Supporting Information for

Pd-Catalyzed Oxidative C–H Arylation of (Poly)fluoroarenes with Aryl Pinacol Boronates and Experimental and Theoretical Studies of its Reaction Mechanism

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Table of Contents

1. General Information

Unless otherwise noted, all reagents were purchased from Sigma-Aldrich were checked for purity by GC-MS and used as received. Acetonitrile (Honeywell, HPLC grade), dimethyl sulfoxide (Acros, ≥ 99.8%), dry dimethylformamide (Sigma Aldrich, anhydrous 99.8%), and wet dimethylformamide (Merck, ACS grade) were used as received.

GC-MS analyses were performed using an Agilent 7890A gas chromatograph (column: DB-5MS 5% phenylmethylsiloxane, 30 m, Ø 0.25 mm, film 0.25 μm; *injector: 200 °C; oven: 40 °C (2 min), 40 °C to 280 °C (20 °C min^{-1}) (5 min) *; carrier gas: He (1 mL min^{-1}) equipped with an Agilent 5977B GC/MSD operating in EI mode. Infrared spectra were recorded on a Nicolet 380 FT-IR spectrometer as solids, using an ATR unit, and are reported in cm^{-1}.

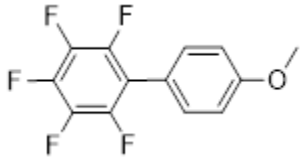
NMR spectra were recorded at 298 K using an Agilent DD2 (^{1}H NMR, 500 MHz; ^{13}C NMR, 125 MHz; ^{19}F NMR, 470 MHz) or a Bruker Avance I 500 (^{1}H NMR, 500 MHz; $^{13}C\{^{1}H\}$ NMR, 125 MHz; $^{13}C\{^{19}F\}$ NMR, 125 MHz; ^{19}F NMR, 470 MHz) spectrometer. ^{1}H NMR chemical shifts are reported relative to TMS and were referenced via residual proton resonances of the corresponding deuterated solvent ($CDCl_3$: 7.26 ppm), ^{13}C NMR, $^{13}C\{^{1}H\}$, $^{13}C\{^{19}F\}$ spectra are reported relative to TMS via the carbon signals of the deuterated solvent ($CDCl_3$: 77.16 ppm), ^{19}F NMR spectra are reported relative to external $CFCl_3$.

2. Experimental Procedures and Characterization of Products

General Procedure

In air, into a flask that was equipped with a magnetic stirring bar containing 3 mL of DMF, was added the corresponding (poly)fluoroarene (0.6 mmol), aryl-Bpin (0.4 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), and Ag_2O (139 mg, 0.60 mmol, 1.5 equiv). After capping the flask with a stopper, the suspension was stirred for 15 h at 100 ˚C. After cooling to room temperature, the solvent was evaporated *in vacuo* and the residue was purified by column chromatography on silica gel (hexane) to obtain the corresponding product.

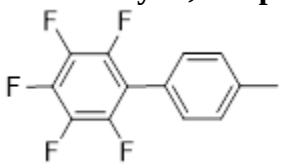
Synthesis of 2,3,4,5,6-pentafluoro-4'-methoxy-1,1'-biphenyl (3a)



Compound **3a** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 2-(4-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2f**) (94 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3f** was obtained as a white solid (101 mg, 92%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ = 7.36 (*m*, 2H, Ar-H), 7.03 – 7.00 (*m*, 2H; Ar-H), 3.87 (*s*, 3H; CH_3); **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$) δ = 160.4, 144.2 ($^1J_{F,C}$ = 244 Hz), 140.1 ($^1J_{F,C}$ = 251 Hz), 137.9 ($^1J_{F,C}$ = 250 Hz), 131.6, 118.5, 114.4, 55.5; **^{13}C{^{19}F} NMR** (125 MHz, $CDCl_3$) δ = 144.2, 140.1, 137.9, 131.5 (*dd*, $^2J_{H,C}$ = 161 Hz, $^3J_{H,C}$ = 7 Hz), 118.4 (*t*, $^3J_{H,C}$ = 7 Hz), 115.7, 114.3 (*dd*, $^2J_{H,C}$ = 161 Hz, $^3J_{H,C}$ = 5 Hz), 55.4 (*q*, $^2J_{H,C}$ = 144 Hz); **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.6 – -162.5 (*m*, 2F), -156.5 (*t*, $^3J_{F,F}$ = 21 Hz, 1F), -143.6 (*dd*,

$^{3}J_{F,F}$ = 23 Hz, $^{4}J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 10.199 min] m/z: 274 $[M]^{+}$. Spectroscopic data match those in the literature.[S1]

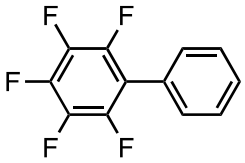
Synthesis of 2,3,4,5,6-pentafluoro-4'-methyl-1,1'-biphenyl (3b)



Compound **3b** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 4,4,5,5-tetramethyl-2-(*p*-tolyl)-1,3,2-dioxaborolane (**2b**) (87 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3b** was obtained as a white solid (101 mg, 98%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.32 (*s*, 4H; Ar-H), 2.44 (*s*, 3H; CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 144.3 (*dm*, $^{1}J_{F,C}$ = 247 Hz), 140.3 (*dm*, $^{1}J_{F,C}$ = 253 Hz), 139.5, 137.9 (*dm*, $^{1}J_{F,C}$ = 250 Hz), 130.0, 129.5, 123.5, 116.1 (*td*, $^{2}J_{F,C}$ = 17 Hz, $^{3}J_{F,C}$ = 4 Hz), 21.5; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.6 – -162.5 (*m*, 2F), -156.2 (*t*, $^{3}J_{F,F}$ = 21 Hz, 1F), -143.4 (*dd*, $^{3}J_{F,F}$ = 23 Hz, $^{4}J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 9.173 min] m/z: 258 $[M]^{+}$. Spectroscopic data match those in the literature.[S1]

Synthesis of 2,3,4,5,6-pentafluoro-1,1'-biphenyl (**3c**)

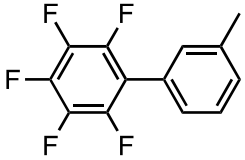


Compound **3c** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 4,4,5,5-tetramethyl-2-phenyl-

1,3,2-dioxaborolane (**2c**) (82 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3c** was obtained as a white solid (78 mg, 80%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.51 – 7.42 (*m*, 5H; Ar-H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 144.3 (*dm*, $^1J_{F,C}$ = 250 Hz), 140.5 (*dm*, $^1J_{F,C}$ = 253 Hz), 138.0 (*dm*, $^1J_{F,C}$ = 254 Hz), 130.3, 129.4, 128.9, 126.5, 116.1; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.2 – -162.3 (*m*, 2F), -155.6 (*t*, $^2J_{F,F}$ = 21 Hz, 1F), -143.2 (*dd*, $^3J_{F,F}$ = 21 Hz , $^4J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 8.535 min] m/z: 254 $[M]^+$. Spectroscopic data matched those in the literature.[S1]

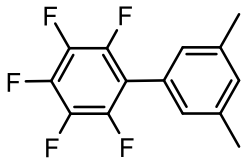
Synthesis of 2,3,4,5,6-pentafluoro-3'-methyl-1,1'-biphenyl (3d)



Compound **3d** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 4,4,5,5-tetramethyl-2-(*m*-tolyl)-1,3,2-dioxaborolane (**2d**) (87 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3d** was obtained as a white solid (75 mg, 72%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.39 (*t*, $^4J_{H,H}$ = 8 Hz, 1H; Ar-H), 7.28 (*d*, $^3J_{H,H}$ = 8 Hz, 1H; Ar-H), 7.23 (*d*, $^3J_{H,H}$ = 11 Hz, 2H; Ar-H), 2.43 (*s*, 3H; CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 144.3 (*dm*, $^1J_{F,C}$ = 247 Hz), 140.4 (*dm*, $^1J_{F,C}$ = 252 Hz), 137.9 (*dm*, $^1J_{F,C}$ = 251 Hz), 138.6, 130.8, 130.2, 128.7, 127.3, 126.3, 116.2 (*td*, $^2J_{F,C}$ = 17 Hz, $^3J_{F,C}$ = 4 Hz), 21.4; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.5 – -162.4 (*m*, 2F), -155.9 (*t*, $^3J_{F,F}$ = 21 Hz, 1F), -143.1 (*dd*, $^3J_{F,F}$ = 23 Hz, $^4J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 9.064 min] m/z: 258 $[M]^+$. Spectroscopic data match those in the literature.[S1]

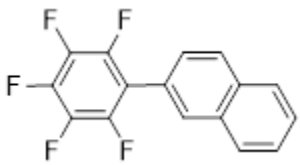
Synthesis of 2,3,4,5,6-pentafluoro-3',5'-dimethyl-1,1'-biphenyl (**3e**)



Compound **3e** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 2-(3,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2a**) (93 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3a** was obtained as a white solid (55 mg, 50%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.09 (*s*, 1H; Ar-H), 7.01 (*s*, 2H; Ar-H), 2.37 (*s*, 6H; CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 144.2 (*dm*, $^1J_{F,C}$ = 247 Hz), 140.2 (*dm*, $^1J_{F,C}$ = 253 Hz), 138.4, 137.8 (*dm*, $^1J_{F,C}$ = 250 Hz), 131.0, 127.8, 126.2, 116.3 (*td*, $^2J_{F,C}$ = 18 Hz, $^3J_{F,C}$ = 4 Hz), 21.3; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.6 – -162.5 (*m*, 2F), -156.1 (*t*, $^3J_{F,F}$ = 21 Hz, 1F), -142.9 (*dd*, $^3J_{F,F}$ = 23 Hz, $^4J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 9.744 min] m/z: 272 $[M]^+$. Spectroscopic data match those in the literature.[S2]

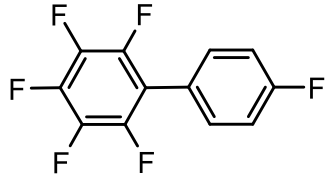
Synthesis of 2-(perfluorophenyl)naphthalene (3g)



Compound **3g** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 4,4,5,5-tetramethyl-2-(naphthalen-2-yl)-1,3,2-dioxaborolane (**2g**) (102 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3g** was obtained as a white solid (100 mg, 85%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.97 - 7.95 (*d*, $^3J_{H,H}$ = 8 Hz, 1H; Ar-H), δ = 7.93 (*s*, 1H; Ar-H), δ = 7.91 - 7.89 (*m*, 2H; Ar-H), δ = 7.59 - 7.54 (*m*, 2H; Ar-H), δ = 7.51 - 7.49 (*d*, $^3J_{H,H}$ = 8 Hz, 1H; Ar-H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 144.4 (*dm*, $^1J_{F,C}$ = 253 Hz), 140.6 (*dm*, $^1J_{F,C}$ = 256 Hz), 138.0 (*dm*, $^1J_{F,C}$ = 252 Hz), 133.4, 133.1, 130.2, 128.5, 128.4, 127.8, 127.3, 127.1, 126.8, 123.8, 116.1 (*td*, $^2J_{F,C}$ = 17 Hz, $^3J_{F,C}$ = 4); **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -162.1 (*m*, 2F), -155.4 (*t*, $^3J_{F,F}$ = 21 Hz, 1F), -143.0 (*dd*, $^3J_{F,F}$ = 23 Hz, $^4J_{F,F}$ = 8 Hz, 2F); **GC-MS**: [t = 11.873 min] m/z: 294 $[M]^+$. Spectroscopic data match those in the literature.[S3]

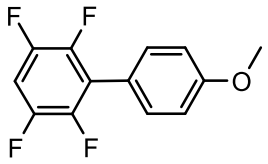
Synthesis of 2,3,4,4',5,6-hexafluoro-1,1'-biphenyl (3h)



Compound **3h** was synthesized following the general procedure and using the following chemicals and conditions: C_6F_5H (**1a**) (101 mg, 0.60 mmol), 2-(4-fluorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2h**) (102 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (139 mg, 0.60 mmol, 1.5 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3h** was obtained as a white solid (53 mg, 50%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.46 - 7.37 (*m*, 2H; Ar-H), δ = 7.26 – 7.13 (*m*, 2H; Ar-H); **^{13}C{^{1}H} NMR** (126 MHz, CDCl3) δ = 163.3 (*d*, $^{1}J_{F,C}$ = 250 Hz), 144.3 (*dm*, $^{1}J_{F,C}$ = 248 Hz), 140.6 (*dm*, $^{1}J_{F,C}$ = 254 Hz), 138.0 (*dm*, $^{1}J_{F,C}$ = 251 Hz), 132.2 (*dt*, $^{2}J_{F,C}$ = 8 Hz, $^{3}J_{F,C}$ = 2 Hz), 122.4, 116.1 (*d*, $^{2}J_{F,C}$ = 22 Hz), 115.1 (*td*, $^{2}J_{F,C}$ = 17 Hz, $^{3}J_{F,C}$ = 4 Hz); **^{19}F NMR** (188 MHz, $CDCl_3$) δ = -162.0 (*m*, 2F), -155.2 (*t*, $^{3}J_{F,F}$ = 21 Hz, 1F), -143.3 (*m*, 2F), -111.3 (*m*, 1F); **GC-MS**: [t = 8.413 min] m/z: 262 $[M]^+$. Spectroscopic data match those in the literature.[S1]

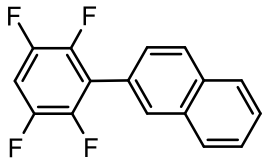
Synthesis of 2,3,5,6-tetrafluoro-4'-methoxy-1,1'-biphenyl (3i)



Compound **3i** was synthesized following the general procedure and using the following chemicals and conditions: 1,2,4,5-tetrafluorobenzene (**1b**) (90 mg, 0.60 mmol), 2-(4-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**3i**) (102 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (93 mg, 0.40 mmol, 1 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3f** was obtained as a white solid (70 mg, 68%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.42 – 7.40 (*d*, $^{3}J_{H,H}$ = 9 Hz, 2H; Ar-H), 7.05 – 7.02 (*m*, 3H; Ar-H), 3.87 (*s*, 3H, CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 160.2, 146.4 (*dm*, $^{1}J_{F,C}$ = 247 Hz), 143.9 (*ddt*, $^{1}J_{F,C}$ = 246 Hz, $^{2}J_{F,C}$ = 14 Hz, $^{3}J_{F,C}$ = 4 Hz), 131.6 (*t*, $^{4}J_{F,C}$ = 2 Hz), 121.4 (*t*, $^{2}J_{F,C}$ = 16), 119.7 (*t*, $^{3}J_{F,C}$ = 2 Hz), 114.2, 104.4 (*t*, $^{2}J_{F,C}$ = 22 Hz), 55.4; **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -139.4 (*m*, 2F), -144.3 (*m*, 2F); **GC-MS**: [t = 10.456 min] m/z: 256 $[M]^+$. Spectroscopic data match those in the literature.[S4]

Synthesis of 2-(2,3,5,6-tetrafluorophenyl)naphthalene (3j)



Compound **3j** was synthesized following the general procedure and using the following chemicals and conditions: 1,2,4,5-tetrafluorobenzene (**1b**) (90 mg, 0.60 mmol), 2-(4-naphthyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2j**) (102 mg, 0.40 mmol), $Pd(OAc)_2$ (4 mg, 0.02 mmol, 5 mol%), Ag_2O (93 mg, 0.40 mmol, 1 equiv.), and DMF (3 mL), 100 °C, 15 h. After column chromatography (hexane), product **3f** was obtained as a white solid (73 mg, 66%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.99 - 7.98 (*m*, 2H; Ar-H), 7.91 (*d*, $^3J_{H,H}$ = 8 Hz, 2H; Ar-H) 7.59 - 7.54 (*m*, 3H; Ar-H), 7.14 - 7.07 (*m*, 1H; Ar-H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 146.4 (*dm*, $^1J_{F,C}$ = 248 Hz), 144.0 (*ddt*, $^1J_{F,C}$ = 247 Hz, $^2J_{F,C}$ = 14 Hz, $^3J_{F,C}$ = 4 Hz), 133.3, 133.1, 130.1 (*t*, $^3J_{F,C}$ = 2 Hz), 128.4, 128.3, 127.8, 127.1 (*m*), 126.7, 121.6 (*t*, $^2J_{F,C}$ =16 Hz), 105.0 (*t*, $^2J_{F,C}$ = 23 Hz); **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -143.6 - -143.7 (*m*, 2F), δ = -139.0 - -139.1 (*m*, 2F); **GC-MS**: [t = 12.122 min] m/z: 278 $[M]^+$. Spectroscopic data match those in the literature.[S5]

3. A Test for C-H activation of pentafluorobenzene with Pd/Ag catalyst

In air, into a Schlenk tube equipped with stirring bar was added C_6F_5H (0.4 mmol), $Pd(OAc)_2$ (50 mol%), Ag_2O (0.4 mmol) and DMF (4mL) then the vial was capped with stopper. The suspension was then stirred at 100 °C for 15 h. After cooling to room temperature, the solution was monitored by ^{19}F NMR spectroscopy. The ^{19}F NMR

spectrum of the reaction mixture is shown below, indicating the formation of *cis*-[Pd(DMF)$_2$(C$_6$F$_5$)$_2$] (δ = -115.9, -162.7, and -165.2). However, we did not see any chemical shifts typical of Ag-C$_6$F$_5$ complexes. For example, the ^{19}F NMR chemical shifts for [Ag(Xphos)(C$_6$F$_5$)] are δ = -106.9 to -107.1 (2F), -161.5 (1F), and -163.4 to -163.3 (2F).[S6]

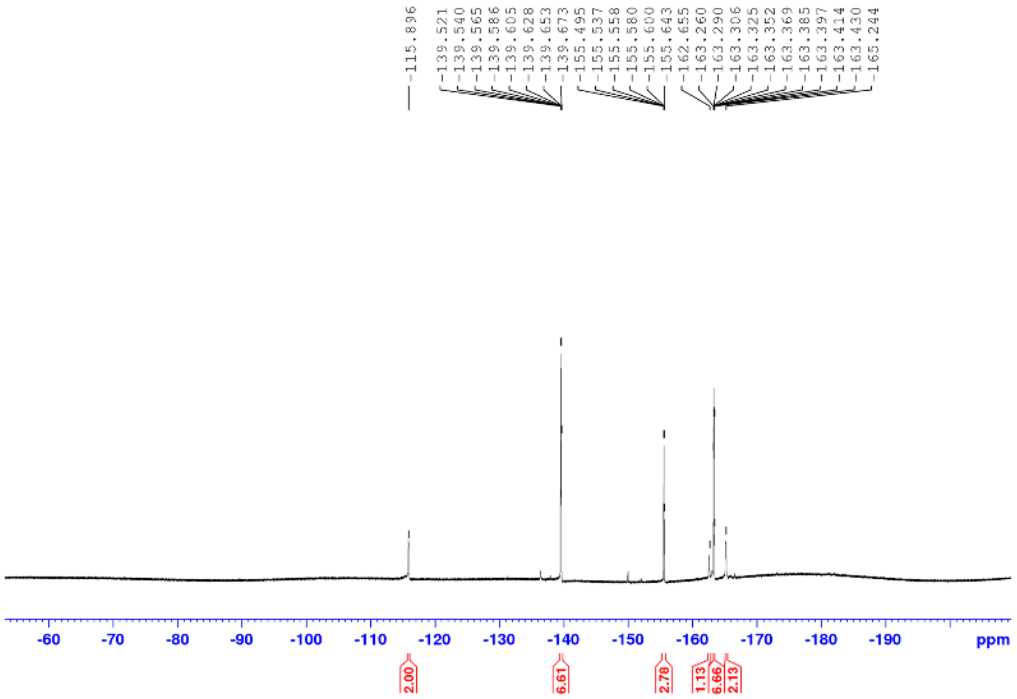
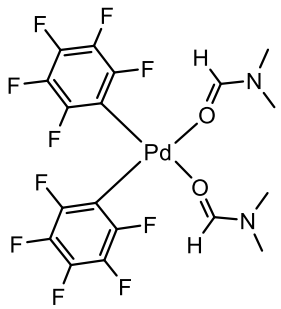


Figure S1. ^{19}F NMR spectrum of the reaction between C$_6$F$_5$H, Pd(OAc)$_2$, and Ag$_2$O, in DMF.

4. Attempt to Isolate *cis*-[Pd(DMF)$_2$(C$_6$F$_5$)$_2$] (5a)



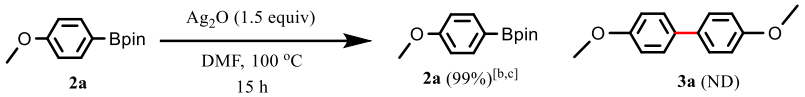
In air, into a dried vial containing 5 mL of DMF solvent and equipped with a stirring bar was added Pd(OAc)$_2$ (45 mg, 0.20 mmol) and the mixture was stirred until homogenous.

Then, C_6F_5H (50 mg, 0.6 mmol) and Ag_2O (139 mg, 0.60 mmol) were added to the solution and the vial was sealed. The suspension was then stirred at 80 °C for 16 h. After cooling to room temperature, the insoluble material was filtered through nylon syringe filter. The DMF solvent was evaporated under reduced pressure at 40 °C. Then the residue was diluted with DCM and the precipitate was removed via filtration and the filtrate was evaporated in air at room temperature until dry. The resulting solid was collected to give the product as a yellow sticky solid (87 mg, 74%). Colorless single crystals suitable for X-ray diffraction were grown via vapor diffusion of a DCM solution placed in a larger vessel containing toluene at room temperature.

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.71 (*s*, 2H, CHO), 2.96 (*s*, C*H*$_3$), 2.89 (*s*, CH_3); **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -164.0 (*m*, $4F_m$), -161.0 (*m*, $2F_p$), -117.7 – -116.9 (*m*, $4F_o$); **IR** (KBr, [cm^{-1}]) = 1660 ($\nu_{C=O,}$ DMF).

Due to the difficulty of finding a suitable solvent to separate unreacted $Pd(OAc)_2$ with **5a**, we were unable to obtain a good clean elemental analysis, and its poor solubility in organic solvents did not allow us to obtain a nice ^{13}C NMR spectrum. However, the trend in chemical shifts of signals in the ^{19}F NMR spectrum is similar to those of reported $[Pd(L)_2(C_6F_5)_2]$ *e.g.*, L = MeCN,[S7] THF,[S8] CO,[S8] NH_3[S9] *e.g.*, for *cis*-$[Pd(MeCN)_2(C_6F_5)_2]$, $^{19}F\{^1H\}$ NMR (376 MHz) δ = -117.6 – -117.7 (*m*, $4F_o$), -162.9 (*t*, $^3J_{F\text{-}F}$ = 19 Hz, $2F_p$), and -165.9 – -166.1 (*m*, $4F_m$).[S7]

5. Reaction of Ag_2O with 4-MeO-C_6H_4-Bpin (**2a**)[a]



2a **2a** (99%)[b,c] **3a** (ND)

[a]Reaction conditions: Into a Schlenk tube, was added **2a** (0.2 mmol), Ag_2O (1.5 equiv), and DMF (2 mL). Afterwards, the tube was capped, and the reaction was stirred for 15 h at 100 ˚C. After cooling to room temperature, the reaction mixture was injected into a GCMS with mesitylene as an internal standard to check the remaining amount of 4-MeO-C_6H_4-Bpin (**2a**). [b]GCMS of the reaction conducted in dry DMF and under inert atmosphere (Figure S2). [c]GCMS of the reaction conducted in wet DMF and in air (Figure S3).

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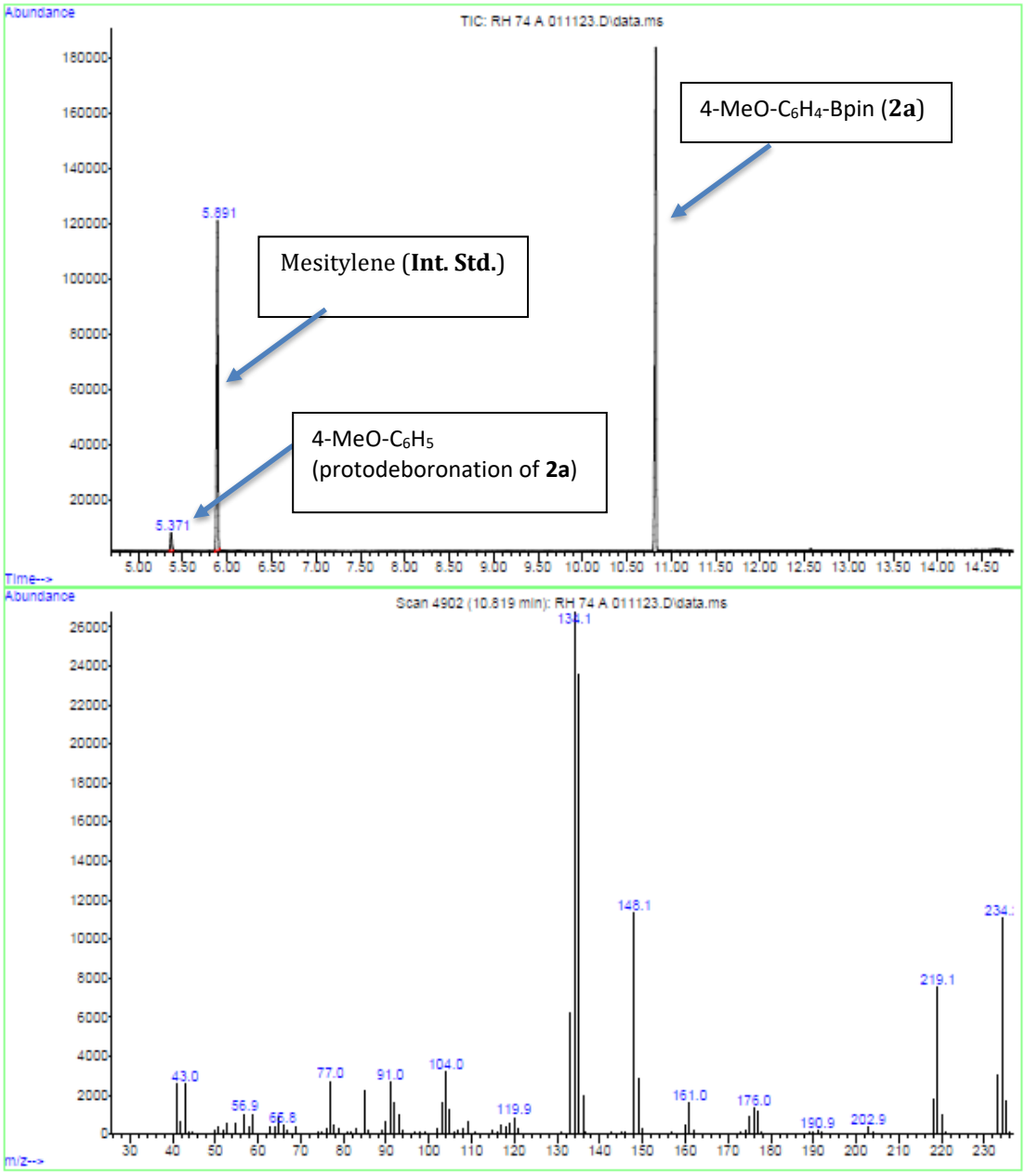


Figure S2. GCMS of a reaction mixture of Ag_2O with 4-MeO-C_6H_4-Bpin (**2a**) in anhydrous DMF under an inert atmosphere, using mesitylene as an internal standard.

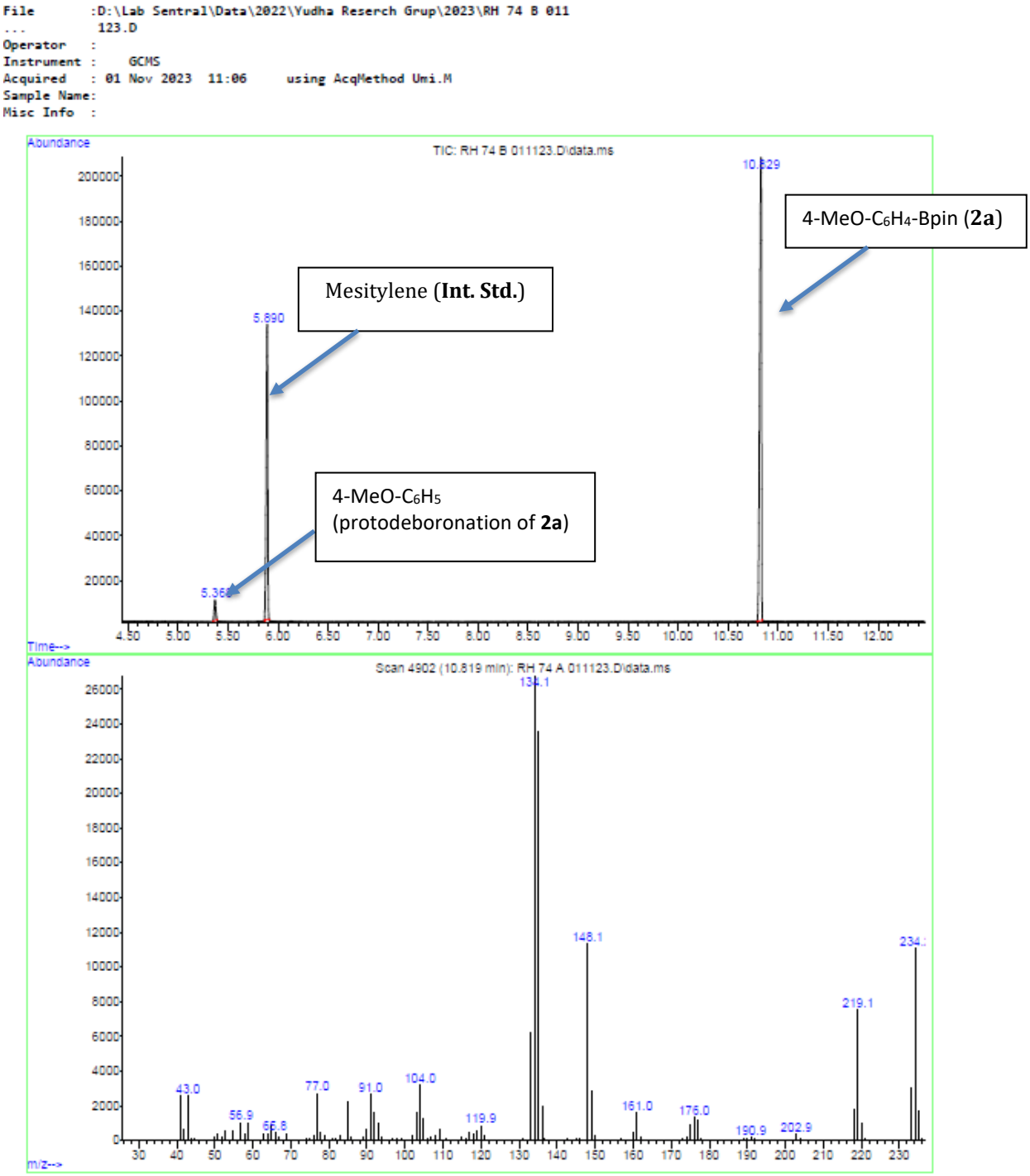


Figure S3. GCMS of a reaction mixture of Ag_2O with 4-MeO-C_6H_4-Bpin (**2a**) in wet DMF in air, using mesitylene as an internal standard.

6. Test for the Possibility of C–H Activation of C_6F_5H with Ag_2O

Into a J-Young's NMR tube wrapped in foil, under an N_2 atmosphere, were added C_6F_5H (0.2 mmol, 34 mg), Ag_2O (0.1 mmol, 23 mg) and dry DMF (1 mL). After sealing the tube, the reaction mixture was placed in an ultrasonic bath for 10 h. We repeated the reaction on a larger scale in a Schlenk tube: C_6F_5H (0.4 mmol, 67 mg), Ag_2O (0.2 mmol, 46 mg), and dry DMF (6 mL) at 100 °C, for 24 h. Afterwards, both reaction mixtures were examined by ^{19}F NMR spectroscopy, with no indication of the formation of an Ag-C_6F_5 complex; only C_6F_5H was observed.

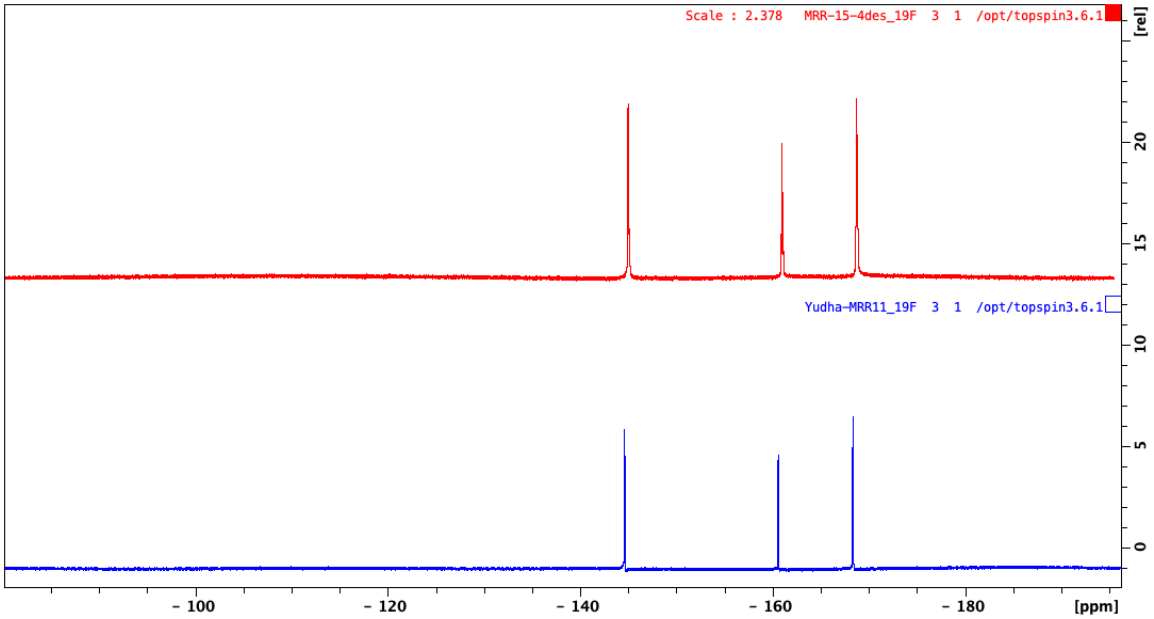
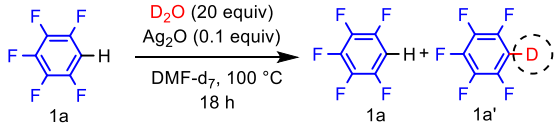


Figure S4. ^{19}F NMR spectra of the reaction mixture between C_6F_5H and Ag_2O, in DMF at room temperature (top) or 100 °C (bottom).

7. H/D exchange of C_6F_5H with D_2O in the presence of Ag_2O



Into a J. Youngs NMR tube, open to the air, were added C_6F_5H (179 µmol, 1.0 equiv), D_2O (3.58 mmol, 20.0 equiv), Ag_2O (17.9 µmol, 0.1 equiv), and DMF-d_7 (0.7 mL). After capping with a stopper, the reaction was heated at 100 °C, for 18 h. Afterwards, the reaction mixture was examined by ^{1}H, ^{2}H, $^{13}C\{^{19}F\}$, and ^{19}F NMR spectroscopy and GC-MS. C_6F_5D was observed in 87% conversion based on the *ortho*-F signal in the ^{19}F NMR spectrum. Notably, no indication of the formation of an Ag-C_6F_5 complex was observed.

Characterization data of C_6F_5D in the reaction mixture: **^{1}H NMR** (500 MHz, DMF-d_7) δ = 7.75; **^{2}H NMR** (500 MHz, DMF-d_7) δ = 7.76; **^{13}C{^{19}F} NMR** (125 MHz, DMF-$_{d7}$) δ = 146.7, 141.8, 138.0, 102.1 (*t*, $^{1}J_{C,D}$ = 26 Hz); **^{19}F NMR** (470 MHz, $CDCl_3$) δ = -140.4 (*m*, $2F_o$), -156.3 (*m*, $2F_p$), -164.1 (*m*, $1F_m$); **GC-MS**: [t = 0.78 min] m/z: 169 $[M]^+$.

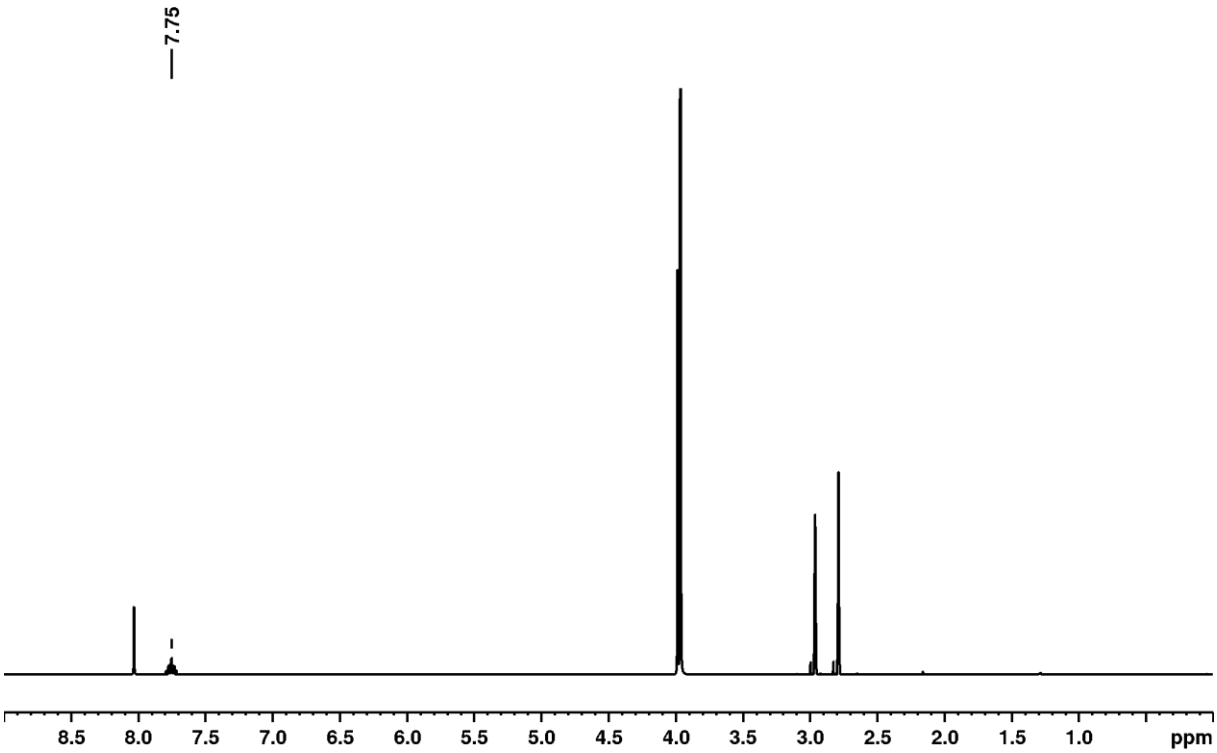


Figure S5: ^{1}H NMR spectrum (500.1 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C.

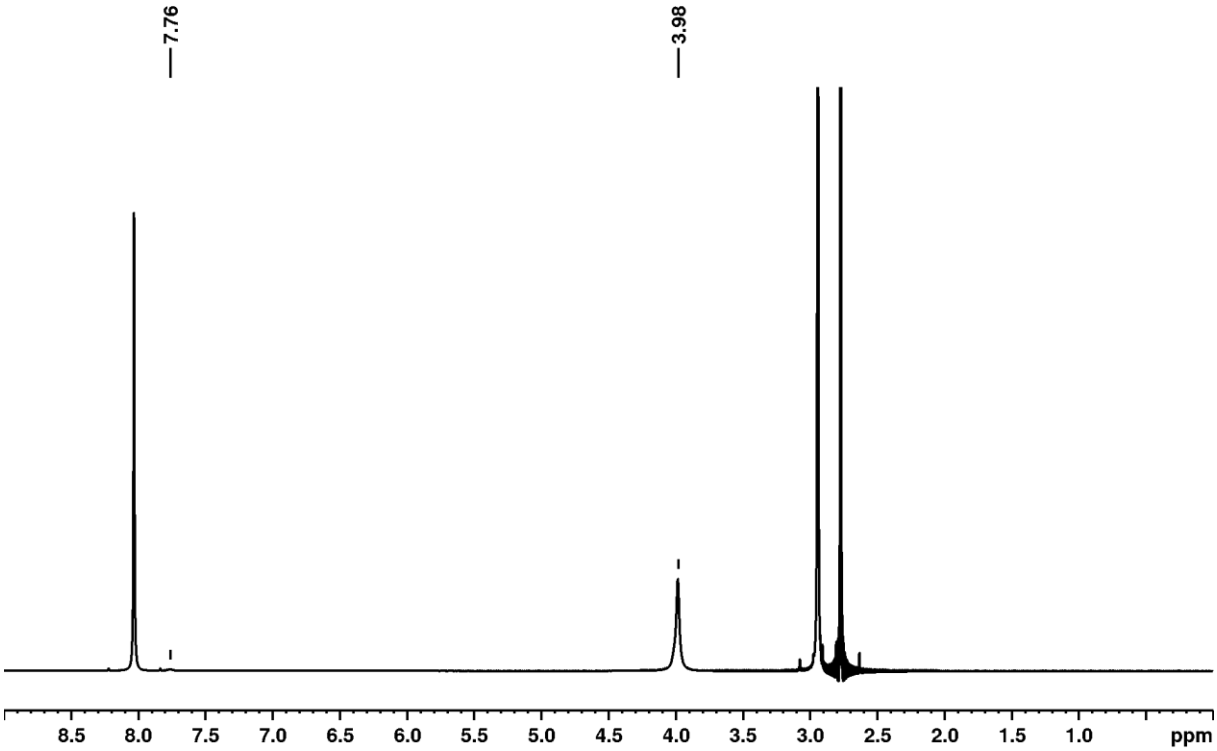


Figure S6: ^{2}H NMR spectrum (76.8 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C.

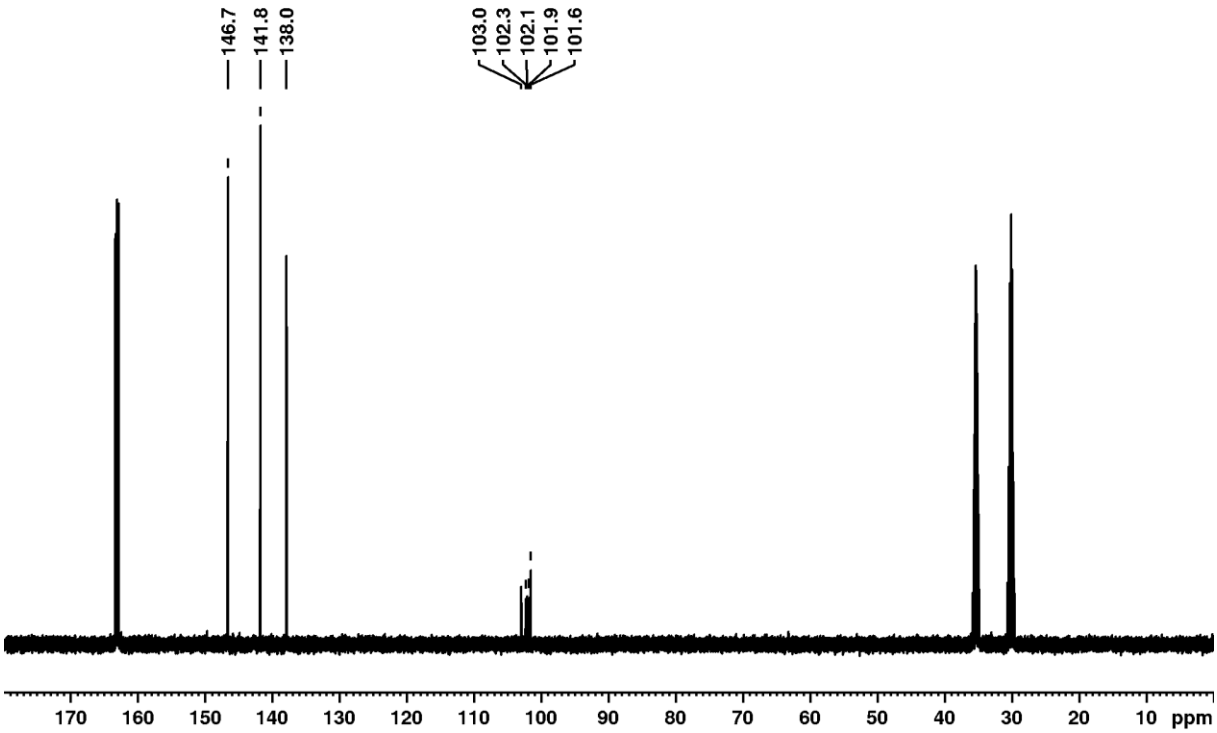


Figure S7: $^{13}C\{^{19}F\}$ NMR spectrum (125.8 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C.

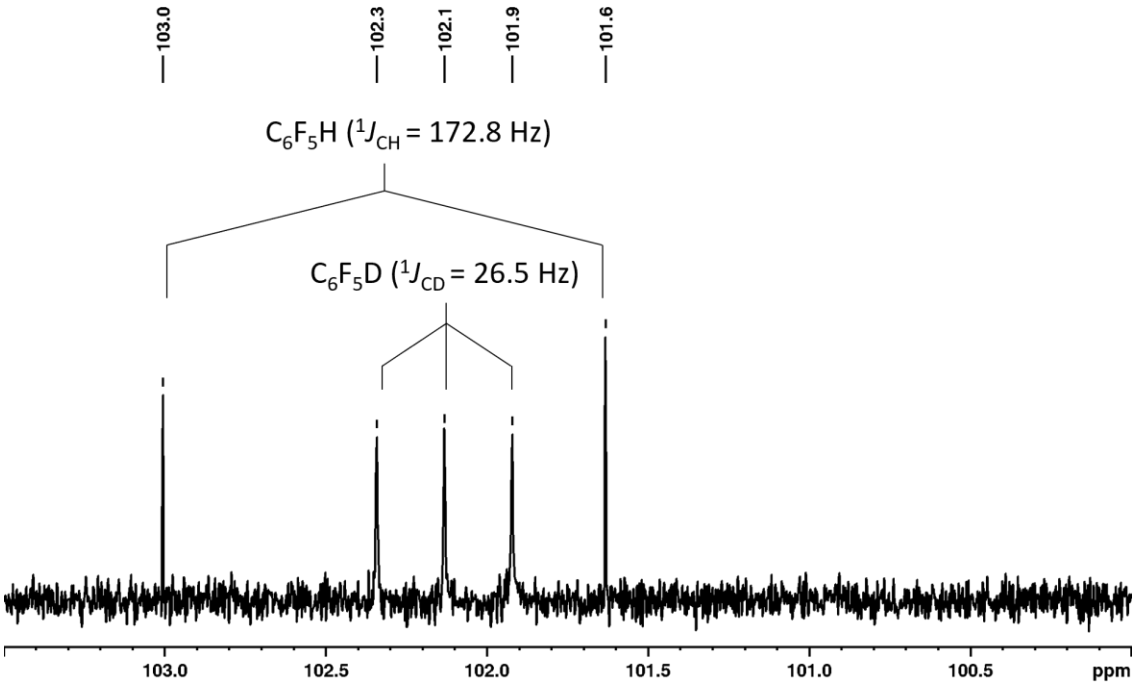


Figure S8: Excerpt from the $^{13}C\{^{19}F\}$ NMR spectrum (125.8 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C with coupling constants.

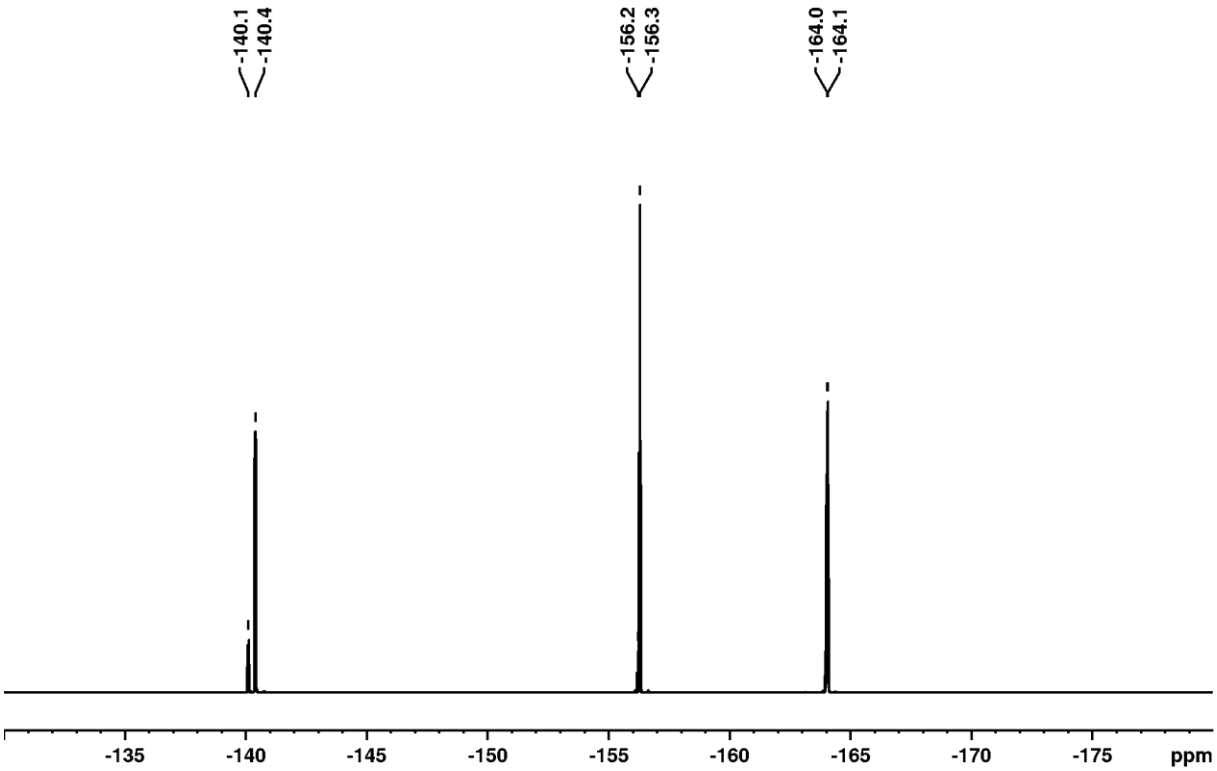


Figure S9: ^{19}F NMR spectrum (470.6 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C.

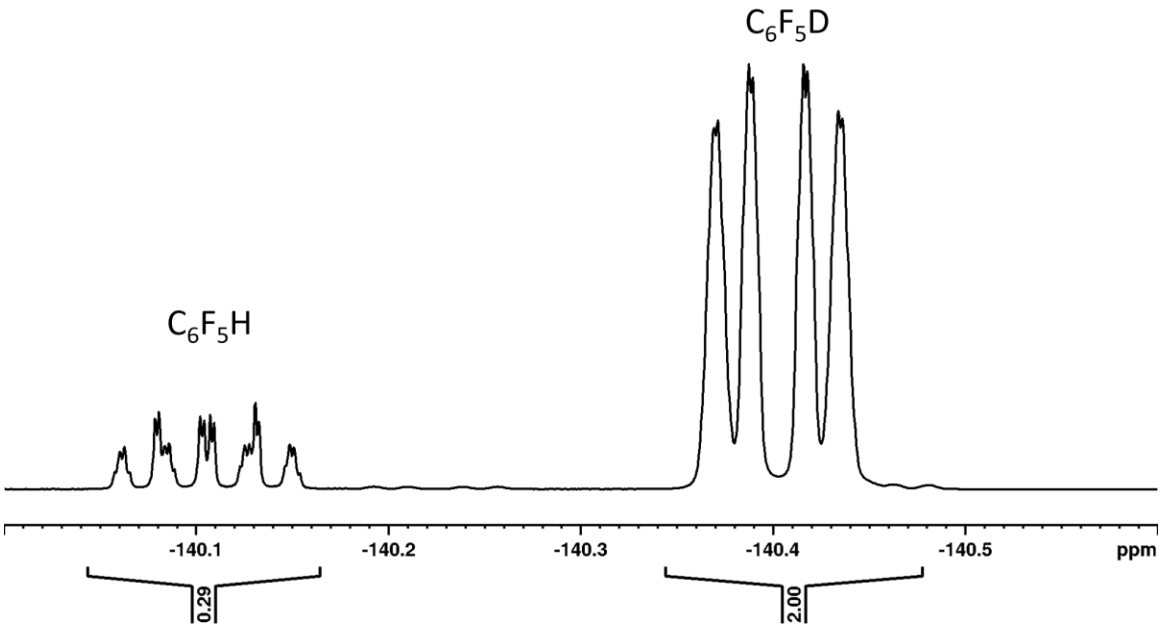


Figure S10: Excerpt from the ^{19}F NMR spectrum (470.6 MHz, DMF-d_7, 298 K) of the reaction mixture after 18 h at 100 °C.

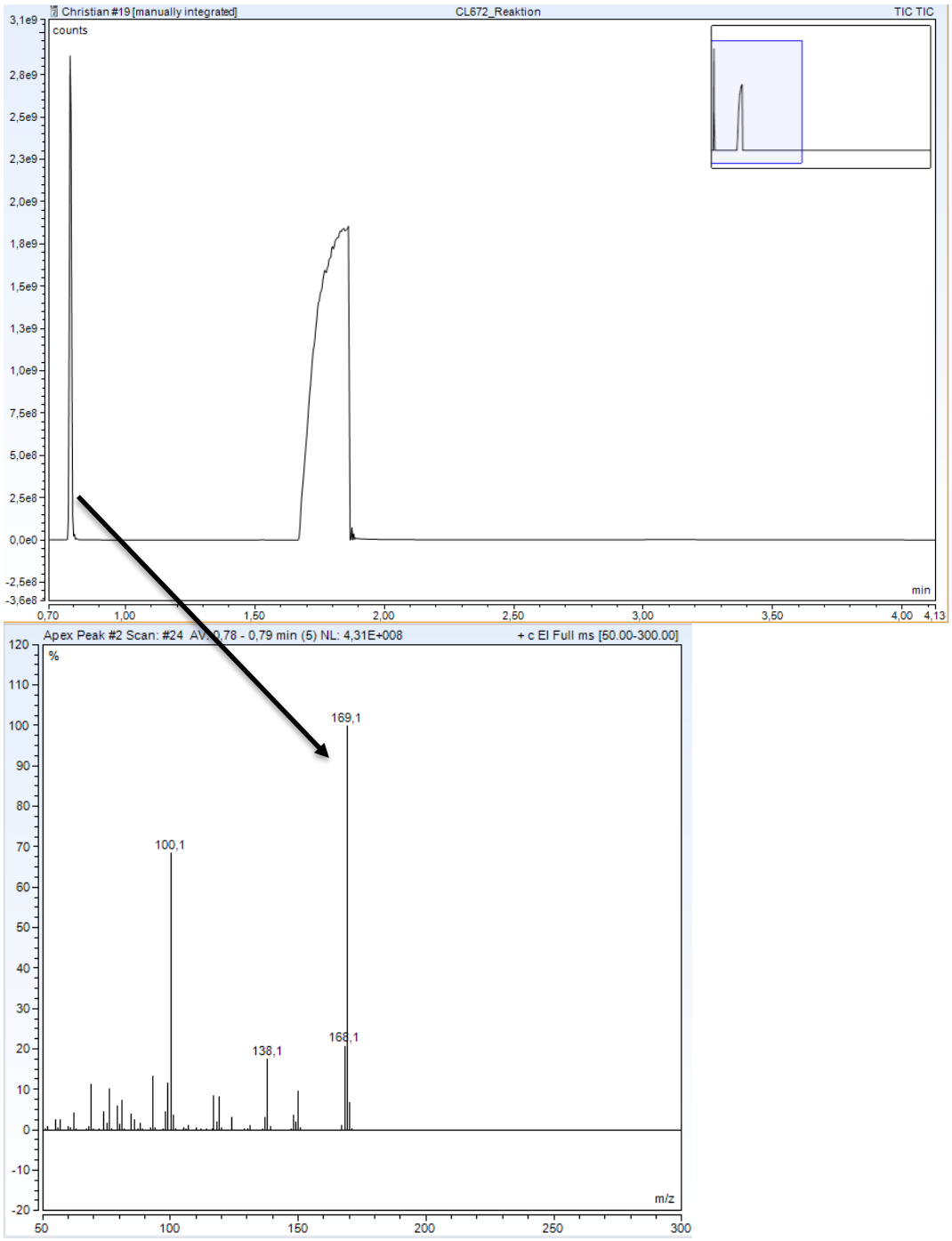


Figure S12: GC-MS spectrum of the reaction mixture after 18 h at 100 °C indicating the formation of of C_6F_5D.

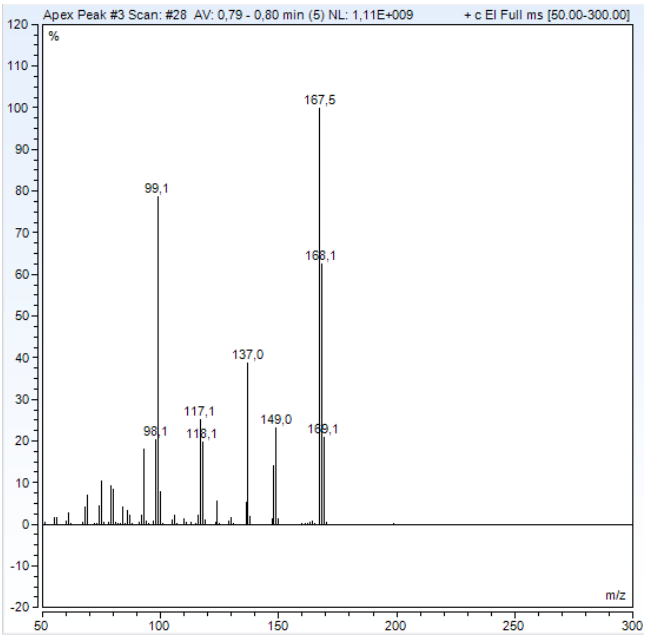


Figure S13: MS spectrum of C_6F_5H as a reference.

8. ^{1}H, $^{13}C\{^{1}H\}$, ^{19}F, $^{9}F\{^{1}H\}$, $^{11}B\{^{1}H\}$ NMR Spectra and GC-MS Data

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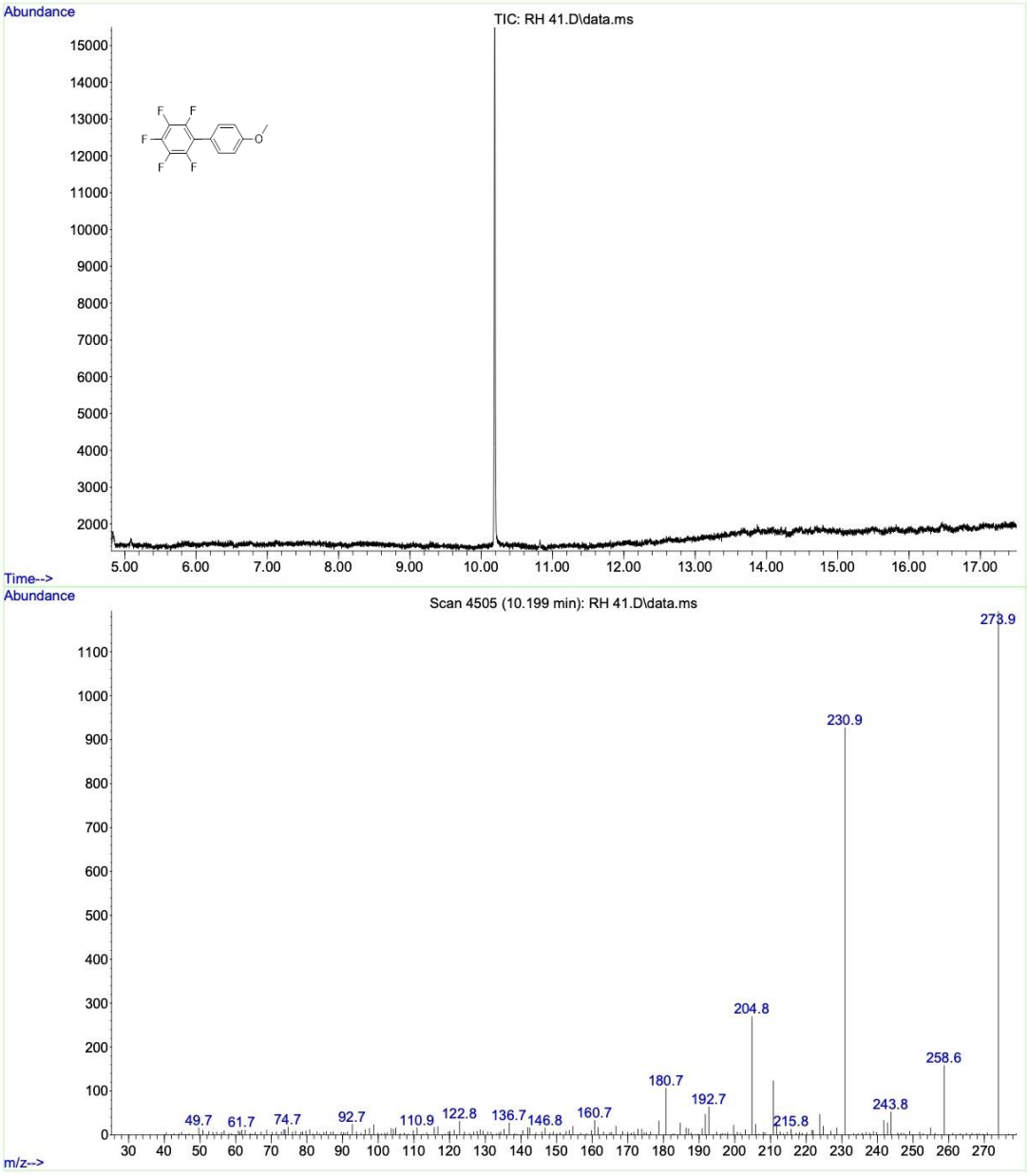
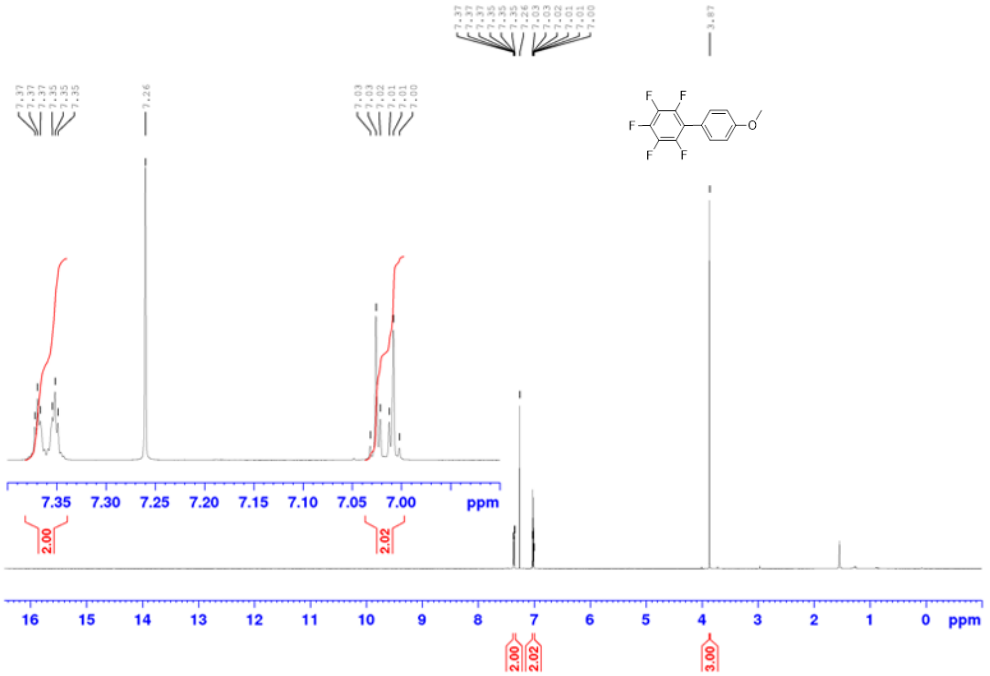
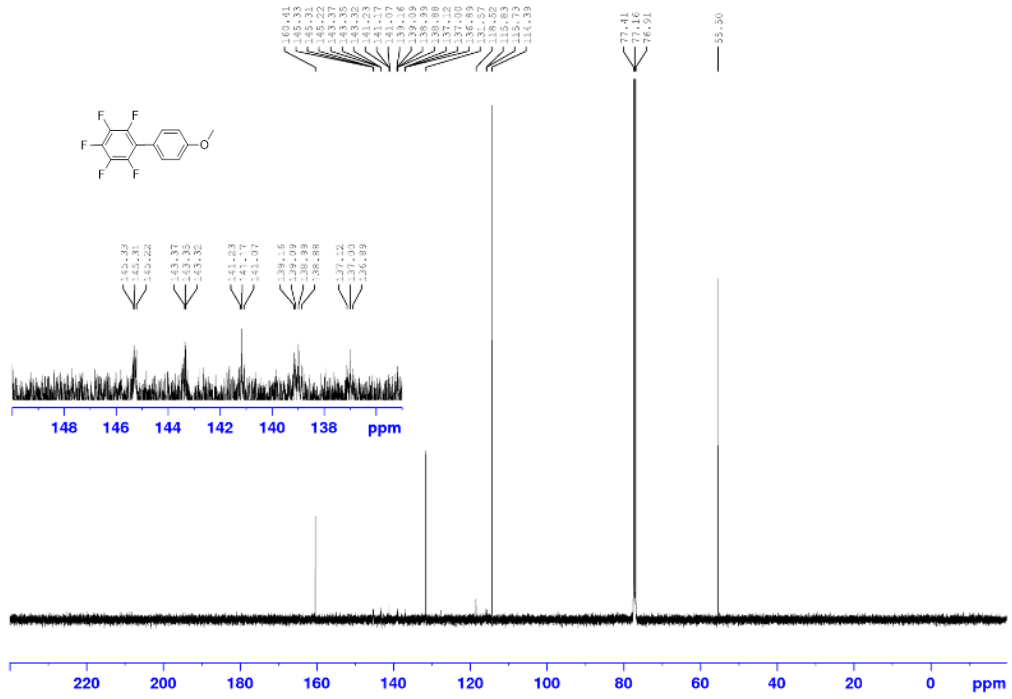


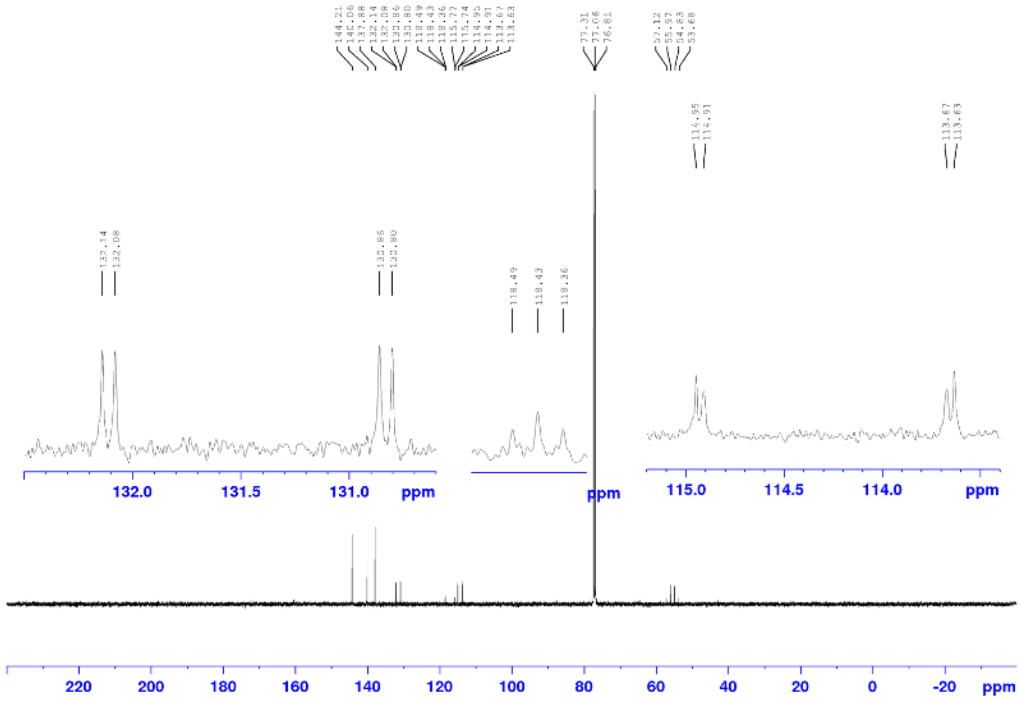
^{1}H NMR of 3a (500 MHz, $CDCl_3$)



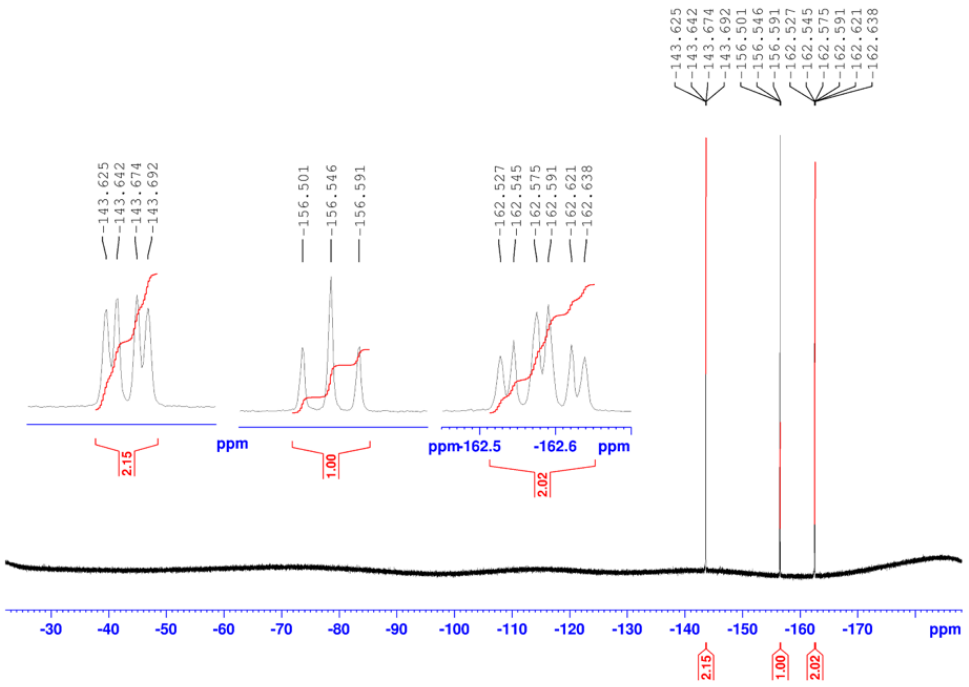
^{13}C{^{1}H} NMR of 3a (125 MHz, $CDCl_3$)



$^{13}C\{^{19}F\}$ NMR of 3a (125 MHz, $CDCl_3$)



^{19}F NMR of 3a (470 MHz, $CDCl_3$)



GC-MS of 3b

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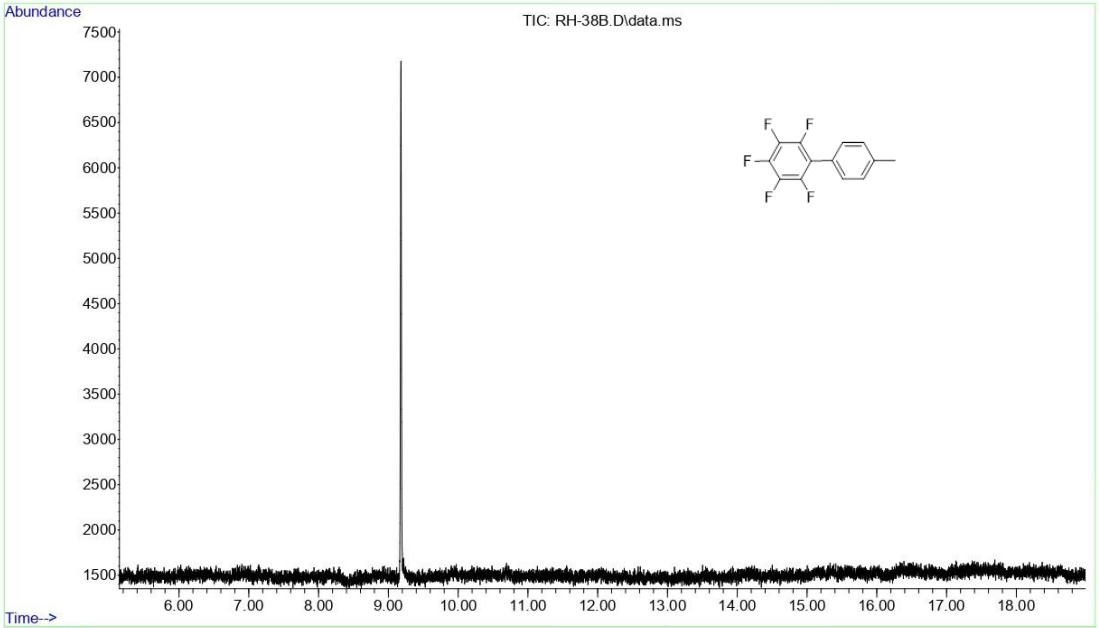
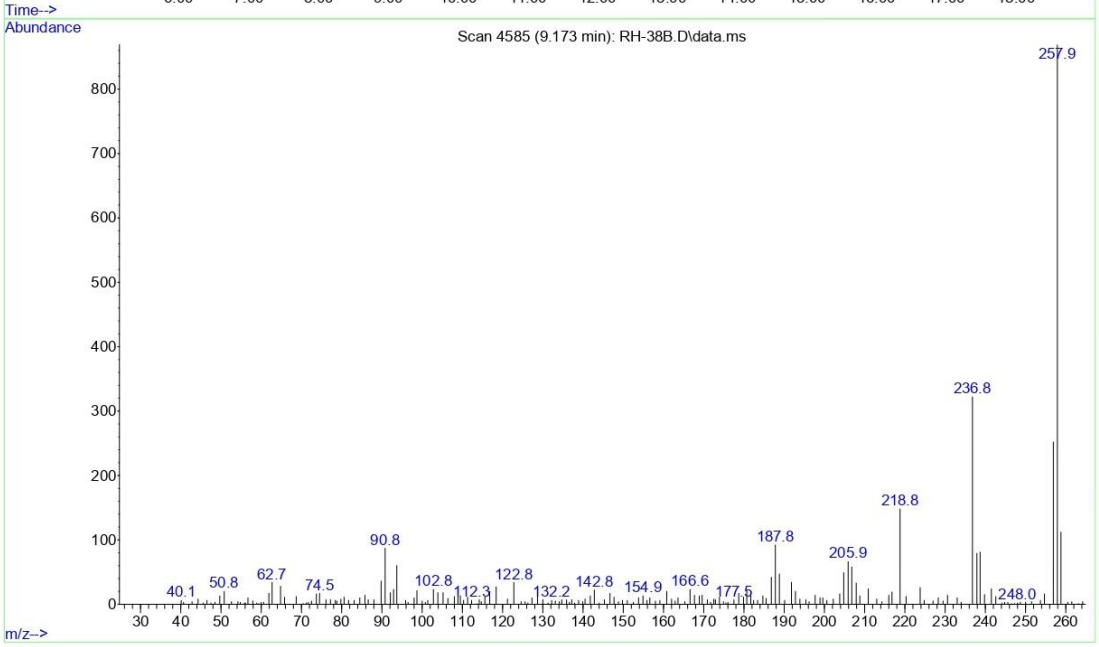
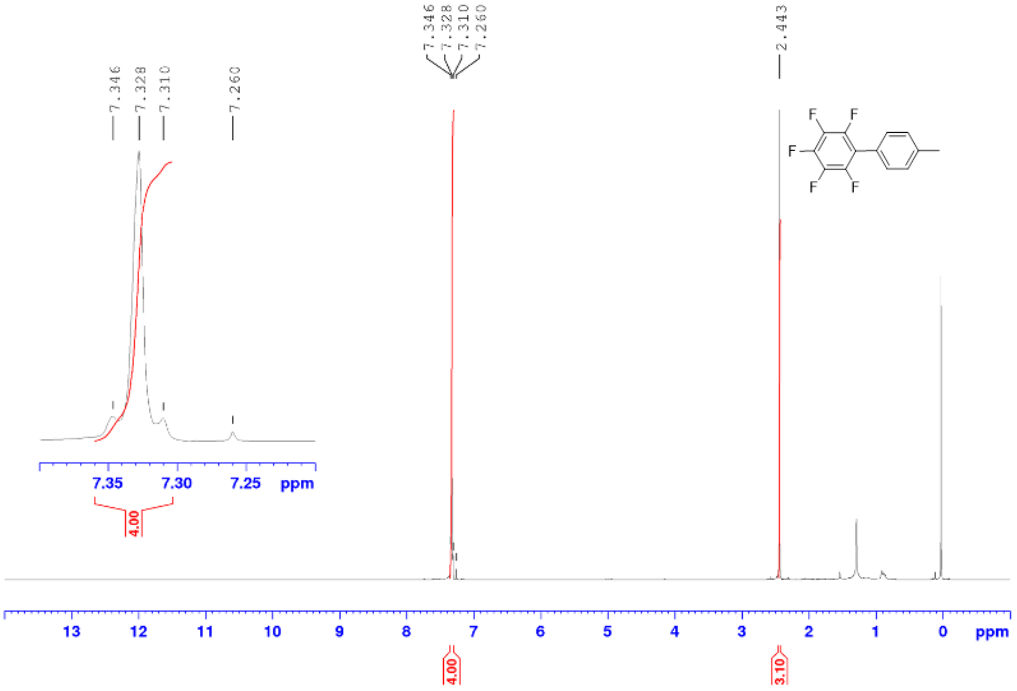
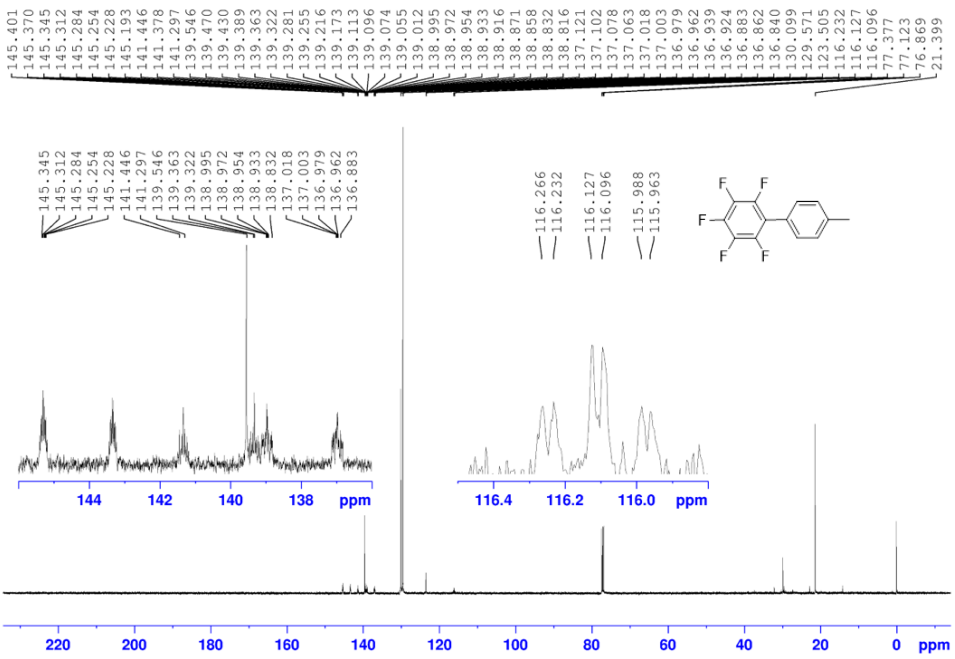




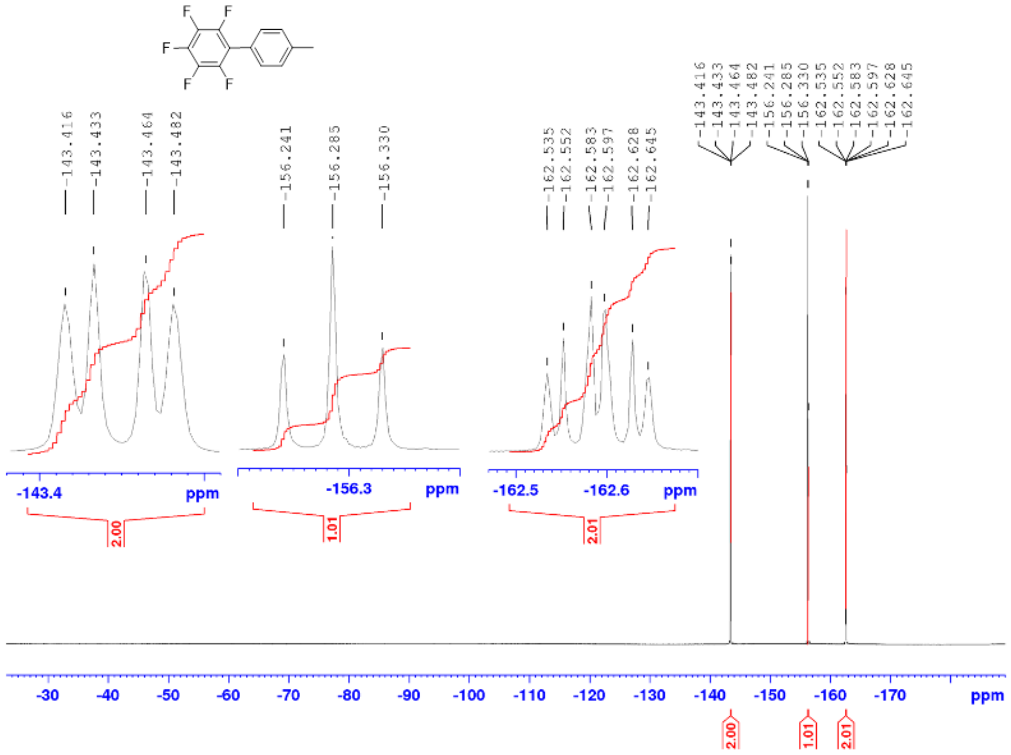
^{1}H NMR Spectrum of 3b (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3b (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3b (470 MHz, $CDCl_3$)



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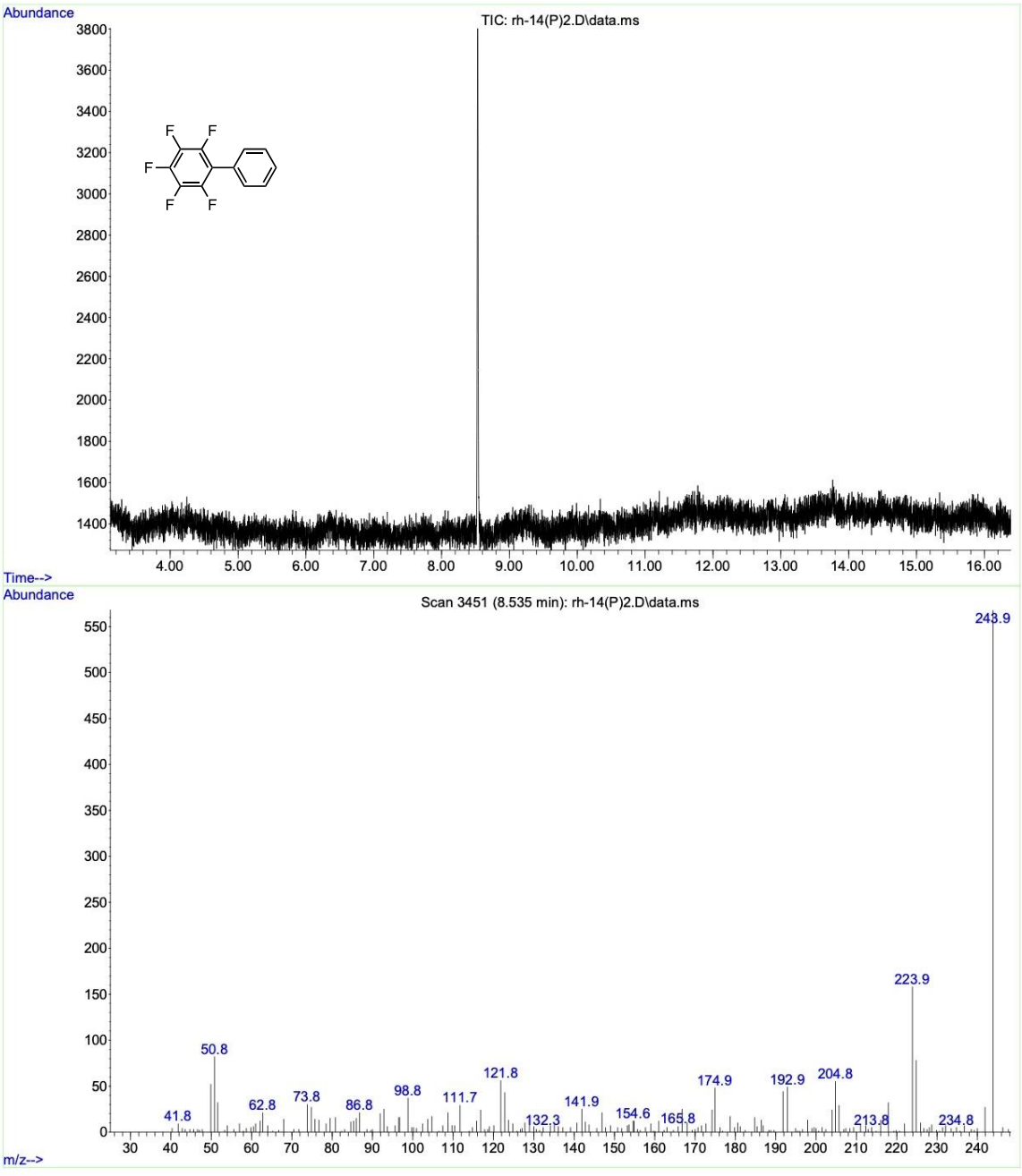
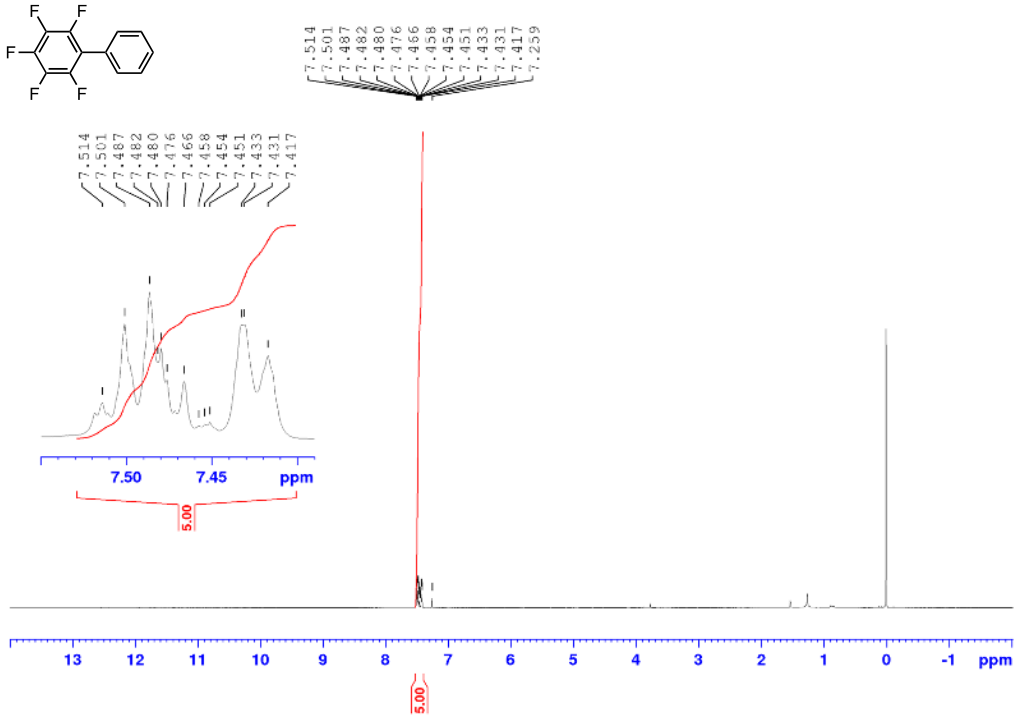
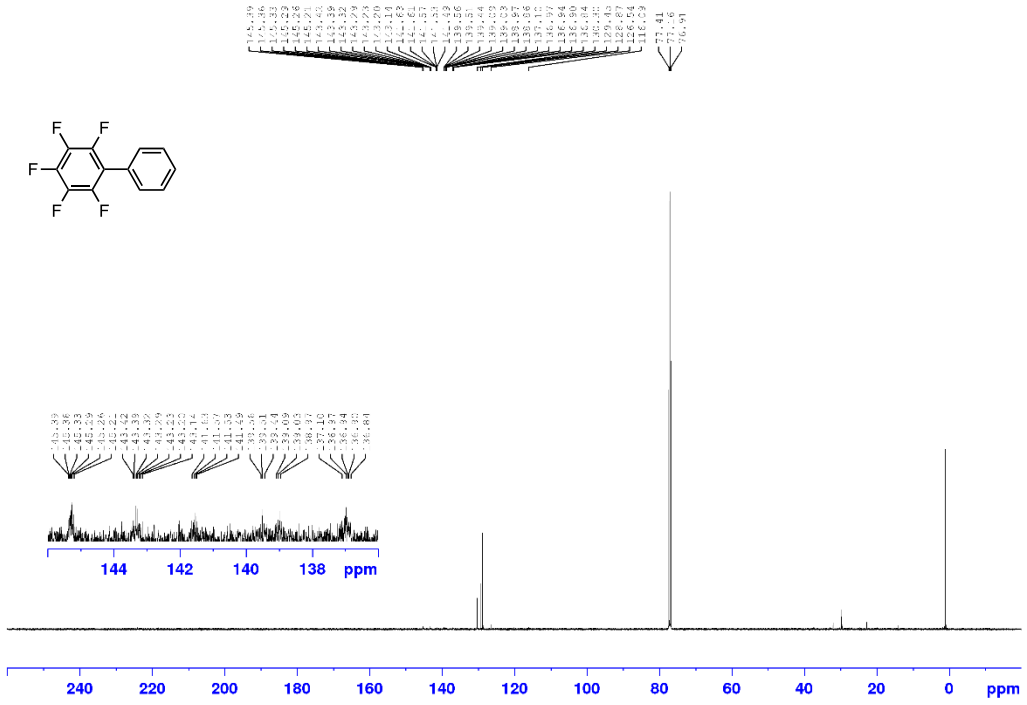


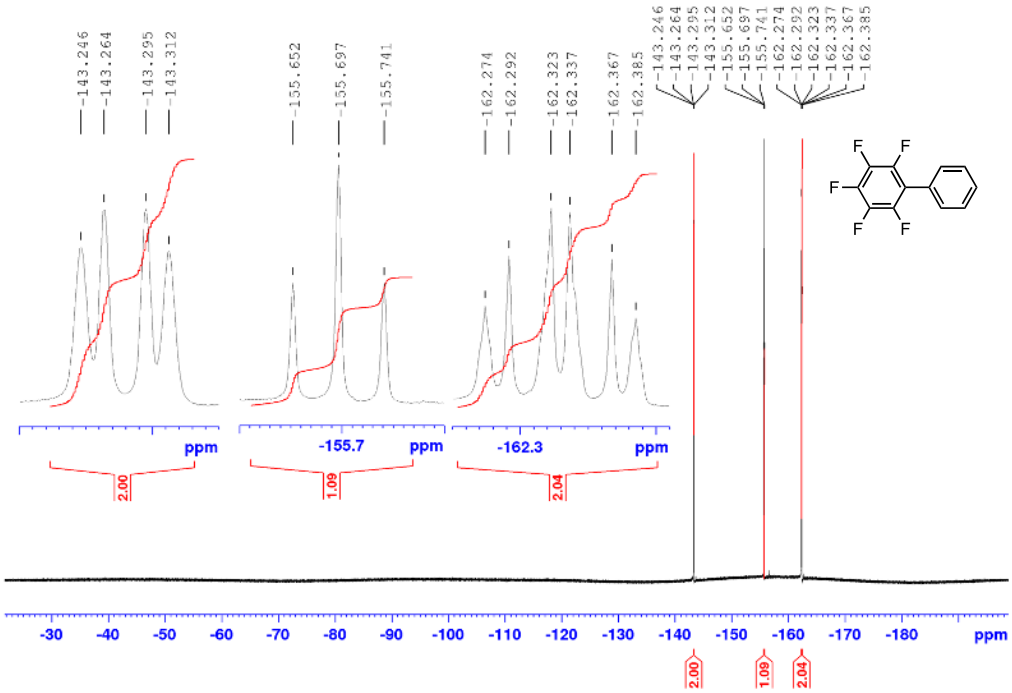
^{1}H NMR Spectrum of 3c (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3c (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3c (470 MHz, $CDCl_3$)



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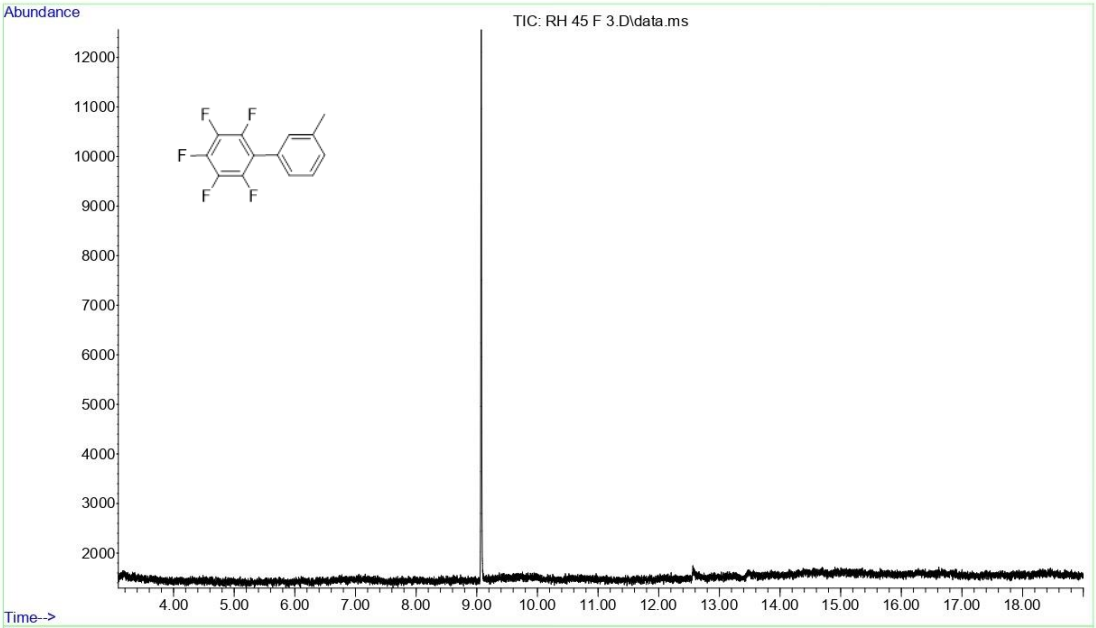
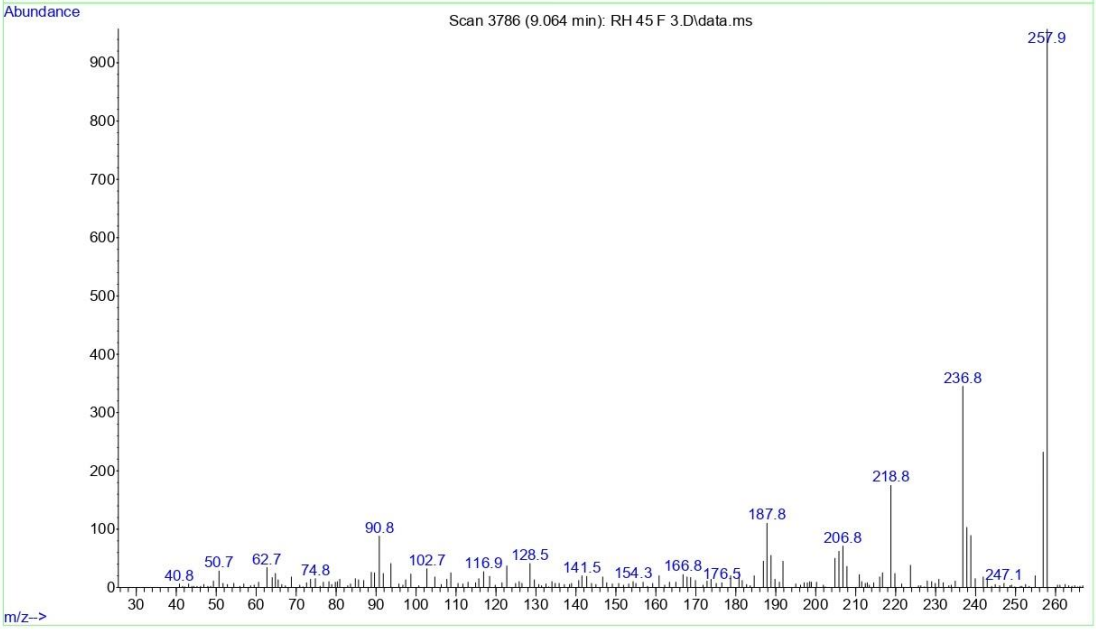
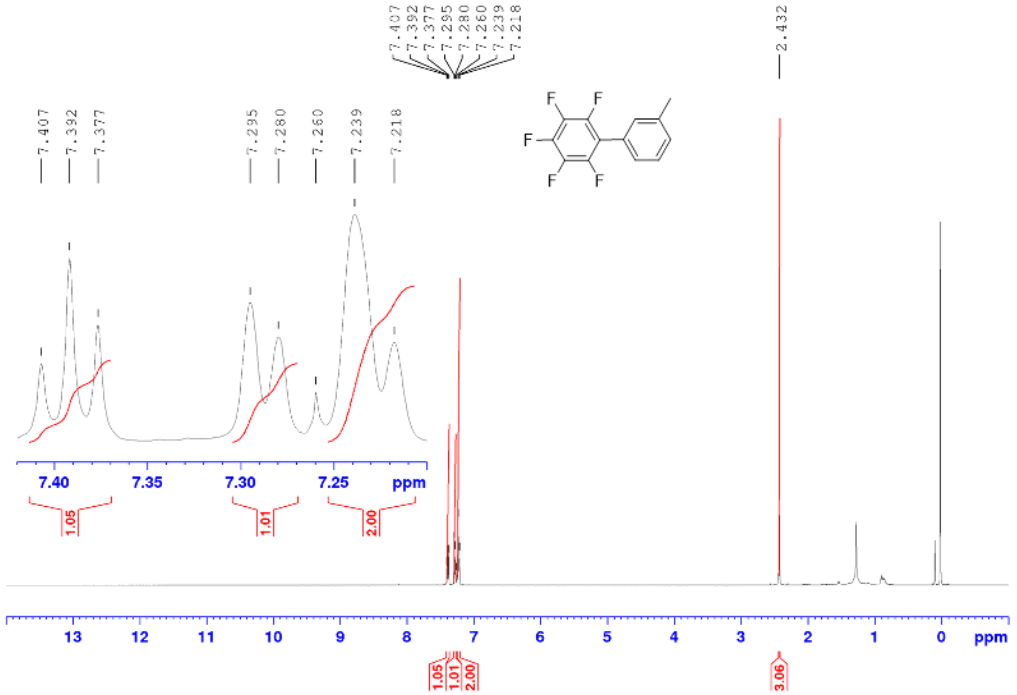
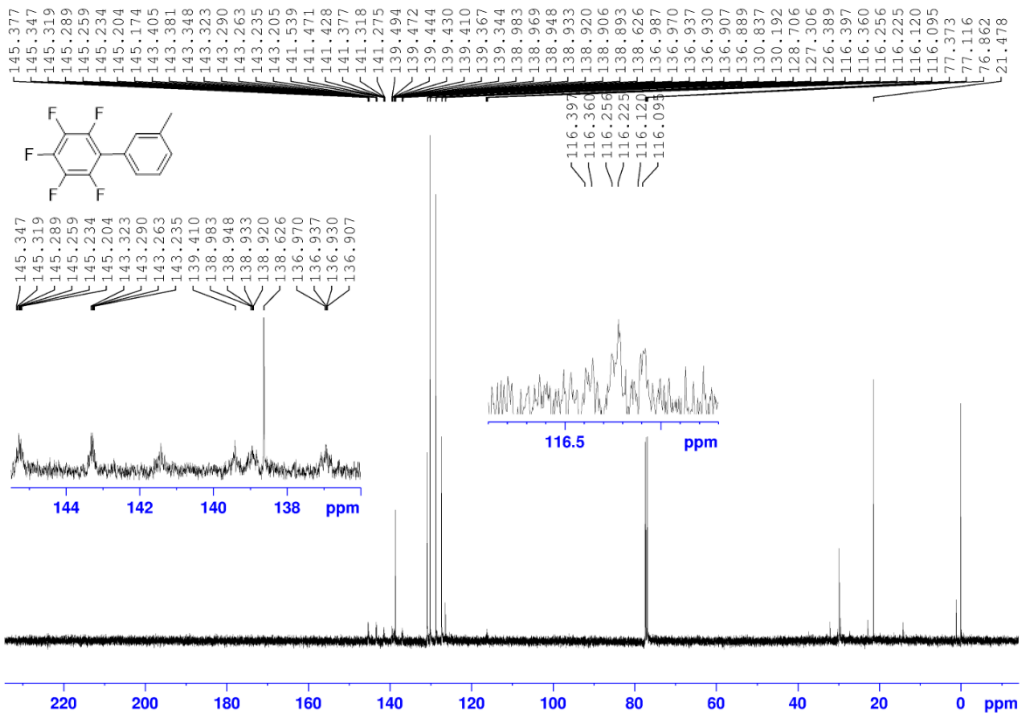




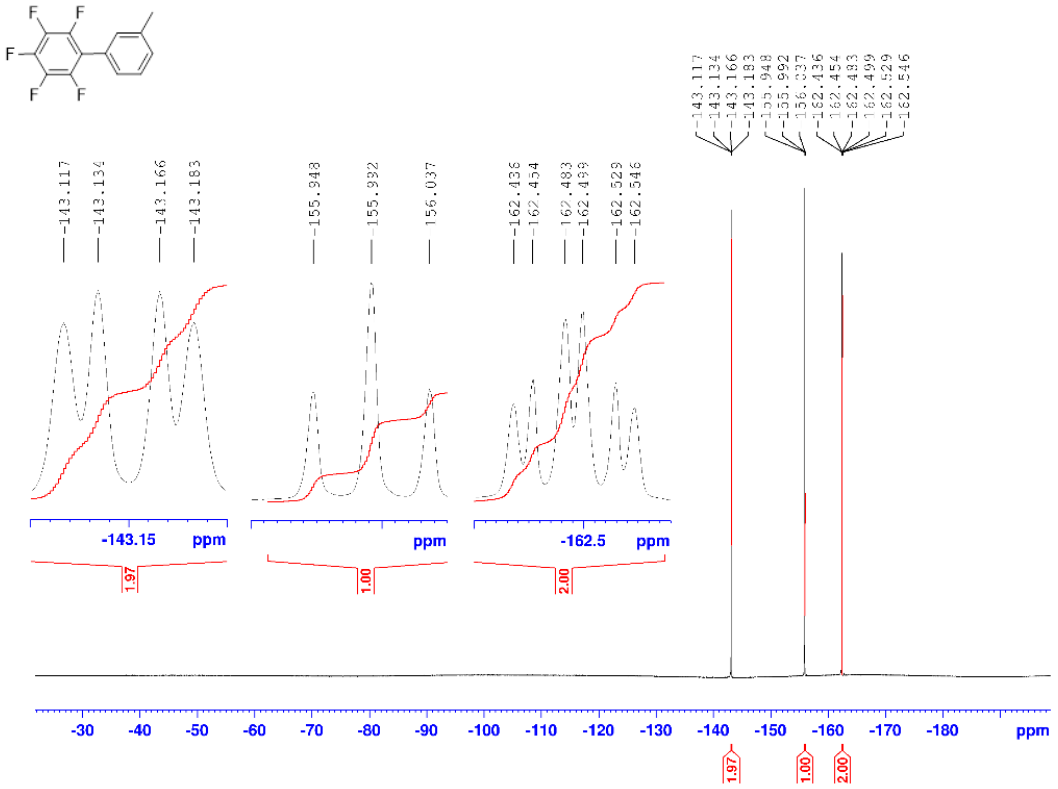
^{1}H NMR Spectrum of 3d (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3d (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3d (470 MHz, $CDCl_3$)



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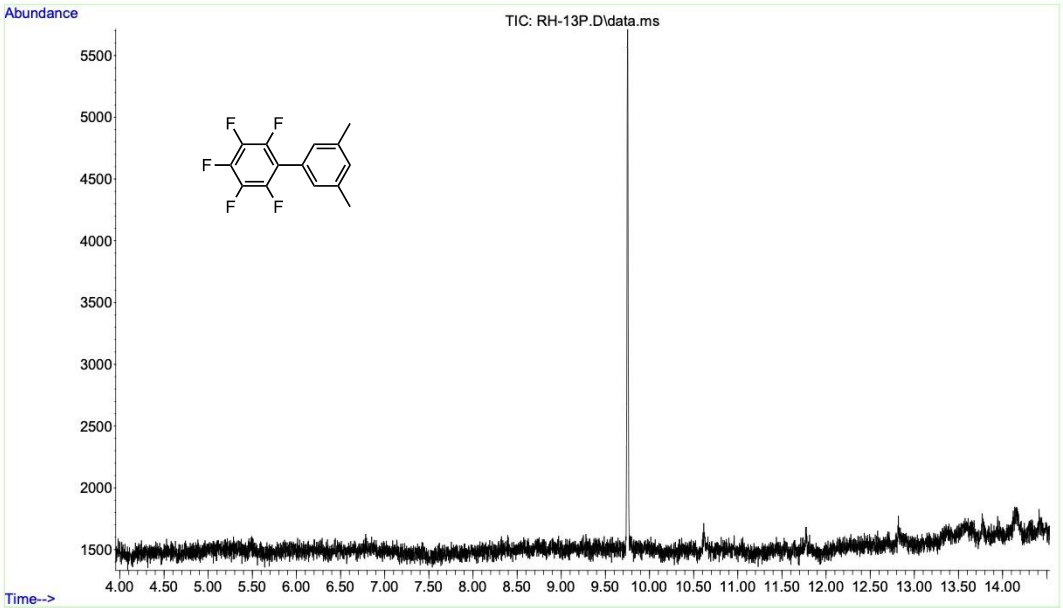
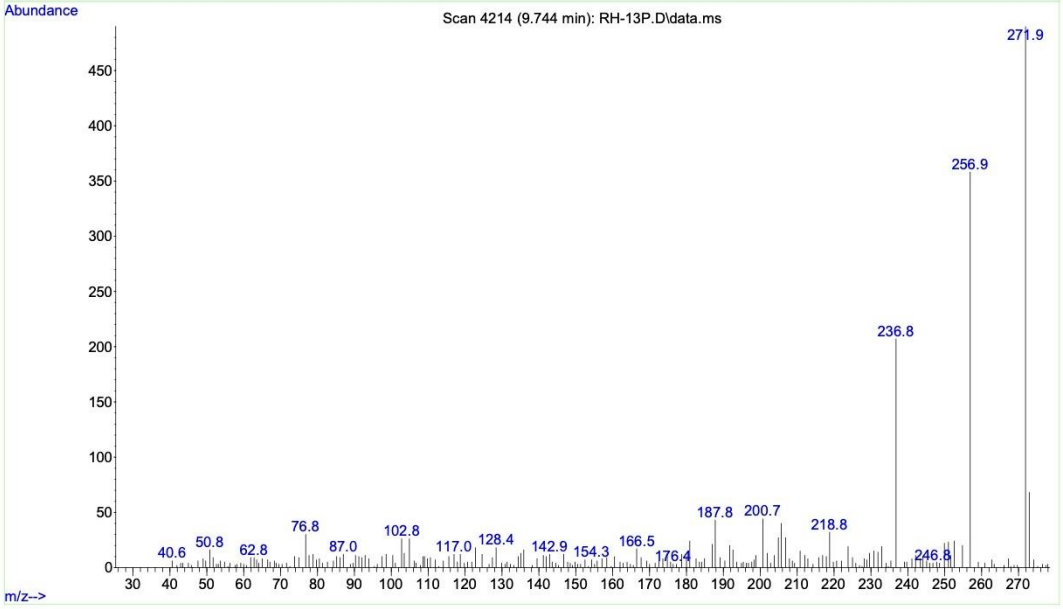
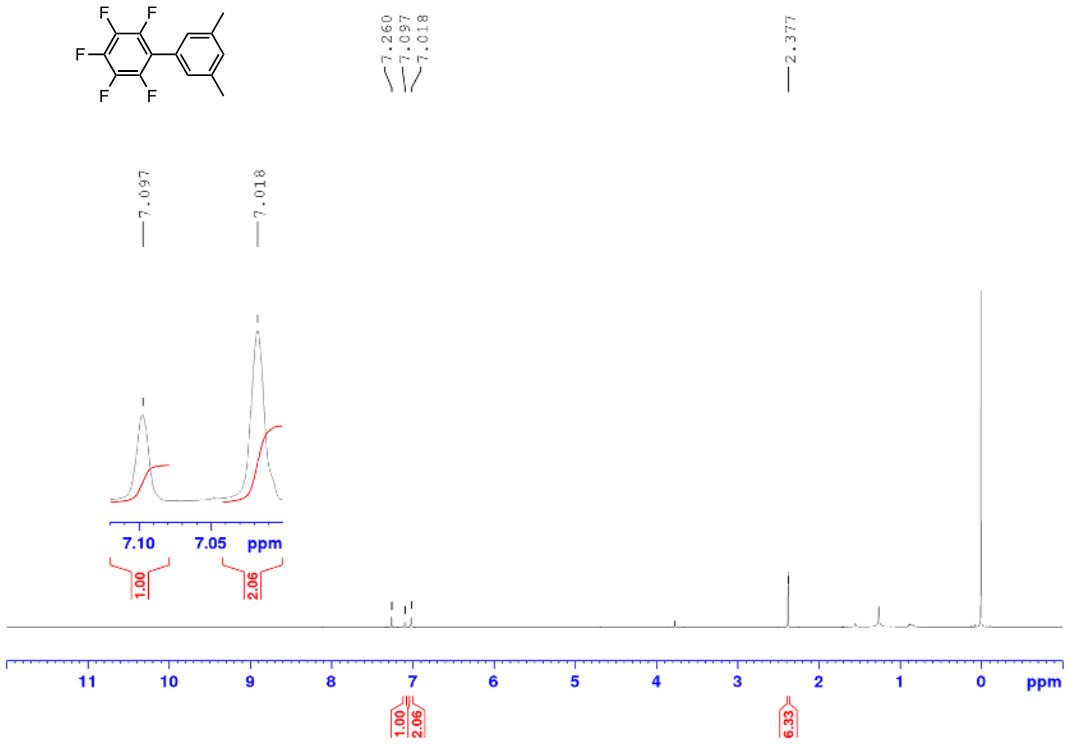
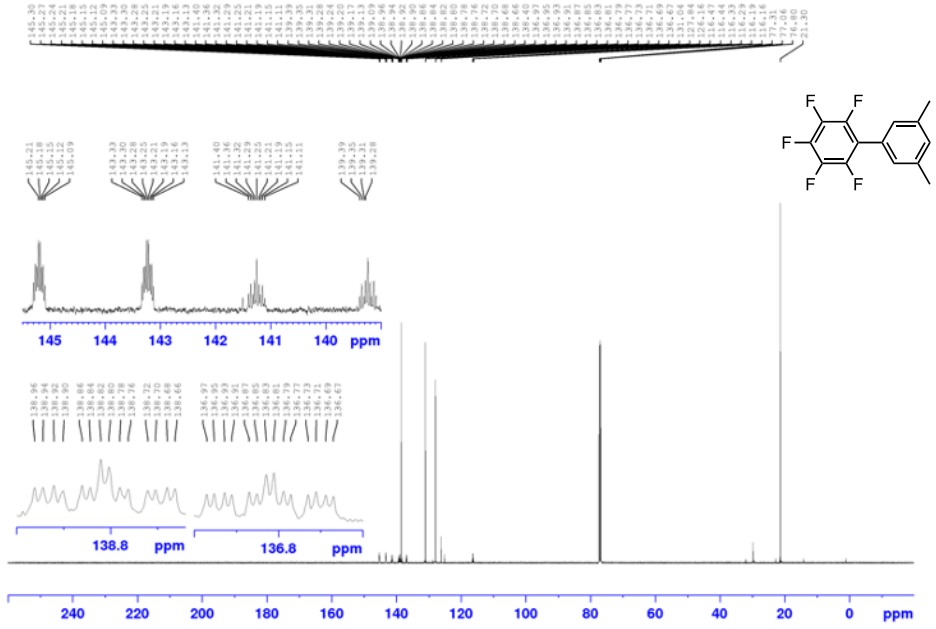




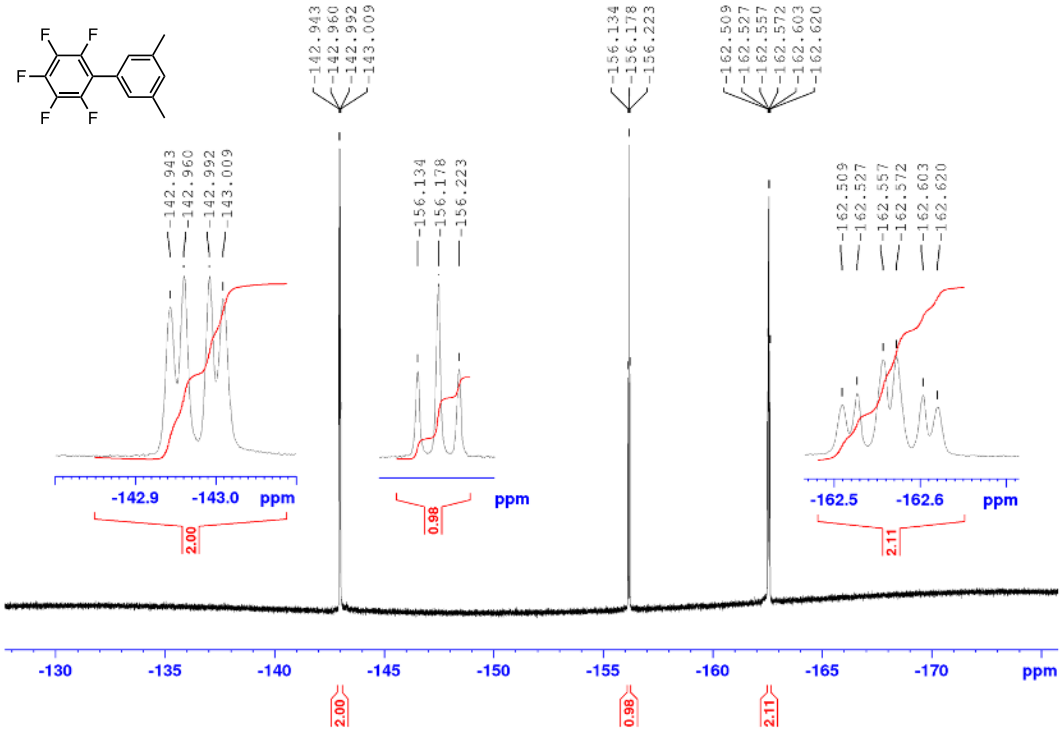
1H NMR Spectrum of 3e (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3e (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3e (470 MHz, $CDCl_3$)



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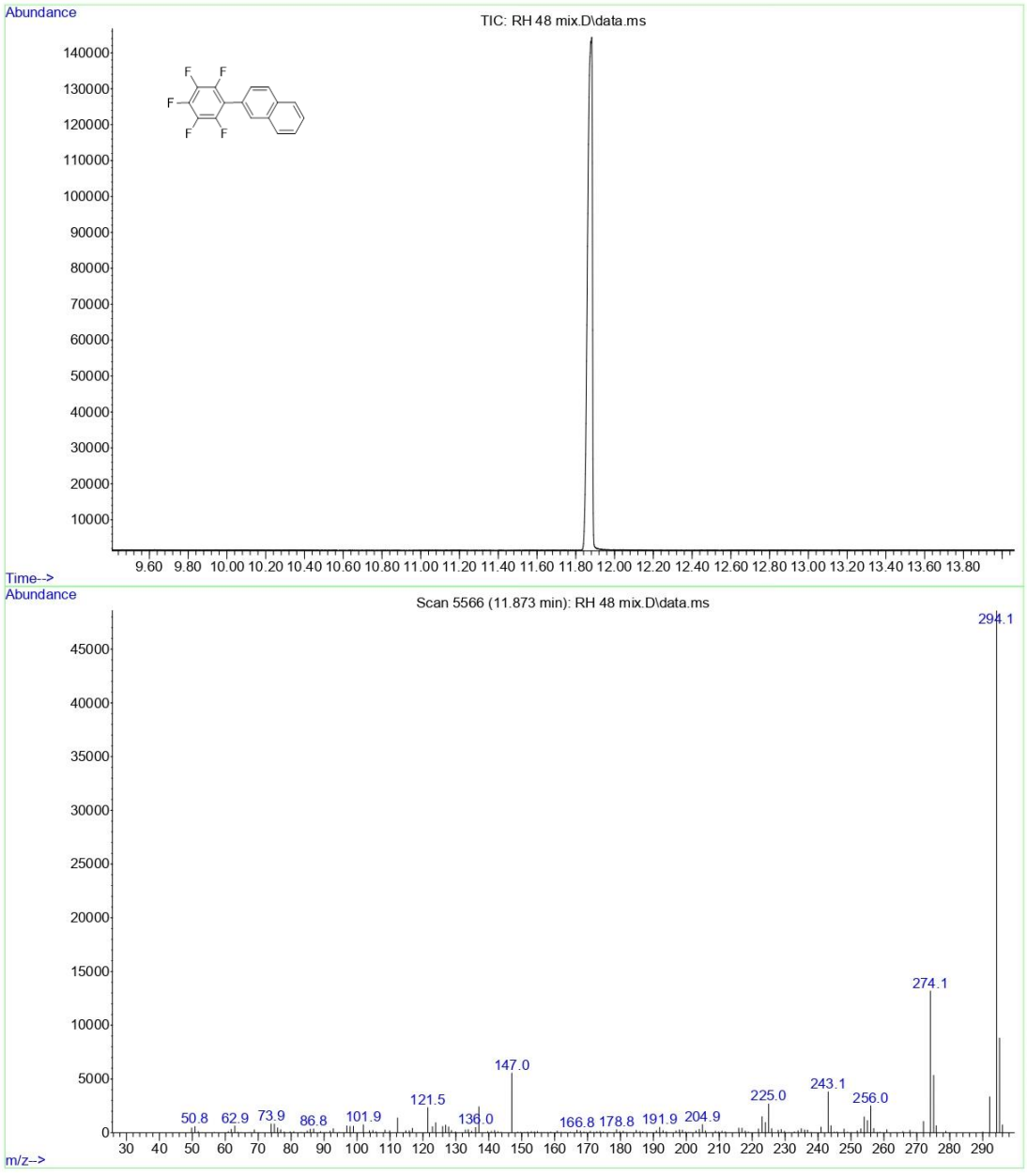
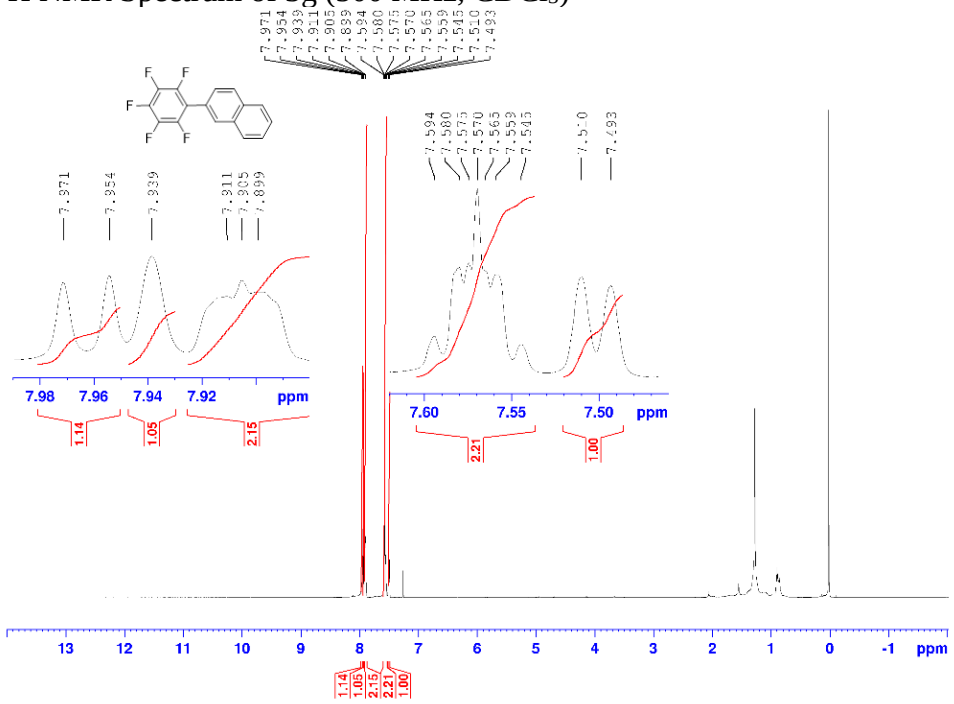
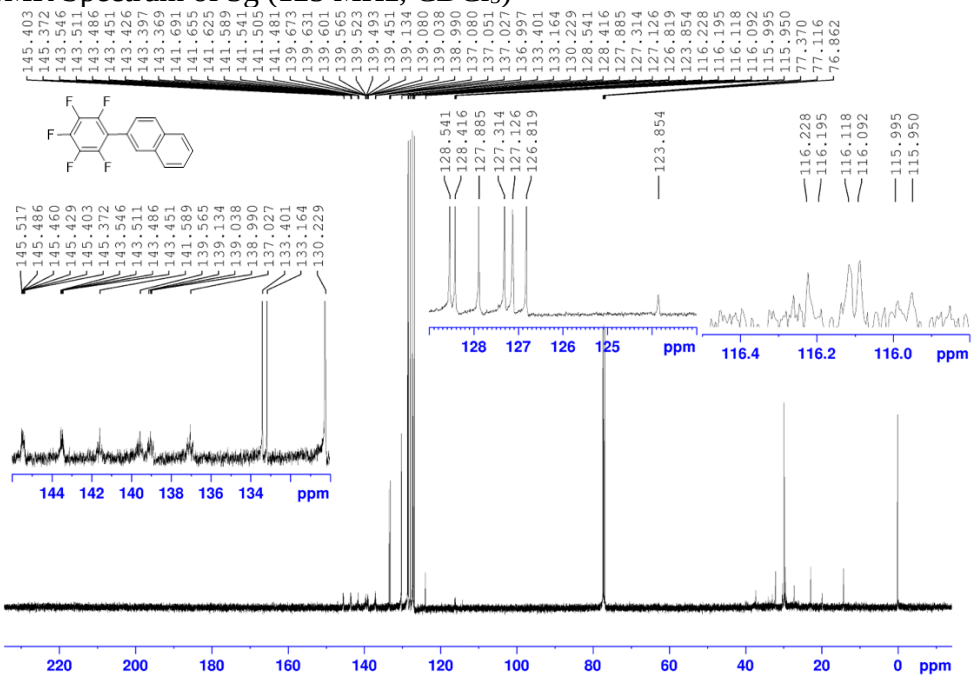


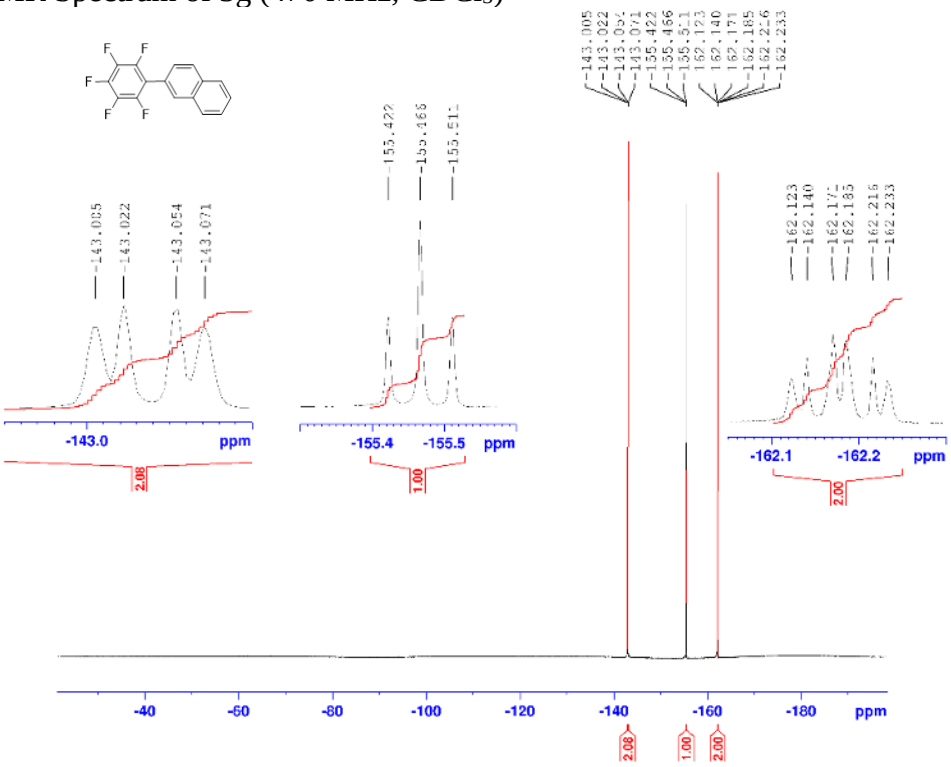
^{1}H NMR Spectrum of 3g (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3g (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3g (470 MHz, $CDCl_3$)



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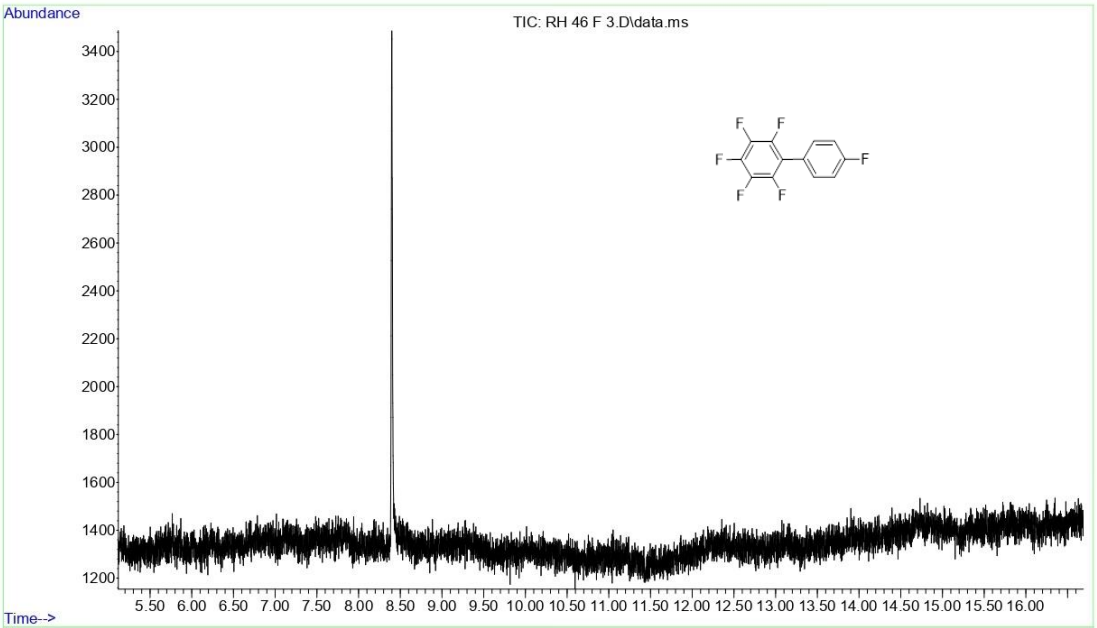
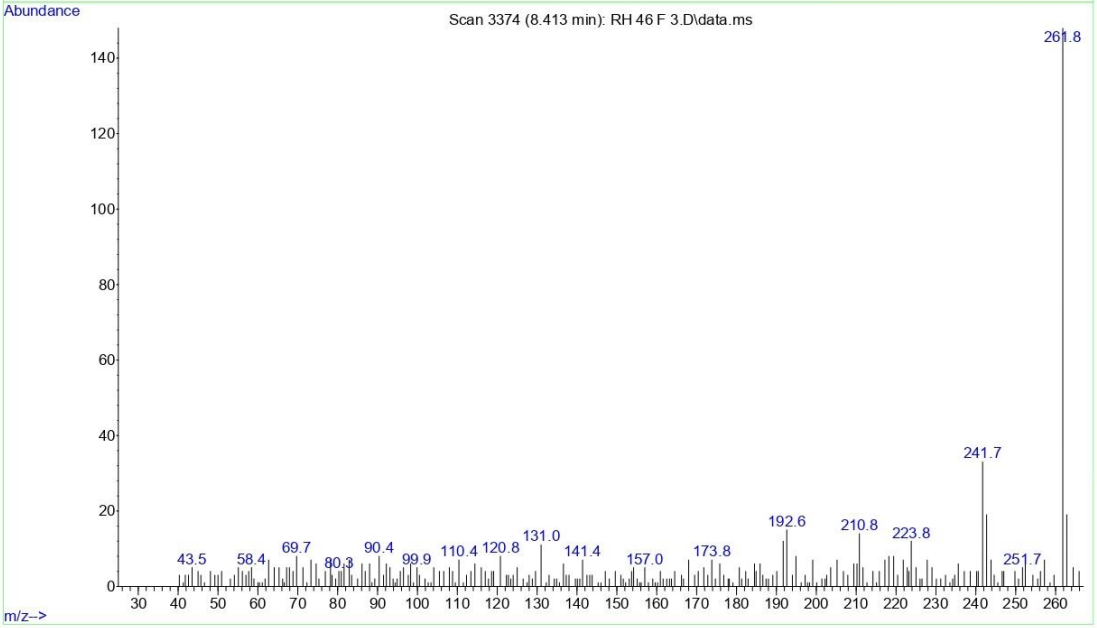
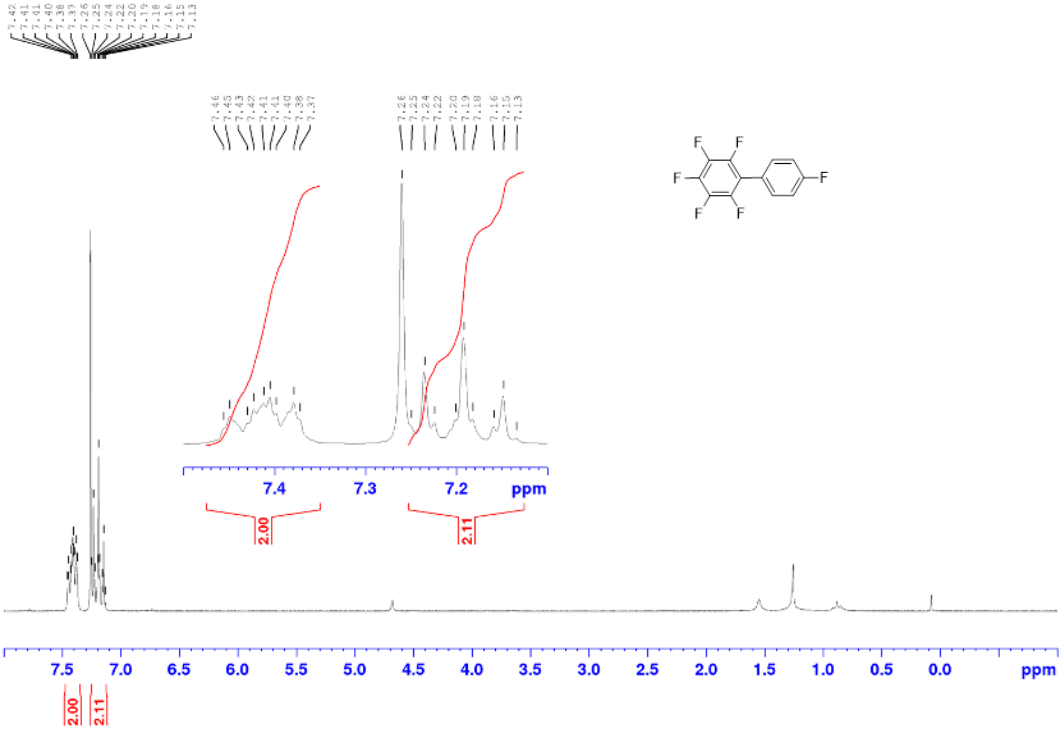
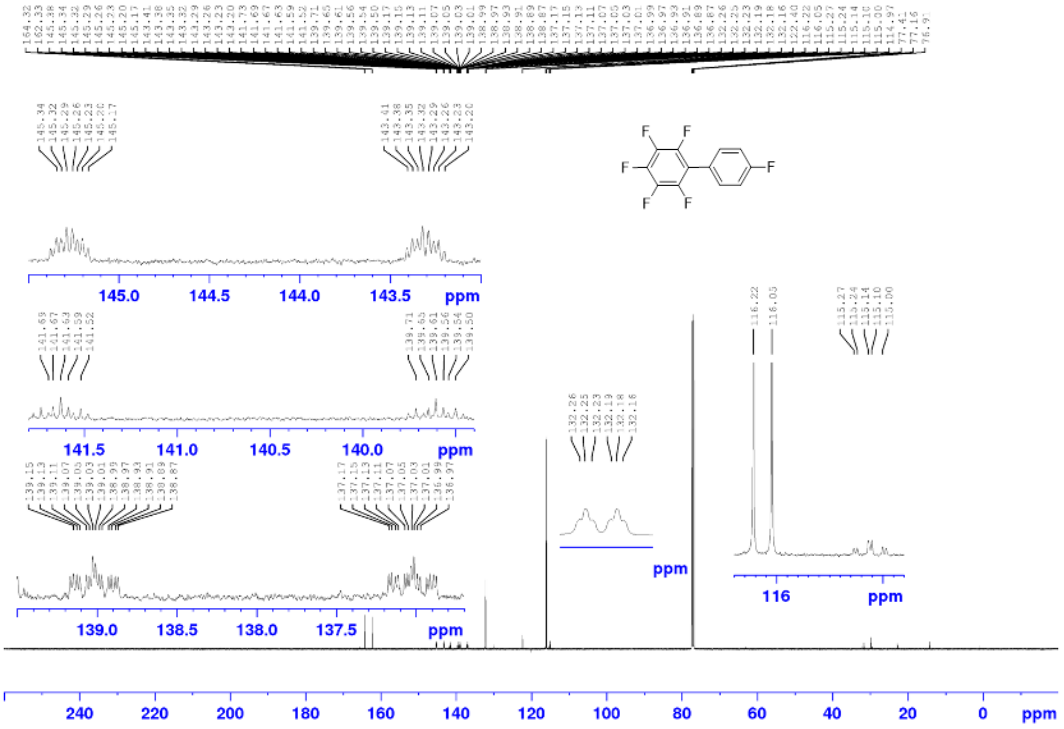




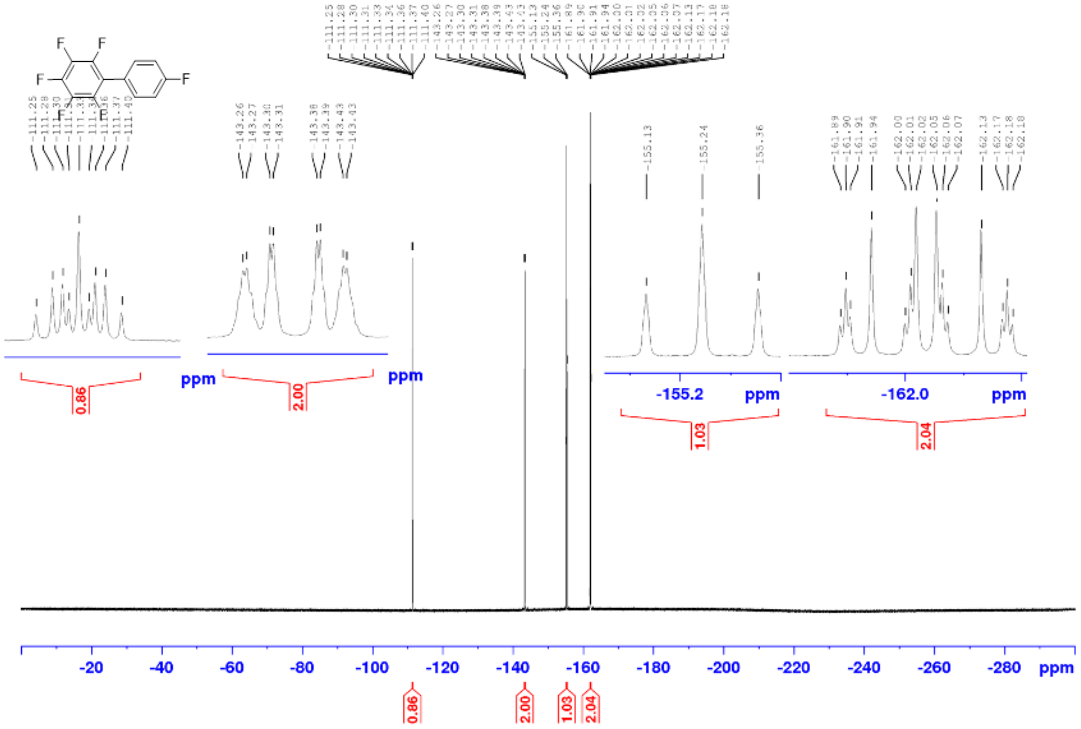
^{1}H NMR Spectrum of 3h (188 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3h (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3h (188 MHz, $CDCl_3$)



GC-MS of 3i

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Sample Name:
Misc Info  :
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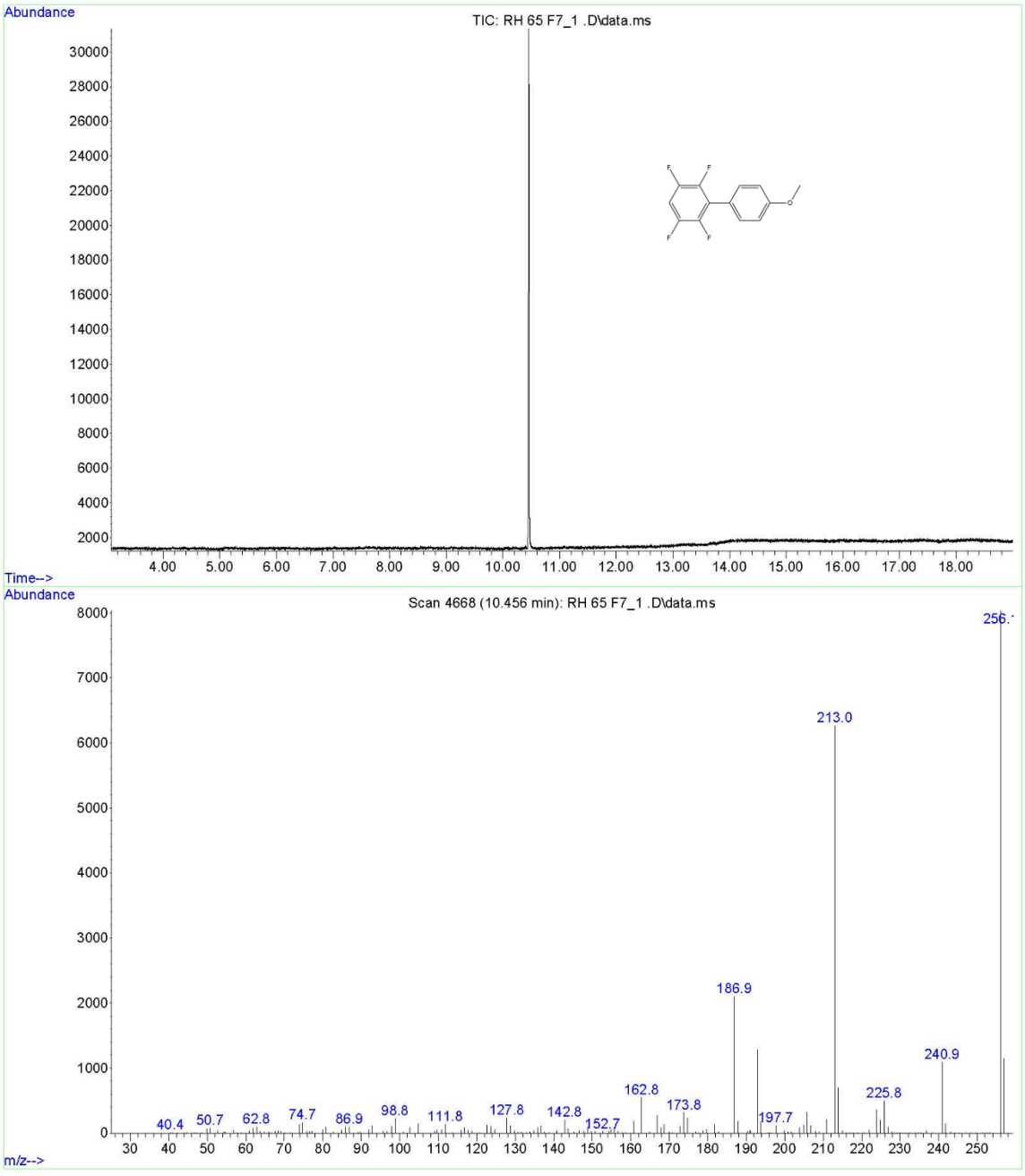
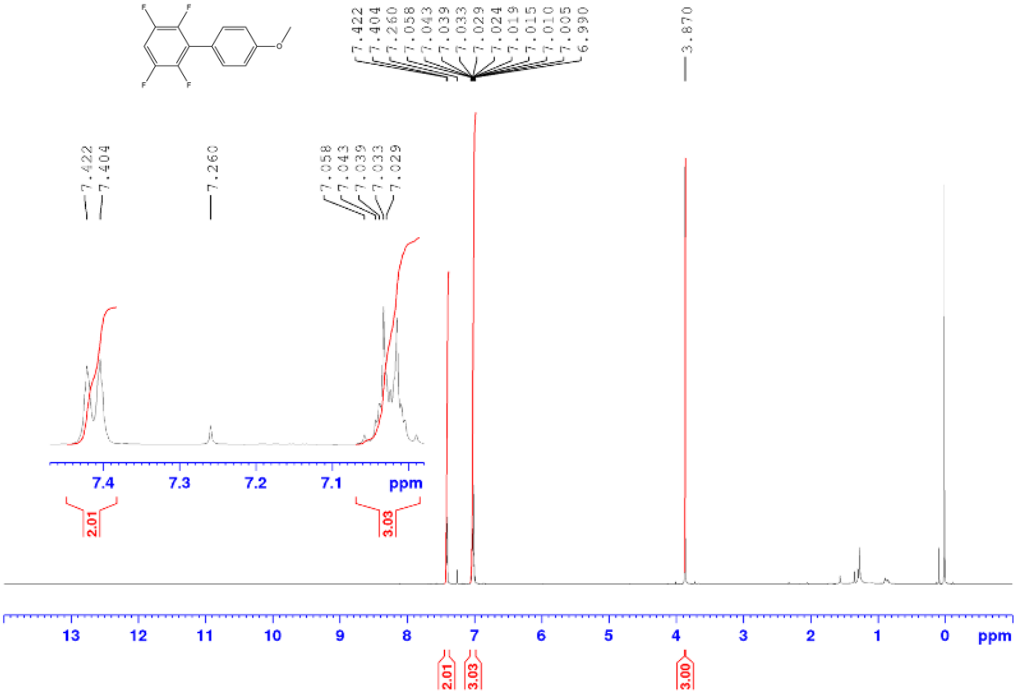
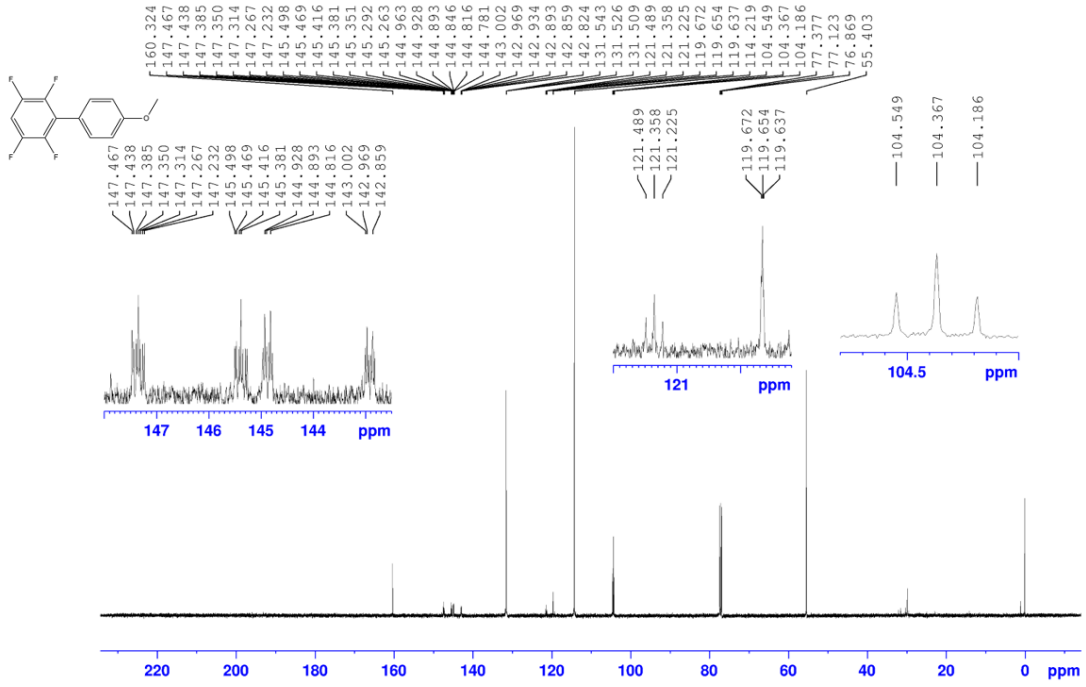


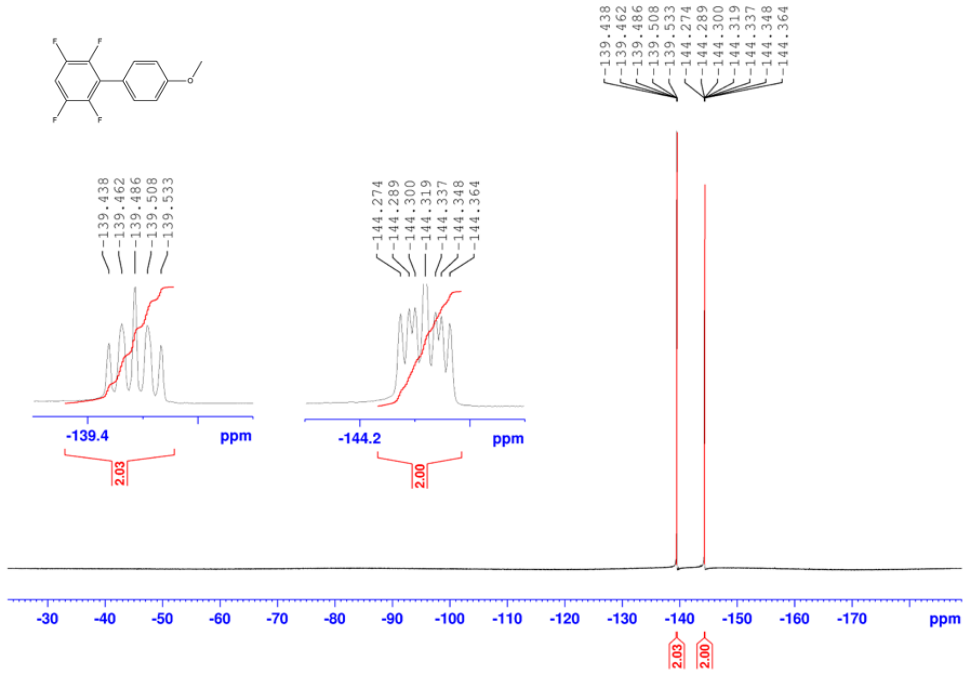
^{1}H NMR Spectrum of 3i (500 MHz, $CDCl_3$)



^{13}C NMR Spectrum of 3i (125 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 3i (470 MHz, $CDCl_3$)



GC-MS of 3j

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Sample Name:
Misc Info  :
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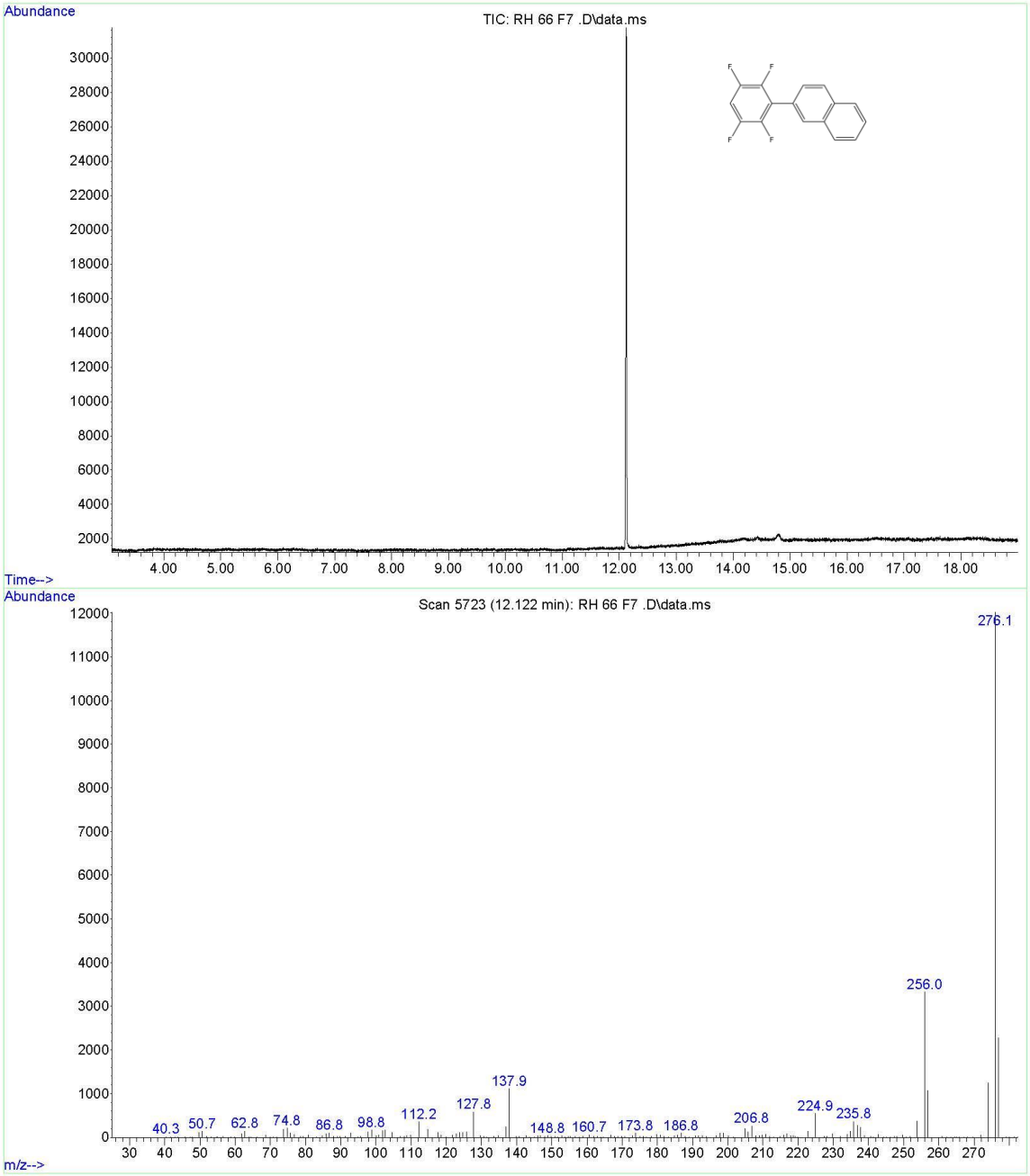
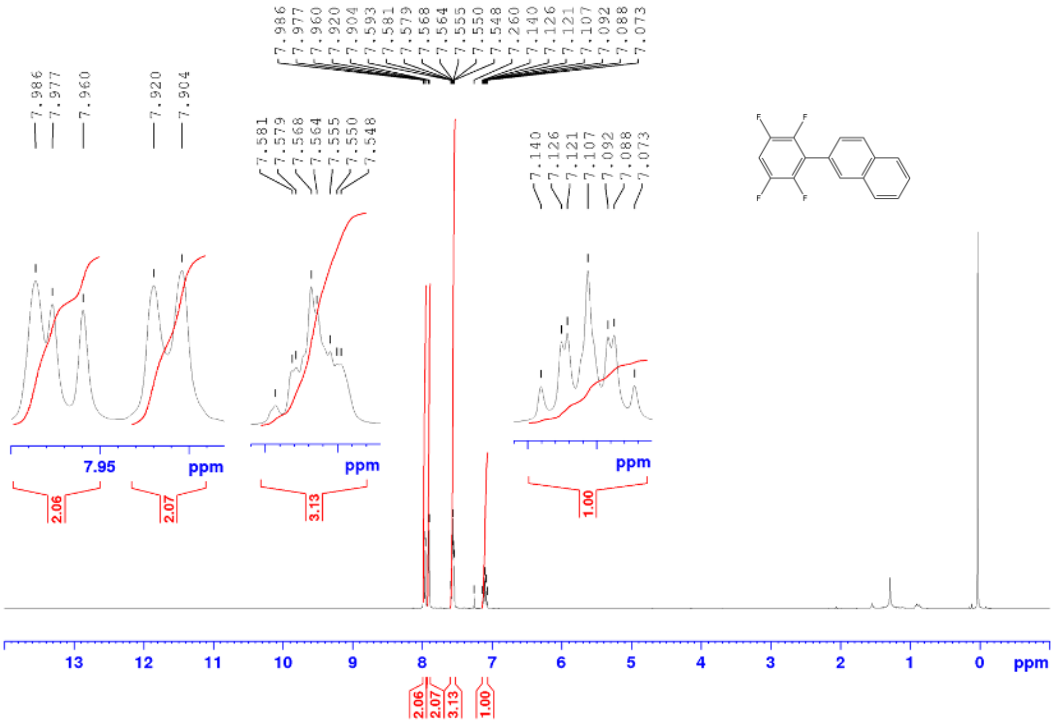
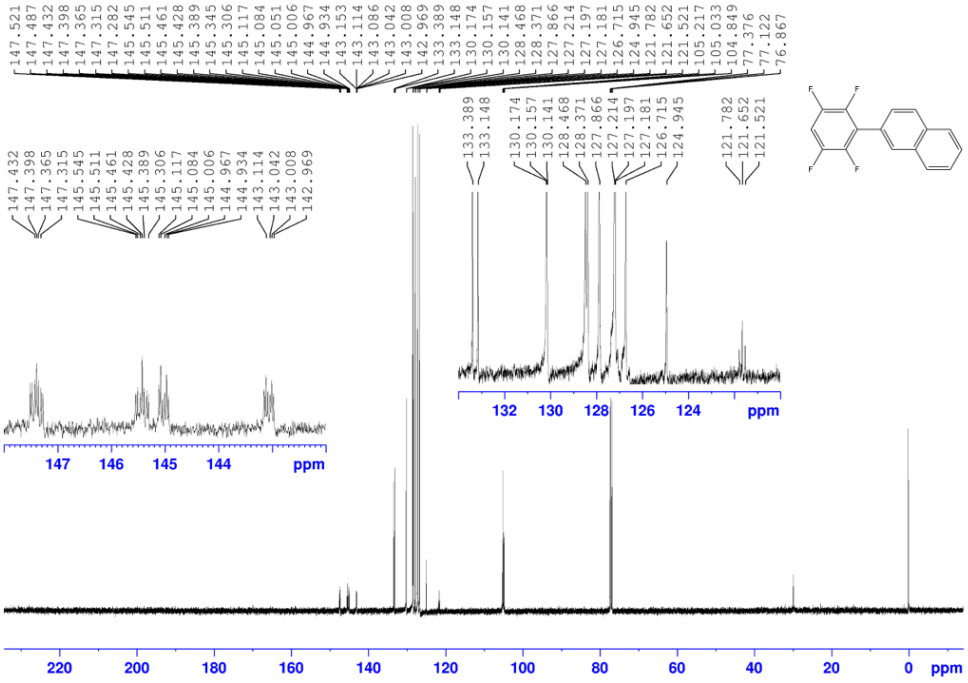


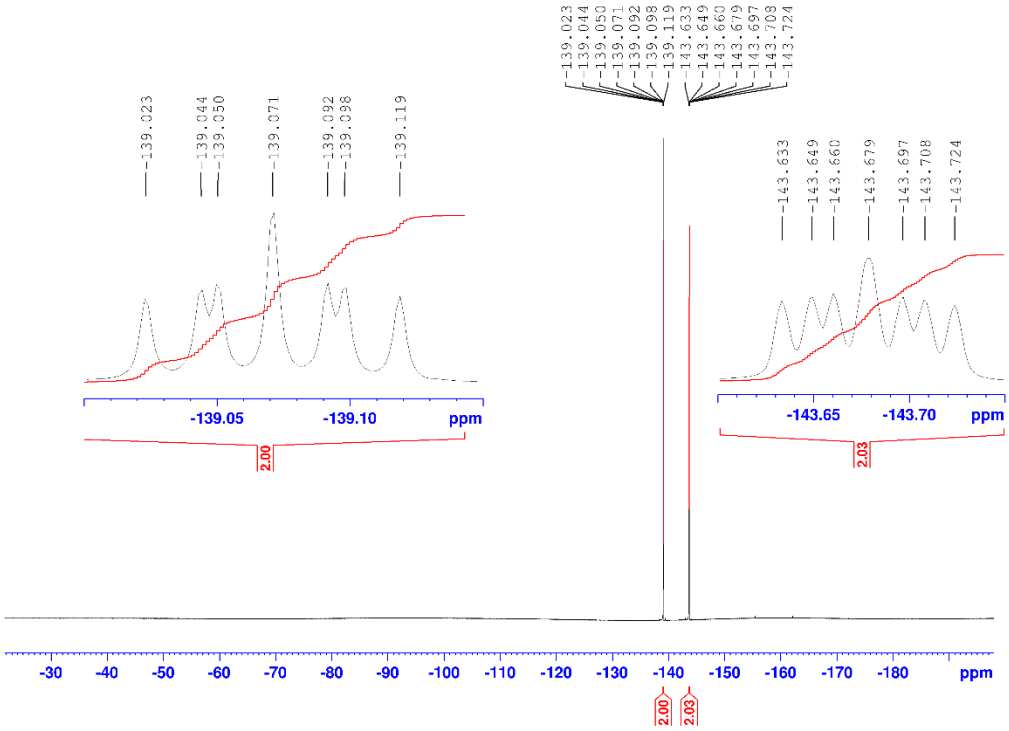
^{1}H NMR Spectrum of 3j (500 MHz, $CDCl_3$)



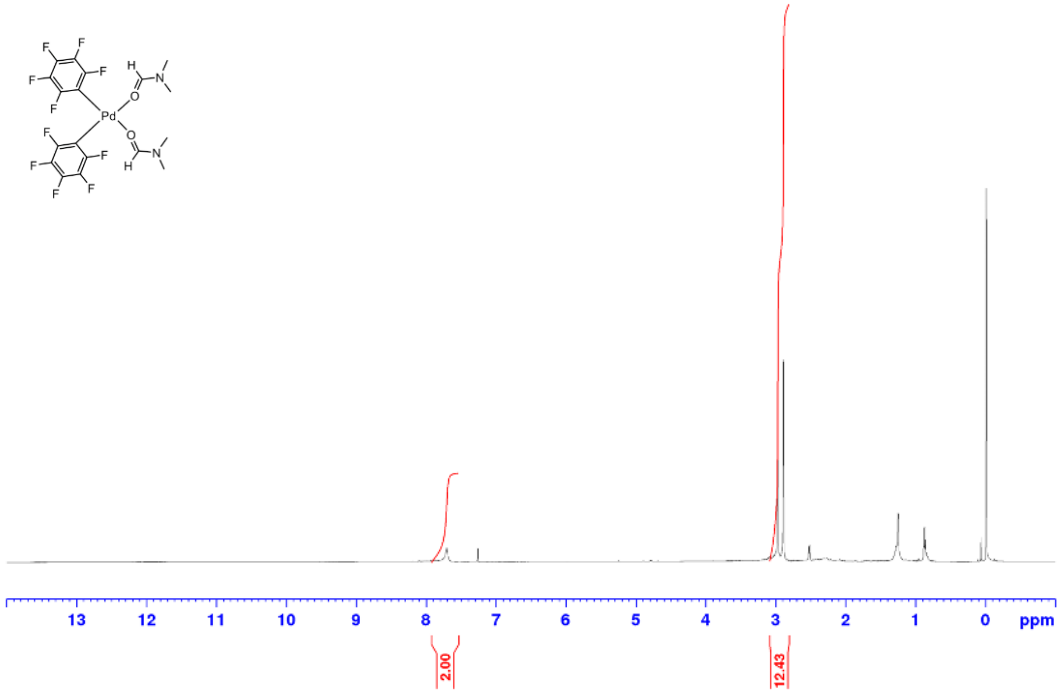
^{13}C NMR Spectrum of 3j (125 MHz, $CDCl_3$)



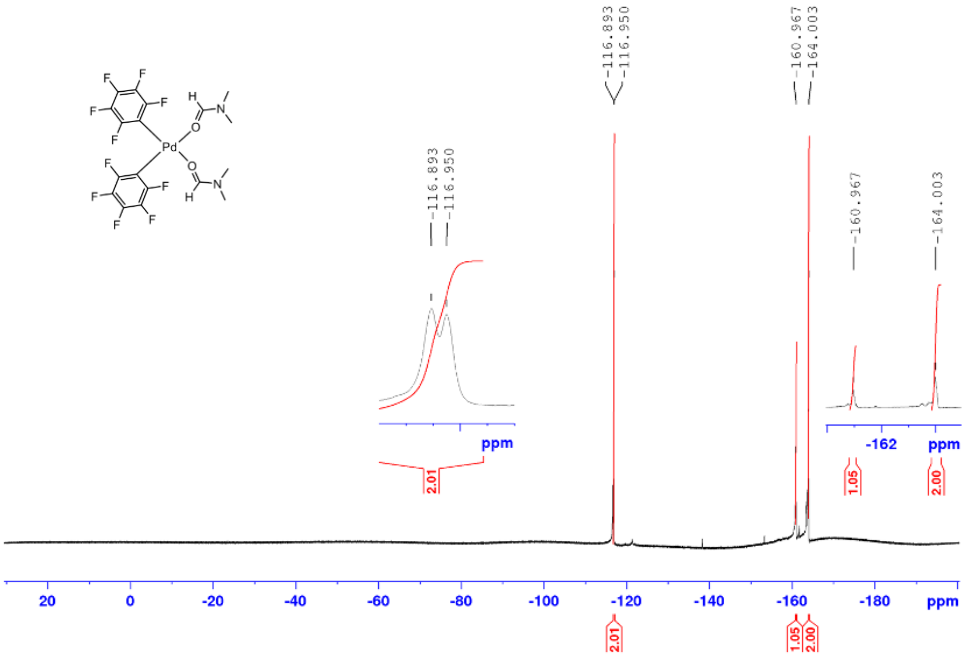
^{19}F NMR Spectrum of 3j (470 MHz, $CDCl_3$)



^{1}H NMR Spectrum of 5a (500 MHz, $CDCl_3$)



^{19}F NMR Spectrum of 5a (470 MHz, $CDCl_3$)



9. X-ray Crystallography

Crystal structure determination. Crystals suitable for single-crystal X-ray diffraction were selected, coated in perfluoropolyether oil, and mounted on a MiTeGen sample holder. Diffraction data for **5a** were collected on a Rigaku Oxford Diffraction XtaLAB Synergy diffractometer with a semiconductor HPA-detector (HyPix-6000) and multi-layer mirror monochromated Cu-K_α radiation. The crystals were cooled using an Oxford Cryostreams low-temperature device. Data were collected at 100 K. The images were processed and corrected for Lorentz-polarization effects and absorption as implemented in the CrysAlis^{Pro} software from Rigaku Oxford Diffraction. The structure was solved using the intrinsic phasing method (SHELXT)[S10] and Fourier expansion technique. All non-hydrogen atoms were refined in anisotropic approximation, with hydrogen atoms 'riding' in idealized positions, by full-matrix least squares against F^2 of all data, using SHELXL[S11] software and the SHELXLE graphical user interface.[S12] Diamond[S13] software was used for graphical representation. Crystal data and experimental details are listed in Table S1; full structural information has been deposited with the Cambridge Crystallographic Data Centre. CCDC-2327275.

Table S1: Single-crystal X-ray diffraction data and structure refinement of **5a** $[Pd(DMF)_2(C_6F_5)_2]$

Data	**5a**
CCDC number	2327275
Empirical formula	$C_{21}H_{21}F_{10}N_2O_2Pd$
Formula weight / $g \cdot mol^{-1}$	629.80
T / K	100(2)
Radiation, λ / Å	CuK_α 1.54184
Crystal size / mm^3	0.07 × 0.14 × 0.22
Crystal color, habit	colorless block
μ / mm^{-1}	6.998
Crystal system	monoclinic
Space group	$P2_1/c$
a / Å	15.2616(2)
b / Å	16.0078(2)
c / Å	10.4878(2)
α / °	90
β / °	106.261(2)
γ / °	90
Volume / $Å^3$	2459.72(7)
Z	4
ρ_{calc} / $g \cdot cm^{-3}$	1.701
$F(000)$	1252
θ range / °	3.016 – 67.066
Reflections collected	24921
Unique reflections	4393
Parameters / restraints	316 / 5
GooF on F^2	1.033
R_1 [I>2σ(I)]	0.0468
wR^2 (all data)	0.1232
Max. / min. residual electron density / $e \cdot Å^{-3}$	3.821 / -1.245

10. Computational Details

The mechanistic study was conducted using quantum chemistry-based density functional methods. All density functional theory (DFT) calculations were performed using ORCA Version 5.0.3.[S14-S16] All possible intermediates were optimized using the B3LYP[S17-S18] functional with van der Waals correction from Grimme and Becke-Johnson damping factor (vdW-D3BJ)[S19] in combination with the def2-SVP basis set.[S20-S22] Subsequently, energy corrections were carried out by performing a single-point calculation with the same functional as the geometry optimization, but using the def2-TZVP basis set.[S20-S22] In this work, we did the simulation in DMF as the solvent. To model the solvent, we employed the CPCM[S23] and SMD[S24] implicit solvent methods for geometry optimization and energy correction, respectively. To estimate the transition state (TS), we implemented a combination of the Nudged Elastic Band and Saddle Point Optimization (NEB-TS).[S25]

11. Reaction Energy

Table 1. Density functional theory (DFT) calculation of the reaction free energy (ΔG) and energy barrier first ($\Delta G^{\ddagger}$) from transmetallation and concerted metalation deprotonation (CMD) reaction.

No	Reaction	ΔG (kcal/mol)	$\Delta G^{\ddagger}$ (kcal/mol)
1	$(DMF)_2Pd(OH)_2 \rightarrow (DMF)Pd(OH)_2$ (Int. 1) + DMF	7.88	0.00
2	$(DMF)Pd(OH)_2 + C_6F_5H \rightarrow (DMF)Pd(OH)_2 - C_6F_5H$	6.02	0.00
3	$(DMF)Pd(OH)_2$ + ArBpin → $(DMF)Pd(OH)_2$ - ArBpin (Int. 2)	-3.79	0.00
4	$(DMF)Pd(OH)_2 - C_6F_5H \rightarrow (DMF)Pd(Ar_F)(OH) - H_2O$	-11.21	27.38
5	$(DMF)Pd(OH)_2$ - ArBpin → (DMF)Pd(Ar)(OH) - pinBOH (Int. 3)	-10.98	4.58
6	(DMF)Pd(Ar)(OH) - pinBOH (Int. 3) + $C_6F_5H \rightarrow$ (DMF)Pd(Ar)(OH) - C_6F_5H (Int.4) + pinBOH	-0.51	0.00
7	(DMF)Pd(Ar)(OH) - C_6F_5H (Int.4) → $(DMF)Pd(Ar)(Ar_F) - H_2O$ (Int. 5)	-25.72	5.87

8	(DMF)Pd(Ar)(Ar_F) - H_2O (Int. 5) → (DMF)Pd(Ar)(Ar_F) (Int. 6) + H_2O	0.52	0.00
9	(DMF)Pd(Ar)(Ar_F) (Int. 6) → (Ar - Ar_F) - Pd(DMF) (Int. 7)	1.63	15.24
10	(DMF)Pd(Ar)(OH) - pinBOH (Int. 3) + ArBpin → (DMF)Pd(Ar)(OH) - ArBpin + pinBOH	-6.43	0.00
11	(DMF)Pd(Ar)(OH) - ArBpin → (DMF)Pd(Ar)(Ar) - pinBOH	-26.73	18.55
12	(DMF)Pd(Ar)(Ar) - pinBOH → (DMF)Pd(Ar)(Ar) + pinBOH	-5.47	0.00
13	(DMF)Pd(Ar)(Ar) → (Ar - Ar) - PdDMF	-9.99	15.40

* Int. = Intermediate

12. Relaxed Geometry

$(DMF)_2Pd(OH)_2$ (Intermediate 1)

Pd	0.53620903552062	1.97583546473690	-0.30676626098315
O	2.12277908003295	3.11264655740164	-0.41853129240366
O	1.67008900049711	0.42253216896719	-0.76797197511683
O	-0.60830402420084	3.66872630501201	0.24814453980592
O	-1.19393112752734	0.77358659616146	-0.18576452943786
C	-1.84096208500723	3.60685676474601	0.44971446868788
C	-1.11348995157017	-0.47136899861130	-0.29760561189237
N	-2.15580040075326	-1.28928293049770	-0.20128826584388
H	-0.13022432199792	-0.93593266574877	-0.48815435882465
C	-3.50394341539125	-0.79691426773944	0.04690018696242
C	-1.99197084233821	-2.72923109616974	-0.34057375537907
N	-2.59198761018363	4.65213848470179	0.78503872286903
H	-2.38057014357791	2.64952991776336	0.35627164625815
C	-2.02888459274257	5.98469059929137	0.95179997999959

C	-4.02272593723964	4.50262605377631	1.00861370872661
H	-4.31605937068186	3.45599122124368	0.85220659196869
H	-4.58486199042416	5.14303690561336	0.30991841763548
H	-4.27920413820968	4.79863148703848	2.03864707764457
H	-0.95502959930812	5.95565097876448	0.73683014274166
H	-2.18993251434425	6.33244870570105	1.98501612295466
H	-2.52518006070352	6.68790996340037	0.26395105493814
H	-0.93438360951532	-2.96735960552184	-0.51384205526468
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H	-3.48771583942743	0.29597328003433	0.12405660544730
H	-3.89206009946587	-1.22647117030523	0.98442345218613
H	-4.16929104937864	-1.09780633734266	-0.77814763369500
H	1.56346645473788	0.32441919368991	-1.72804020482007
H	2.80306753063331	2.45755926237645	-0.64560074808661

(DMF)Pd(OH)$_2$

Pd	0.64429003143394	1.85149405487235	0.16942722578734
O	2.17395189718411	3.03772708857793	0.01803528188204
O	1.55638251207891	0.41132082969548	-0.76724550507281
O	-1.08471476888916	0.69769705573688	0.33920262915567
C	-1.18966410835249	-0.36819875767535	-0.31525276850535
N	-2.23149528572289	-1.18444489888676	-0.23586312982624
H	-0.37898913743178	-0.67622763295895	-0.99693628447611
C	-3.35617120572510	-0.91624632134634	0.65025659211625
C	-2.29081862521629	-2.39808453521803	-1.03950027464340
H	-1.38847565397958	-2.47708179903106	-1.65999900935721

H	-3.17758199759829	-2.37479485982431	-1.69280128494961
H	-2.35925129514732	-3.28142122721565	-0.38481442365433
H	-3.16563864176210	0.00510128979211	1.21147878561719
H	-3.48309673759032	-1.75687434823210	1.35082968652367
H	-4.28039225367555	-0.80688589597838	0.06078388173601
H	2.37697935916738	0.83457002995427	-1.07292977672893
H	2.84742591122656	2.71013992773791	0.63572837439581

(DMF)Pd(OH)$_2$ - C_6F_5H

Pd	1.27890255588836	1.72020937881212	1.02119978479612
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O	1.56949620185143	1.10731577142948	-0.81235525937272
O	-0.59483013795453	0.81073813015231	1.06818156059400
C	-1.04184626319421	0.19805543828226	0.06831232509551
N	-2.27129348140617	-0.29404862079530	0.00698424515463
H	-0.40922484626915	0.06606377426770	-0.82538176964139
C	-3.20265346830422	-0.14849588618725	1.11920321537003
C	-2.73015205217600	-1.02640033900525	-1.16617143435822
H	-1.92710132993742	-1.06805657685145	-1.91323988405517
H	-3.60202675802185	-0.51794308670867	-1.60424240131667
H	-3.01665879033322	-2.05168075444259	-0.88356723144197
H	-2.86036757509204	0.65886686418250	1.77656358420524
H	-3.26652598811863	-1.08845075299553	1.69157828230587
H	-4.19748259700160	0.09753213671867	0.72328695216854
H	2.23006937137961	1.71879548380640	-1.17688806945672
H	3.67609173878906	2.07023503877877	0.93611841769081
C	-1.71899011494907	3.58992760310417	-0.20292837957558

C	-2.50961850752858	2.79125760099644	-1.02969409177754
C	-2.00979589328366	2.38523138977032	-2.26811898257110
C	-0.45352964166844	3.99996522521330	-0.62438735022581
C	0.02735955852448	3.56579643308927	-1.85929936004183
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F	-2.16325402928576	3.94326947890374	1.00003415446504
F	-3.71001434911998	2.38373435211289	-0.61282267922546
F	0.29785585594383	4.75978728557302	0.17362126562444
F	1.26026084271714	3.92535796745866	-2.22088743181323
F	-2.77333373992589	1.59889390129820	-3.03379610975078
H	-0.35252090269173	2.42696799691434	-3.65515229455324

(DMF)PdAr$_F$OH - H$_2$O

Pd	1.03997325465275	1.61287476838960	-0.03235169599804
O	2.60804585079627	2.66247575586620	-0.48609748591731
O	0.55563356109548	0.12718375681106	-3.13345897096805
O	-0.50724103418328	0.31576661248116	0.49239745779577
C	-1.05718838644849	-0.44246305317361	-0.34758856529192
N	-2.14454655934889	-1.15287806949811	-0.08301315983082
H	-0.64787347013632	-0.54936997366483	-1.36644485415750
C	-2.81354006500947	-1.08794753569721	1.20966659299158
C	-2.71741254703090	-2.04181915967050	-1.08494966940021
H	-2.12533510750180	-1.99199744447443	-2.00805636212345
H	-3.75502112155876	-1.74281062803781	-1.30287907780271
H	-2.72107047505948	-3.07864968028450	-0.71255492075329
H	-2.32970532839516	-0.32723369679742	1.83196668243814
H	-2.75899421786717	-2.06700543571176	1.71217812132513

H	-3.87329501336587	-0.82780486433940	1.06091986566731
H	1.41313371835002	0.25542897775508	-2.69919888010126
H	2.62230904168567	3.46622340396289	0.05616329194379
C	-1.88691731799268	5.35347600207452	-0.71166429522154
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C	-1.22172558405380	3.09514115374462	-1.22938859178547
C	-0.85547583733625	5.42120015327270	0.22611372731775
C	-0.01692368211230	4.32002009632712	0.40896217747527
C	-0.18079029884106	3.13233143624160	-0.30423868059441
F	-2.68640070688733	6.40245009973876	-0.90438159834472
F	-3.05852861318388	4.10619989737141	-2.34212095249513
F	-0.67681782060212	6.53915834285970	0.93305586019366
F	0.97096338376532	4.44941558340159	1.31446908318981
F	-1.45165409538459	1.98997811238005	-1.97171048909703
H	0.09039562572387	0.95831831023128	-2.94954170980769

(DMF)PdAr$_F$OH - H$_2$O (TS)

Pd	2.01998210824212	-0.06357577267701	1.02970053273401
O	3.64953536895775	0.93573852482392	1.03579581911270
O	2.32990529284269	-0.64723359581471	-1.07747709356578
O	0.31768576834815	-1.19239392859703	1.29116686864186
C	-0.10152293078724	-1.99120193888026	0.41525399257575
N	-1.16165471723325	-2.76404172618463	0.58138659432549
H	0.41795530479577	-2.08599165459628	-0.55183248358551
C	-1.94702210168782	-2.73820633042835	1.80916332232691
C	-1.59032129131480	-3.68707931119678	-0.46165830202122
H	-0.91304257639706	-3.61818098359253	-1.32278481467533

H	-2.61398005720244	-3.43980740033995	-0.78399968880760
H	-1.58099137910040	-4.71843758541731	-0.07506929329233
H	-1.54117674378981	-1.97964520569781	2.48705297378825
H	-1.91089475339273	-3.72647684677619	2.29439102655274
H	-2.99502276040138	-2.49973537194844	1.56992608438129
H	3.24563329919469	-0.38890488385980	-1.28581955437953
H	3.56910740827244	1.68506114022998	0.42194126870445
C	-0.72176362686009	3.90706183677262	-0.37768805466425
C	-1.33239214128078	2.65643939522570	-0.50057686695350
C	-0.52849698477420	1.53661480936658	-0.72351706950795
C	0.66754021849046	4.01243386976559	-0.47096592710907
C	1.40562671658116	2.85024848824833	-0.69781964828757
C	0.85426092601885	1.58587903602063	-0.81925441219907
F	-1.46354678749754	4.99769058813395	-0.16320442429876
F	-2.66713294789339	2.56558796976286	-0.41568326742347
F	1.24949626800391	5.21382802512715	-0.35482401681808
F	2.76023628362156	3.01479909159627	-0.78376986562057
F	-1.18208776177633	0.35065484956132	-0.84306563896580
H	1.76408459801971	0.22887491137221	-1.22676806096806

(DMF)Pd(OH)$_2$ - ArBpin (Intermediate 2)

Pd	0.47697906221160	1.20737690371894	1.76097404584514
O	1.82990284664464	2.62652713961723	1.93412752074659
O	0.40092507973884	1.71209738039741	-0.14301547440948
O	-0.97608553730734	-0.28102857420996	1.38851832369993
C	-0.90981739915064	-0.88022148826952	0.28803474094764
N	-1.43319590745157	-2.08061986201427	0.07283922538857

H	-0.39386985525542	-0.40974629713058	-0.56583003398062
C	-2.08362954664790	-2.83665686870039	1.13443844518495
C	-1.34595077056901	-2.71499009759550	-1.23487286715987
H	-0.82042493839910	-2.05165622823434	-1.93400919626792
H	-2.35583905252570	-2.92365836498228	-1.62225252851830
H	-0.79480121999388	-3.66541362709235	-1.15406707431466
H	-2.09312437114570	-2.24065828887494	2.05348027110230
H	-1.53262254397775	-3.77493121109258	1.30828280654991
H	-3.11654067104841	-3.08183693757686	0.84118228905260
H	1.14382586285386	2.33358143518881	-0.21555381805764
H	2.40096814207090	2.38099655414319	2.67792403334640
C	1.17448304741100	1.92258884312550	4.90539653603354
C	0.27736056669852	1.00585865057422	4.28955267907460
C	0.77999230563883	-0.17399150475478	3.72470123090861
C	2.54319674105854	1.63374421135429	4.93538772381400
C	3.02583373847767	0.46041881995684	4.32400700811584
C	2.17643707272408	-0.45487553257655	3.70140019476518
O	0.61157592707449	3.02914220139324	5.41875031317978
H	-0.79567440530853	1.18864749164466	4.37717022919203
H	3.24659042072178	2.31660064438751	5.41100721249264
H	4.10448947270418	0.28172519817895	4.32385267798837
H	0.08130670427374	-0.92757403986569	3.36258024272859
B	2.67114689107666	-1.65632497626221	2.85690437883614
O	1.80047334956715	-2.47144349428728	2.17992742130735
O	3.98387482868941	-1.96352444339446	2.63098743646460
C	2.58081502775802	-3.23087320171795	1.21512272480866

C	4.01852535673783	-3.20432893191549	1.86338785783206
C	2.50374889003001	-2.46779843917907	-0.10910856999620
C	1.96661038055102	-4.61519320056475	1.06528536518241
C	4.24645550698805	-4.33867031068777	2.86331625897735
C	5.16665181904331	-3.13164101335059	0.86733581157509
H	1.86558167068513	-5.12129044309266	2.03434578459214
H	2.58434666793230	-5.23996220962579	0.40226015678761
H	0.96472753190117	-4.52567664286132	0.61767156486525
H	3.41600253114236	-4.41094304562828	3.58126371576912
H	5.17187174607453	-4.13886906186429	3.42412069077858
H	4.35291795451619	-5.30609716279653	2.35142883153701
H	2.92388853961157	-1.45498444264001	-0.01571232197935
H	1.44891288550163	-2.37324475720836	-0.40080012387039
H	3.03623393791504	-2.99959727727620	-0.91042065467175
H	5.11044334478929	-2.22493943163572	0.25065130001994
H	5.15367122590446	-4.01076065192733	0.20492573774897
H	6.12585836536213	-3.12275555904988	1.40716253339512
C	1.44305500519098	4.01131639923313	6.02534927875667
H	0.77632446686777	4.81669056393820	6.35764693685576
H	2.17287701124000	4.41116115450463	5.30201742355364
H	1.98026439340173	3.59662732858027	6.89447183342481

(DMF)PdArOH - BpinOH (Intermediate 3)

Pd	0.51914320660565	-0.14815885802807	0.38305073823395
O	0.06348472472346	-0.22540329008488	-1.64813991506585
O	2.62510986874723	-0.11055022093758	-0.01226610263655
O	-1.49174658699927	-0.20602677831991	0.86323840974758

C	-2.33026571450626	-0.29207768129695	-0.07168624848430
N	-3.63837222499746	-0.35982560049448	0.13598813074716
H	-1.96044329898116	-0.31550685268368	-1.11245613988333
C	-4.20983113705343	-0.34145110160855	1.47610704470272
C	-4.56575979128137	-0.45018732724422	-0.98315966412079
H	-4.00674737075034	-0.45508665220169	-1.92807262080920
H	-5.25428364867120	0.41011995092500	-0.97442458018155
H	-5.15975030891139	-1.37526136419015	-0.90878893856171
H	-3.40141064493895	-0.29790788356517	2.21424048493435
H	-4.81019226999219	-1.25110778933488	1.63663052489500
H	-4.86539507296645	0.53666028986707	1.59203148550124
H	2.99730867105308	0.78262747983485	0.07144446516521
H	0.03074845599767	0.69703479077917	-1.94559778107209
C	1.54315067311646	-0.19951645315812	5.11919955712728
C	0.68014709524806	-1.15925319565342	4.56108166553371
C	0.37845799825543	-1.12845569181410	3.19883798406909
C	2.09354438215367	0.78761611653056	4.29114326653651
C	1.79036548940449	0.79086005296937	2.91946587635749
C	0.93203139064083	-0.15621834799723	2.34188185320316
O	1.78659138815820	-0.30939470618843	6.45628207922982
H	0.25550361557287	-1.92316676696824	5.21817979738600
H	2.76749194159343	1.54615401124919	4.69094586375963
H	2.25184697998525	1.56671526249489	2.29922900572427
H	-0.30718842529068	-1.88146282524946	2.79808003904800
B	3.35835488589305	-1.08268520240669	0.65367157999083
O	2.95233368977695	-2.37872936546605	0.66347235026597

O	4.52835394055009	-0.83122985024828	1.29467532207076
C	4.06212781094324	-3.15472589927692	1.21516303635591
C	4.86636210254060	-2.05876309479262	2.02186722317642
C	4.83894970022876	-3.72015859457370	0.02631622842991
C	3.49462338598572	-4.27872198689514	2.06903354146349
C	4.35723297416142	-1.87915474797348	3.45026889346269
C	6.37629381443739	-2.23762281143081	2.00589145911540
H	2.78893638083075	-3.89918592339784	2.81946494364618
H	4.30753653806102	-4.81230807584755	2.58459987214332
H	2.96459656911778	-4.99876573287296	1.42730589845827
H	3.26588734332042	-1.76172756612309	3.47622917121462
H	4.80532969202410	-0.97071763264850	3.87843663524442
H	4.63797866956077	-2.73569023903116	4.07968969907834
H	5.26660250820076	-2.91730106301366	-0.59267911629697
H	4.15176508962308	-4.30957514278840	-0.59874803230397
H	5.65465851433575	-4.37766794562163	0.35989823963985
H	6.78166491701224	-2.19753131854909	0.98632677279658
H	6.64666618652462	-3.20505392512168	2.45590408753559
H	6.84944856868022	-1.44033586480927	2.59888330351101
C	2.67815070706597	0.60888192389876	7.05898730714201
H	2.74226241469084	0.33472658245464	8.12063542669662
H	2.31243017615394	1.64783497828738	6.97646698489249
H	3.68548403436450	0.55275993061714	6.60930289118300

(DMF)PdArOH - BpinOH (TS23)

Pd	-0.42110098744633	1.45642677739838	-2.09348275400251
O	-0.84286651384035	2.25495052429778	-3.89440646387616

O	1.50675287093925	0.88640447024364	-2.45120195085575
O	-2.33472037156242	1.96026499989435	-1.51008368131013
C	-3.22993583998987	1.10455658309499	-1.31394790301173
N	-4.44894437196639	1.40609305279667	-0.88556863394501
H	-3.04981597481395	0.03240185569604	-1.49222741348068
C	-4.84643246285965	2.77901295151447	-0.60311508928955
C	-5.44492918122925	0.36662952610289	-0.66432372295712
H	-5.01689051921893	-0.61592758039644	-0.90260831786278
H	-6.32419167806406	0.54405095037851	-1.30374173471457
H	-5.76783084463260	0.37430280483561	0.38894313590406
H	-4.01930676712902	3.45544659896020	-0.84428814734014
H	-5.10888514314584	2.87954664297855	0.46228391453188
H	-5.72790145554503	3.04053986153689	-1.20951423373115
H	2.11391869306972	1.63693781555619	-2.33654677443364
H	-0.18137800865211	1.89011578117641	-4.50184059575094
C	-0.71556708281696	0.77430559494175	2.56101285651074
C	-1.18018656933048	-0.24654933375929	1.70372198798449
C	-0.78742561888612	-0.26289940540080	0.37360171669951
C	0.14560876735721	1.76674814056397	2.05828360897910
C	0.50978935130634	1.73211340200943	0.71067032009574
C	0.06781480940781	0.72473141281594	-0.17273629885897
O	-1.14552891074614	0.71943983772724	3.83810765882713
H	-1.84208481756394	-1.01178173635490	2.11627781638542
H	0.52315760287652	2.56120608189279	2.70212212986336
H	1.17407195431428	2.51848613790086	0.33722318351073
H	-1.14030321618393	-1.07443734116078	-0.26847680687790

B	1.56309886596421	-0.01638651083361	-1.29022575901112
O	1.21410656650916	-1.35436518464056	-1.54030553948163
O	2.76208300062699	0.06237526419022	-0.56537475595630
C	2.32458619431542	-2.17944608744013	-1.12851260948104
C	3.06905069761015	-1.26068768474577	-0.08026045254874
C	3.17291057945267	-2.46467832930132	-2.37292547604857
C	1.78640664924626	-3.48467877567713	-0.55371650748839
C	2.51683746681961	-1.39928806631738	1.34276864131512
C	4.58476393324399	-1.43060877150606	-0.05788663491775
H	1.05486938690490	-3.30257924986852	0.24485545198948
H	2.60667345710502	-4.09679692020132	-0.14748126450765
H	1.29000718805925	-4.06364212535597	-1.34819332826106
H	1.42301251781616	-1.31533649214695	1.36386178882110
H	2.93327915058419	-0.58998606746321	1.96151138183776
H	2.80675981552564	-2.36080164718914	1.79164720589477
H	3.58649449979285	-1.53628222114371	-2.79418213152447
H	2.53220182499752	-2.93150739723951	-3.13671681217597
H	4.00473900935750	-3.15056136030415	-2.15352398487584
H	5.03488856705404	-1.17929770479661	-1.02748632761631
H	4.85422806093566	-2.46694242327478	0.19885857716085
H	5.02007784072423	-0.76588816214744	0.70449906465416
C	-0.72611517671290	1.71910759388625	4.75637728954078
H	-1.19698007167513	1.47381698807385	5.71696957669842
H	-1.05322447925048	2.72225822211284	4.43474792061209
H	0.37035674134539	1.71908670608877	4.87655687837685

(DMF)Pd(Ar)(OH) - C_6F_5H (Intermediate 4)

Pd	-0.24818903089925	-1.54335448008079	0.92236286403671
O	-0.76005708538439	-2.17633393308850	-1.01099740340364
O	-1.96268126562975	-0.29525711976972	1.03068483805527
C	-2.77501414612031	-0.35786321325087	0.07291268021241
N	-3.91172996795629	0.32564739759131	0.03573540545636
H	-2.53841975200016	-1.01117961550810	-0.78687466161300
C	-4.31582439914712	1.21645384920385	1.11557211255721
C	-4.81197030689235	0.21342670319713	-1.10364737674566
H	-4.39826009201334	-0.49191790758479	-1.83624431428620
H	-4.94230910234599	1.19745711944041	-1.58202831744633
H	-5.79833430604291	-0.14796688578423	-0.77111804864655
H	-3.55722522865996	1.19851938700401	1.90581879756865
H	-5.28502382396478	0.88944947069572	1.52487873455309
H	-4.42574231805231	2.24331758498682	0.73148239421496
H	-0.35055122834183	-1.54506588350986	-1.62291549818889
C	1.02611222345331	-0.40804884034004	5.43251210080967
C	0.16937977080461	-1.49509635762590	5.18772920513200
C	-0.25167813447090	-1.78126111281824	3.88800218800739
C	1.42687311471061	0.40435242812540	4.36165815451264
C	0.99414901042362	0.10103973508974	3.06059893560063
C	0.17867455427161	-1.00588674671793	2.79645916517176
O	1.40895827827793	-0.22032563742995	6.72605353920666
H	-0.14345892633860	-2.11501510113504	6.03199207610375
H	2.08031758638666	1.26278619962686	4.52041629949479
H	1.33886386717608	0.73852786682897	2.23989521127026

H	-0.89855210413725	-2.64966191994115	3.72666200465729
C	2.31156200607771	0.82928109664390	7.02050478859555
H	2.50330828698441	0.78500356140407	8.10096810180909
H	1.88572042122230	1.81697940968809	6.77006165461135
H	3.26566988823371	0.70732179559184	6.47773815026506
F	2.77857241504350	-1.19178706666337	-0.38250947174949
C	2.49390006200168	-1.95287505613768	0.67057843323246
C	1.51694437971710	-2.96474499953662	0.56752811244276
H	1.08322184630445	-3.21774148315613	-0.40644988178702
C	3.19387893711988	-1.74091917065529	1.85604392368554
F	4.05358549184588	-0.73335235601163	1.97219092293430
C	1.31915111216592	-3.80586264877187	1.68231652142334
F	0.44696571238941	-4.80650452976533	1.60976041418285
C	2.94902427144487	-2.57231677969518	2.94959459381826
C	2.01354435094995	-3.60806127300155	2.87076388185643
F	3.56606135165095	-2.33656686127242	4.09674622766668
F	1.76496227974132	-4.35535662586578	3.94196254072120

(DMF)Pd(Ar)(Ar_F) - H_2O (Intermediate 5)

Pd	0.06916633095361	-1.35025384643696	1.35789682635982
O	-0.24237174168108	-2.14862304049701	-0.71727782931599
O	-1.77210179137804	-0.22280106844932	1.12240442081693
C	-2.63188318978726	-0.47640701152429	0.25382950309680
N	-3.83052616011784	0.10204987834236	0.20198799560463
H	-2.43811102576469	-1.21585627194096	-0.54287935542166
C	-4.24495631240734	1.09191724126341	1.18587545580992
C	-4.77611028754942	-0.21775853772434	-0.85691411779841

H	-4.34489162084030	-0.97314106404356	-1.52731088727286
H	-5.01324784413230	0.68661926636881	-1.44044554916029
H	-5.71082915784335	-0.61013019644673	-0.42490571483408
H	-3.47645845938623	1.17560637526393	1.96241838121770
H	-5.19962814060210	0.78377020785918	1.64082376140458
H	-4.38814370656008	2.07165936365677	0.70125859904748
H	0.13792728457537	-1.54461452480272	-1.37723882257278
C	0.38820783796192	0.45239789394616	5.81243304578421
C	-0.76257535094154	-0.22110330697020	5.36825937907614
C	-0.81192994394563	-0.76276548526449	4.08287355616906
C	1.48696812362701	0.56752373029146	4.94918913363499
C	1.42666232000552	0.00698156175533	3.66280711689162
C	0.28127038337421	-0.65707179195588	3.19880671756875
O	0.34531067625432	0.95370533386818	7.07940024773958
H	-1.61426955532270	-0.30524036419119	6.04878741266602
H	2.39564621758688	1.08340248577627	5.26205927932324
H	2.30032029993515	0.10726205862642	3.01519706845482
H	-1.72899819675413	-1.26588976866064	3.76414002714551
C	1.47404489441689	1.64981233429757	7.57220825969395
H	1.22568305945678	1.96859257395138	8.59356989807862
H	1.70243512089146	2.54134561904696	6.96142316062662
H	2.37023237161956	1.00488965856732	7.60355614734843
F	3.12681415124198	-0.67586988902887	0.71825219066370
C	2.99603334223893	-1.92880229988439	1.21053534100385
C	1.74603808106152	-2.40564099333182	1.60083502841714
H	0.25524410931904	-2.97485935796986	-0.83237676912924

C	4.16470054713248	-2.68729473354204	1.30301627971006
F	5.34420163997255	-2.19482475729557	0.90417540425674
C	1.72348401098165	-3.70100868068199	2.11433759020164
F	0.56246854957949	-4.24988024459725	2.53288743979318
C	4.09791062282222	-3.98376243661120	1.81524384307566
C	2.86703587837477	-4.49464277954804	2.22900681268421
F	5.20304930393995	-4.73008207774278	1.90466455064924
F	2.79894732769074	-5.73607105373918	2.72595917148989

(DMF)Pd(Arl)(Ar_F) - H_2O (TS45)

Pd	-0.24207834045157	-0.62804622224829	-1.12878632647601
O	-0.57238104914860	-1.69257997990925	-3.00170303020083
O	-2.00897145479342	0.54482582898556	-1.12192692633407
C	-2.75941050303073	0.44216887109677	-2.12368226255015
N	-3.87279232818630	1.14506149139088	-2.28263324814274
H	-2.50913714632804	-0.26378920518054	-2.93525085568252
C	-4.32448455721550	2.10737036205327	-1.28579769626506
C	-4.69938199472338	0.98379876690444	-3.47155416119404
H	-4.24893941314054	0.23959204245630	-4.14146368708632
H	-4.78381693227135	1.94493418540286	-4.00334281254730
H	-5.70992958703342	0.65029219892176	-3.18649607523627
H	-3.61097985658022	2.13398539628574	-0.45498500718846
H	-5.31852226436614	1.81562183414034	-0.91101641102477
H	-4.40041461064181	3.10709007899977	-1.74217935022974
H	-0.25953587327560	-1.12062042889183	-3.72214080798757
C	0.71267782057973	0.77037530314065	3.37681798044706
C	-0.57821163443512	0.36721189413893	2.99257913285306

C	-0.84078236775842	0.00621180687379	1.67085331104745
C	1.73151959532792	0.81071285655233	2.41404439169375
C	1.45419466960636	0.43587341993047	1.08940327687550
C	0.17561948607756	0.02166270724073	0.69638342228595
O	0.87722468084496	1.09915337207750	4.68770882476155
H	-1.36642149141899	0.34575268843928	3.74993788426404
H	2.74264317777492	1.12366496512204	2.67673481322784
H	2.27364854873534	0.47019226230129	0.36748535074091
H	-1.85685923757793	-0.29216710123346	1.39845349158006
C	2.15598043099912	1.51444172360416	5.12971964441098
H	2.06337041687237	1.72502465995802	6.20361111035925
H	2.48909061582968	2.42947143446740	4.60896009650306
H	2.91458300691658	0.72584431722826	4.98021197690432
F	2.48601596594058	-0.33704327479825	-3.05548353951373
C	2.64655810365854	-1.10728797736339	-1.97473049922467
C	1.57131534595450	-1.87654590066029	-1.50495505231615
H	0.63565345055968	-2.03852532652359	-2.33118440415200
C	3.89146525178400	-1.10853062067218	-1.35594999757456
F	4.90101541394692	-0.36904147350947	-1.81145500157280
C	1.80806119383216	-2.68788071584804	-0.38754910784439
F	0.83258405722462	-3.45610530207944	0.10467077421861
C	4.07718125388148	-1.91301919389195	-0.22536645728674
C	3.03471611514101	-2.70202567789888	0.27132791524419
F	5.25391909744009	-1.92036796575635	0.38304453960498
F	3.23401294344898	-3.44675810124738	1.35768478060834

(DMF)Pd(Ar)(Ar_F) (Intermediate 6)

Pd	-0.17054451290274	-2.19401763261392	1.40199717991844
O	-2.07543864483831	-1.36205670081389	0.90002576744445
C	-2.51390617736288	-0.24958740580339	1.26576516232599
N	-3.71569960361029	0.22108785287509	0.94762488147546
H	-1.90956823463767	0.42045067555769	1.90066000188313
C	-4.64376242744415	-0.53416345451633	0.11739254996474
C	-4.16377959497375	1.52070634923066	1.42835511785022
H	-3.38071490518072	1.98131951180801	2.04534572284277
H	-5.07693908482448	1.40392520070427	2.03375598406888
H	-4.38953780446573	2.18290048715419	0.57720365922784
H	-4.17947952749708	-1.48110297200610	-0.17926756140858
H	-4.89969315603941	0.05033643542382	-0.78085033842034
H	-5.56959300974865	-0.73578739268058	0.67983041371052
C	0.39831601356457	0.78075973545900	5.09469108406773
C	-0.63335903736541	-0.17414853003522	5.07601399699515
C	-0.75031317549889	-1.06868024320031	4.01199231051892
C	1.31632240346630	0.82072780974977	4.03449200607271
C	1.19824956935958	-0.08780478657812	2.97064858894874
C	0.15887942562138	-1.02266226593078	2.94117417525762
O	0.42889006415190	1.61112179888853	6.17081490547661
H	-1.33926062131018	-0.19950848896208	5.91001270371588
H	2.13176071354141	1.54462353285448	4.02382819210626
H	1.93222416136742	-0.05140394199335	2.16335777038989
H	-1.56493541476304	-1.79709201409662	4.02054271481799
C	1.45361454643757	2.58486122958167	6.25429860241145

H	1.29116495333604	3.12979351172957	7.19377253694878
H	1.40847392269150	3.29608872084750	5.41086855100124
H	2.45491020929165	2.11985631555750	6.27381276981796
F	2.77123652184883	-1.75364050152161	0.25869858416917
C	2.75887446653667	-2.72827317762206	1.19360602104303
C	1.56802588050181	-3.08240906632708	1.82707583874160
C	3.98407322153540	-3.33202173025214	1.48386943149230
F	5.10387479288786	-2.97282209779104	0.84457048123671
C	1.66843536468385	-4.06999147969755	2.80769492676027
F	0.57930937330278	-4.45630531574381	3.50343075035499
C	4.03989570860955	-4.32301458526394	2.46472707229661
C	2.87264036385780	-4.69827126686187	3.13139380982284
F	5.20144053104182	-4.91232538828485	2.75946779978123
F	2.92878272482769	-5.64497872882501	4.07591583487041

(DMF)Pd - ArAr_F (Intermediate 7)

Pd	-0.23970310854619	-1.76482839120416	1.46336883943465
O	-2.23632162016775	-1.35227515096716	0.24346490699585
C	-3.29326656551238	-1.06430586735851	0.83051000431985
N	-4.44274270144328	-0.76084232762465	0.21650297376007
H	-3.35799027278969	-1.03953182011245	1.93505489591501
C	-4.54728331869171	-0.74018034104243	-1.23424205230000
C	-5.63997308900460	-0.43525659246621	0.97493316150156
H	-5.42454538455811	-0.48391912830491	2.05096849602316
H	-6.44844485334959	-1.14659482194854	0.73891988723846
H	-5.98656563849182	0.58095256740375	0.72473847521766
H	-3.57849014278829	-1.01199879382723	-1.66857049503762

H	-4.83671806660035	0.26626806958286	-1.57859136553494
H	-5.31502005026617	-1.45737568834052	-1.56759474562426
C	1.52363223858842	1.41139722878971	5.60516822246031
C	0.38008538437894	0.64618439712497	5.30507616186468
C	0.47384896857110	-0.46028016786950	4.47163236341107
C	2.76126570462731	1.04123596191366	5.05506477866445
C	2.84259490038401	-0.07400211661445	4.21667871704623
C	1.70939396401451	-0.83985104145982	3.90765786232359
O	1.33736397944422	2.47303445581249	6.42126644373500
H	-0.57772454328953	0.94533408813971	5.73618024557442
H	3.66613165481682	1.60804491974196	5.27252546585194
H	3.81429771221241	-0.34922684094224	3.80247807898918
H	-0.42462936562178	-1.03626687058572	4.23802591272793
C	2.45289823020428	3.27852809566987	6.77056115465214
H	2.07166240579057	4.06617073099923	7.43324889711682
H	2.91013526093692	3.74151943693505	5.87942969556653
H	3.22047283760412	2.69282600221445	7.30484615619597
F	3.12676468896065	-0.87427791089960	1.39452093802013
C	2.58916917399218	-2.01786102484809	1.83134806183870
C	1.81944046113498	-2.03117929977088	3.02238713562317
C	2.89602856262777	-3.18626322561022	1.12696142687184
F	3.62427491578406	-3.12498495585453	0.01207504150447
C	1.31957830988566	-3.29840411297605	3.41755209473233
F	0.62693853676798	-3.41136364267746	4.55387025829038
C	2.41880840467582	-4.41636369103937	1.57809733119740
C	1.61822760437344	-4.47072801644275	2.72033678639433

F	2.68141896073065	-5.52556720087997	0.89101864041598
F	1.13782586061443	-5.64129691266016	3.14114914702100

(DMF)Pd - ArAr$_F$ (TS67)

Pd	-0.28822611961780	-0.84768816348089	-0.93153690667739
O	-2.11839838267852	-0.34578862451701	-1.96036616476443
C	-2.99161211819953	0.48798068638534	-1.64692948330410
N	-4.09585091471865	0.71918603701027	-2.35559078675702
H	-2.89861683493615	1.10538991530766	-0.73451789748070
C	-4.37925584300682	-0.00281048549434	-3.58753663080377
C	-5.07652594118317	1.70419648629366	-1.92336227457044
H	-4.74936741156544	2.16959293431465	-0.98416437722348
H	-6.05391370221481	1.22084719967534	-1.76388013866536
H	-5.19386418554901	2.48604285273439	-2.69106528583167
H	-3.56139071003996	-0.70152933233923	-3.79547768304407
H	-4.47936981644811	0.70844327886655	-4.42307510861026
H	-5.32451677979662	-0.55999093880130	-3.48619071526404
C	1.31632027508542	1.55668980536793	2.78851624324513
C	0.58308310998976	0.37222992311333	2.98410484431004
C	0.36694519900818	-0.51241739932081	1.93353041647812
C	1.82734951713538	1.83653712691408	1.51141571627051
C	1.60642223053860	0.94540172366182	0.45674381790718
C	0.86742117363553	-0.24261867912582	0.63609889242433
O	1.47890380346350	2.35287522505258	3.87342749987930
H	0.18675430013886	0.16068069630323	3.98021728742450
H	2.40011605497649	2.74446441152880	1.32115198994219
H	2.02868482898329	1.18282233284643	-0.51813932266278

H	-0.19175660578091	-1.42704916524096	2.12413445247688
C	2.21454465026704	3.55725689598461	3.73553696933132
H	2.22135083910665	4.03358544607260	4.72464563780089
H	1.74197969480937	4.23893307694059	3.00727663099815
H	3.25387442444242	3.36204177891257	3.41918607748468
F	2.74241237804106	-0.44188892006551	-1.89309624127749
C	2.58370857231875	-1.57151678918397	-1.17972075614353
C	1.43516693493997	-1.75199476222678	-0.38131796096499
C	3.60930946122204	-2.50870446482067	-1.26974015735146
F	4.67965250004806	-2.27262270321110	-2.03470315359220
C	1.36519978144827	-3.00206913484499	0.26818187178162
F	0.29387905150633	-3.31785854622485	1.01918645396796
C	3.50520746051356	-3.71944683572898	-0.58338311747398
C	2.37305639725854	-3.96002913749821	0.19620279849118
F	4.46966870161844	-4.63574688264517	-0.67815362867669
F	2.25165402523996	-5.12342686851582	0.84239019092586

(DMF)Pd(Ar)(OH) - ArBpin

Pd	-0.18523149221345	-0.90737623463245	0.66103835492993
O	-0.42159158771774	-0.29223012975628	-1.33599965836134
O	-1.85595407229992	0.35963415629513	1.13325687193523
C	-2.44535105487672	0.92661402049932	0.18033801082556
N	-3.48995188584176	1.73159144548206	0.34430542826941
H	-2.08785916312572	0.75814442326243	-0.85184543546087
C	-4.03808692855899	2.03067609235562	1.65984113401209
C	-4.12993078187354	2.36377560300498	-0.80029616923570
H	-3.62765244760534	2.05214011904159	-1.72545024922980
H	-4.07239516198891	3.46065784900620	-0.71001089992242
H	-5.19148377862942	2.07218439479602	-0.85010491703044

H	-3.47627159432330	1.47968549605326	2.42212151570537
H	-5.09920785984252	1.73641584551893	1.69800969993892
H	-3.96717966124829	3.11234873622636	1.85852516121415
H	0.00043331918282	-0.91566776780490	-1.94115539446032
C	0.33338900546922	-1.89349846405335	5.35370038553396
C	-0.61812733306838	-2.59304608245936	4.59070085944813
C	-0.80052995491439	-2.28877421673351	3.24001692481126
C	1.07250318997767	-0.86561038803350	4.75200305265939
C	0.87477342174824	-0.57418240099913	3.39276569369339
C	-0.03853819489241	-1.28989219810286	2.61029733842795
O	0.46358438372572	-2.27336883797065	6.65797815668639
H	-1.19561496053815	-3.38517717432492	5.07518382753013
H	1.80662373845013	-0.29238526080558	5.31943144527044
H	1.47931176059274	0.21985734279883	2.94440432620916
H	-1.52959367729736	-2.86917295310663	2.66547266799843
C	1.45818016015467	-1.64860796430396	7.44602681845950
H	1.41885650847912	-2.12166206847557	8.43655106642503
H	1.27323160394001	-0.56530643387590	7.55700779081951
H	2.46569789489125	-1.79150750273358	7.01587509788887
H	0.02029859465595	-2.40692867566415	-4.94083999885282
H	3.81068364810101	-0.51213422961005	1.01596434937949
H	2.20480118723418	-0.99579994105888	-0.78567436166788
H	1.36743825883447	-4.33733188209944	-4.28001470274341
C	-0.80688131559498	-2.66090709358742	-4.26061336982385
H	4.33905510531626	-0.02470017409994	3.27238937564857
H	5.63187166177492	-0.91921271874319	2.39913566166071
H	-1.21944679848000	-1.72790645636112	-3.85516081924539
C	3.15985503354144	-1.38098753407502	1.10430787374266
C	2.20314633065089	-1.62629520784775	0.10586110722349
O	0.62579061339361	-2.81466660563041	-2.31282449450012
C	4.94331773938248	-0.94707547343625	3.25991842687122

H	-1.58787904660291	-3.17091478169916	-4.84479587523830
C	0.49835524834470	-4.73838475385503	-3.73732140878945
C	-0.29845315897066	-3.57257583720240	-3.15186082739956
H	-0.11029111215748	-5.32350832642834	-4.44190912949229
H	5.52285774583851	-1.01821143439830	4.18887775938578
H	0.86478502286376	-5.41041615891216	-2.94719813050830
B	0.40429328996058	-3.17903896442424	-1.00897011041307
C	1.30371938613899	-2.72701998321509	0.18356268083367
C	3.25564324224908	-2.25327861532436	2.19318794180426
O	4.11139950451278	-2.09939330941659	3.21832876517848
H	-2.10295956392719	-1.99673059225879	-1.74903762962564
C	-1.39991689045189	-4.02294418420218	-2.11480033110873
C	-2.52150982029238	-2.99453951787043	-1.94821702632571
H	-3.16161216967114	-2.95236504336696	-2.84132389479925
O	-0.65685671879555	-4.02979647734645	-0.85929407312492
C	1.44742835790508	-3.60005222490552	1.30911820252800
C	2.40909354089845	-3.38823299419153	2.26851668370967
H	-2.46480338344128	-5.45624883690251	-3.33922992131840
C	-1.97215177214884	-5.41220734997463	-2.35579290060329
H	-1.19459041297398	-6.18652249161729	-2.31679858571523
H	-3.14510422101486	-3.28905290067853	-1.09015727798567
H	2.51436461545071	-4.05341913479203	3.12777157828051
H	0.78114593596725	-4.46081269946285	1.39661378357294
H	-2.72450107424724	-5.63902684150914	-1.58521822552967

(DMF)Pd(Ar)(Ar) - pinBOH

Pd	0.36205534360859	-0.63941287100451	1.28567467877240
O	0.54759930962232	-0.40142457910249	-0.97887848473862
O	-1.47839632929352	0.58701898631626	1.05324721908594
C	-2.34815529275923	0.28505727762884	0.21495428243166
N	-3.45585018782134	0.99591227174456	-0.00943593853441
H	-2.25157926129441	-0.61683332792978	-0.41669261746254

C	-3.74269209046136	2.21684937732616	0.72760188949888
C	-4.42352368104466	0.57979425009961	-1.01253859544266
H	-4.08632566065364	-0.34904201835857	-1.49062073158169
H	-4.53392129137616	1.35959748743553	-1.78381775936951
H	-5.40751035134165	0.40820194978560	-0.54656099589374
H	-2.94131973864571	2.39876861539776	1.45255688524040
H	-4.70389797231462	2.11920426257465	1.25777002718111
H	-3.81193929236109	3.06991546051579	0.03292353046567
H	1.30309247094218	0.12415203780094	-1.28236263868513
C	-0.29894624416624	-0.80702088625522	6.07283298838502
C	0.23967055356882	-1.92865514481089	5.42125001267557
C	0.47283326506561	-1.90602812041494	4.04467907501348
C	-0.60866913899631	0.33253800535167	5.31713494525072
C	-0.38155057703784	0.33220550968177	3.93139105485131
C	0.16446377275918	-0.77534300069269	3.25690272068029
O	-0.48541612323726	-0.91590844295006	7.41990323979881
H	0.47489434529231	-2.81492464984602	6.01731282944698
H	-1.03077229756897	1.22169561023892	5.78758797308736
H	-0.65915958171529	1.22732979281204	3.36909679354328
H	0.90795617588770	-2.79277018048372	3.57970050286592
C	-1.03060932042148	0.18586484174587	8.11946948994670
H	-1.09586690948914	-0.11189311010264	9.17479134960075
H	-2.04106437595007	0.44259110655139	7.75423161389475
H	-0.38861184777021	1.08083286458108	8.03627718599878
H	0.71507660902582	-2.54110871300297	-5.64296334581377
H	5.20285940082316	-1.95157766317377	2.59477791440873
H	3.18161366728270	-0.57951041960448	2.74981053906502
H	2.11504668411964	-3.52151582237535	-3.89752692149776
C	-0.21574772427755	-2.69032065997226	-5.07520597156656
H	6.41100835644527	-3.94701731144157	2.86609376979683
H	7.02243603858642	-2.94277158352697	1.51134326985787

H	-0.88067548639606	-1.83924524851951	-5.27192548623040
C	4.32857186936395	-2.23314771042207	2.00615055938008
C	3.16781156880050	-1.44525584201621	2.08248612443880
O	0.62213610322622	-1.54407832154087	-3.10865630444345
C	6.59596849651920	-3.92639828997695	1.77718015263936
H	-0.69865682411740	-3.60856878272607	-5.44247792272221
C	1.20751130912234	-3.85660817572431	-3.37349134822216
C	0.10339546063064	-2.82277471915220	-3.59382774039860
H	0.91808751218519	-4.83890473717052	-3.77340505285318
H	7.31951517731232	-4.71219897996817	1.52109989924398
H	1.44967828499758	-3.96848924911888	-2.30682288556381
B	0.14654991823540	-1.38697601105854	-1.84372353641149
C	2.00965052002146	-1.74340496318067	1.34582700023183
C	4.34876366128982	-3.36967309112241	1.18487665453190
O	5.41986637608557	-4.20284940752929	1.04193967107345
H	-2.27661734954032	-1.36183051340188	-3.49909623237704
C	-1.15986129713944	-3.04701821311379	-2.66630967373107
C	-2.43604761005416	-2.41439964232372	-3.22099869732590
H	-2.79818180405795	-2.96002236379451	-4.10382866198397
O	-0.80052328029943	-2.29450601384121	-1.46754686879442
C	2.05732390162723	-2.89754254844481	0.53170715682085
C	3.19821047983150	-3.69764200692077	0.44856018082663
H	-1.58587153221426	-5.10595905912356	-3.17582227973900
C	-1.40834219078376	-4.49651323786242	-2.27673896311549
H	-0.55819208066865	-4.91996537559862	-1.72613825060132
H	-3.21741089846458	-2.45249453287984	-2.44722146629233
H	3.21722280924935	-4.58742210360980	-0.18710179818950
H	1.18190082471965	-3.18990527711783	-0.05427702168762
H	-2.30186462251392	-4.55959678527961	-1.63744898876182

(DMF)Pd(Ar)(Ar) - pinBOH (TS)

Pd	0.01479166387463	0.94057370470665	0.25689701284506

O	-0.19458618762676	1.21434507427194	-1.84671756908125
O	-1.68133786072427	2.17839944091185	0.63444145517924
C	-2.45272090761822	2.41046792895037	-0.39001250926122
N	-3.52764786666630	3.16438423569177	-0.30168732227300
H	-2.19722142379134	1.99103304614335	-1.35978667356706
C	-3.91452402229571	3.84779390567902	0.92009267507461
C	-4.35704362054292	3.38679606544503	-1.48134111693418
H	-3.95850698829529	2.81602007327948	-2.32961419483726
H	-4.36792160674312	4.45875490170306	-1.73883199046292
H	-5.39105417702528	3.06161346331751	-1.28009752701664
H	-3.20966816178941	3.57869504583745	1.71784742471662
H	-4.93442273978580	3.55365880034223	1.21093708137579
H	-3.88982141204280	4.93693658858496	0.75759092725819
H	0.51643140971433	1.39693140710393	-2.47990376045221
C	0.32898721386572	0.17732583599295	4.99344059156548
C	-0.14033342792849	-0.82990594785579	4.16819829174257
C	-0.25753242593740	-0.64863096752329	2.78754685311552
C	0.70354681970885	1.42388780361123	4.43217313447240
C	0.60605560302262	1.58275537959806	3.03172296059861
C	0.14325156462578	0.57491187360198	2.19477921963774
O	0.37647081964967	-0.11507555726849	6.32413026513026
H	-0.43102496312048	-1.78213792082770	4.63879992569297
H	1.04179724260156	2.24734926095010	5.04611262843213
H	0.89337736829283	2.55912335997374	2.61340616510004
H	-0.68288124422152	-1.45362529864106	2.19489054103828
C	0.85726911783396	0.85789851869609	7.22363962398494
H	0.83650285329963	0.40223671919977	8.22159281768838
H	0.21855656059729	1.75906770218963	7.21789579417382
H	1.89240171500816	1.15062999529629	6.97442003329558
H	0.10557197814702	-0.74195818766803	-5.95293539059705
H	4.44977395747407	0.94964548874851	0.65442470423010

H	2.52787035916960	1.48745383241782	-0.64966016365736
H	1.57086893030254	-2.37981277018630	-4.88259000581170
C	-0.72666005354328	-0.95958490208227	-5.26501659703413
H	5.57679938816717	0.31557634039753	2.57940722270438
H	6.42802362008674	-0.06276492144023	1.04632742813990
H	-1.27144654016291	-0.02390388808702	-5.08259702825354
C	3.66727956370110	0.18531934716637	0.52994272854010
C	2.53042035862774	0.46670458611734	-0.25260906511260
O	0.65229445678456	-0.65749465874299	-3.24302930529672
C	6.00282838105615	-0.49531328124282	1.96730769030757
H	-1.41151713115544	-1.64804919808944	-5.79383906794306
C	0.71166367899087	-2.77345417774876	-4.31830380758387
C	-0.19450557788055	-1.59085296029807	-3.96589627683814
H	0.21482923892602	-3.53952690204083	-4.93400912817565
H	6.79973367682048	-1.00144754049119	2.53013462262170
H	1.09162542562033	-3.24294234893549	-3.40030742590343
B	0.33249585858907	-0.62232890224532	-1.85644888089996
C	1.49190748834538	-0.51003559941768	-0.54549882362539
C	3.88347421638342	-1.09196171420408	1.04712882017652
O	5.00728393979634	-1.47969404249551	1.68218307725140
H	-2.31931016897346	-0.01705360006607	-3.06540918919291
C	-1.33058953544171	-1.94493478452952	-2.92254440695577
C	-2.59176117218137	-1.07945344027794	-3.06159405890716
H	-3.17211882707615	-1.30287254654331	-3.97244459224364
O	-0.69801525706922	-1.59345949993659	-1.65156956088533
C	1.70759185200862	-1.74355545861948	0.17299997900890
C	2.85094422140881	-2.05788446813086	0.88087647499032
H	-2.18367117400333	-3.70367659476596	-3.92732346227502
C	-1.76167961703439	-3.42403701910518	-2.94295180312284
H	-0.93192968666043	-4.11049343515473	-2.72994003979459
H	-3.24509392027421	-1.27206518113007	-2.19654653730260

H	3.01631387088991	-3.06606631331371	1.28014869151149
H	0.93219590775435	-2.50935777288550	0.08849349605759
H	-2.55468262353374	-3.60087792393470	-2.19887307635998

(DMF)Pd(Ar)(Ar)

Pd	-1.25446760298808	-0.05767560183188	3.16694545092642
O	-2.86365284338350	-0.48245763191376	1.75292229691885
C	-2.74002760603071	-1.12868395792046	0.69371105959145
N	-3.74383037270204	-1.41193888305748	-0.13573530624088
H	-1.75877211412744	-1.52399501486269	0.37570545107084
C	-5.10727515259150	-0.97980185055416	0.13506216235405
C	-3.51785997165926	-2.17120393387130	-1.35641123022362
H	-2.45706017501885	-2.44420503695735	-1.43373515566010
H	-3.80049812677483	-1.57084393681536	-2.23635640076109
H	-4.12600211706689	-3.09028143021515	-1.35023187418606
H	-5.13165812459517	-0.42793524731833	1.08135077616721
H	-5.77150702018516	-1.85670228453306	0.20106432704614
H	-5.46451979217847	-0.33078918862379	-0.68072450091464
C	1.73880100965948	1.36585804913711	6.67346242081190
C	0.61984899699974	0.56367670763375	6.95452312379264
C	-0.20418636791311	0.11529613897482	5.92064831297838
C	2.01570510172646	1.70890032713691	5.34150704633621
C	1.17677390923924	1.24663530288865	4.31567566275639
C	0.04312721137007	0.45580619850929	4.57121562714819
O	2.49049016421516	1.75320011607506	7.74148861072385
H	0.41770398695965	0.29601058426264	7.99523808586234
H	2.87814597359670	2.32698405412578	5.08905333782454
H	1.43179498677396	1.52099524994600	3.28744495712479
H	-1.05876673565392	-0.51755227940331	6.17874050990926
C	3.64376384685774	2.54041888565182	7.51139310822791
H	4.09697118579360	2.72786378643144	8.49415283411872
H	3.39084167675674	3.50674016393715	7.04023021498128

H	4.37406305656461	2.01522502274213	6.87060735636694
H	2.93574763938912	-2.47367992868557	1.40246950649161
H	1.70511261043231	-0.51748586340051	2.21019533460826
H	3.94728734214780	-4.57576251966993	1.64570507068963
H	3.31752979674803	-4.30267195399700	-0.01233128744608
C	1.91588025505308	-2.60700115687673	1.76524483716810
C	1.20352686338947	-1.48689109752915	2.22397313081783
C	3.24722137114280	-4.95142562357647	0.87864388400916
H	3.53364679780061	-5.97477390840434	0.60128281050995
C	-0.11280190629265	-1.59723043596646	2.68966150743886
C	1.31654074288463	-3.87470401316196	1.78590465382168
O	1.92191441154997	-5.02168508583108	1.37068938306677
C	-0.70012019298947	-2.87874154691082	2.70943984004497
C	0.00158180896859	-4.00076804460032	2.26517714591847
H	-0.45783555353386	-4.99263548663615	2.27982359234238
H	-1.72505897033463	-3.01341764432783	3.06533232546613

(Ar - Ar) - PdDMF

Pd	-0.64793428569754	-0.16141842757151	2.98386995971358
O	-2.65703116941025	0.19325145383298	1.76804233122086
C	-3.13061842371549	-0.63729486744413	0.97522689840440
N	-4.26938946414048	-0.46579844524888	0.29248032476010
H	-2.62883377749700	-1.60325747266772	0.77380762776930
C	-5.06462576553770	0.74389923265903	0.43624604597212
C	-4.76523079946783	-1.48251507188912	-0.62058515757940
H	-4.07625142457749	-2.33780413926849	-0.63739720378967
H	-4.85110643191419	-1.07224129701073	-1.64027515854205
H	-5.76110345346916	-1.83180849702340	-0.30141267283165
H	-4.56893534002580	1.41806834376582	1.14392847967460
H	-6.07125395042841	0.49317312616398	0.80934276378938
H	-5.16926121325848	1.24577855353774	-0.53954320988784

C	1.05561350280522	1.20028491983888	6.19663153334690
C	0.63401272196900	-0.09360532695330	6.56729562058984
C	0.78632972949011	-1.16402635300426	5.69836975582119
C	1.62607946820533	1.39727469110339	4.93416793513568
C	1.78583215314098	0.30755074691549	4.05771813379886
C	1.38731219181011	-1.00584586434681	4.41887498788859
O	0.86213955228327	2.17838855259469	7.11527072519980
H	0.18792501065108	-0.23354318250541	7.55446415959859
H	1.95661190747585	2.38362031309105	4.60994819413620
H	2.28565018881943	0.48021772141524	3.10260621866874
H	0.47817161515791	-2.15822360042776	6.02718033495243
C	1.27957216536786	3.49771156390036	6.80788030781476
H	1.03874834631523	4.11341805121867	7.68435720148965
H	0.74674685155783	3.89568971699775	5.92695621403807
H	2.36612549620690	3.54368614195136	6.61861185700203
H	3.89943169722988	-3.24271729619117	1.17016517349822
H	3.43246179032305	-1.32732274007056	2.61848475532924
H	4.44117672926920	-5.47344995643061	0.70796594973085
H	3.37218157328636	-4.76264951724087	-0.54761844617611
C	3.03766631718818	-3.28422419597551	1.83639495119387
C	2.76301764419331	-2.18891765903743	2.66252479391850
C	3.46365159350945	-5.56642409799360	0.20354874786381
H	3.40897853719320	-6.54026314648258	-0.30054798421481
C	1.67233914572475	-2.17956834690323	3.54681511013084
C	2.21499133018077	-4.41933149951833	1.88600378745702
O	2.39378184952669	-5.53292274273644	1.13267775505620
C	0.85992629322425	-3.33433125776703	3.58358547206915
C	1.12240965209113	-4.43180720654053	2.77311426242707
H	0.48209864723228	-5.31647263736304	2.80187060844892

H	-0.01127820228885	-3.36353828337389	4.24108085511181

(Ar - Ar) - PdDMF (TS)

Pd	-1.03396731659550	0.82921970871490	0.16117087420408
O	-2.77326995887642	0.93966904405375	-1.14784251339333
C	-2.86634047596282	0.16713206810895	-2.12269649253957
N	-3.94953356175681	0.04337127432300	-2.88899175925061
H	-2.02535523657786	-0.48740371275195	-2.41459636875610
C	-5.16297050310247	0.80027756639668	-2.62228274065525
C	-3.95189137986481	-0.85420412286025	-4.03347832809289
H	-2.97744714994421	-1.35492969695794	-4.11230096650851
H	-4.13829107948768	-0.28701555349706	-4.95980233133954
H	-4.74047219761323	-1.61574930111705	-3.92223051433191
H	-5.00926785021285	1.42662532806577	-1.73620009285302
H	-6.00285680792377	0.10929108034308	-2.44432691623508
H	-5.40925332633015	1.43779188923970	-3.48653489587000
C	1.48284024069457	2.42099049437670	3.72754690642003
C	0.56353032079090	1.38444939734840	3.97620596596913
C	0.02946989985338	0.63855948719537	2.92406313287448
C	1.85893395761833	2.69858061363955	2.40381251847699
C	1.31727597822368	1.94577021268635	1.35827415399819
C	0.37651891559512	0.92054735947723	1.58334600376157
O	1.95550112390284	3.09714269582166	4.80882266840731
H	0.26642506137837	1.18857543207810	5.00943797858376
H	2.55566130966139	3.50352947231540	2.17074525180400
H	1.62654934894766	2.18798397750699	0.33863761355645
H	-0.68643081530494	-0.15679528591976	3.14906708248004
C	2.90366309481609	4.13172950430680	4.60408859188292
H	3.15635207387472	4.52876798803380	5.59621686426751
H	2.49161213571470	4.94771784225450	3.98452852908692

H	3.82240625967046	3.75210664910341	4.12288491346816
H	3.21254956581923	-1.61156779394164	-1.48575483581048
H	2.21346367069575	0.37321446095006	-0.49603759123140
H	4.11691692329659	-3.80713900976784	-1.44035654679722
H	3.31572977536222	-3.39466001526190	-2.99246480669114
C	2.24208008521770	-1.70370586001195	-0.99767762250980
C	1.66340712764643	-0.56607785706489	-0.42299550833178
C	3.30169533458543	-4.08596059508266	-2.13156218770110
H	3.47415383290348	-5.10891331898508	-2.49274514748750
C	0.42488477890129	-0.60928913828725	0.23939075358334
C	1.57310529123562	-2.93537925250250	-0.94065756521501
O	2.04238447372295	-4.09272280737952	-1.48178653532932
C	-0.21255057670996	-1.87200984605166	0.32942492214853
C	0.33399373271280	-3.00307493455745	-0.27924580374883
H	-0.20166004324006	-3.95573120529819	-0.26483025341868
H	-1.17954603333817	-1.97071423904358	0.82973359912466

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