O	2.73616	-2.96695	0.68391
O	0.69999	3.61431	-0.68002
S	-2.96532	-0.39242	0.19514
S	0.88924	2.41786	0.11151
S	2.35711	-1.60097	0.39853
Au	-0.33294	-0.28172	-0.43237

Zero-point correction= 0.160004 (Hartree/Particle)
Thermal correction to Energy= 0.179112
Thermal correction to Enthalpy= 0.180056
Thermal correction to Gibbs Free Energy= 0.110940
Sum of electronic and zero-point Energies= -2126.064446
Sum of electronic and thermal Energies= -2126.045338
Sum of electronic and thermal Enthalpies= -2126.044394
Sum of electronic and thermal Free Energies= -2126.113510
E(RM06L) = -2126.79040970



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H	-2.76372	-2.48128	3.13045
H	-1.54154	-1.63551	4.14114
H	-0.55535	4.13383	-1.09750
H	-1.99121	3.08817	-0.84502
H	-1.80397	4.60372	0.10193
H	1.50570	0.35484	-2.62651
H	-0.06365	-1.27914	-3.58332
H	-0.28924	-3.53999	-2.56750
H	1.06905	-4.12913	-0.57199
H	2.64694	-2.50163	0.37492
H	4.11989	2.72154	-0.90037
H	3.64016	1.84120	-2.36287
H	2.40361	2.41461	-1.21389
H	4.02574	1.02012	2.09153
H	2.30882	1.27732	1.72356
H	2.90233	-0.35542	2.08679
H	5.32173	-1.47633	-0.02076
H	5.51372	-0.65595	-1.58055
H	6.06146	0.13354	-0.08715
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C	-2.01745	-1.68566	3.16029
C	-1.28309	3.76945	-0.37147
C	2.21549	-0.94690	-1.06035
C	1.43126	-0.63215	-2.17705
C	0.53535	-1.55554	-2.72036
C	0.40689	-2.81800	-2.14974
C	1.17481	-3.15260	-1.03464
C	2.06559	-2.22529	-0.50212
C	3.40900	1.99417	-1.30376
C	3.14929	0.59076	1.59600
C	5.28433	-0.50344	-0.52155
O	-1.67811	0.58030	-1.41598
O	0.18609	-0.86490	1.93243
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S	-0.76155	-2.07601	1.96836
S	-3.23861	0.25215	-1.40813
S	-0.40064	2.89705	0.90545
Ge	3.51482	0.31668	-0.30602
Au	-0.66655	-0.03021	0.19780

Zero-point correction= 0.364468 (Hartree/Particle)
Thermal correction to Energy= 0.398574
Thermal correction to Enthalpy= 0.399518
Thermal correction to Gibbs Free Energy= 0.294071
Sum of electronic and zero-point Energies= -4551.946305
Sum of electronic and thermal Energies= -4551.912199
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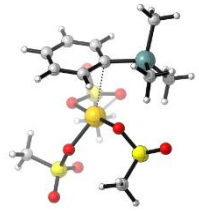
Sum of electronic and thermal Free Energies= -4552.016701
E(RM06L) = -4555.17044479



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H	-2.49616	-1.08731	2.48600
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H	-1.88955	4.54445	0.35324
H	1.43740	0.51184	-2.40977
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H	0.26678	-3.57170	-3.00408
H	1.40252	-4.20043	-0.88668
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H	3.54832	1.36730	2.37779
H	1.83139	1.25015	1.95932
H	2.71516	-0.20252	2.44505
H	4.96252	-1.50046	0.64150
H	5.35464	-0.82446	-0.95182
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C	-2.06670	-2.07611	2.65358
C	-1.50950	3.75770	-0.30114
C	2.09357	-0.85286	-0.86156
C	1.41796	-0.51781	-2.06082
C	0.76919	-1.49019	-2.83238
C	0.77250	-2.81303	-2.41476
C	1.42047	-3.17045	-1.22671
C	2.06604	-2.20784	-0.46877
C	3.51173	2.01289	-1.02779
C	2.79386	0.73853	1.89444
C	5.04090	-0.57279	0.06581
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O	0.28895	-1.14900	1.87675
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O	-3.50887	0.05436	0.87335
O	-1.18218	-1.91700	0.15199
O	-4.44835	1.40943	-1.02164
O	0.26375	1.80489	-0.45208
O	-0.79407	2.22011	1.73560
O	0.89819	3.81870	0.76632
S	-0.65819	-2.26353	1.59221
S	-3.59693	0.33057	-0.55368
S	-0.22017	2.91324	0.58856
Ge	3.33449	0.39681	0.05140
Au	-0.48524	-0.01956	-0.14683

Zero-point correction= 0.364351 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.398586
Thermal correction to Gibbs Free Energy= 0.297146
Sum of electronic and zero-point Energies= -4551.937231
Sum of electronic and thermal Energies= -4551.903940
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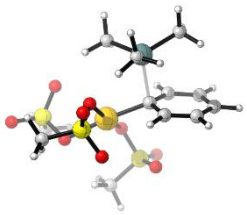
Sum of electronic and thermal Free Energies= -4552.004436
E(RM06L) = -4555.16944888



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H	3.40741	1.33170	-1.77272
H	4.83911	0.60142	-0.96265
H	4.51360	0.25529	-2.69009
H	-3.00357	3.63153	-0.86104
H	-3.76801	1.15598	2.57633
H	-4.08701	-1.82431	0.67408
H	-3.77605	-2.94707	-0.66447
H	-2.52669	-2.69594	0.57444
H	-0.57074	-1.84656	-2.15472
H	-1.93719	-1.78267	-3.30018
H	-0.96610	-0.32904	-2.98711
H	-4.86048	-0.50391	-2.27646
H	-4.72340	0.72744	-1.01206
H	-3.89122	0.95966	-2.56972
H	-1.89422	-0.32578	1.93420
H	-1.18067	2.12102	-1.55331
H	-4.28751	3.15325	1.20548
C	2.90078	2.71337	1.19623
C	1.72310	-3.21800	1.59833
C	4.06358	0.46105	-1.71728
C	-1.76670	1.89482	-0.66887
C	-2.78326	2.74532	-0.27612
C	-3.50291	2.47207	0.88975
C	-3.21738	1.34914	1.66209
C	-2.17931	0.50245	1.29235
C	-1.45473	0.73737	0.09595
C	-3.31501	-2.20722	0.00124
C	-1.38731	-1.22832	-2.53056
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O	1.07445	1.92383	-0.51068
O	-0.14741	-1.83418	0.34840
O	-0.87514	-3.53750	1.91994
O	1.16626	4.30418	-0.00605

O	0.16937	-1.41859	2.76976
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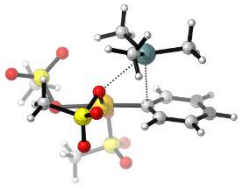
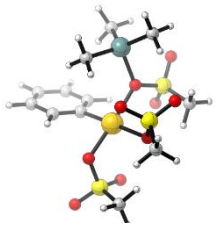
O	2.49596	-0.50084	0.12280
O	3.93042	-2.09933	-1.07597
O	1.96772	-1.03543	-2.22661
S	0.11502	-2.48093	1.76877
S	1.23250	3.00435	0.63672
S	3.06551	-0.94512	-1.25748
Ge	-2.65875	-0.78099	-1.13502
Au	0.47109	0.06950	0.02825

Zero-point correction= 0.366377 (Hartree/Particle)
Thermal correction to Energy= 0.399663
Thermal correction to Enthalpy= 0.400607
Thermal correction to Gibbs Free Energy= 0.299546
Sum of electronic and zero-point Energies= -4551.968599
Sum of electronic and thermal Energies= -4551.935312
Sum of electronic and thermal Enthalpies= -4551.934368
Sum of electronic and thermal Free Energies= -4552.035429
E(RM06L) = -4555.19913442



H	4.02843	0.43730	0.56254
H	4.62214	1.64076	-0.63557
H	4.89787	1.91307	1.11437
H	1.46589	-2.26066	2.16359
H	0.51402	-3.55861	2.96777
H	0.74423	-3.55571	1.17628
H	4.06579	-0.81835	-1.98973
H	4.59358	-2.21695	-0.99060
H	4.03130	-2.47610	-2.67155
H	-1.82856	4.42760	-1.37946
H	-3.67777	2.36258	1.90445
H	-4.59966	-0.09578	0.85673
H	-4.93734	-1.51434	-0.16495
H	-3.67298	-1.62555	1.07925
H	-1.90159	-2.66872	-1.42917
H	-2.45496	-1.87031	-2.94641
H	-0.88881	-1.44683	-2.21015
H	-4.38250	0.58270	-2.70170
H	-3.91766	1.88138	-1.58239
H	-2.78303	1.34493	-2.85512
H	-1.93377	0.61839	1.79394
H	-0.10703	2.66661	-1.53283
H	-3.60740	4.29571	0.34776
C	4.22036	1.49406	0.36811
C	0.62219	-2.94414	2.07182
C	3.90942	-1.87523	-1.76872
C	-0.91221	2.57862	-0.81269
C	-1.87189	3.57437	-0.70972
C	-2.87491	3.49877	0.26315
C	-2.91980	2.41784	1.12909
C	-1.95656	1.40240	1.04335
C	-0.95234	1.48939	0.06955
C	-4.14976	-0.95653	0.35959
C	-1.92203	-1.73755	-1.99634
C	-3.54542	1.02446	-2.14340
O	1.80248	1.61825	-0.60678
O	-0.77634	-1.28966	0.51502
O	-1.99843	-2.92256	1.80282
O	2.85643	3.73162	0.03796
O	-0.91258	-0.99288	2.98207
O	2.10433	2.10525	1.80889
O	2.21952	-1.19892	0.07626
O	2.03541	-3.48700	-0.85637
O	1.34661	-1.49823	-2.20872
S	-0.87536	-2.00203	1.93073
S	2.66834	2.36551	0.48931
S	2.23461	-2.08114	-1.19143
Ge	-2.90364	-0.40604	-1.00658
Au	0.56839	0.17832	0.07625

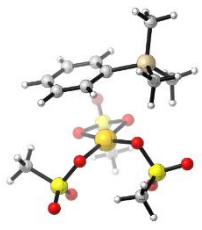
Zero-point correction= 0.366113 (Hartree/Particle)
Thermal correction to Energy= 0.398640
Thermal correction to Enthalpy= 0.399585
Thermal correction to Gibbs Free Energy= 0.300266
Sum of electronic and zero-point Energies= -4551.963424
Sum of electronic and thermal Energies= -4551.930897
Sum of electronic and thermal Enthalpies= -4551.929953
Sum of electronic and thermal Free Energies= -4552.029271
E(RM06L) = -4555.19650578



H	3.38502	-2.05325	0.40603
H	4.61447	-1.49136	-0.78475
H	5.02674	-1.56448	0.95867
H	-0.12300	-2.06455	2.34366
H	-1.57232	-2.30701	3.39060
H	-1.62276	-2.69709	1.62238
H	2.39819	-3.58098	-1.63125
H	1.76721	-4.66512	-0.34456
H	1.11046	-4.76862	-2.00811
H	1.00972	4.52423	-2.53300
H	-0.22609	5.85775	-0.84189
H	-1.00209	4.78098	1.25676
H	-3.05720	2.48325	0.04674
H	-4.45095	2.04011	-0.95581
H	-4.35601	1.46991	0.73500
H	-4.31743	-1.71264	0.12112
H	-4.34492	-1.69036	-1.66247
H	-2.94576	-2.38392	-0.81372

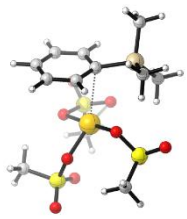
H	-2.57722	0.49454	-3.24782
H	-1.37361	1.47962	-2.38869
H	-1.10654	-0.28238	-2.62440
H	-0.58493	2.37559	1.65163
H	1.45908	2.12263	-2.13504
C	4.23192	-1.38744	0.23165
C	-1.21141	-2.04381	2.39393
C	1.52082	-4.10328	-1.24670
C	0.89556	2.69953	-1.41035
C	0.64708	4.05436	-1.62398
C	-0.04347	4.80101	-0.67308
C	-0.48294	4.19870	0.50154
C	-0.25396	2.84051	0.72976
C	0.41573	2.11680	-0.24571
C	-3.77996	1.68911	-0.16425
C	-3.70775	-1.59842	-0.77682
C	-1.84747	0.49637	-2.42912
O	2.53079	0.37662	-0.66884
O	-1.38057	-0.12882	0.52509
O	-3.21468	-0.33922	2.15376
O	4.71648	1.20294	0.07852
O	-0.97398	0.54040	2.89231
O	3.03033	0.38323	1.76560
O	0.96247	-2.04343	0.22961
O	-0.88510	-3.60485	-0.30680
O	0.03442	-2.08696	-2.05268
S	-1.76542	-0.38620	2.11078
S	3.65802	0.28733	0.45340
S	0.27578	-2.89127	-0.84876
Ge	-2.83205	0.12498	-0.80518
Au	0.65766	0.13286	-0.01134

Zero-point correction= 0.366289 (Hartree/Particle)
Thermal correction to Energy= 0.399747
Thermal correction to Enthalpy= 0.400691
Thermal correction to Gibbs Free Energy= 0.299019
Sum of electronic and zero-point Energies= -4552.008330
Sum of electronic and thermal Energies= -4551.974873
Sum of electronic and thermal Enthalpies= -4551.973928
Sum of electronic and thermal Free Energies= -4552.075601
E(RM06L) = -4555.23328047



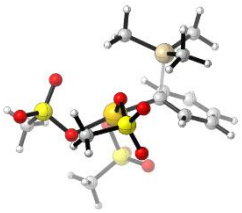
H	-2.60980	-1.38690	-3.24880
H	-2.31654	-2.24185	-1.69439
H	-3.99408	-1.99034	-2.28045
H	-2.13101	-0.84040	2.92362
H	-2.26928	-2.61215	3.20006
H	-1.11313	-1.64060	4.17471
H	-0.77891	4.10003	-1.15804
H	-2.09912	2.92073	-0.86693
H	-2.04796	4.46027	0.05771
H	1.65834	0.48109	-2.67822
H	0.19372	-1.28326	-3.56018
H	0.16478	-3.53391	-2.49923
H	1.60977	-3.98000	-0.52856
H	3.08453	-2.22494	0.34821
H	4.11763	2.96594	-1.01239
H	3.65399	2.06448	-2.46316
H	2.41961	2.55138	-1.27662
H	4.17294	1.46246	1.84167
H	2.42871	1.40076	1.55084
H	3.31150	-0.08300	1.94658
H	5.59709	-1.00399	-0.14328
H	5.66034	-0.23830	-1.73744
H	6.18421	0.65834	-0.30060
C	-2.98533	-1.57512	-2.24241
C	-1.59814	-1.75172	3.20338
C	-1.45442	3.67532	-0.41455
C	2.50782	-0.73037	-1.10507
C	1.67136	-0.49846	-2.20698
C	0.83390	-1.49704	-2.70914
C	0.81489	-2.75382	-2.11285
C	1.63223	-3.00792	-1.01165
C	2.46440	-2.00752	-0.51893
C	3.44607	2.18858	-1.39414
C	3.36953	0.86325	1.39739
C	5.44600	-0.05899	-0.67796
O	-1.54594	0.44890	-1.41401
O	0.50080	-0.75665	1.92237
O	0.39231	-3.25579	2.28848
O	-3.45385	-0.28253	0.00791
O	-1.03598	-1.99999	0.62535
O	-3.80449	0.94007	-2.16772
O	0.32309	1.78971	0.03676
O	-1.34895	2.24406	1.80811
O	0.53045	3.85569	1.31828
Si	3.69110	0.59003	-0.43554
S	-0.33120	-2.04826	1.99623
S	-3.06904	-0.02190	-1.37217
S	-0.46830	2.91411	0.85771
Au	-0.45602	-0.03436	0.19174

Zero-point correction= 0.365709 (Hartree/Particle)
Thermal correction to Energy= 0.399043
Thermal correction to Enthalpy= 0.399987
Thermal correction to Gibbs Free Energy= 0.297659
Sum of electronic and zero-point Energies= -2766.674712
Sum of electronic and thermal Energies= -2766.641377
Sum of electronic and thermal Enthalpies= -2766.640433
Sum of electronic and thermal Free Energies= -2766.742761
E(RM06L) = -2767.77648099



H	-3.70354	-1.25132	-2.49980
H	-2.94343	-2.14216	-1.13290
H	-4.70587	-1.79092	-1.11513
H	-2.25458	-1.23866	2.46439
H	-2.41499	-3.02191	2.35112
H	-1.41632	-2.30534	3.65858
H	-1.18128	4.15681	-1.18130
H	-2.32207	2.92011	-0.55440
H	-2.03791	4.43419	0.36909
H	1.62825	0.66687	-2.38284
H	0.58968	-1.12105	-3.73053
H	0.74694	-3.48648	-2.98560
H	1.89516	-4.03692	-0.85367
H	2.91527	-2.27060	0.49948
H	4.30668	2.87980	-0.53725
H	3.85045	1.99918	-2.00148
H	2.60008	2.72905	-0.96232
H	3.67221	1.59574	2.31600
H	1.96601	1.40260	1.89989
H	2.90906	-0.00506	2.38993
H	5.20040	-1.10652	0.65234
H	5.52863	-0.42246	-0.94818
H	5.93101	0.49713	0.51126
C	-3.72153	-1.43474	-1.42490
C	-1.75788	-2.19607	2.62771
C	-1.59227	3.68498	-0.28798
C	2.35966	-0.64756	-0.82137
C	1.67582	-0.36110	-2.03159
C	1.10360	-1.37574	-2.80900
C	1.19237	-2.69523	-2.39048
C	1.84845	-3.00811	-1.19428
C	2.41879	-2.00483	-0.42937
C	3.55789	2.20280	-0.96463
C	2.95030	0.93198	1.82563
C	5.19280	-0.18051	0.06638
O	-1.99825	0.52222	-1.16055
O	0.53623	-1.09037	1.90180
O	0.26660	-3.58676	1.65743
O	-3.32634	-0.16654	0.84608
O	-0.84530	-1.94733	0.14358
O	-4.34120	1.11031	-1.06418
O	0.32549	1.87405	-0.43752
O	-0.77944	2.18828	1.74285
O	0.79462	3.92001	0.80283
Si	3.48833	0.62938	0.05490
S	-0.32104	-2.26704	1.59056
S	-3.41215	0.10446	-0.58183
S	-0.24997	2.93401	0.60737
Au	-0.28219	-0.00408	-0.14314

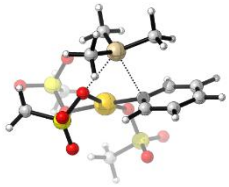
Zero-point correction= 0.365666 (Hartree/Particle)
Thermal correction to Energy= 0.398240
Thermal correction to Enthalpy= 0.399185
Thermal correction to Gibbs Free Energy= 0.300510
Sum of electronic and zero-point Energies= -2766.665027
Sum of electronic and thermal Energies= -2766.632453
Sum of electronic and thermal Enthalpies= -2766.631509
Sum of electronic and thermal Free Energies= -2766.730184
E(RM06L) = -2767.77499151



H	-2.28194	2.19765	-1.60905
H	-2.53100	3.64831	-0.58244
H	-1.87860	3.83150	-2.24195
H	-2.72441	-1.91993	-1.46727
H	-2.46437	-3.35451	-2.52943
H	-2.43241	-3.52783	-0.74189
H	-2.94858	2.09812	1.54218
H	-4.43907	1.70924	0.61062
H	-4.36794	1.37373	2.36911
H	1.71771	1.68037	1.74668
H	3.65517	2.97327	0.94047
H	4.01759	0.34513	-2.45309
H	2.03277	-0.92049	-1.69820
H	4.52996	-1.51548	2.67411
H	4.75332	-0.35848	1.35794
H	3.92118	0.13998	2.84451
H	1.96970	-3.23459	-0.13584
H	3.66804	-2.70191	-0.22008
H	3.09569	-3.63089	1.17060
H	1.52580	-2.10168	3.53863
H	0.86875	-0.49767	3.17917
H	0.20887	-1.91912	2.36025
H	4.80520	2.29222	-1.14468
C	-1.91226	3.19343	-1.35715
C	-2.20765	-2.87261	-1.58424
C	-3.79495	1.41623	1.44115
C	2.23433	1.37492	0.84261
C	3.32148	2.09705	0.39640
C	3.96206	1.71018	-0.78383
C	3.52770	0.60829	-1.52228
C	2.42450	-0.10732	-1.09380
C	1.77943	0.21070	0.14215
C	4.05617	-0.68397	2.13766
C	2.81198	-2.85622	0.44589
C	1.12930	-1.46534	2.73718
O	-0.43846	2.02624	0.46667
O	-0.17462	-1.95834	-0.17000
O	0.24221	-3.84760	-1.64119
O	0.16186	4.30604	-0.15041
O	-0.14550	-1.56621	-2.61586

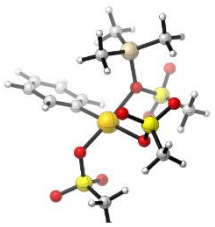
O	0.57392	2.42967	-1.77043
O	-2.36240	0.01267	-0.21738
O	-4.25234	-1.12287	0.87077
O	-2.19445	-0.52736	2.18596
Si	2.43810	-1.30804	1.41509
S	-0.45588	-2.57214	-1.60204
S	-0.24919	3.04124	-0.73300
S	-3.14527	-0.21388	1.11610
Au	-0.28486	0.04876	0.04691

Zero-point correction= 0.367061 (Hartree/Particle)
Thermal correction to Energy= 0.399821
Thermal correction to Enthalpy= 0.400765
Thermal correction to Gibbs Free Energy= 0.301763
Sum of electronic and zero-point Energies= -2766.690405
Sum of electronic and thermal Energies= -2766.657645
Sum of electronic and thermal Enthalpies= -2766.656701
Sum of electronic and thermal Free Energies= -2766.755703
E(RM06L) = -2767.79575700



H	3.20374	0.71641	1.53014
H	4.25565	1.64546	0.41254
H	3.91548	2.28115	2.05314
H	1.07333	-3.21793	1.02083
H	0.20630	-4.10588	2.32291
H	-0.43939	-4.11406	0.64957
H	3.59635	0.17464	-1.68701
H	4.65934	-0.94793	-0.76634
H	4.31829	-1.25506	-2.49850
H	-0.43424	2.61831	-1.58121
H	-2.28966	4.24059	-1.45968
H	-4.13607	1.93445	1.65949
H	-2.27873	0.32892	1.58018
H	-4.57570	0.04478	-2.68042
H	-4.94705	0.68428	-1.06620
H	-3.70468	1.45986	-2.07742
H	-3.17819	-3.03348	-0.29493
H	-4.02342	-1.87669	0.71959
H	-4.70741	-2.29603	-0.86784
H	-2.20046	-1.59547	-3.29096
H	-1.26238	-0.14046	-2.92976
H	-0.79165	-1.68670	-2.20437
H	-4.13303	3.92206	0.17162
C	3.51596	1.71270	1.21136
C	0.09994	-3.53371	1.39915
C	3.91834	-0.86112	-1.56264
C	-1.26382	2.44602	-0.90461
C	-2.30105	3.36336	-0.82009
C	-3.34004	3.18432	0.10097
C	-3.34645	2.07476	0.92802
C	-2.31064	1.13072	0.85129
C	-1.26031	1.33031	-0.05896
C	-4.14062	0.50433	-1.78009
C	-3.77490	-2.12027	-0.31584
C	-1.64387	-1.07106	-2.49905
O	1.56776	1.62396	-0.54853
O	-0.99970	-1.38414	0.35028
O	-2.19510	-2.49003	2.19624
O	2.54681	3.80151	-0.08169
O	-0.09272	-1.20545	2.65437
O	1.11070	2.68642	1.65940
O	2.02872	-1.15994	0.20317
O	2.90437	-3.19638	-0.84705
O	1.47558	-1.61051	-2.15833
Si	-2.89041	-0.73692	-1.17211
S	-0.85721	-2.08913	1.79019
S	2.09582	2.59761	0.59111
S	2.48742	-1.82686	-1.11377
Au	0.34223	0.12840	0.00878

Zero-point correction= 0.366755 (Hartree/Particle)
Thermal correction to Energy= 0.398905
Thermal correction to Enthalpy= 0.399849
Thermal correction to Gibbs Free Energy= 0.301974
Sum of electronic and zero-point Energies= -2766.677484
Sum of electronic and thermal Energies= -2766.645334
Sum of electronic and thermal Enthalpies= -2766.644390
Sum of electronic and thermal Free Energies= -2766.742265
E(RM06L) = -2767.78648999

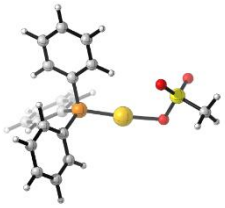


H	2.98101	-2.21426	0.65702
H	4.30350	-1.83581	-0.50401
H	4.63535	-1.83932	1.25928
H	-0.89402	-2.23975	1.98924
H	-2.28267	-2.18343	3.14964
H	-2.55729	-2.43779	1.38040
H	2.03482	-4.09181	-1.03483
H	0.88754	-4.85530	0.11707
H	0.64466	-5.03981	-1.64851
H	1.38267	1.98340	-2.23324
H	1.12485	4.41351	-2.64736
H	0.07980	5.86495	-0.92576
H	-0.70149	4.88244	1.21592
H	-0.47861	2.45087	1.62582
H	-4.22479	2.30729	-1.41655
H	-4.16079	2.00775	0.33546
H	-2.77409	2.74434	-0.49891
H	-4.73870	-1.06181	-1.69338
H	-3.46391	-2.05289	-0.95969

H	-4.60299	-1.13341	0.07171
H	-2.56593	0.32819	-3.35209
H	-1.23212	1.21534	-2.60364
H	-1.22909	-0.57105	-2.61988
C	3.89149	-1.63720	0.48634
C	-1.93728	-1.95908	2.13807
C	0.99673	-4.37627	-0.85693
C	0.89792	2.61606	-1.49751
C	0.75979	3.98528	-1.71902
C	0.17633	4.79799	-0.75047
C	-0.26536	4.24912	0.44957
C	-0.14628	2.87855	0.68642
C	0.41448	2.09175	-0.30786
C	-3.57535	2.00198	-0.58709
C	-4.02915	-1.11897	-0.85920
C	-1.85658	0.32107	-2.51370
O	2.40008	0.21179	-0.59857
O	-1.62745	0.01520	0.36357
O	-3.43730	0.22681	2.05948
O	4.61435	0.88582	0.20161
O	-1.01757	0.44562	2.73165
O	2.79375	0.32700	1.85566
O	0.57141	-2.08476	0.27381
O	-1.39253	-3.29649	-0.61945
O	0.23803	-2.22333	-2.16884
Si	-2.85712	0.32232	-0.94739
S	-2.05807	-0.20159	1.96425
S	3.46415	0.09231	0.58374
S	-0.00647	-2.90287	-0.89379
Au	0.48526	0.09971	-0.04646

Zero-point correction= 0.367012 (Hartree/Particle)
Thermal correction to Energy= 0.399978
Thermal correction to Enthalpy= 0.400923
Thermal correction to Gibbs Free Energy= 0.300710
Sum of electronic and zero-point Energies= -2766.739062
Sum of electronic and thermal Energies= -2766.706096
Sum of electronic and thermal Enthalpies= -2766.705151
Sum of electronic and thermal Free Energies= -2766.805364
E(RM06L) = -2767.84006887

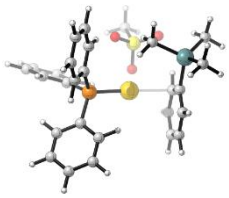
Bond Activation with Au(I)



H	2.75358	0.01769	-2.45291
H	1.15648	-2.84939	0.33111
H	3.90466	-1.80319	-3.65959
H	2.32254	-4.66451	-0.87297
H	3.69847	-4.14616	-2.87346
H	-0.94806	1.36718	-1.66770
H	3.16028	1.99405	-0.49381
H	-0.84557	3.38575	-3.06369
H	3.24380	4.02163	-1.90174
H	1.24370	4.72189	-3.19276
H	0.55287	1.32406	2.50741
H	3.87734	-0.64482	0.60930
H	1.98181	1.85449	4.45198
H	5.29791	-0.11674	2.56063
H	4.35700	1.13365	4.48461
H	-5.84677	-1.37491	0.41244
H	-6.08661	-0.37618	-1.05498
H	-4.95496	-1.76621	-1.09488
C	1.89146	-1.29352	-0.97225
C	2.66360	-1.00449	-2.09905
C	1.76915	-2.61810	-0.53689
C	3.31138	-2.03252	-2.77984
C	2.42302	-3.63937	-1.21528
C	3.19448	-3.34695	-2.33857
C	1.11388	1.52733	-1.00800
C	-0.01719	1.92751	-1.72871
C	2.28723	2.28861	-1.06977
C	0.03752	3.07544	-2.51475
C	2.33325	3.43191	-1.85891
C	1.20847	3.82414	-2.58284
C	2.12473	0.31460	1.42600
C	1.59523	1.01511	2.51504
C	3.46139	-0.09175	1.44629
C	2.39911	1.31247	3.60929
C	4.26108	0.20497	2.54684
C	3.73205	0.90671	3.62624
C	-5.37107	-0.96699	-0.48036
O	-3.14467	-0.85946	0.81397
O	-4.60891	1.14773	0.88662
O	-3.35438	0.56558	-1.19590
P	1.04734	0.00511	-0.01111
S	-4.04457	0.11804	0.02330
Au	-1.10778	-0.50487	0.49140

Zero-point correction= 0.332574 (Hartree/Particle)
Thermal correction to Energy= 0.356946
Thermal correction to Enthalpy= 0.357890
Thermal correction to Gibbs Free Energy= 0.271766

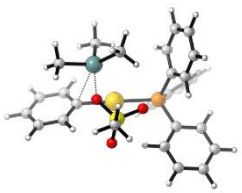
Sum of electronic and zero-point Energies= -1834.846443
Sum of electronic and thermal Energies= -1834.822071
Sum of electronic and thermal Enthalpies= -1834.821127
Sum of electronic and thermal Free Energies= -1834.907251
E(RM06L) = -1835.72401779



H	-1.78391	2.04524	-1.59110
H	-4.26228	0.47422	1.56183
H	-3.35515	3.92573	-1.87747
H	-5.81897	2.37313	1.28205
H	-5.37327	4.09940	-0.44444
H	-4.67594	-0.98318	-0.46812
H	-0.81465	-2.86461	-0.71368
H	-5.73410	-3.05336	-1.28984
H	-1.88448	-4.94641	-1.50975
H	-4.34808	-5.04502	-1.80549
H	-0.71321	1.33416	2.19668
H	-2.65920	-2.50650	1.99086
H	-0.53000	1.09642	4.65261
H	-2.45058	-2.74264	4.44164
H	-1.39089	-0.94306	5.77984
H	2.71556	0.94040	-1.33218
H	3.07887	-3.26426	-0.46774
H	1.63911	0.40016	-3.48514
H	2.13063	-3.79737	-2.67445
H	1.35540	-1.98545	-4.18299
H	5.00150	-2.05668	2.73608
H	3.75065	-3.05139	1.97775
H	5.25012	-2.68276	1.09718
H	4.45282	1.66595	0.43718
H	5.49728	1.00820	1.71514
H	5.72686	0.48085	0.03438
H	1.79136	0.87523	1.80904
H	1.42681	-0.80742	2.25943
H	2.56755	0.14573	3.23054
H	1.10132	5.37028	0.27073
H	1.32751	5.16165	-1.49424
H	-0.30511	4.98950	-0.77091
C	-2.95689	1.09994	-0.04153
C	-2.69240	2.08509	-0.99607
C	-4.07924	1.21496	0.78764
C	-3.56784	3.15845	-1.13940
C	-4.95014	2.28752	0.63656
C	-4.69658	3.25739	-0.33189
C	-2.67564	-1.79093	-0.51456
C	-4.06073	-1.85025	-0.68570
C	-1.89604	-2.91270	-0.82220
C	-4.65777	-3.01880	-1.15167
C	-2.49728	-4.08130	-1.27557

C	-3.87947	-4.13539	-1.44199
C	-1.71182	-0.56654	1.94248
C	-1.11055	0.45111	2.69397
C	-2.19401	-1.71556	2.57145
C	-1.00246	0.31004	4.07233
C	-2.07650	-1.84772	3.95334
C	-1.48295	-0.83649	4.70288
C	2.90720	-1.12979	-0.68600
C	2.49851	-0.10083	-1.57157
C	2.75876	-2.45159	-1.11497
C	1.92485	-0.41156	-2.82235
C	2.21882	-2.75918	-2.36624
C	1.78539	-1.74711	-3.21526
C	4.50277	-2.27851	1.78737
C	4.98018	0.77038	0.78006
C	2.21639	-0.05053	2.21211
C	0.76458	4.83477	-0.61855
O	0.56774	2.44360	-1.63557
O	2.50033	2.91158	-0.16881
O	0.22343	2.70591	0.79740
P	-1.82471	-0.31285	0.14104
S	1.05017	3.08608	-0.36887
Ge	3.67580	-0.65309	1.06451
Au	0.22382	0.01722	-0.85640

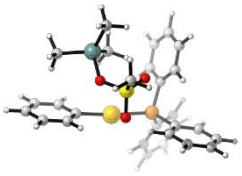
Zero-point correction= 0.538366 (Hartree/Particle)
Thermal correction to Energy= 0.576884
Thermal correction to Enthalpy= 0.577828
Thermal correction to Gibbs Free Energy= 0.461391
Sum of electronic and zero-point Energies= -4260.714658
Sum of electronic and thermal Energies= -4260.676140
Sum of electronic and thermal Enthalpies= -4260.675195
Sum of electronic and thermal Free Energies= -4260.791632
E(RM06L) = -4264.09226695



H	0.84239	-1.38919	-2.35644
H	4.62061	-0.38613	-0.53052
H	2.02535	-2.71706	-4.04993
H	5.79198	-1.75439	-2.21391
H	4.50130	-2.91939	-3.98620
H	4.18925	1.19887	1.39161
H	1.41258	2.71580	-1.52451
H	5.44672	3.31761	1.28970
H	2.67417	4.83223	-1.62095
H	4.69565	5.14422	-0.21280
H	2.54386	-2.48449	0.75591
H	1.63343	1.29466	2.59398
H	2.81134	-3.50001	2.99355
H	1.88229	0.27318	4.82632
H	2.47439	-2.13062	5.03397
H	-3.01541	-0.56168	-1.90822
H	-2.27592	3.19591	0.04808
H	-5.18618	0.29752	-2.71378
H	-4.44562	4.04116	-0.74328
H	-5.92580	2.58911	-2.11130
H	-1.97879	1.43428	3.56282
H	-0.70356	1.86154	2.40449
H	-2.38004	2.39708	2.12055
H	-4.42849	-1.10834	0.94423
H	-4.48219	-0.38206	2.57724
H	-4.54080	0.66328	1.13362
H	-0.34724	-1.83996	2.07846
H	-0.89510	-1.07156	3.59604
H	-1.88197	-2.34111	2.79613
H	-1.87363	-4.67476	0.31578
H	-2.84026	-4.36584	-1.16276
H	-1.14991	-4.94346	-1.30166
C	2.65355	-0.78461	-1.33537
C	1.92687	-1.44069	-2.33101
C	4.04858	-0.89951	-1.29819
C	2.59796	-2.20577	-3.28263
C	4.71011	-1.66770	-2.24740
C	3.98311	-2.32057	-3.24269
C	2.71957	1.80444	-0.06838
C	3.85929	1.98748	0.72160
C	2.30047	2.84094	-0.90907
C	4.56584	3.18508	0.66876
C	3.01090	4.03580	-0.96456
C	4.14406	4.20967	-0.17465
C	2.09788	-0.52502	1.52749
C	2.42765	-1.87531	1.64508
C	1.89541	0.24316	2.67963
C	2.56283	-2.44679	2.90771
C	2.03752	-0.33044	3.93716
C	2.37026	-1.67890	4.05194
C	-2.48595	1.24457	-0.86095
C	-3.32382	0.44606	-1.65306
C	-2.90945	2.54652	-0.55013
C	-4.54898	0.93181	-2.10359
C	-4.13622	3.03070	-0.99698
C	-4.96357	2.21824	-1.76889
C	-1.75675	1.58513	2.49778
C	-4.12113	-0.25601	1.54883
C	-1.21626	-1.48882	2.63693
C	-1.84352	-4.33348	-0.72024
O	-1.25816	-2.21398	-2.15620
O	-2.29189	-1.90810	0.06484
O	0.06827	-2.64827	-0.10436
P	1.78113	0.23039	-0.10022
S	-1.25880	-2.64364	-0.74785
Ge	-2.18325	-0.13526	1.62142
Au	-0.55303	0.66217	-0.46542

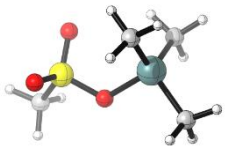
Zero-point correction= 0.537710 (Hartree/Particle)
Thermal correction to Energy= 0.575371
Thermal correction to Enthalpy= 0.576315
Thermal correction to Gibbs Free Energy= 0.464820

Sum of electronic and zero-point Energies= -4260.681704
Sum of electronic and thermal Energies= -4260.644043
Sum of electronic and thermal Enthalpies= -4260.643099
Sum of electronic and thermal Free Energies= -4260.754595
E(RM06L) = -4264.07124623



H	0.80022	-1.09107	-2.31565
H	4.59035	-1.55527	-0.31938
H	1.47109	-2.77847	-3.97333
H	5.25228	-3.25290	-1.98153
H	3.69930	-3.87298	-3.81523
H	4.46720	-0.21630	1.83331
H	2.91161	2.54851	-1.06998
H	6.45917	1.21266	2.12522
H	4.90984	3.97511	-0.77713
H	6.68859	3.31194	0.82230
H	1.62310	-2.84259	0.61753
H	1.94287	0.84901	2.80007
H	1.07810	-4.02828	2.71222
H	1.40576	-0.34206	4.89473
H	0.96690	-2.78707	4.85813
H	-2.29991	1.23010	-2.38899
H	-1.32763	3.58301	1.07562
H	-4.40107	2.47831	-2.64006
H	-3.43846	4.81262	0.83206
H	-4.99481	4.27758	-1.03104
H	-1.91101	-0.55212	3.24894
H	-0.90099	-0.96061	1.84510
H	-1.47233	0.71282	2.06825
H	-5.44736	0.35669	0.37583
H	-5.13508	0.74604	2.08422
H	-4.20479	1.55578	0.79819
H	-3.22769	-3.28063	1.59886
H	-4.35209	-2.51342	2.73440
H	-4.86987	-2.81952	1.06614
H	-3.46451	-3.75547	-0.90213
H	-3.77172	-2.93005	-2.46766
H	-2.38687	-4.05511	-2.30104
C	2.64885	-1.20894	-1.20396
C	1.77900	-1.55428	-2.23998
C	3.90277	-1.82524	-1.11566
C	2.15799	-2.51519	-3.17504
C	4.27724	-2.78012	-2.05263
C	3.40343	-3.12676	-3.08341
C	3.56468	1.05939	0.34480
C	4.56767	0.69406	1.24899
C	3.69567	2.24884	-0.37913
C	5.68736	1.50245	1.41843
C	4.81885	3.05302	-0.21138
C	5.81534	2.68073	0.68688
C	1.85360	-0.92534	1.57374
C	1.60061	-2.29727	1.55479
C	1.77183	-0.22434	2.78301
C	1.28144	-2.96208	2.73687
C	1.46329	-0.89314	3.96088
C	1.21597	-2.26507	3.93887
C	-1.62461	2.30661	-0.64434
C	-2.52789	2.02440	-1.68393
C	-1.99051	3.32569	0.25189
C	-3.72498	2.72415	-1.82457
C	-3.18821	4.02954	0.11998
C	-4.06105	3.73174	-0.92324
C	-1.73151	-0.34086	2.18888
C	-4.67148	0.61467	1.10087
C	-4.01964	-2.53105	1.69125
C	-3.00864	-3.31705	-1.79113
O	-1.42767	-1.36130	-2.51459
O	-2.97094	-0.97850	-0.65397
O	-1.01485	-2.46367	-0.29584
P	2.09555	0.01724	0.02715
S	-1.95112	-1.96538	-1.29959
Ge	-3.32947	-0.77660	1.18684
Au	0.11687	1.25416	-0.42932

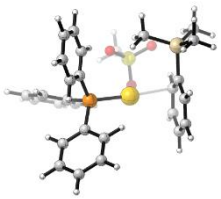
Zero-point correction= 0.537908 (Hartree/Particle)
Thermal correction to Energy= 0.576480
Thermal correction to Enthalpy= 0.577424
Thermal correction to Gibbs Free Energy= 0.461971
Sum of electronic and zero-point Energies= -4260.722862
Sum of electronic and thermal Energies= -4260.684290
Sum of electronic and thermal Enthalpies= -4260.683346
Sum of electronic and thermal Free Energies= -4260.798799
E(RM06L) = -4264.10023022



H	2.20962	2.09156	-1.03382
H	0.56783	1.76466	-1.64676
H	3.41687	-0.02210	1.35398
H	2.24103	-1.14499	2.06685
H	1.52195	-2.41743	-0.78933
H	0.77988	-1.39456	-2.04429
H	2.07350	0.60416	2.33430
H	0.78552	2.47116	-0.03389
H	2.53714	-1.32547	-1.75500
H	-3.86528	-0.85297	0.20410
H	-2.56607	-2.07617	0.37896
H	-2.93392	-0.95063	1.73137
C	1.20194	1.76528	-0.75707
C	2.36093	-0.16006	1.60760
C	1.55802	-1.44032	-1.27885
C	-2.89246	-1.07117	0.64826
O	-1.55912	-0.14694	-1.44040
O	-0.43173	-0.34950	0.75284

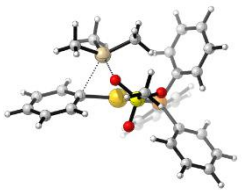
O	-2.12012	1.43930	0.41502
S	-1.73259	0.10693	-0.01425
Ge	1.26470	-0.01760	0.01007

Zero-point correction= 0.165534 (Hartree/Particle)
Thermal correction to Energy= 0.179361
Thermal correction to Enthalpy= 0.180305
Thermal correction to Gibbs Free Energy= 0.124267
Sum of electronic and zero-point Energies= -2857.968049
Sum of electronic and thermal Energies= -2857.954222
Sum of electronic and thermal Enthalpies= -2857.953278
Sum of electronic and thermal Free Energies= -2858.009316
E(RM06L) = -2860.50716276



H	-1.39158	2.05221	-1.66743
H	-4.09312	0.73436	1.41793
H	-2.81259	4.03114	-2.05475
H	-5.49724	2.73214	1.03880
H	-4.86455	4.38203	-0.70372
H	-4.51949	-0.72659	-0.64197
H	-0.79695	-2.88279	-0.67073
H	-5.68094	-2.72546	-1.50225
H	-1.97165	-4.89178	-1.50634
H	-4.41729	-4.81675	-1.92983
H	-0.51480	1.30864	2.20935
H	-2.78460	-2.34424	1.92765
H	-0.47561	1.08073	4.67311
H	-2.72385	-2.57099	4.38786
H	-1.57365	-0.86030	5.76725
H	3.02634	0.72993	-1.09227
H	3.16896	-3.46743	-0.11175
H	2.03302	0.17965	-3.27706
H	2.30271	-4.01344	-2.34688
H	1.67381	-2.20921	-3.93018
H	4.93442	-2.17242	3.09227
H	3.71650	-3.17466	2.29882
H	5.27037	-2.86416	1.49897
H	4.62320	1.37524	0.70725
H	5.54410	0.71551	2.06912
H	5.87672	0.14084	0.42478
H	1.96177	0.73355	1.93626
H	1.52180	-0.91677	2.41961
H	2.67201	0.01680	3.39350
H	1.42045	5.24970	0.30785
H	1.66048	5.05250	-1.45667
H	0.02812	4.84063	-0.74210
C	-2.68509	1.22965	-0.14368
C	-2.31608	2.17047	-1.10849
C	-3.82727	1.44261	0.63741
C	-3.10645	3.29935	-1.30848
C	-4.61282	2.57050	0.43009
C	-4.25446	3.49722	-0.54731
C	-2.58333	-1.67652	-0.57873
C	-3.95845	-1.63816	-0.82121
C	-1.87180	-2.85462	-0.83613
C	-4.61342	-2.76629	-1.30856
C	-2.53154	-3.98225	-1.31133
C	-3.90363	-3.93895	-1.54935
C	-1.66356	-0.49891	1.91602
C	-1.01206	0.46887	2.69112
C	-2.27992	-1.59230	2.52682
C	-0.98696	0.33368	4.07413
C	-2.24559	-1.71913	3.91374
C	-1.60098	-0.75772	4.68634
C	3.09635	-1.33147	-0.38077
C	2.77361	-0.30792	-1.31156
C	2.91378	-2.65648	-0.78935
C	2.24558	-0.62582	-2.57990
C	2.41913	-2.97244	-2.05830
C	2.06760	-1.96566	-2.94843
C	4.48756	-2.41566	2.12133
C	5.08224	0.46332	1.10713
C	2.34839	-0.19836	2.36780
C	1.10049	4.70998	-0.58506
O	0.96142	2.31788	-1.61140
O	2.87295	2.82020	-0.12730
O	0.59196	2.56562	0.81788
Si	3.77006	-0.85809	1.33431
P	-1.66438	-0.25568	0.10957
S	1.42243	2.96683	-0.34087
Au	0.45330	-0.07204	-0.77559

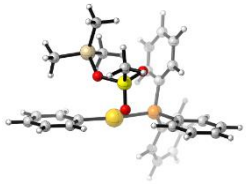
Zero-point correction= 0.539159 (Hartree/Particle)
Thermal correction to Energy= 0.577175
Thermal correction to Enthalpy= 0.578120
Thermal correction to Gibbs Free Energy= 0.463191
Sum of electronic and zero-point Energies= -2475.443613
Sum of electronic and thermal Energies= -2475.405597
Sum of electronic and thermal Enthalpies= -2475.404653
Sum of electronic and thermal Free Energies= -2475.519582
E(RM06L) = -2476.69856075



H	0.59520	-1.43714	-2.25262
H	4.49496	-0.44446	-0.69356
H	1.64999	-2.82496	-3.97974
H	5.53881	-1.87040	-2.41330
H	4.12249	-3.06124	-4.06842
H	4.18119	1.14954	1.28235
H	1.31540	2.68422	-1.53591
H	5.47688	3.24154	1.09768

H	2.61552	4.77409	-1.71615
H	4.70027	5.06201	-0.39873
H	2.45933	-2.50679	0.75330
H	1.63937	1.29375	2.59180
H	2.77913	-3.51158	2.98940
H	1.95496	0.28534	4.82321
H	2.52536	-2.12313	5.02847
H	-3.19664	-0.57666	-1.63141
H	-2.32126	3.14244	0.34231
H	-5.22067	0.43325	-2.61385
H	-4.33850	4.14446	-0.63917
H	-5.81962	2.78617	-2.09951
H	-2.19597	1.34369	3.65858
H	-1.06644	1.98848	2.46327
H	-2.80086	2.36013	2.34218
H	-4.57731	-1.15779	1.19907
H	-4.49259	-0.41794	2.81851
H	-4.74763	0.60438	1.39099
H	-0.47380	-1.66073	2.09885
H	-0.95042	-0.78977	3.57644
H	-1.95046	-2.12180	2.92927
H	-2.14117	-4.55390	0.64041
H	-3.15830	-4.27879	-0.81081
H	-1.50501	-4.94748	-0.98865
C	2.47565	-0.83553	-1.36126
C	1.67823	-1.50494	-2.29193
C	3.86878	-0.96898	-1.40981
C	2.27727	-2.30325	-3.26399
C	4.45821	-1.76951	-2.37957
C	3.66059	-2.43673	-3.30914
C	2.66657	1.76742	-0.12506
C	3.84107	1.93622	0.61507
C	2.23177	2.80035	-0.96190
C	4.56863	3.11829	0.51554
C	2.96336	3.97911	-1.06383
C	4.13229	4.13954	-0.32442
C	2.06718	-0.53586	1.52622
C	2.37973	-1.88993	1.64143
C	1.90556	0.24311	2.67765
C	2.54485	-2.45513	2.90336
C	2.07952	-0.32429	3.93343
C	2.39874	-1.67637	4.04685
C	-2.61741	1.19173	-0.54485
C	-3.44653	0.45244	-1.40408
C	-2.95542	2.53456	-0.29546
C	-4.58817	1.02527	-1.95848
C	-4.09518	3.10672	-0.84968
C	-4.92156	2.34614	-1.67458
C	-2.07649	1.58127	2.59214
C	-4.23246	-0.28820	1.75893
C	-1.32107	-1.26510	2.66250
C	-2.14212	-4.27296	-0.41392
O	-1.52462	-2.25834	-1.98683
O	-2.45346	-1.79825	0.25118
O	-0.12831	-2.65242	0.02576
Si	-2.37206	-0.06096	1.65708
P	1.70013	0.21334	-0.09202
S	-1.47919	-2.61972	-0.56086
Au	-0.62882	0.63367	-0.28857

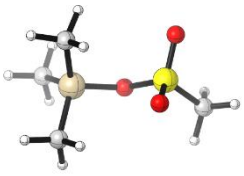
Zero-point correction= 0.539317 (Hartree/Particle)
Thermal correction to Energy= 0.576221
Thermal correction to Enthalpy= 0.577165
Thermal correction to Gibbs Free Energy= 0.467604
Sum of electronic and zero-point Energies= -2475.401364
Sum of electronic and thermal Energies= -2475.364460
Sum of electronic and thermal Enthalpies= -2475.363516
Sum of electronic and thermal Free Energies= -2475.473077
E(RM06L) = -2476.66465502



H	0.57188	-1.10839	-2.28347
H	4.42731	-1.46991	-0.39709
H	1.23417	-2.79305	-3.95085
H	5.08056	-3.16491	-2.06610
H	3.48998	-3.83413	-3.84965
H	4.35612	-0.06559	1.73180
H	2.61102	2.57390	-1.18044
H	6.31364	1.42845	1.91084
H	4.57461	4.06567	-1.00049
H	6.43107	3.49761	0.54651
H	1.63263	-2.82314	0.68033
H	1.78735	0.93750	2.76027
H	1.23563	-3.98545	2.82117
H	1.39923	-0.22971	4.90089
H	1.11780	-2.69766	4.93888
H	-2.60534	1.04806	-2.25048
H	-1.58508	3.54256	1.09939
H	-4.77126	2.19320	-2.43632
H	-3.75864	4.66915	0.92124
H	-5.37314	4.00952	-0.84987
H	-2.04011	-0.56601	3.39353
H	-1.01321	-1.11452	2.05525
H	-1.57737	0.56697	2.10392
H	-5.57074	0.04759	0.76258
H	-5.07238	0.52150	2.39922
H	-4.32055	1.28476	0.98256
H	-3.20514	-3.38548	1.89648
H	-4.29975	-2.57395	3.02076
H	-4.86713	-2.98020	1.39571
H	-3.50545	-3.94139	-0.55549
H	-3.97992	-3.10633	-2.07481
H	-2.55954	-4.19895	-2.05505
C	2.45343	-1.17629	-1.22619
C	1.56234	-1.54979	-2.23409
C	3.72361	-1.76229	-1.17115
C	1.93655	-2.50790	-3.17381
C	4.09307	-2.71548	-2.11188

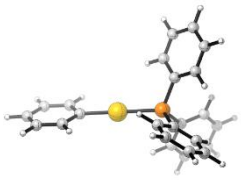
C	3.19814	-3.08981	-3.11433
C	3.36121	1.14279	0.24608
C	4.40735	0.83127	1.12081
C	3.42903	2.31581	-0.51253
C	5.50770	1.67640	1.22657
C	4.53274	3.15670	-0.40833
C	5.57282	2.83780	0.46061
C	1.76965	-0.87054	1.58102
C	1.60512	-2.25558	1.60413
C	1.68473	-0.14466	2.77532
C	1.37035	-2.90816	2.81266
C	1.46067	-0.80041	3.97921
C	1.30156	-2.18536	3.99905
C	-1.90170	2.20401	-0.56886
C	-2.83707	1.85199	-1.55740
C	-2.27172	3.23275	0.31425
C	-4.07035	2.49295	-1.66073
C	-3.50524	3.87784	0.21949
C	-4.41091	3.51000	-0.77197
C	-1.85726	-0.46901	2.31600
C	-4.71479	0.34257	1.37804
C	-3.99937	-2.63313	1.96800
C	-3.14793	-3.48285	-1.47845
O	-1.69568	-1.47500	-2.32375
O	-3.06994	-1.15318	-0.32621
O	-1.04391	-2.58402	-0.16516
Si	-3.38616	-0.95978	1.37454
P	1.91289	0.05068	0.01001
S	-2.07711	-2.11403	-1.07751
Au	-0.11719	1.21926	-0.39333

Zero-point correction= 0.538607 (Hartree/Particle)
Thermal correction to Energy= 0.575898
Thermal correction to Enthalpy= 0.576842
Thermal correction to Gibbs Free Energy= 0.464909
Sum of electronic and zero-point Energies= -2475.460004
Sum of electronic and thermal Energies= -2475.422713
Sum of electronic and thermal Enthalpies= -2475.421768
Sum of electronic and thermal Free Energies= -2475.533702
E(RM06L) = -2476.71311568



H	-2.51558	2.08225	0.68907
H	-0.85759	1.95600	1.30859
H	-3.59472	-0.24803	-1.27993
H	-2.42626	-1.46160	-1.82637
H	-1.80024	-2.21241	1.12771
H	-1.08825	-0.99939	2.20956
H	-2.27155	0.22102	-2.36266
H	-1.13351	2.39630	-0.38212
H	-2.82337	-0.94878	1.83368
H	3.58139	-0.89707	-0.20435
H	2.26534	-2.11321	-0.13808
H	2.55324	-1.17512	-1.64526
C	-1.49527	1.76871	0.43861
C	-2.53733	-0.41781	-1.51417
C	-1.82973	-1.15720	1.41996
C	2.58092	-1.15650	-0.55528
O	1.38200	0.04657	1.47269
O	0.12345	-0.43286	-0.61264
O	1.82843	1.37177	-0.60893
Si	-1.46588	-0.03870	-0.03131
S	1.47818	0.11468	0.02280

Zero-point correction= 0.166500 (Hartree/Particle)
Thermal correction to Energy= 0.179839
Thermal correction to Enthalpy= 0.180783
Thermal correction to Gibbs Free Energy= 0.126253
Sum of electronic and zero-point Energies= -1072.706871
Sum of electronic and thermal Energies= -1072.693532
Sum of electronic and thermal Enthalpies= -1072.692588
Sum of electronic and thermal Free Energies= -1072.747117
E(RM06L) = -1073.12045110

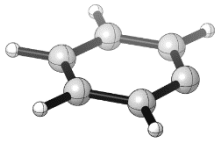


H	-3.41388	0.98596	-1.53243
H	-0.26302	2.60831	0.90590
H	-4.35813	3.25122	-1.81333
H	-1.22047	4.87121	0.63323
H	-3.26920	5.19883	-0.73000
H	-0.20070	-0.60782	-2.68002
H	-3.47462	-1.73975	-0.12876
H	-1.15796	-1.96894	-4.50782
H	-4.41902	-3.10964	-1.95419
H	-3.26845	-3.22595	-4.14874
H	-0.21142	-2.00217	1.89467
H	-3.49582	0.75203	1.53211
H	-1.19103	-2.89193	3.98271
H	-4.46342	-0.13135	3.62663
H	-3.31847	-1.95688	4.85542
H	3.59018	-2.15074	0.06277
H	3.59174	2.14998	-0.05958
H	6.04291	-2.14637	0.06204
H	6.04441	2.14379	-0.06024
H	7.29587	-0.00172	0.00084
C	-1.78365	1.64458	-0.28232
C	-2.93465	1.83365	-1.05173
C	-1.16797	2.74773	0.31957
C	-3.46613	3.11085	-1.21028
C	-1.70512	4.02076	0.16384
C	-2.85437	4.20348	-0.60213
C	-1.78293	-1.06940	-1.28818

C	-1.13284	-1.14546	-2.52502
C	-2.96853	-1.78221	-1.08869
C	-1.66993	-1.91405	-3.55215
C	-3.50003	-2.55485	-2.11754
C	-2.85349	-2.61978	-3.34903
C	-1.79797	-0.57901	1.56468
C	-1.15133	-1.60200	2.26649
C	-2.99289	-0.05135	2.06247
C	-1.70074	-2.09978	3.44317
C	-3.53719	-0.54866	3.24327
C	-2.89378	-1.57333	3.93254
C	3.37486	-0.00025	0.00324
C	4.11132	-1.19637	0.03642
C	4.11217	1.19527	-0.03168
C	5.50503	-1.20163	0.03579
C	5.50583	1.19948	-0.03265
C	6.20900	-0.00134	0.00139
P	-1.04869	-0.00369	0.00117
Au	1.33345	-0.00089	0.00497

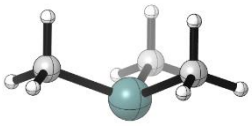
Zero-point correction= 0.370558 (Hartree/Particle)
Thermal correction to Energy= 0.393989
Thermal correction to Enthalpy= 0.394933
Thermal correction to Gibbs Free Energy= 0.310555
Sum of electronic and zero-point Energies= -1402.726776
Sum of electronic and thermal Energies= -1402.703345
Sum of electronic and thermal Enthalpies= -1402.702401
Sum of electronic and thermal Free Energies= -1402.786779
E(RM06L) = -1403.57402539

Bond Dissociation Energies



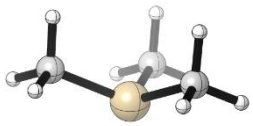
H	2.15056	1.17724	0.00003
H	2.15945	-1.32086	0.00001
H	-2.15942	-1.32091	0.00003
H	-2.15055	1.17723	-0.00001
H	-0.00002	2.40728	0.00003
C	1.21115	0.63074	0.00001
C	1.22396	-0.76928	-0.00003
C	0.00001	-1.39775	0.00001
C	-1.22396	-0.76926	0.00001
C	-1.21117	0.63072	-0.00002
C	0.00001	1.32150	0.00001

Zero-point correction= 0.088670 (Hartree/Particle)
Thermal correction to Energy= 0.092995
Thermal correction to Enthalpy= 0.093939
Thermal correction to Gibbs Free Energy= 0.060651
Sum of electronic and zero-point Energies= -231.382847
Sum of electronic and thermal Energies= -231.378523
Sum of electronic and thermal Enthalpies= -231.377578
Sum of electronic and thermal Free Energies= -231.410867
E(UM06L) = -231.585604085



H	1.68524	-0.76833	1.43540
H	1.81183	-1.80172	-0.00389
H	2.54821	-0.18612	-0.00396
H	-1.50922	-1.07347	1.43538
H	-2.46622	-0.66818	-0.00522
H	-1.43535	-2.11372	-0.00264
H	0.65509	2.46962	-0.00326
H	-1.11236	2.30029	-0.00443
H	-0.17766	1.84306	1.43524
C	1.68955	-0.77036	0.33825
C	-1.51220	-1.07758	0.33823
C	-0.17744	1.84828	0.33807
Ge	0.00003	-0.00011	-0.32406

Zero-point correction= 0.110450 (Hartree/Particle)
Thermal correction to Energy= 0.118256
Thermal correction to Enthalpy= 0.119200
Thermal correction to Gibbs Free Energy= 0.077819
Sum of electronic and zero-point Energies= -2194.314256
Sum of electronic and thermal Energies= -2194.306450
Sum of electronic and thermal Enthalpies= -2194.305506
Sum of electronic and thermal Free Energies= -2194.346887
E(UM06L) = -2196.63151678

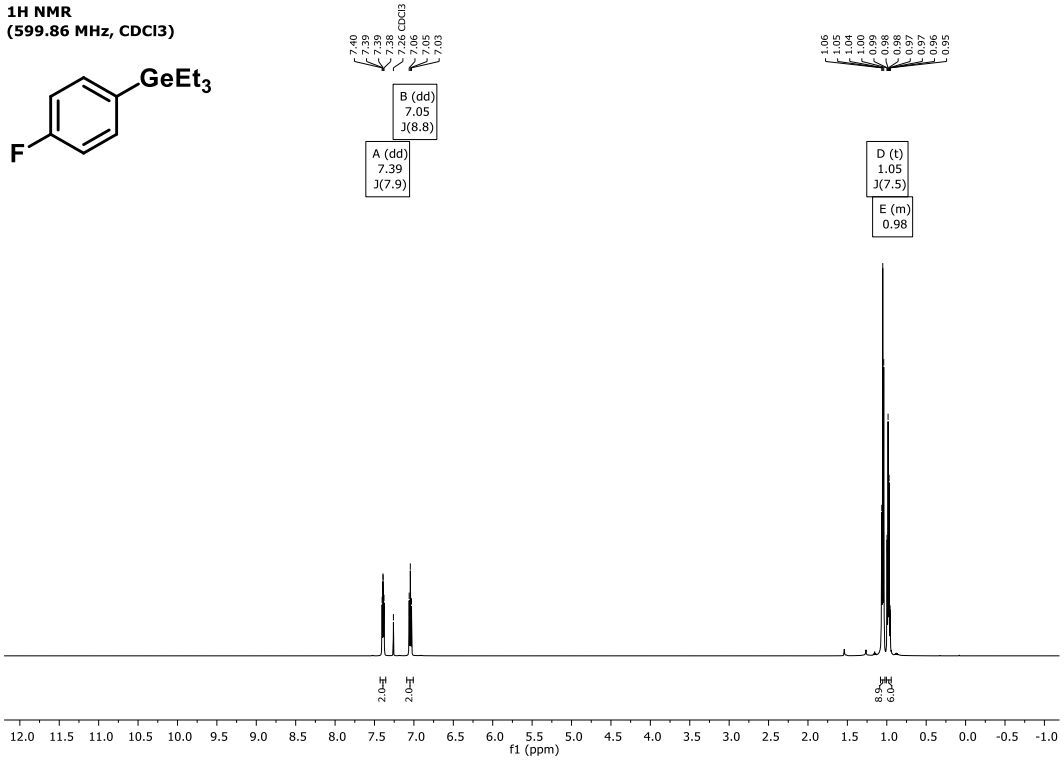


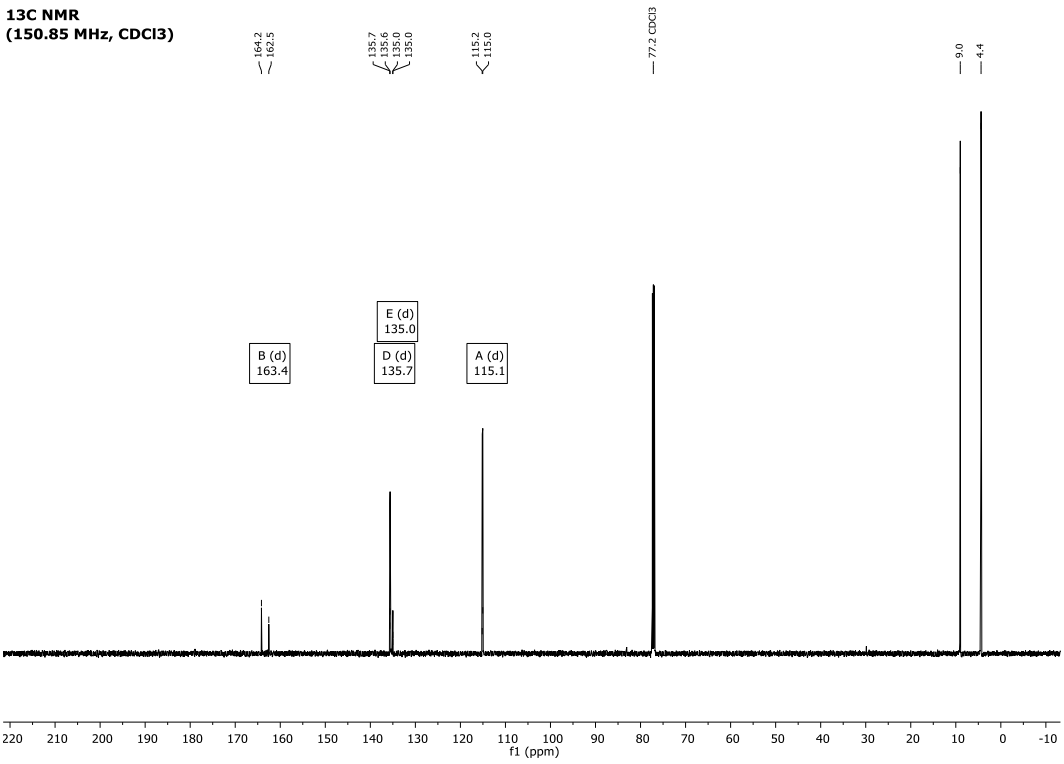
H	0.90410	1.57810	1.27825
H	1.92873	1.58352	-0.16795
H	0.39250	2.46467	-0.16873
H	0.91394	-1.57242	1.27825
H	0.40820	-2.46215	-0.16884
H	1.93875	-1.57121	-0.16783
H	-2.33599	0.87813	-0.16841
H	-2.33044	-0.89284	-0.16851
H	-1.81919	-0.00581	1.27830
C	0.89082	1.55404	0.17994
C	0.90064	-1.54836	0.17994
C	-1.79133	-0.00567	0.18002
Si	-0.00010	-0.00000	-0.43314

Zero-point correction= 0.111386 (Hartree/Particle)
Thermal correction to Energy= 0.118754
Thermal correction to Enthalpy= 0.119699
Thermal correction to Gibbs Free Energy= 0.080355
Sum of electronic and zero-point Energies= -409.034188
Sum of electronic and thermal Energies= -409.026820
Sum of electronic and thermal Enthalpies= -409.025876
Sum of electronic and thermal Free Energies= -409.065219
E(UM06L) = -409.22310245

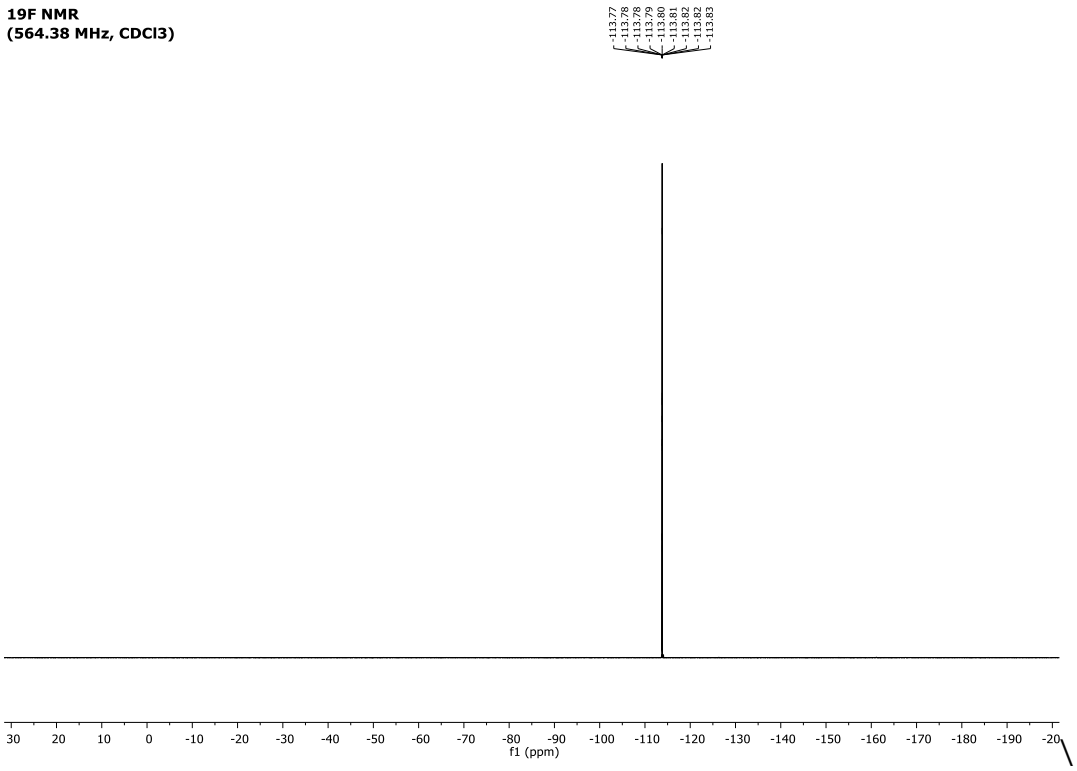
NMR Spectra

Triethyl(4-fluorophenyl)germane

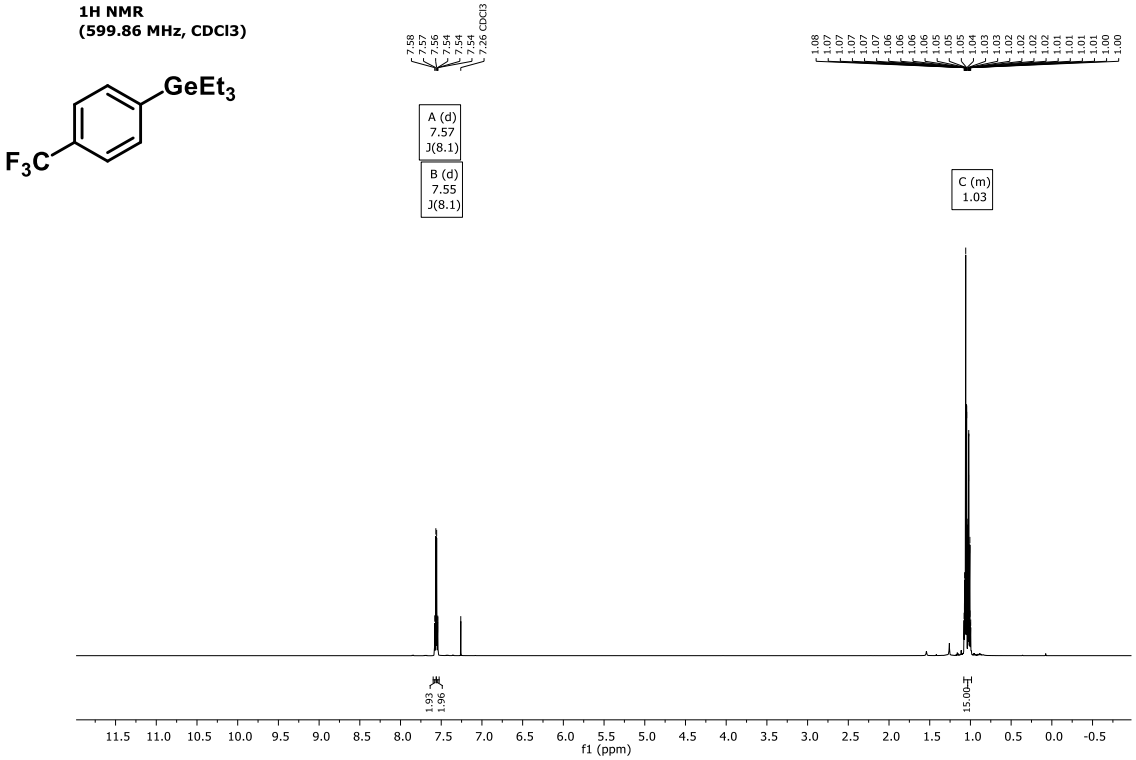


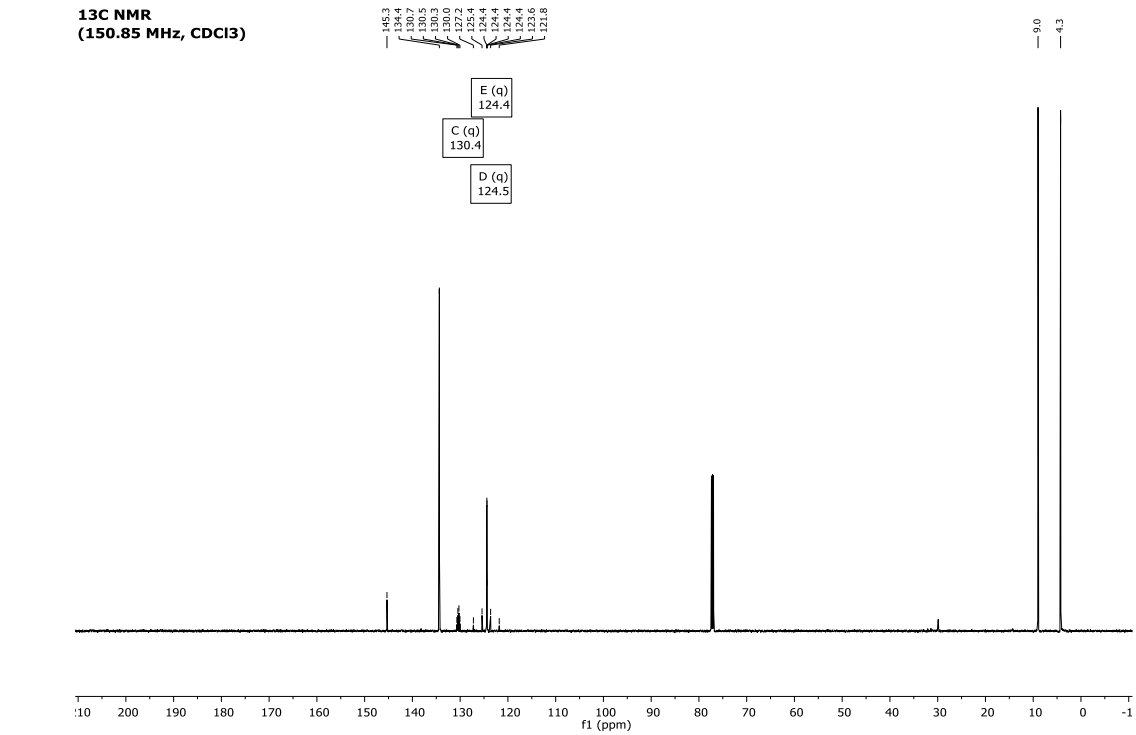


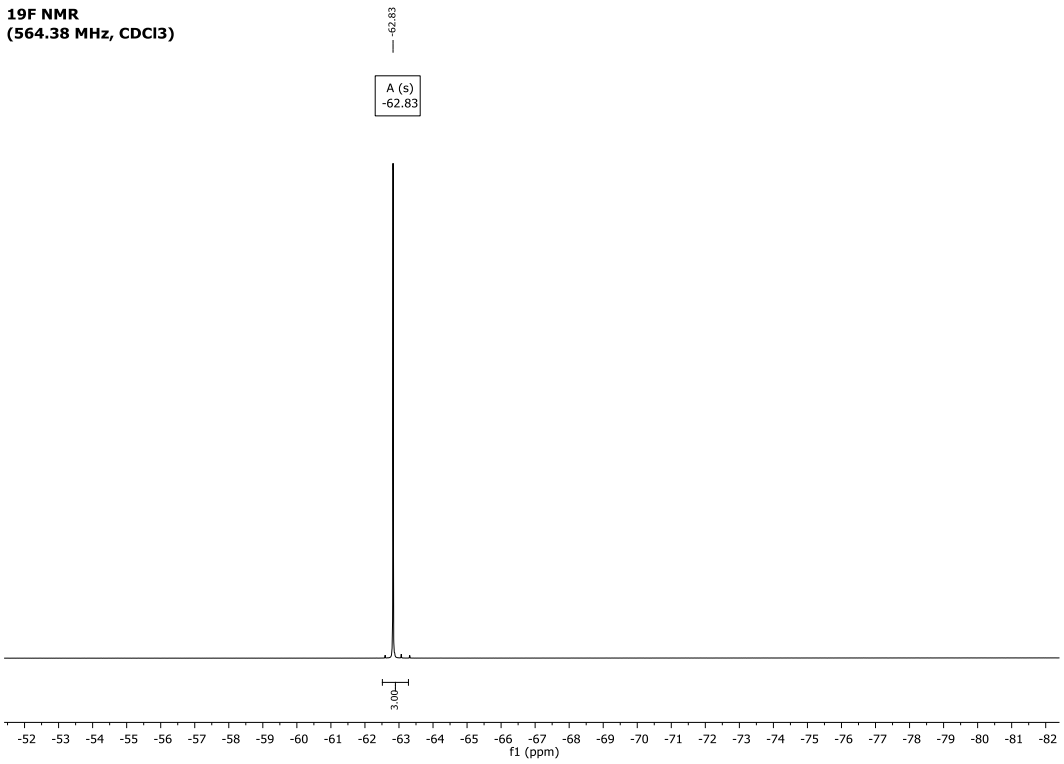
19F NMR
(564.38 MHz, CDCl3)



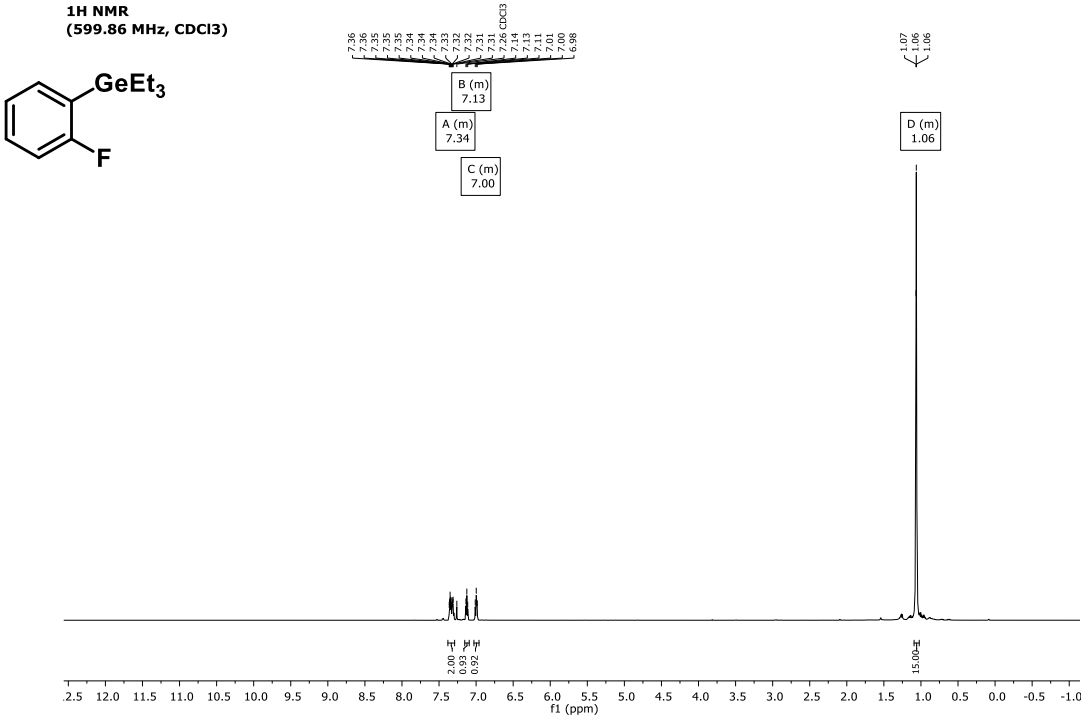
Triethyl(4-(trifluoromethyl)phenyl)germane

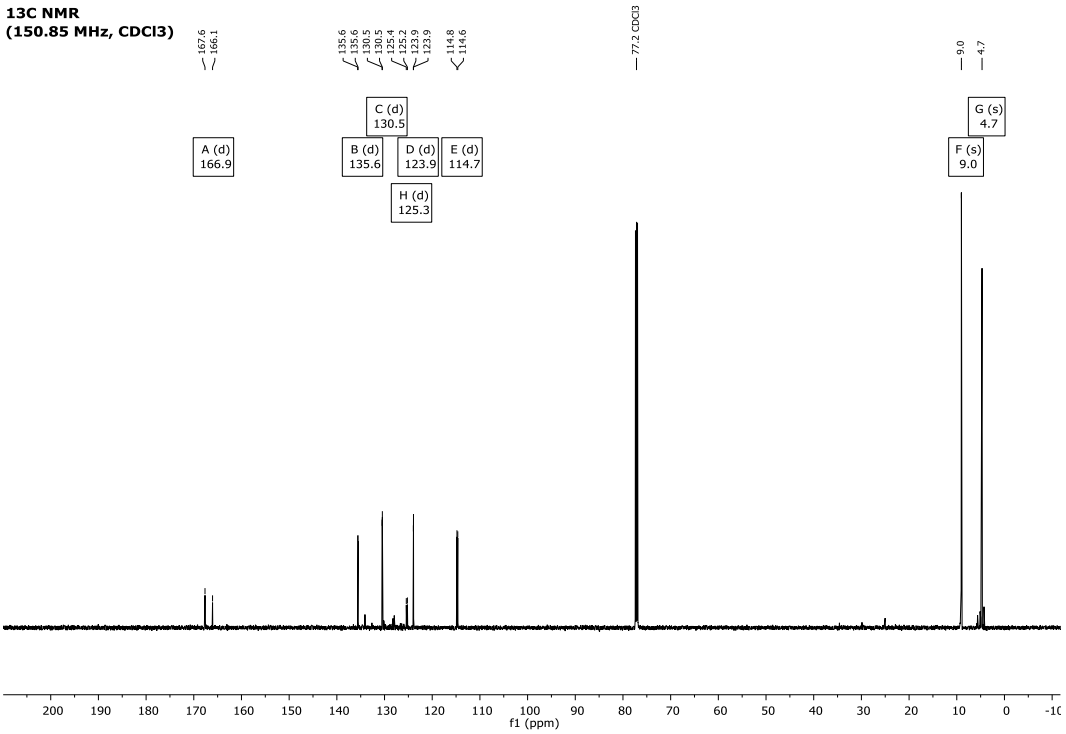




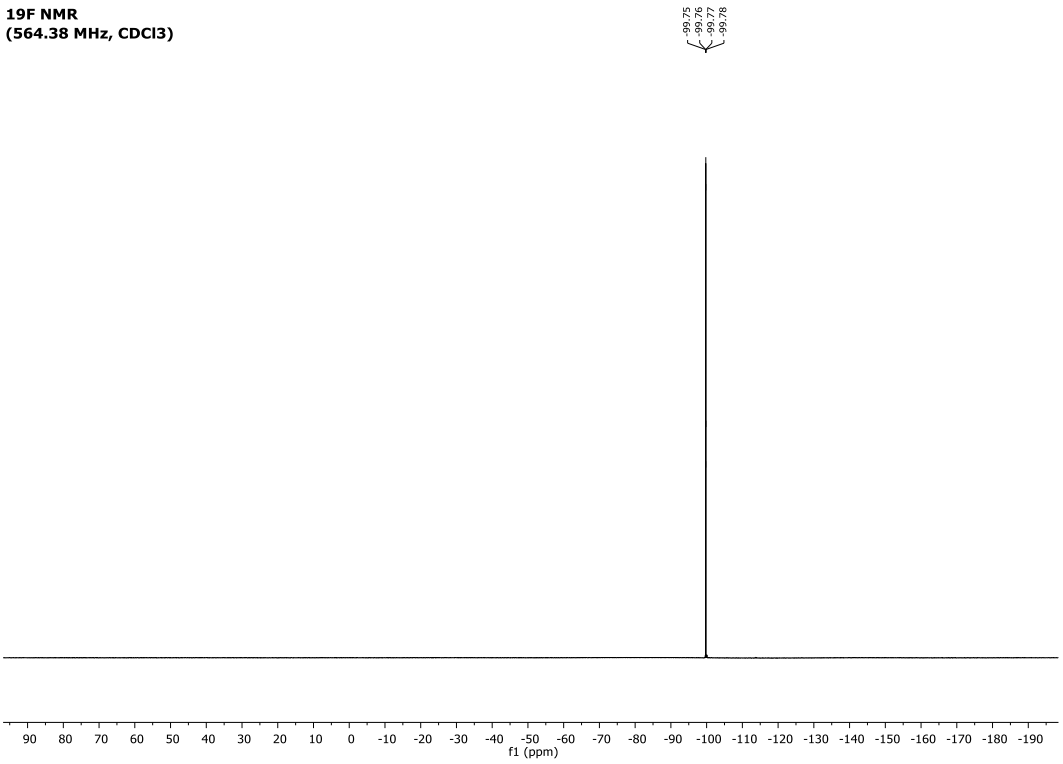

19F NMR
(564.38 MHz, CDCl3)
-62.83
A (s)
-62.83
3.00
-52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 -81 -82
f1 (ppm)

Triethyl(2-fluorophenyl)germane

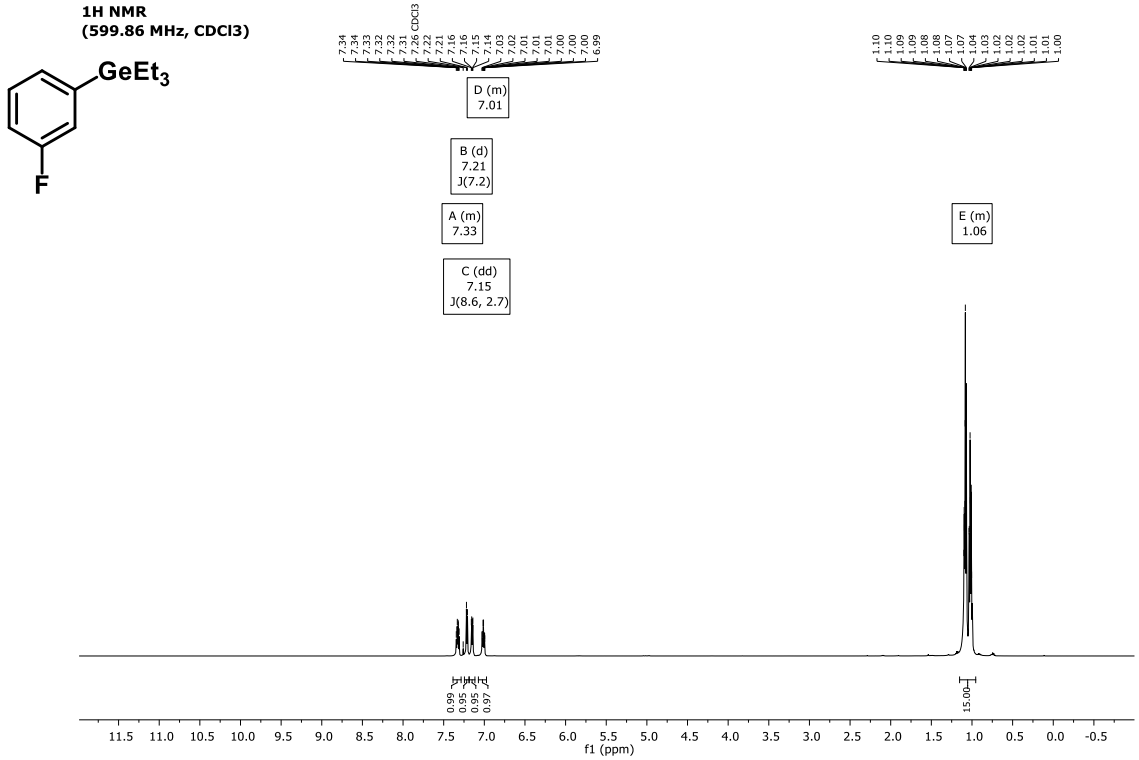


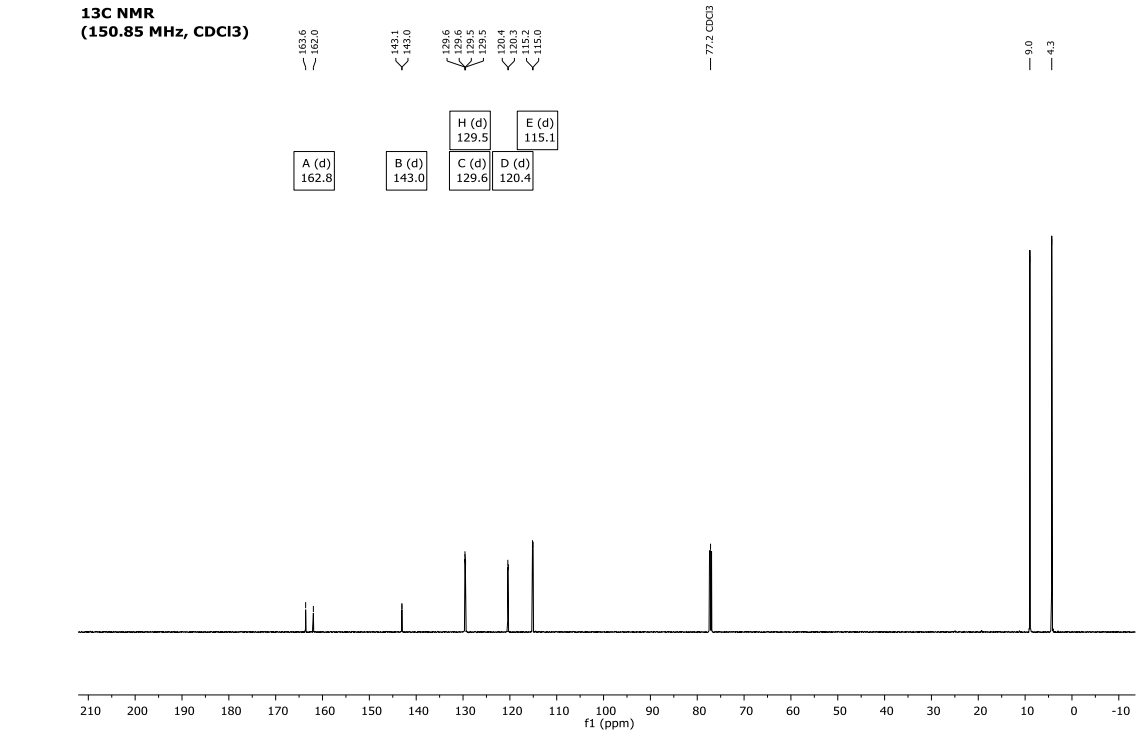


19F NMR
(564.38 MHz, CDCl3)

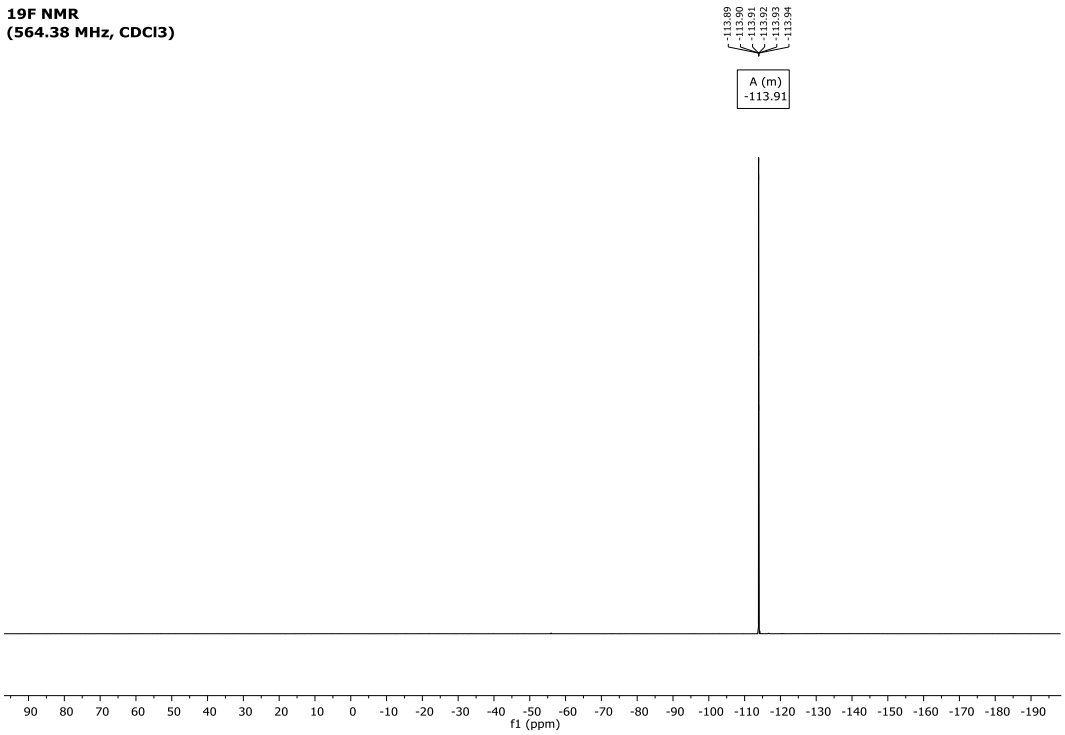


Triethyl(3-fluorophenyl)germane



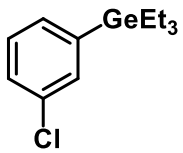


19F NMR
(564.38 MHz, CDCl3)

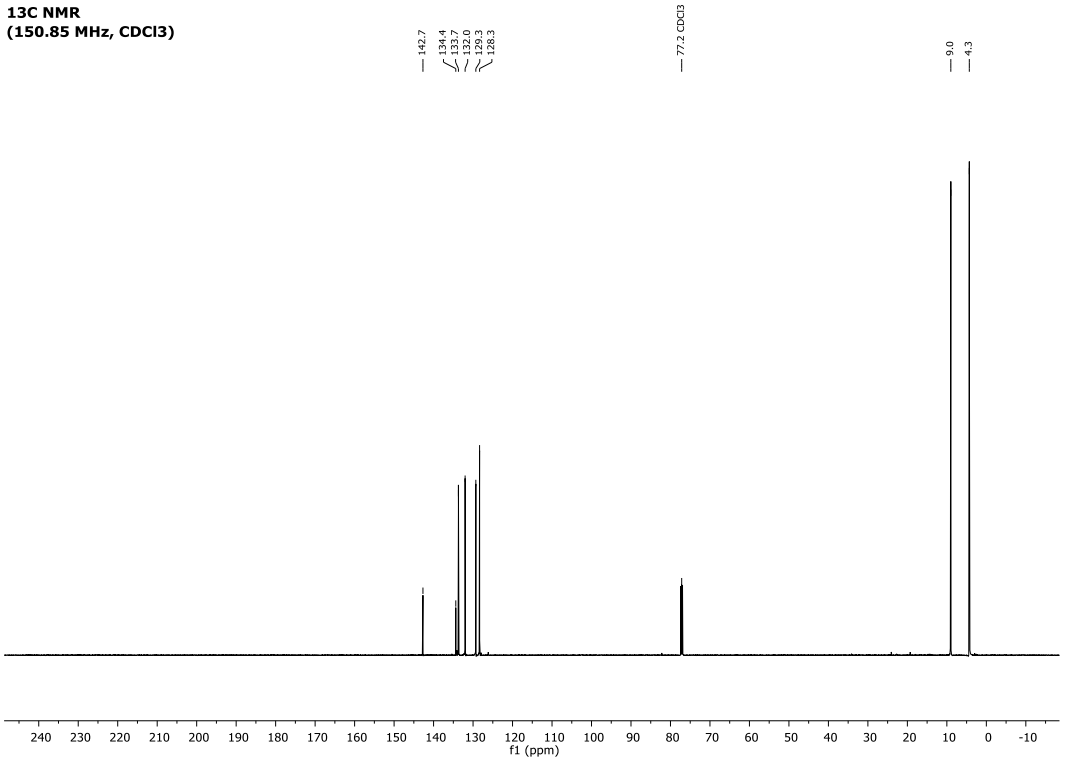


Triethyl(3-chlorophenyl)germane

1H NMR
(599.86 MHz, CDCl3)

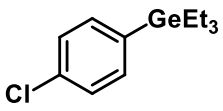


13C NMR
(150.85 MHz, CDCl3)

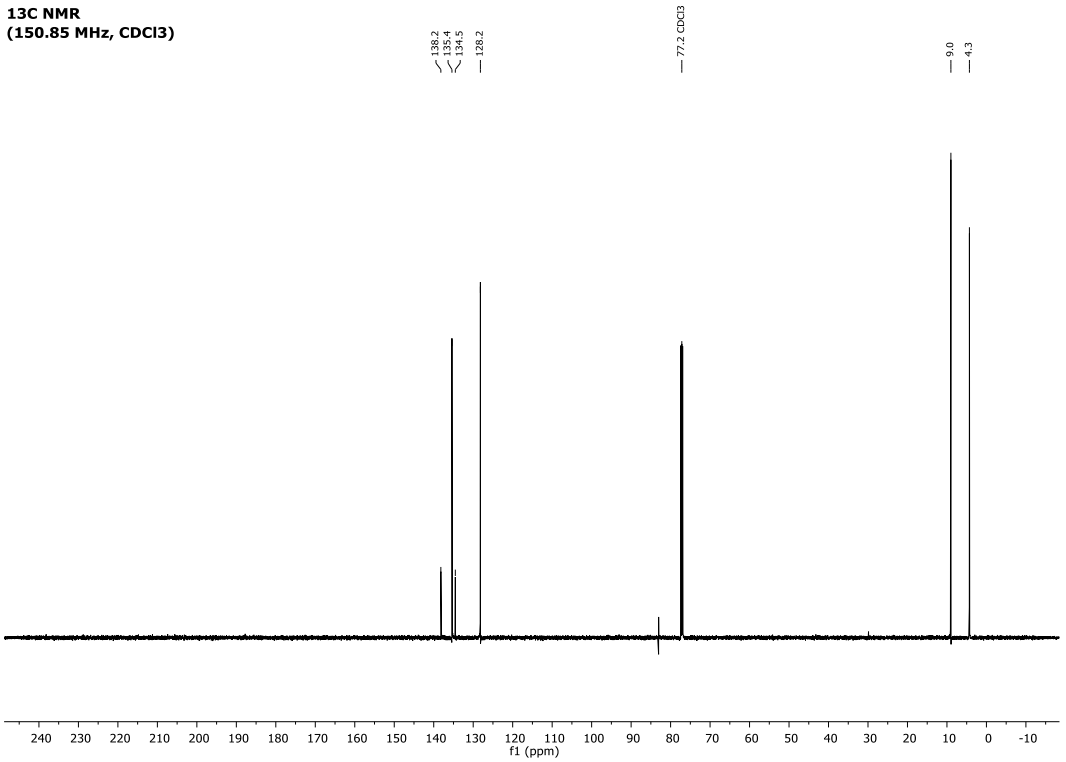


Triethyl(4-chlorophenyl)germane

1H NMR
(599.86 MHz, CDCl3)

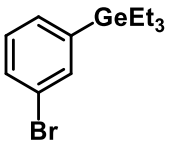


13C NMR
(150.85 MHz, CDCl3)

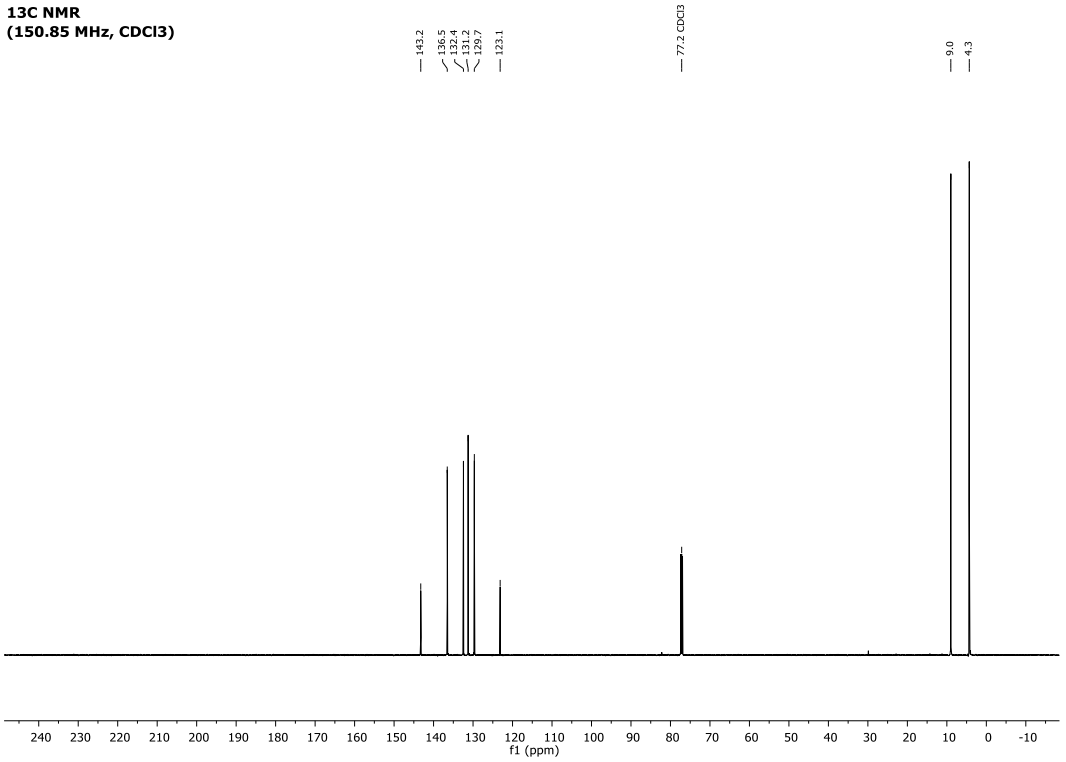


Triethyl(3-bromophenyl)germane

1H NMR
(599.86 MHz, CDCl3)

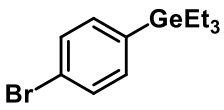


13C NMR
(150.85 MHz, CDCl3)

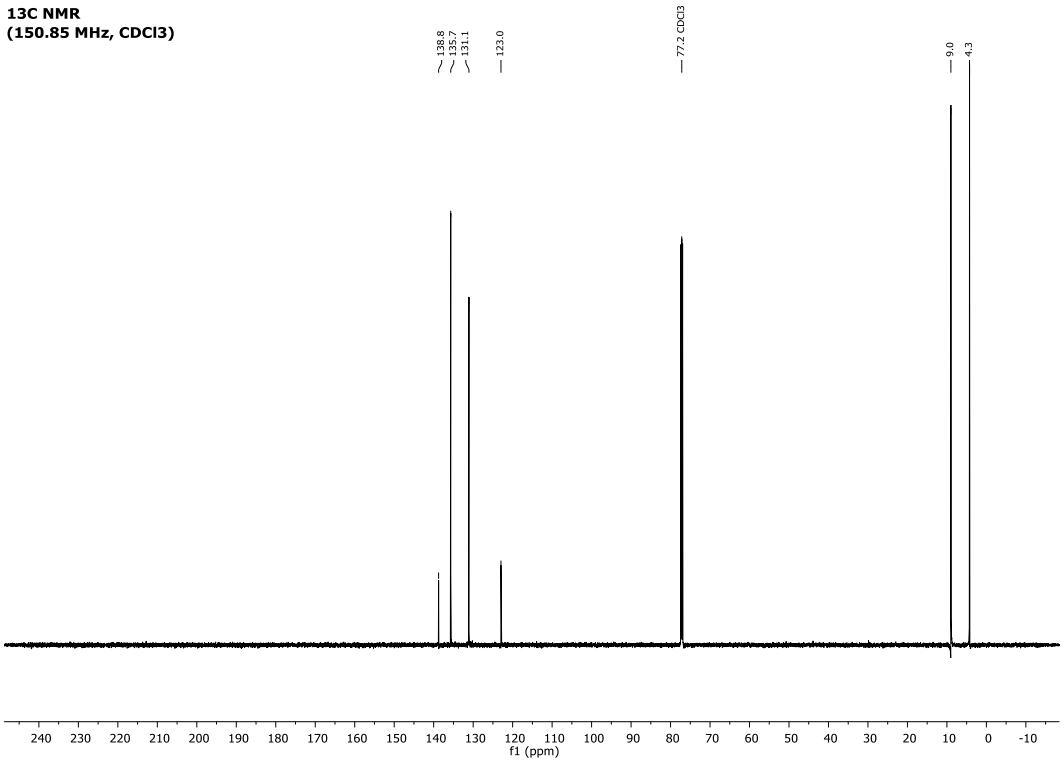


Triethyl(4-bromophenyl)germane

1H NMR
(599.86 MHz, CDCl3)

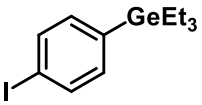


13C NMR
(150.85 MHz, CDCl3)

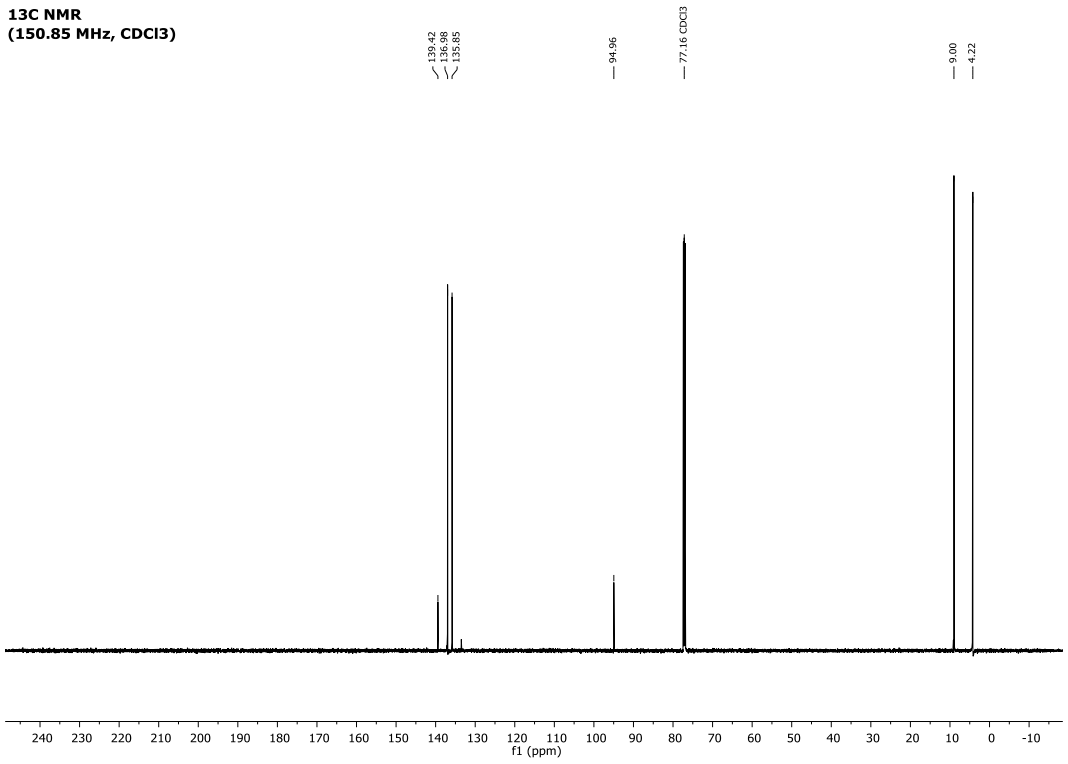


Triethyl(4-iodophenyl)germane

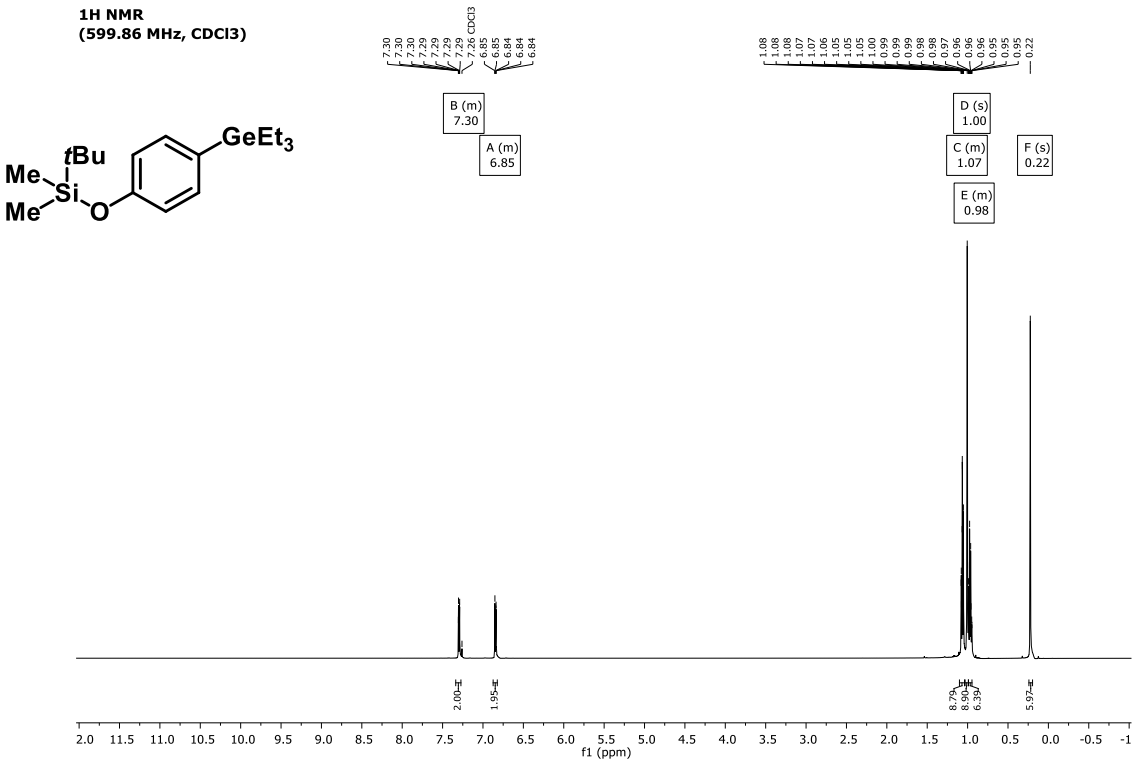
1H NMR
(599.86 MHz, CDCl3)

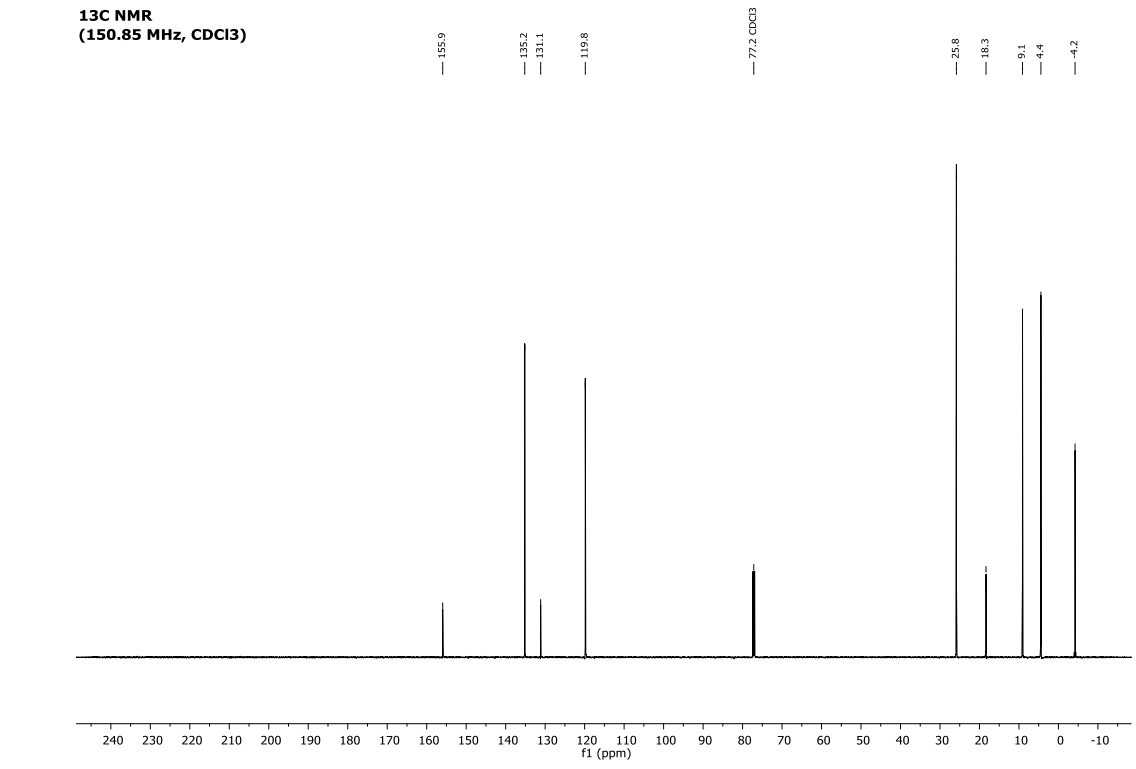


13C NMR
(150.85 MHz, CDCl3)

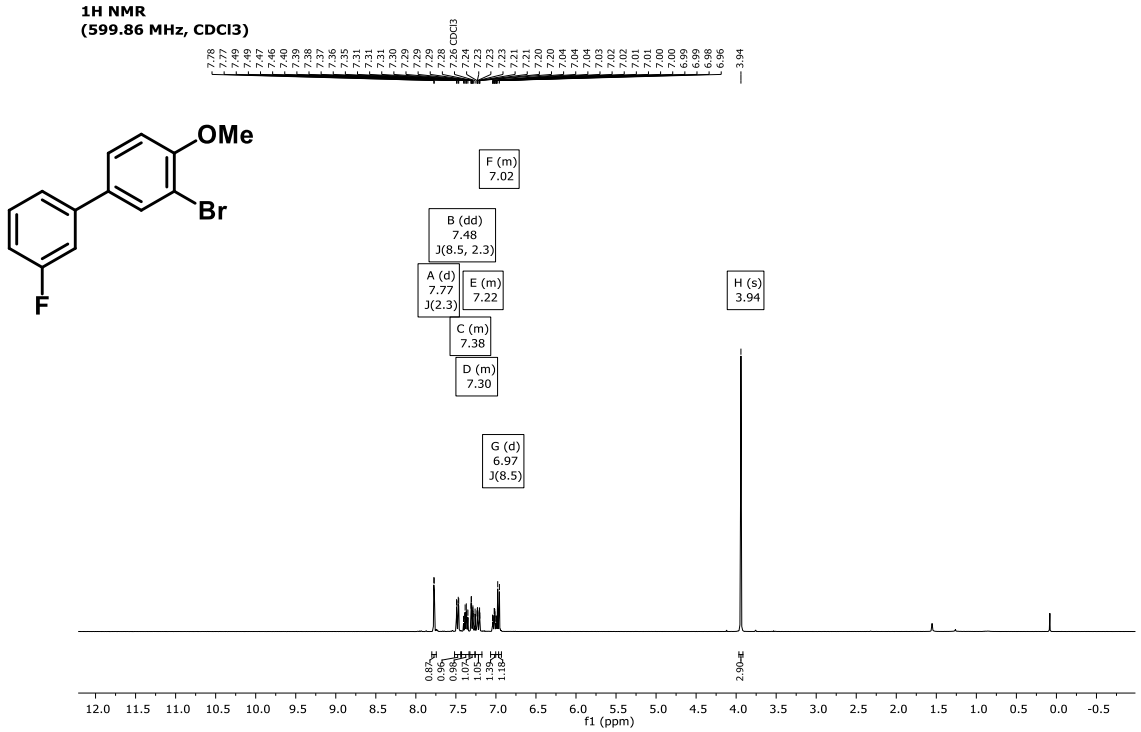


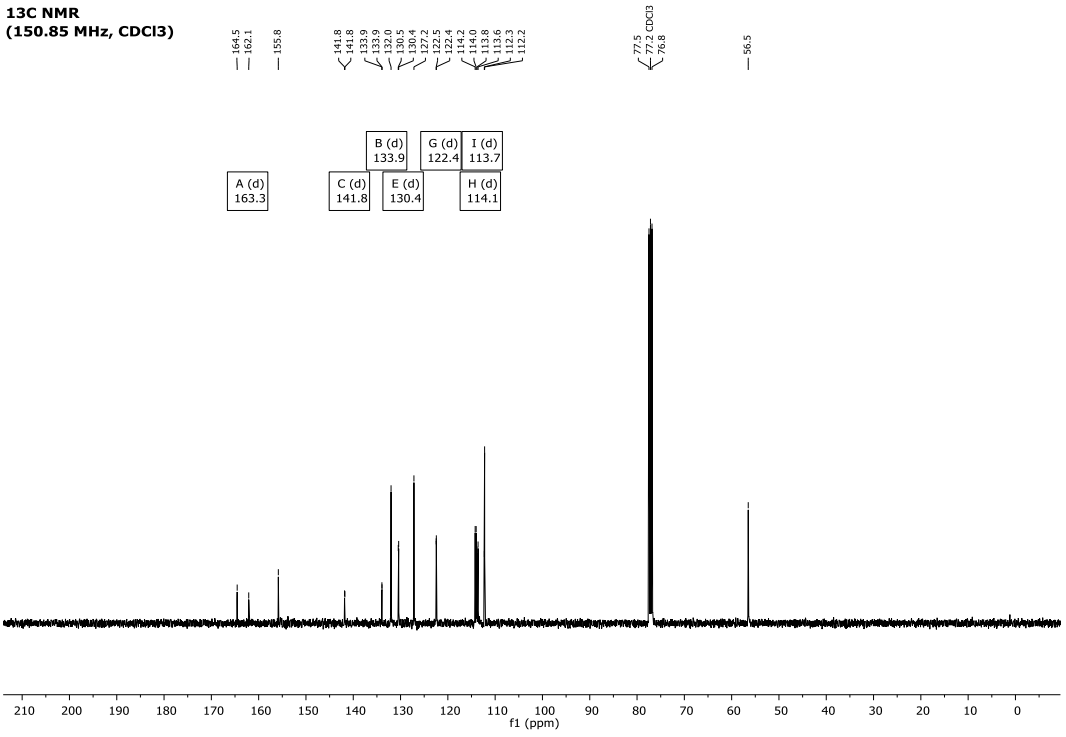
tert-Butyldimethyl(4-(triethylgermyl)phenoxy)silane



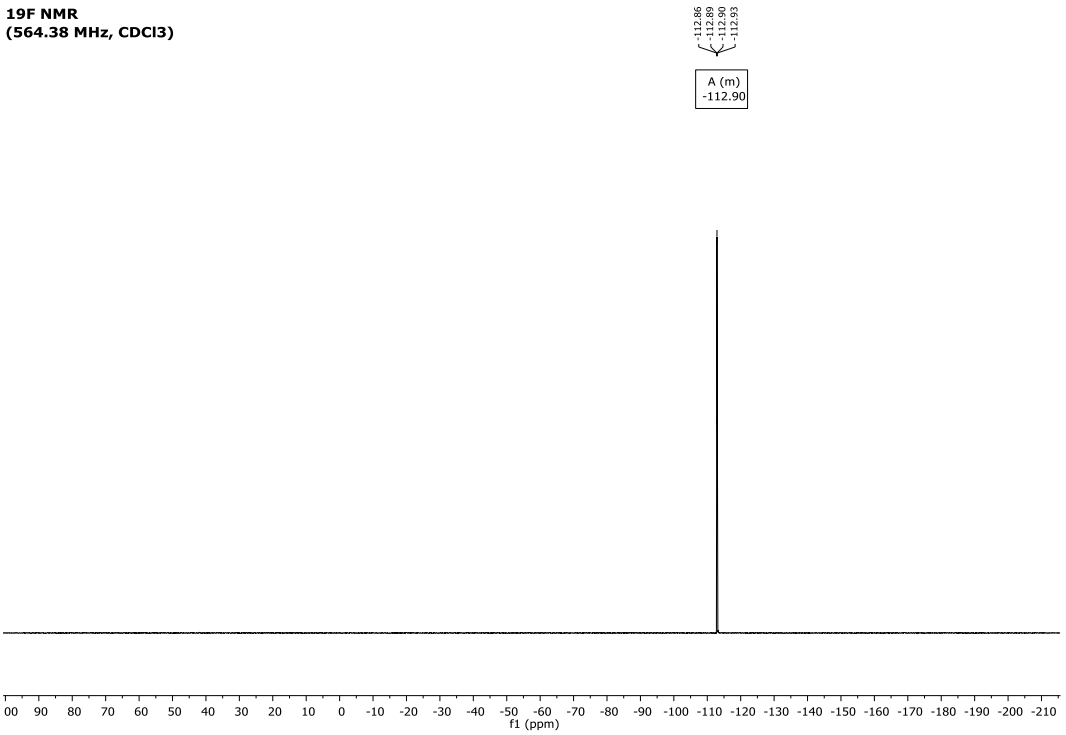


3-Bromo-3'-fluoro-4-methoxy-1,1'-biphenyl

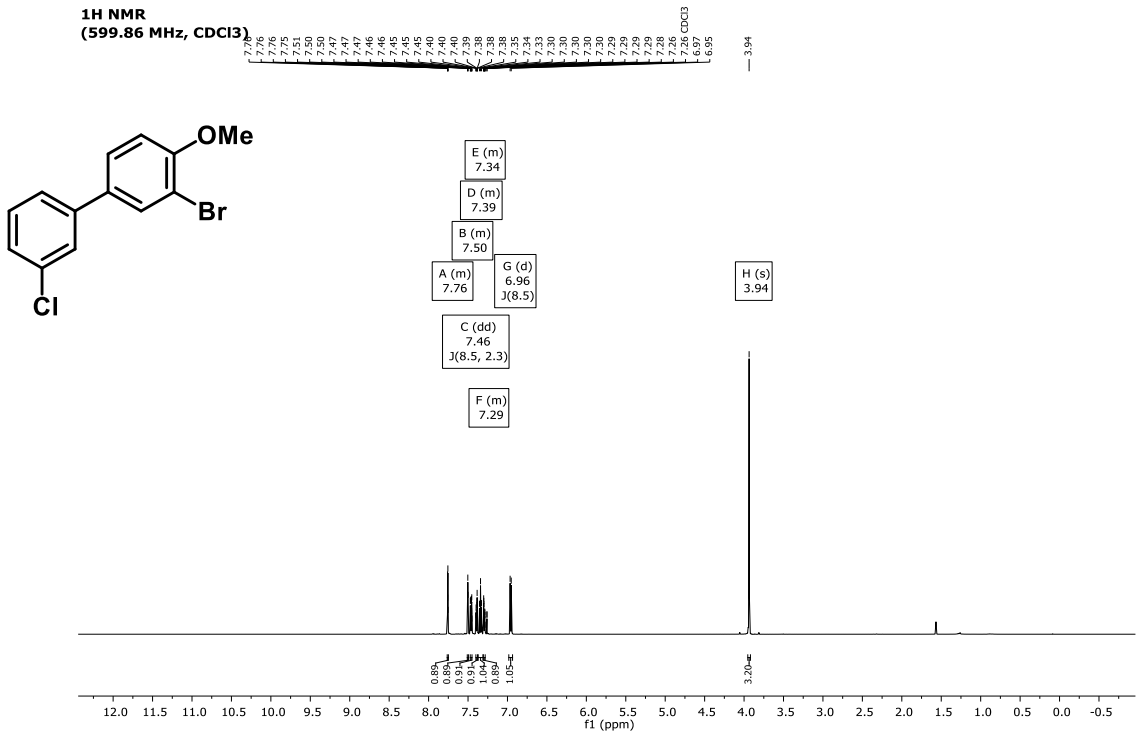


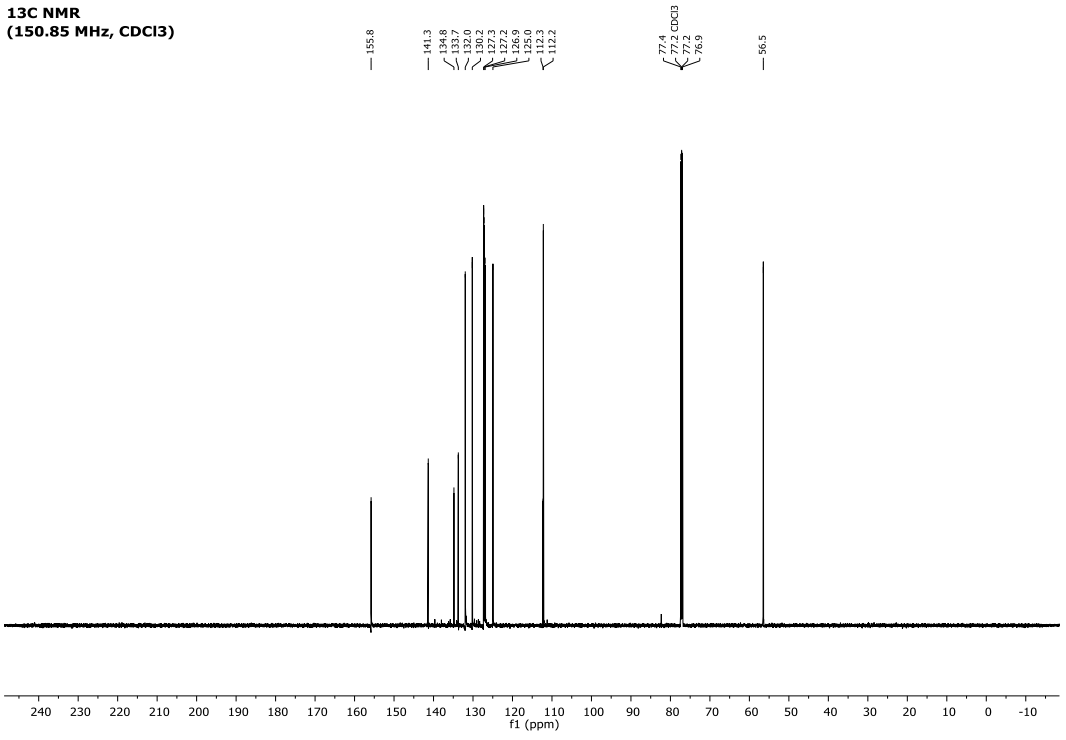


19F NMR
(564.38 MHz, CDCl3)

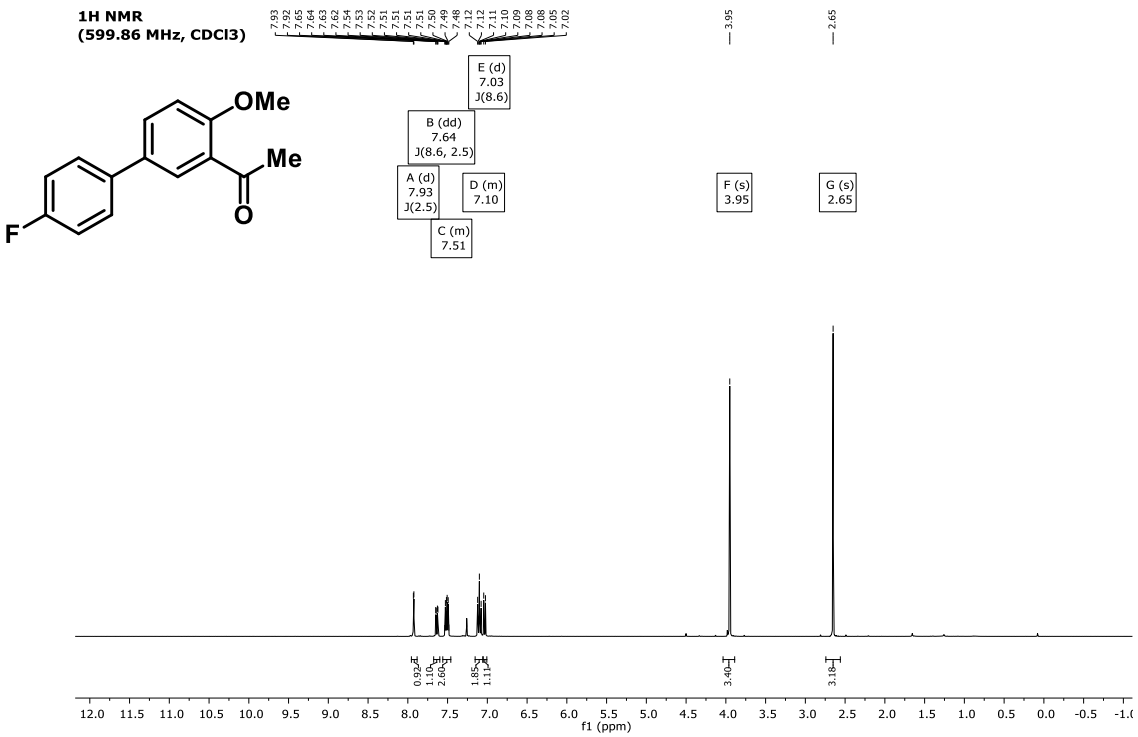


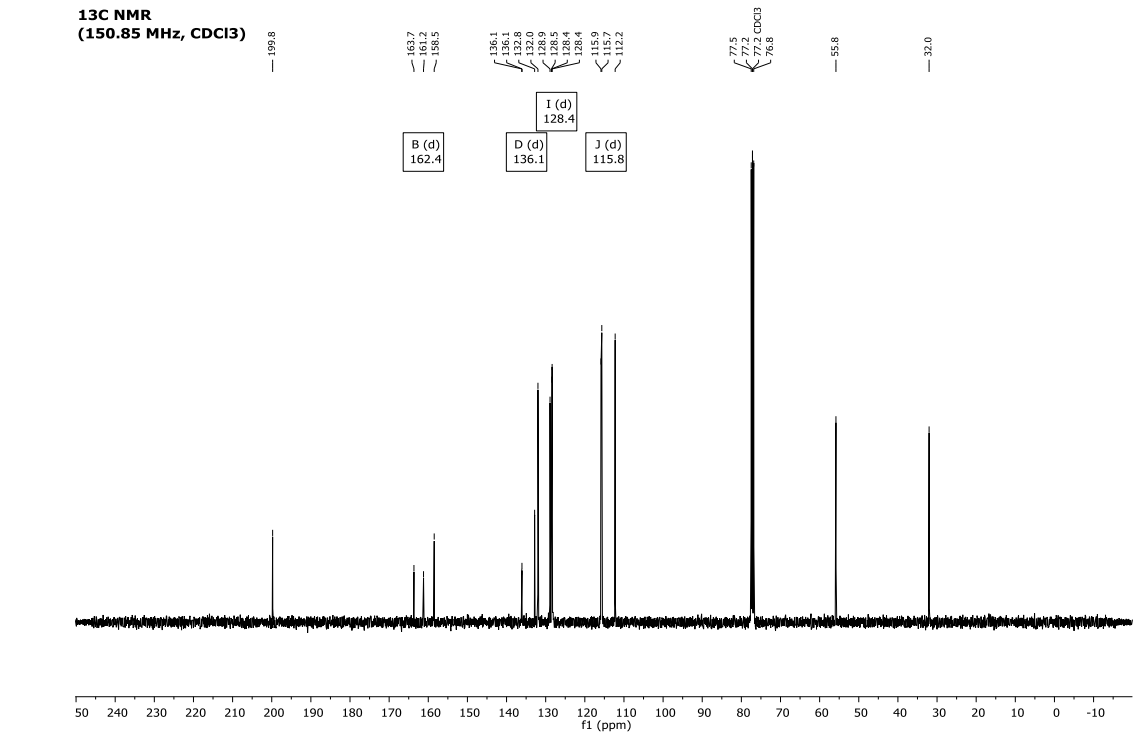
3-Bromo-3'-chloro-4-methoxy-1,1'-biphenyl



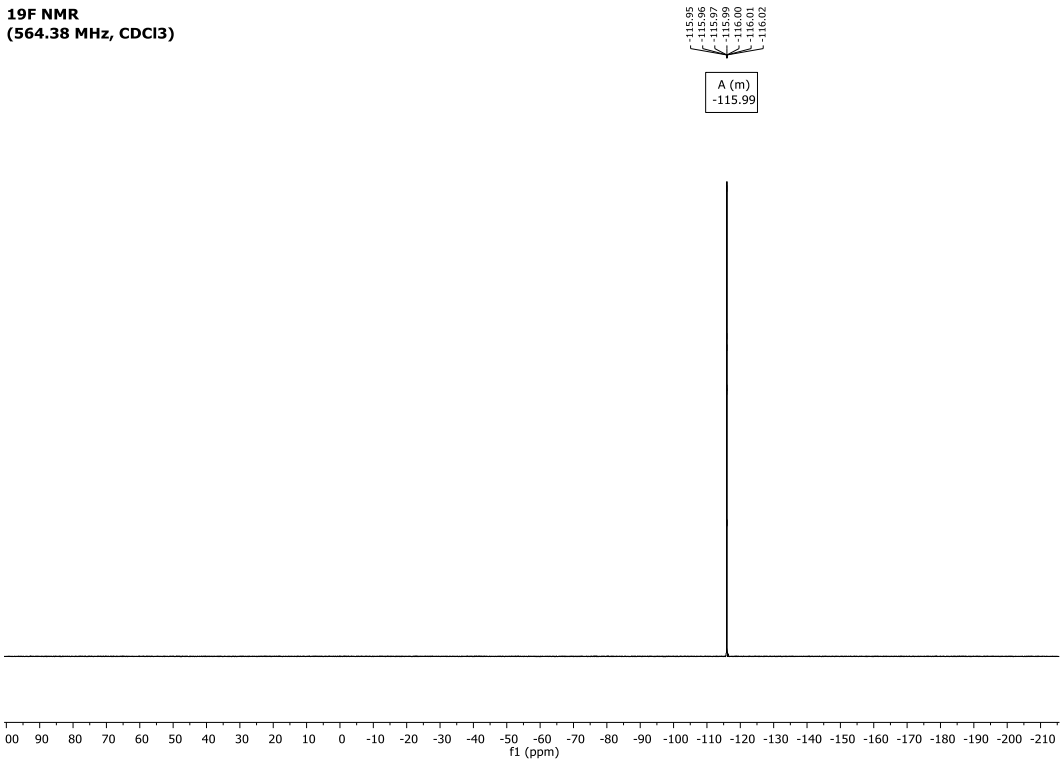


1-(4'-Fluoro-4-methoxy-[1,1'-biphenyl]-3-yl)ethan-1-one

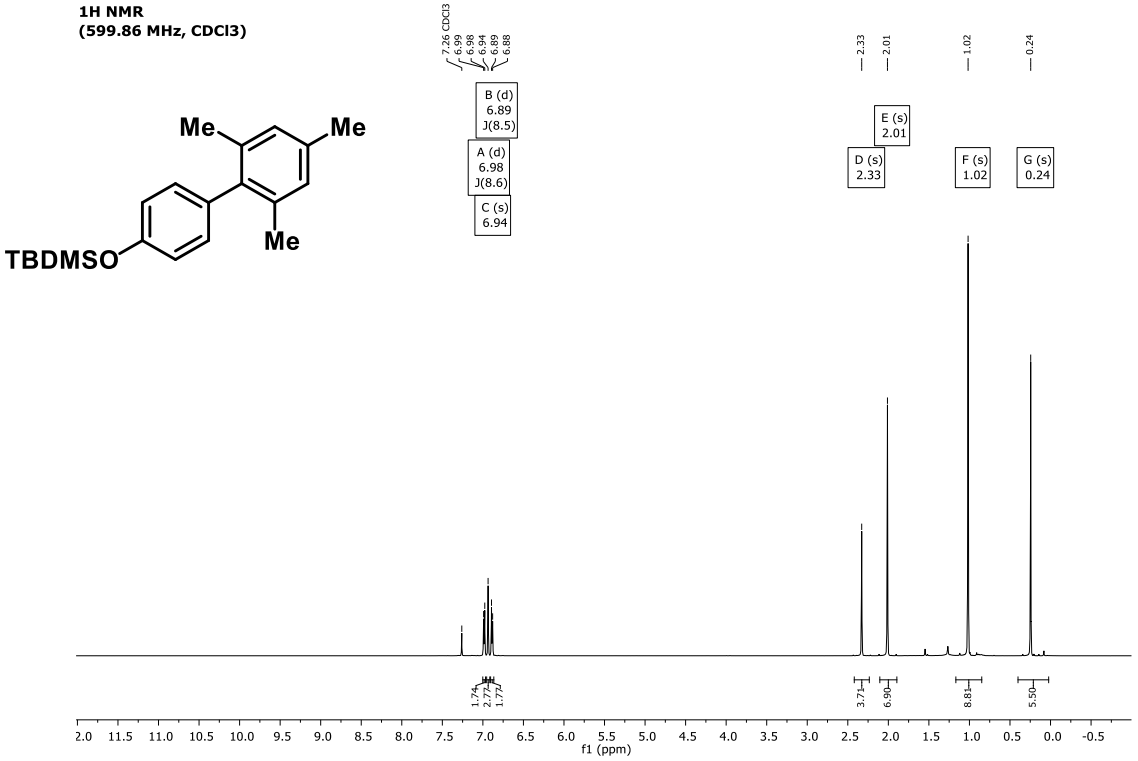


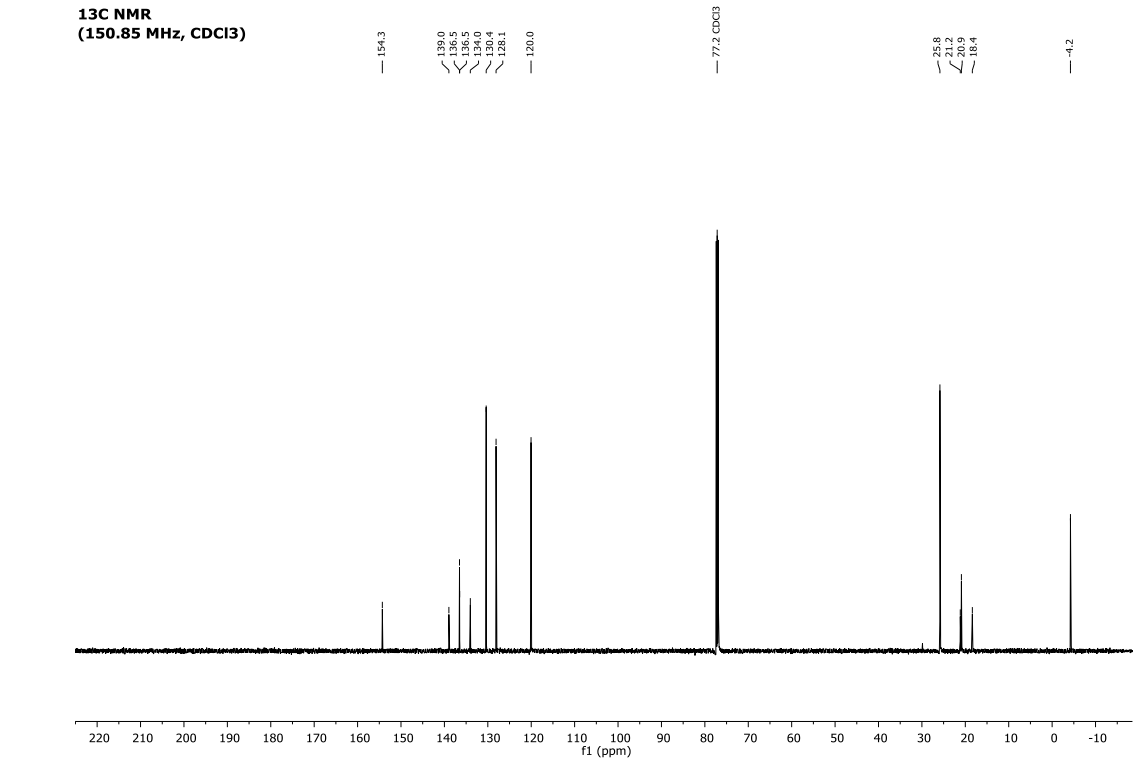


19F NMR
(564.38 MHz, CDCl3)

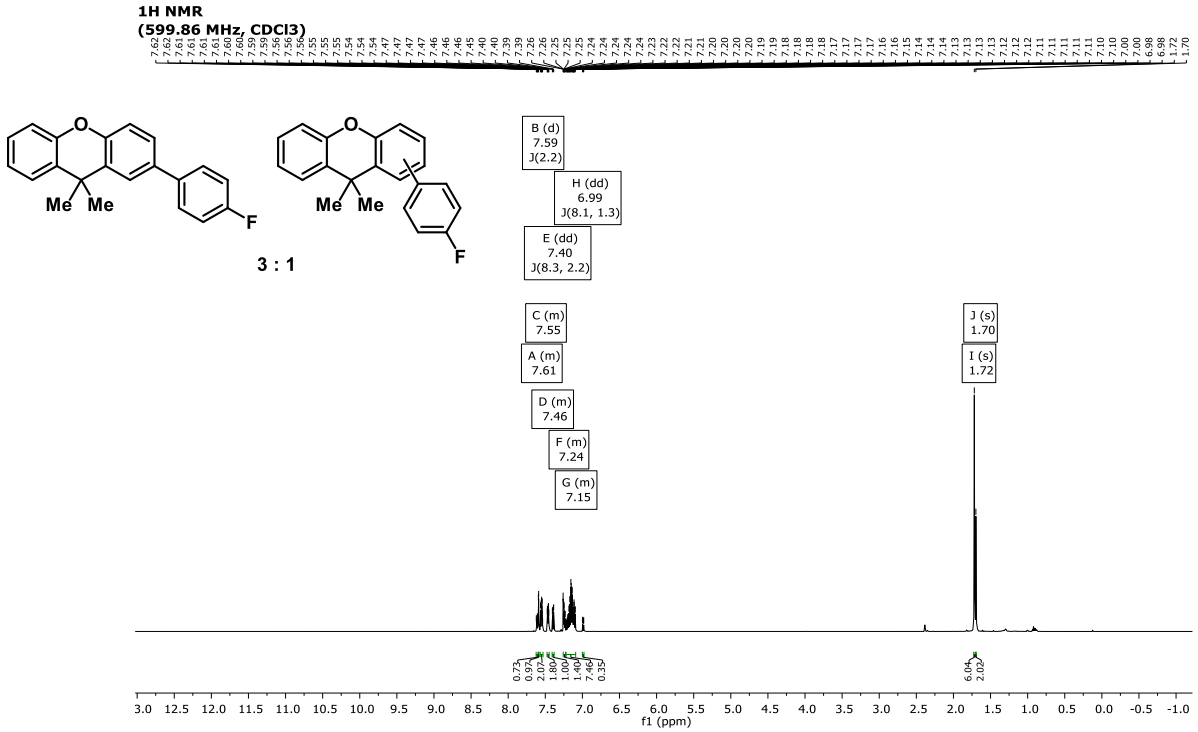


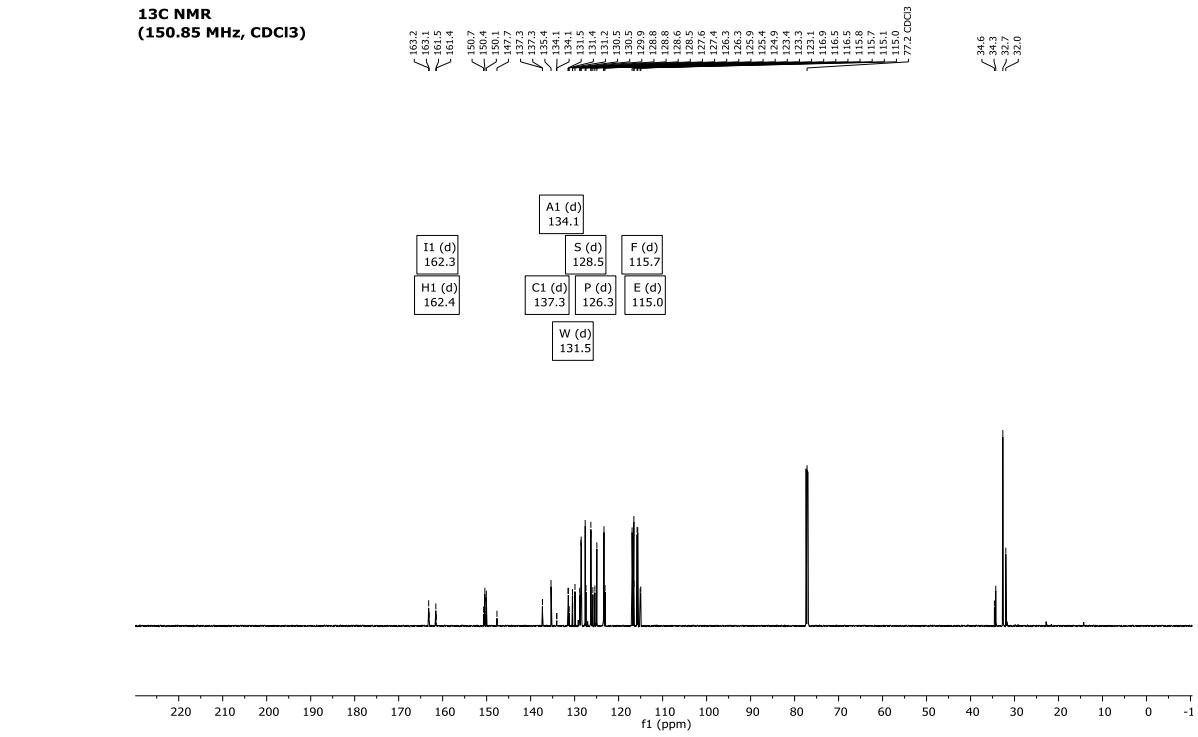
tert-Butyldimethyl((2',4',6'-trimethyl-[1,1'-biphenyl]-4-yl)oxy)silane



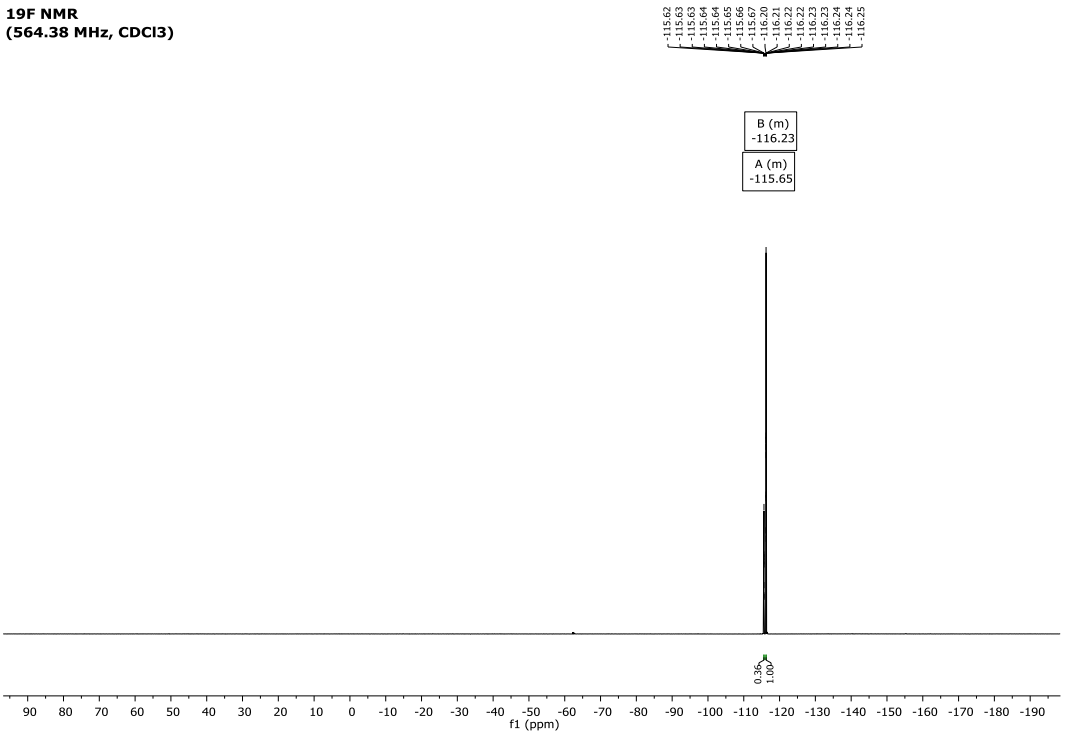


2-(4-Fluorophenyl)-9,9-dimethyl-9H-xanthene

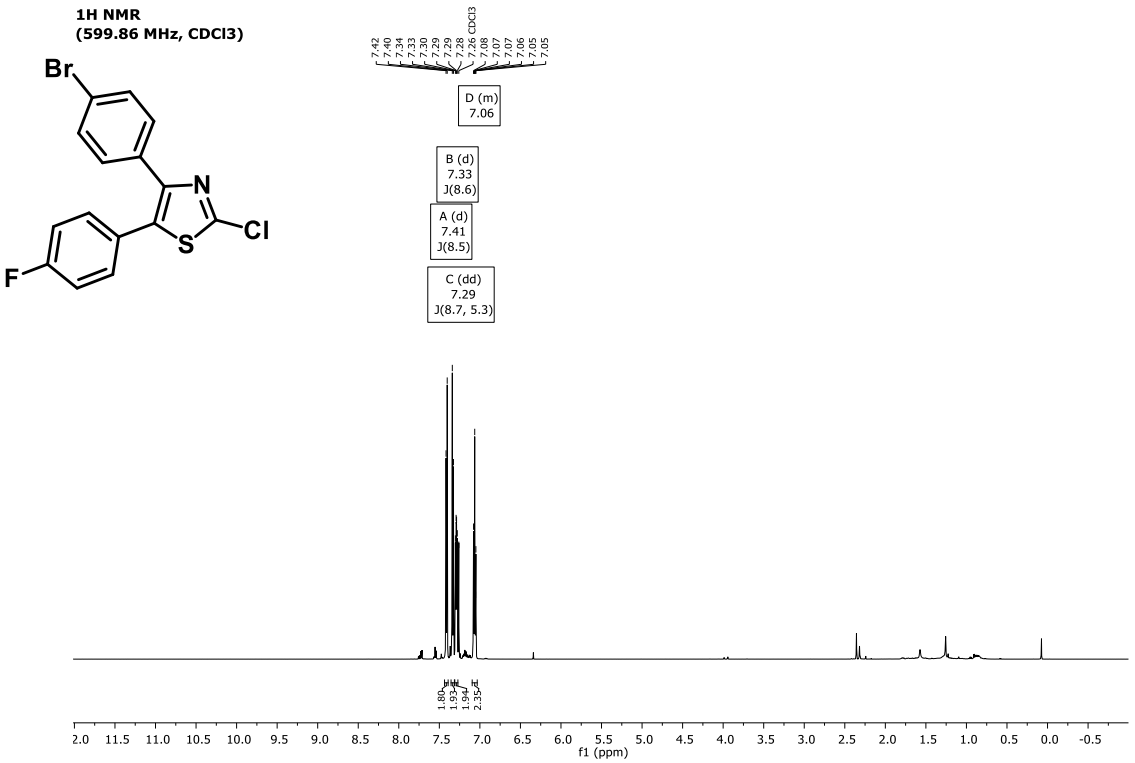


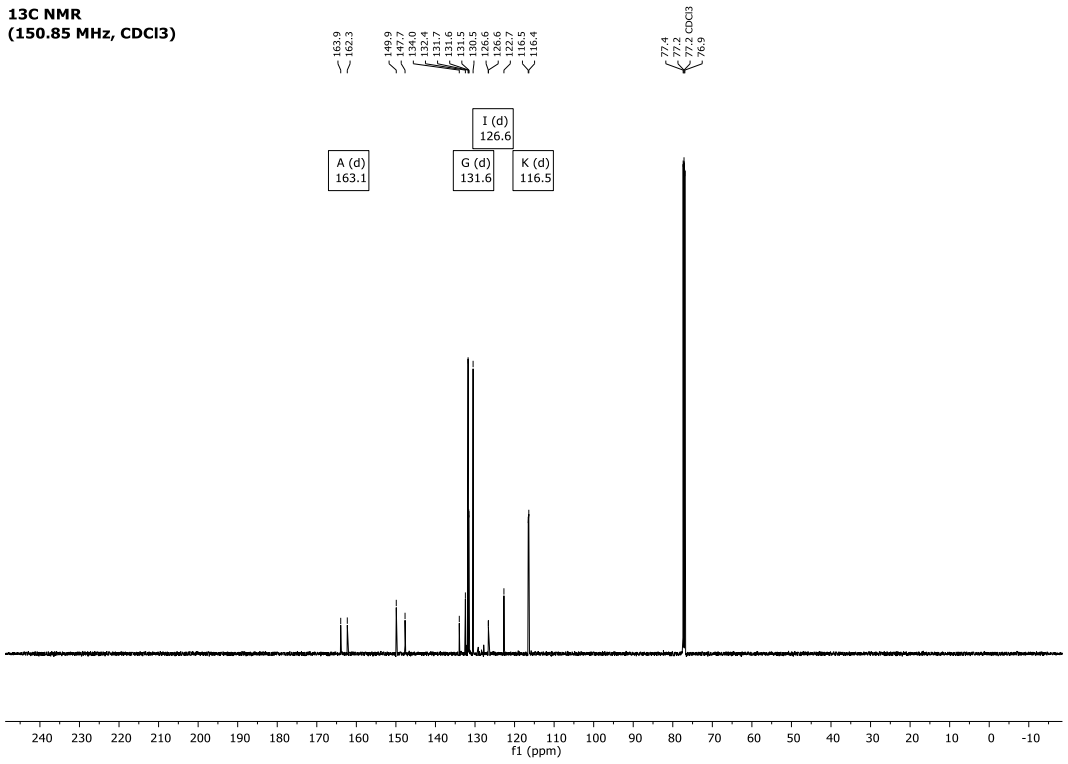


19F NMR
(564.38 MHz, CDCl3)

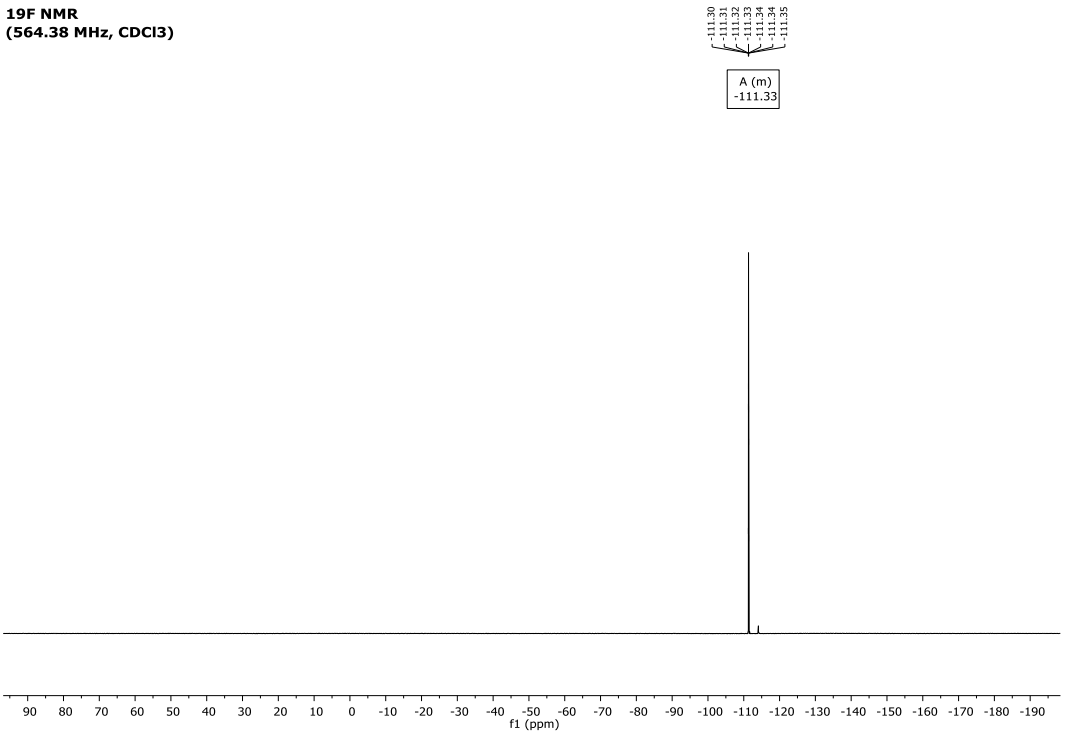


4-(4-Bromophenyl)-2-chloro-5-(4-fluorophenyl)thiazole





19F NMR
(564.38 MHz, CDCl3)



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