Supporting Information for:

Mechanistic and Computational Studies of Oxidatively Induced Aryl–CF_3 Bond-Formation at Pd: Rational Design of Room Temperature Aryl Trifluoromethylation

*Nicholas D. Ball, J. Brannon Gary, Yingda Ye, Melanie S. Sanford**

Department of Chemistry, University of Michigan, 930 N. University Avenue, Ann Arbor, Michigan 48109

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General Procedures

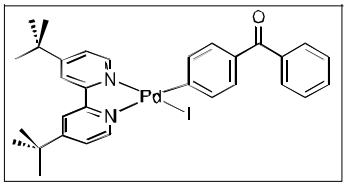
NMR spectra were obtained on a Varian Inova 400 (399.96 MHz for ^{1}H; 376.34 MHz for ^{19}F; 100.57 MHz for ^{13}C), a vnmr500 (500.09 MHz for ^{1}H; 470.56 MHz for ^{19}F; 125.75 MHz for ^{13}C) spectrometer, or an MR400 (400.53 MHz for ^{1}H; 376.87 MHz for ^{19}F; 100.71 MHz for ^{13}C) spectrometer. ^{1}H, ^{19}F and ^{13}C chemical shifts are reported in parts per million (ppm) relative to TMS, with the residual solvent peak used as an internal reference. $CDCl_3$ was referenced to –77.00 ppm in ^{13}C and 7.26 ppm in ^{1}H NMR spectra. ^{19}F NMR spectra are referenced on a unified scale, where the single primary reference is the frequency of the residual solvent peak in the ^{1}H NMR spectrum.[1] ^{1}H and ^{19}F multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), quartet (q), multiplet (m), and broad resonance (br). Elemental analyses were conducted by Atlantic Microlabs in Norcross, Georgia. Mass spectral data were obtained on a Micromass magnetic sector mass spectrometer or on a Micromass LCT mass spectrometer with an electrospray ionization mode.

Materials and Methods

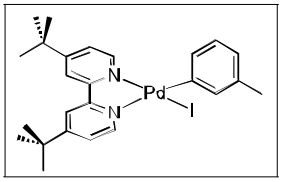
The palladium(II) complexes $Pd(dba)_2$ [dba = dibenzylideneacetone],[2] (dtbpy)$PdCl_2$ [dtbpy = 4,4'-di-*tert*-butyl-2,2'-bipyridyl],[3] (dtbpy)PdI_2, [4](bpy)Pd(Ph)(I) [bpy = 2,2'-bipyridyl],[5] (dtbpy)Pd(Aryl)(CF_3) (Aryl = *p*-FC_6H_4, *p*-$CF_3C_6H_4$ and *p*-$MeOC_6H_4$),[6] (teeda)Pd(Ph)(I) [teeda = *N,N,N',N'*-tetraethylethylenediamine],[7] (dpe)Pd(Ph)(I) [dpe =1,2-dipiperidinoethane],[7] (tmeda)Pd(*p*-FC_6H_4)(CF_3)[6] and (tmeda)Pd(Ph)(CF_3)[6] were prepared according to literature procedures. (dtbpy)Pd^{IV}(*p*-FC_6H_4)(F)(CF_3)(OTf) was prepared according to the literature.[6]All aryl iodides were purchased from commercial sources. Authentic samples of all of the aryl–CF_3 reductive elimination products were purchased from commercial sources. Rupert's reagent ($TMSCF_3$) and 1-fluoro-4-benzotrifluoride were obtained from Matrix Chemicals. The ligands tmeda, teeda, and dtbpy were obtained from Aldrich, while 1,2-bispiperidinoethane was synthesized according to a literature procedure.[8] 1-Fluoro-2,4,6-trimethylpyridinium triflate was obtained from TCI America. Unless otherwise noted, all reagents were used as received. Nitrobenzene-d_5, CD_2Cl_2, CD_3CN and $CDCl_3$ were obtained from Cambridge Isotope Laboratories. All other solvents were obtained from Fisher Chemicals. Tetrahydrofuran, toluene and pentane were purified using an Innovative Technologies (IT) solvent purification system consisting of a copper catalyst, activated alumina, and molecular sieves. Dichloroethane was distilled from CaH_2. Nitrobenzene-d_5 was distilled from P_2O_5 and then stored over 4 Å molecular sieves. All syntheses were conducted using standard Schlenk techniques or in an inert atmosphere glovebox unless otherwise stated.

Experimental Details

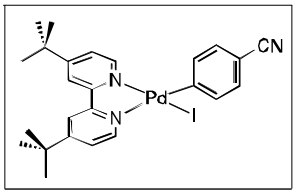
General procedure for the synthesis of (dtbpy)Pd(Aryl)(I): Under nitrogen, $Pd(dba)_2$ (3.0 g, 5.23 mmol, 1 equiv) was weighed into a 250 mL round bottom flask and dissolved in THF (50 mL). The ligand dtbpy (3.7 g, 13.6 mmol, 2.6 equiv) was added, and the resulting mixture was stirred at 25 ºC for 15 min. The aryl iodide (14.6 mmol, 2.8 equiv) was added, and the reaction was heated for 60 ºC for 3 h. In air, the reaction mixture was filtered through a plug of Celite, and the solvent was removed under reduced pressure. The resulting solid was washed with hexanes (3 x 20 mL), 50:50 (v:v) mixture hexanes/diethyl ether (6 x 20 mL) and then diethyl ether (3 x 5 mL) to remove all residual dibenzylidene acetone (dba). The product was then dried *in vacuo*.



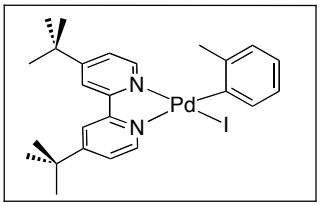
The product (dtbpy)Pd(*p*-PhC(O)C_6H_4)(I) was isolated as an orange solid (2.20 g, 62% yield). ^{1}H NMR ($CDCl_3$): δ 9.45 (d, *J* = 6 Hz, 1H), 7.97 (app. s, 2H), 7.80-7.78 (multiple peaks, 2H), 7.58 (d, *J* = 8 Hz, 2H), 7.53-7.42 (multiple peaks, 7H), 7.30 (dd, *J* = 6 Hz, 2Hz, 1H), 1.40 (s, 9H), 1.35 (s, 9H). ^{13}C NMR ($CDCl_3$): δ 197.68, 169.15, 163.78, 163.66, 155.39, 154.39, 151.72, 150.44, 138.74, 135.98, 132.62, 131.50, 129.91, 128.12, 127.96, 123.60, 123.38, 118.21, 118.08, 35.43(2 overlapping carbons), 30.31, 30.28. HRMS electrospray (m/z): $[M - I + MeCN]^+$ calcd for $C_{33}H_{36}N_3OPd$, 596.1880; Found, 596.1900. Notably, small amounts (~5%) of (dtbpy)Pd$(I)_2$ were observed in the ^{1}H and ^{13}C NMR spectra of most isolated samples of (dtbpy)Pd(*p*-Ph C(O)C_6H_4)(I).



The product (dtbpy)Pd(*m*-$CH_3C_6H_4$)(I) was isolated as an orange solid (0.72 g, 23% yield). ^{1}H NMR ($CDCl_3$): δ 9.50 (d, *J* = 6 Hz, 1H), 7.98 (s, 2H), 7.59 (d, *J* = 6 Hz, 1H), 7.51 (m, 1H), 7.35 (m, 1H), 7.28 (s, 1H), 7.20 (d, *J* = 7 Hz, 1H), 6.93 (t, *J* = 7 Hz, 1H), 6.74 (d, *J* = 7 Hz, 1H), 2.28 (s, 3H), 1.44 (s, 9H), 1.40 (s, 9H). ^{13}C NMR ($CDCl_3$): δ 163.21, 163.16, 155.92, 153.91, 152.57, 150.00, 146.54, 137.20, 136.54, 133.51, 126.99, 124.19, 123.90, 123.65, 118.37, 117.99, 35.61, 35.56, 30.52, 30.39, 21.65. HRMS electrospray (m/z): $[M - I - MeCN]^+$ calcd for $C_{25}H_{31}IN_2Pd$, 506.1782; Found, 506.1798. Notably, small amounts (~4%) of (dtbpy)Pd$(I)_2$ were observed in the ^{1}H and ^{13}C NMR spectra of most isolated samples of (dtbpy)Pd(*m*-$CH_3C_6H_4$)(I).

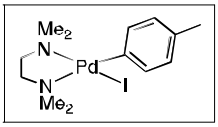


The product (dtbpy)Pd(*p*-CNC_6H_4)(I) was isolated as an orange solid (1.38 g, 66% yield). ^{1}H NMR ($CDCl_3$, 500.09 MHz): δ 9.47 (d, *J* = 6 Hz, 1H), 7.97 (s, 1H), 7.95 (s, 1H), 7.58 (d, *J* = 9 Hz, 2H), 7.50 (dd, *J* = 5 Hz, 2 Hz, 1H), 7.43 (d, *J* = 6 Hz, 1H), 7.34 (dd, *J* = 6 Hz, 2 Hz, 1H), 7.25 (d, *J* = 9 Hz, 2H), 1.41 (s, 9H), 1.38 (s, 9H). ^{13}C NMR ($CDCl_3$, 125.75 MHz): δ 163.78, 163.59, 158.15, 155.94, 153.77, 152.59, 149.26, 137.67, 129.18, 124.02, 123.71, 120.14, 118.64, 118.20, 106.32, 35.55, 35.47, 30.31, 30.18. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{25}H_{28}IN_3Pd$, 626.0255; Found, 626.0256. Notably, small amounts (~5%) of (dtbpy)Pd$(I)_2$ were observed in the ^{1}H and ^{13}C NMR spectra of most isolated samples of (dtbpy)Pd(*p*-CNC_6H_4)(I).

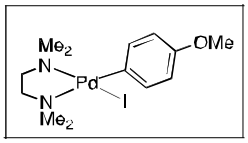


The product (dtbpy)Pd(*o*–tol)(I) was isolated as an orange solid (0.60 g, 19%). ^{1}H NMR ($CDCl_3$,): δ 9.45 (d, *J* = 6 Hz, 1H), 7.94 (s, 2H), 7.48 (d, *J* = 6 Hz, 1H), 7.39-7.34 (multiple peaks, 2H), 7.26 (m, 1H), 6.94 (m, 1H), 6.84-6.82 (multiple peaks, 2H), 2.57 (s, 3H), 1.40 (s, 9H), 1.36 (s, 9H). ^{13}C NMR ($CDCl_3$): δ 163.06, 163.02, 155.86, 153.70, 152.28, 149.18, 147.26, 141.28, 136.10, 128.65, 123.98, 123.82, 123.64, 123.09, 118.33, 117.86, 35.45, 35.41, 30.27, 30.23, 26.90. HRMS-electrospray (m/z): $[M + Na]^+$ calcd for $C_{25}H_{31}IN_2Pd$, 615.0464; Found, 615.0477. Notably, small amounts (~7%) of (dtbpy)Pd$(I)_2$ were observed in the ^{1}H and ^{13}C NMR spectra of most isolated samples of (dtbpy)Pd(*o*–tol)(I).

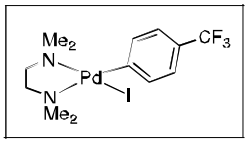
General procedure for the synthesis of (tmeda)Pd(Aryl)(I): Under nitrogen, Pd$(dba)_2$ (2.0 g, 3.48 mmol, 1 equiv) was weighed into a 250 mL round bottom flask and dissolved in THF (50 mL). TMEDA (1.1 g, 9.06 mmol, 2.6 equiv) was added, and the resulting mixture was stirred at 25 ºC for 15 min. The appropriate aryl iodide (9.74 mmol, 2.8 equiv) was added, and the reaction was heated at 60 ºC for 30 min. In air, the reaction mixture was filtered through a plug of Celite, and the solvent was removed under reduced pressure. The resulting solid was washed with hexanes (3 x 20 mL) and then diethyl ether (3 x 50 mL) to remove all residual dibenzylidene acetone (dba). The product was then dried *in vacuo*.



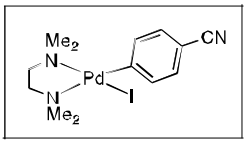
The product (tmeda)Pd(*p*-MeC_6H_4)(I) was isolated as an orange solid (1.18 g, 51% yield). ^{1}H NMR ($CDCl_3$): δ 7.06 (d, *J* = 8 Hz, 2H), 6.72 (d, *J* = 8 Hz, 2H), 2.68-2.66 (multiple peaks, 2H), 2.62 (s, 6H), 2.52-2.49 (multiple peaks, 2H), 2.28 (s, 6H), 2.18 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 139.49, 135.89, 131.43, 127.43, 61.98, 58.10, 49.77, 49.56, 20.48. HRMS electrospray (m/z): $[M - I + MeCN]^+$ calcd for $C_{13}H_{23}IN_2Pd$, 354.1162; Found, 354.1166.



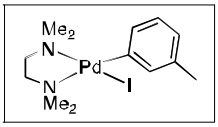
The product (tmeda)Pd(*p*-$MeOC_6H_4$)(I) was isolated as an orange solid (1.23 g, 77% yield). ^{1}H NMR ($CDCl_3$, 500.09 MHz): δ 7.08 (d, *J* = 9 Hz, 2H), 6.61 (d, *J* = 9 Hz, 2H), 3.69 (s, 3H), 2.72-2.70 (multiple peaks, 2H), 2.66 (s, 6H), 2.56-2.54 (multiple peaks, 2H), 2.31 (s, 6H). ^{13}C NMR ($CDCl_3$, 125.75 MHz): δ 156.22, 135.90, 131.70, 112.64, 61.92, 58.09, 54.90, 49.69, 49.53. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{13}H_{23}IN_2OPd$, 478.9788; Found, 478.9782.



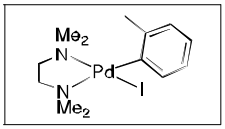
The product (tmeda)Pd(*p*-$CF_3C_6H_4$)(I) was isolated as an orange solid (1.02 g, 39% yield). ^{1}H NMR ($CDCl_3$): δ 7.35 (d, *J* = 8 Hz, 2H), 7.06 (d, *J* = 8 Hz, 2H), 2.59 (s, 6H), 2.45 (app s, 4H), 2.20 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –61.81 (s, 3F). ^{13}C NMR ($CDCl_3$): δ 152.69, 136.48, 124.77 (q, *J* = 271 Hz), 124.56 (q, *J* = 32 Hz), 121.90 (q, *J* = 4 Hz), 61.93, 58.08, 49.76, 49.60. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{13}H_{20}F_3IN_2Pd$, 516.9556; Found, 516.9573.



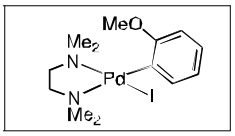
The product (tmeda)Pd(*p*-CNC_6H_4)(I) was isolated as an orange solid (0.95 g scale, 0.51 g, 68% yield). ^{1}H NMR ($CDCl_3$): δ 7.44 (d, *J* = 8 Hz, 2H), 7.13 (d, *J* = 8 Hz, 2H), 2.73 (br. s, 2H), 2.67 (s, 6H), 2.57 (br. s, 2H), 2.31 (6H). ^{13}C NMR ($CDCl_3$): δ 156.99, 137.40, 128.46, 119.99, 105.90, 62.12, 58.31, 49.98, 49.86. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{13}H_{20}IN_3Pd$, 473.9634; Found, 473.9644.



The product (tmeda)Pd(*m*-MeC_6H_4)(I) was isolated as an orange solid (1.24 g, 81% yield). ^{1}H NMR ($CDCl_3$): δ 7.05 (s, 1H), 7.00 (d, *J* = 8 Hz, 1H), 6.77 (m, 1H), 6.58 (d, *J* = 7 Hz, 1H), 2.69 (br multiplet, 2H), 2.63 (s, 6H), 2.53 (br multiplet, 2H), 2.29 (s, 6H), 2.18 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 144.46, 136.77, 135.31, 133.21, 125.86, 123.41, 61.92, 58.03, 49.76, 49.67, 49.49 (2 overlapping carbons), 21.29. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{13}H_{23}IN_2Pd$, 462.9838; Found, 462.9843.

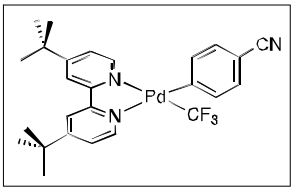


The product (tmeda)Pd(*o*-MeC_6H_4)(I) was isolated as an orange solid (0.52 g, 68% yield). ^{1}H NMR ($CDCl_3$): δ 7.17 (d, *J* = 7 Hz, 1 Hz, 1H), 6.82 (m, 1H), 6.77-6.72 (multiple peaks, 2H), 2.86-2.82 (multiple peaks, 2H), 2.70-2.66 (multiple peaks, 11H), 2.45 (s, 3H), 2.16 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 144.55, 141.63, 135.31, 127.76, 123.62, 122.62, 62.03, 58.09, 50.20 (2 overlapping carbons), 48.77, 48.52, 27.50. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{13}H_{23}IN_2Pd$, 462.9838; Found, 462.9844.

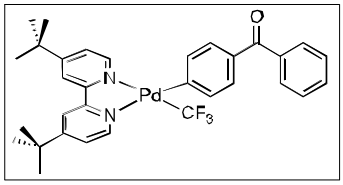


The product (tmeda)Pd(*o*-$MeOC_6H_4$)(I) was isolated as an orange solid (0.61 g, 38% yield). ^{1}H NMR ($CDCl_3$): δ 7.16 (d, *J* = 7 Hz, 1H), 6.82 (t, *J* = 7 Hz, 1H), 6.63 (t, *J* = 7 Hz, 1H), 6.47 (d, 8 Hz, 1H), 3.82 (s, 3H), 2.74-2.62 (multiple peaks, 4H), 2.70 (s, 3H), 2.69 (s, 3H), 2.36 (s, 3H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 161.80, 137.50, 129.74, 123.62, 119.95, 110.13, 61.98, 58.41, 55.75, 50.09 (2 overlapping carbons), 49.73, 49.27. HRMS electrospray (m/z): $[M + I]^+$ calcd for $C_{13}H_{23}IN_2OPd$, 329.0845; Found, 329.0848.

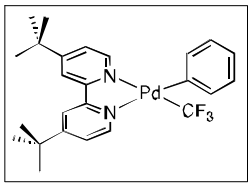
General procedure for the synthesis of (dtbpy)Pd(Aryl)(CF_3): Under nitrogen, (dtbpy)Pd(Aryl)(I) (1 equiv) and CsF (3 equiv) were suspended in THF (0.145 M) in a 25 mL Schlenk flask. This mixture was stirred for 10 min, and then Me_3SiCF_3 (2 equiv) was added. The reaction was stirred vigorously for 3 h at 22 ºC. The solvent was removed under reduced pressure, CH_2Cl_2 (15 mL) was added to dissolve the product, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (2 x 5 mL), the filtrate was concentrated under reduced pressure to (~2 mL), and hexanes (60 mL) was added to precipitate the product. The resulting solid was collected on fritted Büchner funnel, washed with hexanes (3 x 10 mL) and diethyl ether (2 x 2 mL), and dried *in vacuo*. The scale of these syntheses (amount of (dtbpy)Pd(Aryl)(I) starting material) are noted accordingly.



Complex 1b. Product **1b** was isolated as an yellow solid (1.2 g scale, 0.59 g, 54% yield). ^{1}H NMR ($CDCl_3$): δ 9.00 (app. d, *J* = 6 Hz 1H), 7.99 (s, 1H), 7.96 (s, 1H), 7.76 (d, *J* = 8 Hz, 2H), 7.54 (d, *J* = 6 Hz, 1H), 7.50 (d, *J* = 6 Hz, 1H), 7.32 (d, *J* = 8 Hz, 2H), 7.28 (d, *J* = 6 Hz, 1H), 1.43 (s, 9H), 1.36 (s, 9H). ^{19}F NMR ($CDCl_3$): δ –21.25 (s). ^{13}C NMR ($CDCl_3$): δ 168.76, 164.00, 163.81, 155.40, 154.33, 151.71 (br q, *J* = 4 Hz), 150.13, 136.94, 134.57 (q, *J* = 364 Hz), 129.37, 123.71, 123.45, 120.60, 118.33, 118.25, 106.20, 35.46 (2 overlapping carbons), 30.30, 30.23. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{26}H_{28}F_3N_3Pd$, 568.1162; Found, 568.1166.

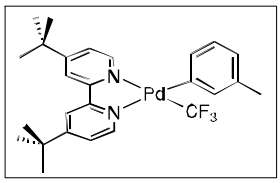


Complex 1d. Product **1d** was isolated as a yellow solid (1.0 g scale, 0.47 g, 51% yield). ^{1}H NMR ($CDCl_3$): δ 9.02 (br multiplet, 1H), 7.98 (s, 1H), 7.94 (s, 1H), 7.83 (d, *J* = 7 Hz, 2H), 7.78 (d, *J* = 8 Hz, 2H), 7.59-7.51 (multiple peaks, 5H), 7.48-7.43 (multiple peaks, 2H), 7.23 (resonance overlaps with $CDCl_3$ peak, 1H), 1.42 (s, 9H), 1.35 (s, 9H). ^{19}F NMR ($CDCl_3$): δ –20.86 (s). ^{13}C NMR ($CDCl_3$): δ 197.68, 169.14 (q, *J* = 11 Hz), 163.78, 163.66, 155.39, 154.39, 151.73 (q, *J* = 5 Hz), 150.44, 138.75, 135.99, 134.15 (q, *J* = 364 Hz), 132.63, 131.50, 129.91, 128.12, 127.96, 123.60, 123.39, 118.21, 118.08, 35.43 (2 carbon resonances overlapping), 30.31, 30.24. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{32}H_{33}F_3N_2OPd$, 605.1596; Found, 605.1603.

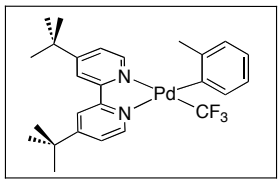


Complex 1e. Product **1e** was isolated as a yellow solid (0.53 g scale, 0.23 g, 47% yield). ^{1}H NMR ($CDCl_3$): δ 8.95 (app. s, 1H), 7.94 (s, 1H), 7.90 (s, 1H), 7.59-7.45 (multiple peaks, 4H), 7.17 (br d, *J* = 4 Hz, 1H), 7.04-7.00 (multiple peaks, 2H), 6.94 (m, 1H), 1.37 (s, 9H), 1.29 (s, 9H). ^{19}F NMR ($CDCl_3$): δ –20.45 (s). ^{13}C NMR ($CDCl_3$): δ 163.40, 163.39, 157.66 (q, *J* = 10 Hz), 155.33, 154.33, 151.62 (q, *J* = 4 Hz), 150.48, 135.90, 135.73 (q, *J* = 369 Hz), 126.86, 123.44, 123.21, 122.94, 118.12, 117.92, 35.36,

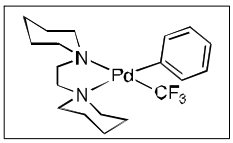
35.34, 30.28, 30.21. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{25}H_{29}F_3N_2Pd$, 543.1215; Found, 543.1223.



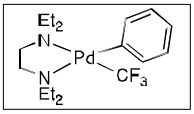
Complex 1i. NOTE: The product is partially soluble in hexanes and diethyl ether; therefore, pentanes (60 mL) was used to precipitate the product. The resulting solid was filtered over a fritted Büchner funnel, washed with pentanes (3 x 10 mL) and dried *in vacuo*. Product **1i** was isolated as a yellow solid (0.72 g scale, 0.35 g, 54% yield). ^{1}H NMR ($CDCl_3$): δ 8.94 (br. d, *J* = 4 Hz, 1H), 7.93 (s, 1H), 7.89 (s, 1H), 7.59 (d, *J* = 6 Hz, 1H), 7.44 (br. d, *J* = 5 Hz, 1H), 7.37 (s, 1H), 7.30 (br. d, *J* = 8 Hz, 1H), 7.17 (br. d, *J* = 6 Hz, 1H), 6.90 (m, 1H), 6.74 (br. d, *J* = 7 Hz, 1H), 2.22 (s, 3H), 1.36 (s, 9H), 1.29 (s, 9H). ^{19}F NMR ($CDCl_3$): δ –20.33 (s). ^{13}C NMR ($CDCl_3$): δ 163.35, 157.41 (q, *J* = 10 Hz), 155.30, 154.31, 151.58 (q, *J* = 4 Hz), 150.55, 135.93 (q, *J* = 364 Hz), 135.73, 136.48, 132.74, 126.48, 123.83, 123.58, 123.41, 123.20, 118.08, 117.89, 35.34, 35.33, 30.27, 30.19, 21.63. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{26}H_{31}F_3N_2Pd$, 557.1372; Found, 557.1383.



Product (dtbpy)Pd(*o*-tol)(CF_3) was isolated as an yellow solid (0.50 g scale, 0.20 g, 45%). ^{1}H NMR ($CDCl_3$): δ 9.05 (br d, *J* = 4 Hz, 1H), 7.98 (s, 1H), 7.93 (s, 1H), 7.58 (d, *J* = 7 Hz, 1H), 7.53 (d, *J* = 6 Hz, 1H), 7.46 (d, *J* = 6 Hz, 1H), 7.22 (m, 1H), 7.03 (d, *J* = 6 Hz, 1H), 6.96-6.89 (multiple peaks, 2H), 2.61 (s, 3H), 1.42 (s, 9H), 1.35 (s, 9H). ^{19}F NMR ($CDCl_3$): δ –20.51 (s). ^{13}C NMR ($CDCl_3$): δ 163.29, 159.17 (*J* = 10 Hz), 155.43, 154.28, 151.71, 151.67, 150.06, 141.58, 136.08 (*J* = 361 Hz), 135.45, 127.90, 123.55 (two overlapping carbons), 123.38, 122.59, 118.03, 117.92, 35.38 (two overlapping carbons), 30.34, 30.26, 26.46. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{26}H_{31}F_3N_2Pd$, 557.1372; Found, 557.1384. Anal. Calc. for $C_{23}H_{31}F_3N_2Pd$: C, 58.37, H, 5.84, N, 5.24; Found: C, 58.29, H, 5.95, N, 5.24. By ^{1}H, ^{19}F, ^{13}C NMR spectroscopy, <5% of (dtbpy)Pd(CF_3)$_2$ was observed.



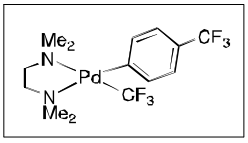
Complex 9. Product **9** was synthesized from (dpe)Pd(Ph)(CF_3) [dpe = 1,2-dipiperidinoethane] according the procedure described for (tmeda)Pd(Aryl)(CF_3). Under nitrogen, (dpe)Pd(Ph)(I) (1.0 g, 1.97 mmol, 1 equiv) and CsF (3 equiv) were suspended in THF (0.145 M) in a 25 mL Schlenk flask. This mixture was stirred for 10 min and then Me_3SiCF_3 (2 equiv) was added. The reaction was stirred vigorously for 6 h at 23 ºC. The solvent was removed under reduced pressure, CH_2Cl_2 (15 mL) was added to dissolve the product, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (2 x 5 mL), the filtrate was concentrated under reduced pressure to (~2 mL), and hexanes (60 mL) was added to precipitate the product. The resulting solid was collected on fritted Buchner funnel, washed with hexanes (3 x 10 mL) and diethyl ether (2 x 2 mL), and dried *in vacuo*. The product was isolated as a pale yellow solid (0.59 g, 67% yield). ^{1}H NMR (CD_2Cl_2): δ 7.42 (d, *J* = 7 Hz, 2H), 6.97-6.93 (multiple peaks, 2H), 6.87 (m, 1H), 3.56-2.63 (multiple peaks, 12H), 1.77-0.99 (multiple peaks, 12H). ^{19}F NMR (CD_2Cl_2): δ –21.02 (s). ^{13}C NMR (CD_2Cl_2): δ 159.27 (q, *J* = 10 Hz), 136.37, 135.14 (q, *J* = 365 Hz), 126.38, 122.59, 54.42, 54.16, 50.82, 49.73, 24.34, 24.11, 19.63, 19.16. HRMS electrospray (m/z): [M + Na]$^+$ calcd for $C_{19}H_{29}F_3N_2Pd$, 471.1215; Found, 471.1203.



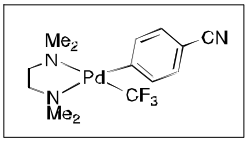
Complex 10. Product **10** was synthesized from (teeda)Pd(Ph)(I) [teeda = teeda = *N,N,N',N'*-tetraethylethylenediamine] according the procedure described for (tmeda)Pd(Ph)(CF_3). Under nitrogen, (teeda)Pd(Ph)(I) (0.4 g, 0.80 mmol, 1 equiv) and CsF (3 equiv) were suspended in THF (0.145 M) in a 25 mL Schlenk flask. This mixture was stirred for 10 min and then Me_3SiCF_3 (2 equiv) was added. The reaction was stirred vigorously for 20 h at 23 ºC. The solvent was removed under reduced pressure, CH_2Cl_2 (15 mL) was added to dissolve the product, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (2 x 5 mL), the filtrate was concentrated under reduced pressure to (~2 mL), and hexanes (60 mL) was added to precipitate the product. The resulting solid was collected on fritted Buchner funnel, washed with hexanes (3 x 10 mL) and diethyl ether (2 x 2 mL), and dried *in vacuo*. The product was isolated as a yellow solid (0.20 g, 56% yield). ^{1}H NMR (CD_2Cl_2): δ 7.42 (d, *J* = 8 Hz, 2H), 6.90 (m, 2H), 6.82 (m, 1H), 3.07-2.98 (multiple peaks, 2H), 2.82-2.73 (multiple peaks, 2H), 2.62 (s, 4H), 2.51-2.39 (multiple peaks, 4H), 1.36 (t, *J* = 7 Hz, 6H), 1.29 (t, *J* = 7 Hz, 6H). ^{19}F NMR (CD_2Cl_2): δ –21.10 (s). ^{13}C NMR (CD_2Cl_2): δ 157.88 (q, *J* = 10 Hz), 134.54 (q, *J* = 366 Hz), 136.26, 126.12 (q, *J* = 12 Hz), 122.46, 51.50, 51.38, 49.82, 48.40, 11.13, 11.06. HRMS electrospray (m/z): [M + Na]$^+$ calcd for $C_{17}H_{29}F_3N_2Pd$, 447.1215; Found, 447.1219.

General procedure for the synthesis of (tmeda)Pd(Aryl)(CF_3) 11: Under nitrogen, (tmeda)Pd(Aryl)(I) (1.0 g, 2.02-2.30 mmol, 1 equiv) and CsF (3 equiv) were suspended in THF (0.145 M) in a 25 mL Schlenk

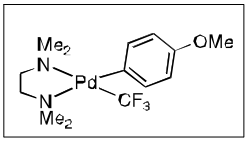
flask. This mixture was stirred for 10 min and then Me_3SiCF_3 (2 equiv) was added. The reaction was stirred vigorously for 3 h at 22 ºC. The solvent was removed under reduced pressure, CH_2Cl_2 (15 mL) was added to dissolve the product, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (2 x 5 mL), the filtrate was concentrated under reduced pressure to (~2 mL), and hexanes (60 mL) was added to precipitate the product. The resulting solid was collected on fritted Buchner funnel, washed with hexanes (3 x 10 mL) and diethyl ether (2 x 2 mL), and dried *in vacuo*. Some substrates were synthesized on a different scale with the same equivalents of materials as described above. These substrates and their scale of synthesis (as determined by amount of (tmeda)Pd(Aryl)(I) used) are noted accordingly.



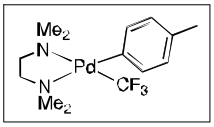
Complex 11b. Product **11b** was isolated as a yellow solid (0.37 g, 42% yield). ^{1}H NMR ($CDCl_3$): δ 7.61 (d, *J* = 8 Hz, 2H), 7.19 (d, *J* = 8 Hz, 2H), 2.69 (s, 6H), 2.59 (app. s, 4H), 2.20 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –21.14 (s, 3F), –61.67 (s, 3F). ^{13}C NMR ($CDCl_3$): δ 163.82 (q, *J* = 11 Hz), 136.05, 133.69 (q, *J* = 365 Hz), 125.19 (q, *J* = 271 Hz), 124.81 (q, *J* = 32 Hz), 122.44, 60.37, 59.84, 49.03, 48.72. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{20}F_6N_2Pd$, 417.0581; Found, 417.0586.



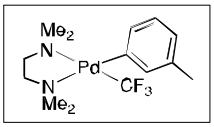
Complex 11c. Product **11c** was isolated as a yellow solid (0.47 scale, 0.21 g, 51% yield). ^{1}H NMR ($CDCl_3$) δ 7.64 (d, *J* = 7 Hz, 2H), 7.22 (d, *J* = 7 Hz, 2H), 2.69 (s, 6H), 2.60 (app. s, 4H), 2.21 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –21.60 (s). ^{13}C NMR ($CDCl_3$): δ 168.37 (q, *J* = 10 Hz), 136.91, 133.12 (q, *J* = 365 Hz), 128.65, 120.55, 105.86, 60.40, 59.96, 49.12, 48.82. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{30}F_3N_3Pd$, 416.0542 Found, 416.0537.



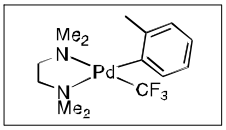
Complex 11d. Product **11d** was isolated as a yellow solid (0.89 g, 34% yield). ^{1}H NMR ($CDCl_3$): δ 7.33 (d, *J* = 8 Hz, 2H), 6.64 (d, *J* = 8 Hz, 2H), 3.72 (s, 3H), 2.67 (s, 6H), 2.56 (app. s, 4H), 2.20 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –20.80 (s). ^{13}C NMR ($CDCl_3$): δ 155.94, 144.95 (q, *J* = 11 Hz), 135.65, 134.74 (q, *J* = 365 Hz), 112.24, 60.23, 59.63, 54.80, 48.87, 48.52. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{23}F_3N_2Pd$, 421.0695; Found, 421.0699.



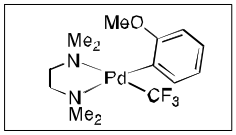
Complex 11f. Product **11f** was isolated as a yellow solid (0.51 g, 57% yield). ^{1}H NMR ($CDCl_3$): δ 7.33 (d, *J* = 8 Hz, 2H), 6.81 (d, *J* = 8 Hz, 2H), 2.67 (s, 6H), 2.56 (br multiplet, 4H), 2.22 (s, 6H), 2.20 (s, 3H). ^{19}F NMR ($CDCl_3$): δ –20.86 (s). ^{13}C NMR ($CDCl_3$): δ 151.74 (q, *J* = 11 Hz), 135.52, 134.93 (q, *J* = 365 Hz), 131.37, 127.17, 60.33, 59.66, 48.91, 48.63, 20.85. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{23}F_3N_2Pd$, 363.0864; Found, 363.0863.



Complex 11g. Product **11g** was isolated as a yellow solid (0.37 g, 42% yield). ^{1}H NMR ($CDCl_3$): δ 7.30 (s, 1H), 7.24 (d, *J* = 7 Hz, 1H), 6.85 (m, 1H), 6.70 (d, *J* = 7 Hz, 1H), 2.65 (s, 6H), 2.54 (app. s, 4H), 2.23 (s, 3H), 2.19 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –20.82 (s). ^{13}C NMR ($CDCl_3$): δ 156.30 (q, *J* = 10 Hz), 136.49, 134.92 (q, *J* = 365 Hz), 135.05, 132.83, 125.82, 123.48, 60.40, 59.70, 48.96, 48.70, 21.54. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{23}F_3N_2Pd$, 405.0746; Found, 405.0758.

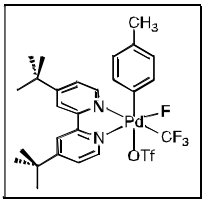


Complex 11h. Product **11h** was isolated as a yellow solid (1.5 g scale, 0.89 g, 59% yield). ^{1}H NMR ($CDCl_3$): δ 7.42 (d, *J* = 7 Hz, 1H), 6.91 (m, 1H), 6.85-6.81 (multiple peaks, 2H), 2.72-2.67 (multiple peaks, 11 H), 2.48-2.45 (multiple peaks, 2H), 2.32 (s, 3H), 2.09 (s, 3H). ^{19}F NMR ($CDCl_3$): δ –20.819 (s). ^{13}C NMR ($CDCl_3$): δ 157.67 (q, *J* = 11 Hz), 141.76, 135.30, 134.98 (q, *J* = 365 Hz), 127.11, 123.01, 122.27, 60.24, 59.56, 49.37, 48.94, 47.93, 47.78, 26.33. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{23}F_3N_2Pd$, 405.0746; Found, 405.0734.

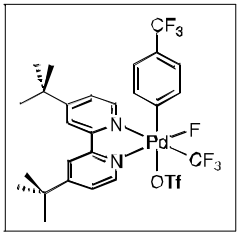


Complex 11i. Product **11i** was isolated as a yellow solid (0.50 g scale, 0.04 g, 10% yield). ^{1}H NMR ($CDCl_3$): δ 7.40 (d, *J* = 7 Hz, 1H), 6.93 (m, 1H), 6.69 (m, 1H), 6.58 (d, *J* = 8 Hz, 1H), 3.82 (s, 3H), 2.73 (s, 3H), 2.69 (s, 3H), 2.65-2.60 (multiple peaks, 2H), 2.53-2.46 (multiple peaks, 2H), 2.25 (s, 3H), 2.21 (s,

3H). ^{19}F NMR ($CDCl_3$): δ –20.74 (s). ^{13}C NMR ($CDCl_3$): δ 162.26, 143.25 (q, *J* = 11 Hz), 136.83, 133.79 (q, *J* = 365 Hz), 123.44, 119.76, 109.70, 60.22, 60.00, 55.61, 49.57, 49.03, 48.48, 48.36. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{14}H_{23}F_3N_2OPd$, 421.0695; Found, 421.0699.

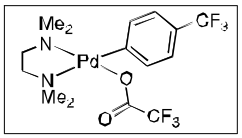


Synthesis of (dtbpy)Pd^{IV}(4-$CH_3C_6H_5$)(CF_3)(F)(OTf), 5. Under N_2, a solution of complex **1g** (60 mg, 0.11 mmol, 1 equiv) in DCE (1 mL) was added to a suspension of 1-fluoro-2,4,6-trimethylpyridium triflate (NFTPT) (45 mg, 0.15 mmol, 1.4 equiv) in DCE (1 mL). An additional 0.8 mL of DCE was added, and the reaction mixture was stirred at 23 °C for 45 min. The solvent was then removed *in vacuo*, and the residue was taken up in a mixture of DCE (0.5 mL) and toluene (2 mL). This suspension was filtered through a plug of Celite, which was washed with additional toluene (0.5 mL). Pentane (10 mL) was then added, and the resulting suspension was sonicated for 5 min. The solids were allowed to settle, and then the solution was removed by decantation. Fresh pentane (10 mL) was added, and the sonication process was repeated. The residue was dried *in vacuo*. The product was recrystallized by vapor diffusion of pentanes into a concentrated DCE solution of **5** at –30 °C. The resulting solid was washed with cold DCE (3 x 2 mL) and dried *in vacuo*, yielding **5** as a yellow solid (21 mg, 27% yield). ^{1}H NMR (CD_3CN): δ 8.93-8.91 (multiple peaks, 2H), 8.53 (s, 1H), 8.46 (s, 1H), 8.40 (m, 1H), 7.95 (m, 1H), 6.87-6.85 (multiple peaks, 2H), 6.81-6.79 (multiple peaks, 2H), 2.24 (s, 3H), 1.55 (s, 9H), 1.47 (s, 9H). ^{19}F NMR (CD_3CN): δ –31.23 (d, *J* = 9 Hz, 3F, Pd–**CF_3**), –79.30 (s, 3F, Pd–**OTf**), –256.42 (br q, 1F, Pd–**F**). Calc. for $C_{27}H_{31}F_7N_2O_3PdS$: C, 46.13, H, 4.42, N, 3.98 Found: C, 45.87, H, 4.51, N, 4.12. Splitting of the aryl–Pd carbon signal by both F and CF_3 groups could not be seen because this signal was in the baseline.

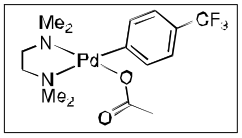


Synthesis of (dtbpy)Pd^{IV}(4-$CF_3C_6H_5$)(CF_3)(F)(OTf), 6. Under N_2, a solution of complex **1c** (60 mg, 0.09 mmol, 1 equiv) in DCE (0.5 mL) was added to a suspension of 1-fluoro-2,4,6-trimethylpyridium triflate (NFTPT) (38 mg, 0.13 mmol, 1.4 equiv) in DCE (0.5 mL). An additional 0.5 mL of DCE was added, and

the reaction mixture was stirred at 23 °C for 45 min. The solvent was then removed *in vacuo*, and the residue was taken up in a mixture of DCE (0.5 mL) and toluene (2 mL). This suspension was filtered through a plug of Celite, which was washed with additional toluene (0.5 mL). Pentane (10 mL) was then added, and the resulting suspension was sonicated for 5 min. The solids were allowed to settle, and then the solution was removed by decantation. Fresh pentane (10 mL) was added, and the sonication process was repeated. The residue was dried *in vacuo*. The product was recrystallized by vapor diffusion of pentanes into a concentrated DCE solution of **6** at –30 °C. The resulting solid was washed with cold DCE (3 x 2 mL) and dried *in vacuo*, yielding **6** as a yellow solid (4.3 mg, 2% yield). ^{1}H NMR (CD_3CN): δ 8.88 (d, *J* = 6 Hz, 1H), 8.85 (d, *J* = 6 Hz, 1H), 8.49 (s, 1H), 8.41 (s, 1H), 8.00 (m, 1H), 7.90 (m, 1 H), 7.32 (d, *J* = 9 Hz, 2H), 7.10 (d, *J* = 9 Hz, 2H), 1.50 (s, 9H), 1.41 (s, 9H). ^{19}F NMR (CD_3CN): δ –30.72 (d, *J* = 8 Hz, 3F, Pd^{IV}–**CF_3**), –63.10 (s, 3F, Pd^{IV}–**ArylCF_3**), –79.35 (s, 3F, Pd^{IV}–**OTf**), –254.55 (br. q, *J* = 10 Hz, 1F, Pd^{IV}–**F**). Anal. Calc. for $C_{27}H_{28}F_{10}N_2O_3PdS$: C, 42.84, H, 3.73, N, 3.70 Found: C, 42.55, H, 3.83, N, 3.78. Splitting of the aryl–Pd carbon signal by F, CF_3 and Aryl-CF_3 groups (qqd) could not be seen by ^{13}C NMR because this signal was in the baseline.



Under N_2, (tmeda)Pd(*p*-CF_3Ph)(I) (500 mg, 1.01 mmol, 1 equiv) and AgTFA (246 mg, 1.11 mmol, 1.1 equiv) were dissolved in CH_2Cl_2 (5 mL) in a 20 mL vial. The reaction was stirred vigorously for 30 min. The solvent was then removed under reduced pressure. CH_2Cl_2 (50 mL) was added, and the resulting suspension was filtered through a plug of Celite. The filtrate was concentrated under reduced pressure to ~2 mL, and hexanes (30 mL) was added to precipitate the product. The resulting solid was collected on a fritted filter, washed with hexanes (50 mL), and dried *in vacuo*. The product was isolated as a pale-yellow solid (430 mg, 88% yield). ^{1}H NMR ($CDCl_3$): δ 7.55 (d, *J* = 8 Hz, 2H), 7.17 (d, *J* = 8 Hz, 2H), 2.76 (m, 2H), 2.59 (m, 2H), 2.58 (s, 6H), 2.50 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –61.83 (s, 3F), –74.51 (s, 3F). ^{13}C NMR ($CDCl_3$): δ 155.10, 134.54, 126.20, 125.79(q, *J* = 32 Hz), 124.88 (q, *J* = 272 Hz), 122.29 (q, *J* = 4 Hz), 115.38 (q, *J* = 292 Hz), 63.63, 57.62, 51.55, 47.78. HRMS electrospray (m/z): $[M – TFA + MeCN]^+$ calcd for $C_{15}H_{20}F_6N_2O_2Pd$, 408.0879; Found, 408.0881.



Under N_2, (tmeda)Pd(*p*-CF_3Ph)(I) (500 mg, 1.01 mmol, 1 equiv) and AgOAc (186 mg, 1.11 mmol, 1.1 equiv) were dissolved in CH_2Cl_2 (5 mL) in a 20 mL vial. The reaction was stirred vigorously for 30 min.

The solvent was then removed under reduced pressure. CH_2Cl_2 (50 mL) was added, and the resulting suspension was filtered through a plug of Celite. The filtrate was concentrated under reduced pressure to ~2 mL, and hexanes (30 mL) was added to precipitate the product. The resulting solid was collected on a fritted filter, washed with hexanes (50 mL), and dried *in vacuo*. The product was isolated as a yellow solid (326 mg, 76% yield). ^{1}H NMR ($CDCl_3$): δ 7.60 (d, *J* = 8 Hz, 2H), 7.14 (d, *J* = 8 Hz, 2H), 2.71 (m, 2H), 2.59 (s, 6H), 2.56 (m, 2H), 2.46 (s, 6H). ^{19}F NMR ($CDCl_3$): δ –61.76 (s). ^{13}C NMR ($CDCl_3$): δ 176.94, 157.53, 135.15, 125.25 (q, *J* = 32 Hz), 125.14 (q, *J* = 272 Hz), 122.09 (q, *J* = 4 Hz), 63.37, 57.92, 51.42, 48.17, 23.83. HRMS electrospray (m/z): $[M + Na]^+$ calcd for $C_{15}H_{23}F_3N_2O_2Pd$, 408.0879; Found, 408.0880.

Procedure for the synthesis of (tmeda)Pd(*p*-CF_3Ph)(CF_3) (**11b**) from (tmeda)Pd(*p*-CF_3Ph)(TFA). Under N_2, (tmeda)Pd(*p*-CF_3Ph)(TFA) (416 mmol, 1 equiv) and CsF (2 equiv) were dissolved in THF (0.04 M) in a 25 mL Schlenk flask. Me_3SiCF_3 (10 equiv) was added. The reaction was stirred vigorously for 2 h at 22 °C. The solvent was then removed under reduced pressure. CH_2Cl_2 (50 mL) was added, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (40 mL), the filtrate was concentrated under reduced pressure to ~5 mL, and hexanes (60 mL) was added to precipitate the product. The resulting solids were collected on a fritted filter, washed with hexanes (50 mL), and dried *in vacuo* to afford **10b** in 56% yield.

Procedure for the synthesis of (tmeda)Pd(*p*-CF_3Ph)(CF_3) (**11b**) from (tmeda)Pd(*p*-CF_3Ph)(OAc). Under N_2, (tmeda)Pd(*p*-CF_3Ph)(OAc) (469 mmol, 1 equiv) and CsF (2 equiv) were dissolved in THF (0.04 M) in a 25 mL Schlenk flask. Me_3SiCF_3 (10 equiv) was added. The reaction was stirred vigorously for 2 h at 22 °C. The solvent was then removed under reduced pressure. CH_2Cl_2 (50 mL) was added, and the resulting suspension was filtered through a plug of Celite. The plug was washed with CH_2Cl_2 (40 mL), the filtrate was concentrated under reduced pressure to ~5 mL, and hexanes (60 mL) was added to precipitate the product. The resulting solids were collected on a fritted filter, washed with hexanes (50 mL), and dried *in vacuo* to afford **10b** in 61% yield.

General procedure for oxidatively induced Aryl–CF_3 coupling from 1a-1i, (dtbpy)Pd(*o*-tol)(CF_3), 9, 10 and 11a-11i. The Pd^{II} trifluoromethyl complex (40 mg, 1 equiv) was dissolved in an appropriate volume of nitrobenzene to make a 0.084 M solution. The solution was added to a 4 mL scintillation vial containing 1-fluoro-2,4,6-trimethylpyridium triflate (2 equiv) and a Teflon®-coated stir bar. The vial was purged with nitrogen, sealed with a Teflon®-lined cap, shaken vigorously, and then stirred at 23 °C for 1 h or 80 °C for 3h. The resulting light to dark brown mixture was cooled to room temperature, 4-fluoroanisole was added as an internal standard (under air), and the reactions were analyzed by ^{19}F NMR spectroscopy. The identities of the organic reductive elimination products were confirmed by comparison to authentic samples of these materials. The authentic sample was spiked into the crude reaction

mixtures, and, in each case, the ^{19}F NMR resonances were coincident. Reactions with complexes **1a-1k**, **11a, 11f and 11g** were conducted on a 50 mg scale.

It is important to note that the optimal conditions for ^{19}F NMR spectroscopic analysis of these reactions were as follows: spectral window of –10 to –150 ppm, relaxation delay = 2 s, and acquisition time = 2 s. These conditions were required due to the faster relaxation time of the standard relative to the trifluoromethylated Arene products.

Procedure to determine rate of reductive elimination from Pd^{IV} complex 4.

In a N_2-filled drybox, complex **4** (14 mg, 0.0198 mmol, 1.0 equiv) was added to a screw-cap NMR tube and dissolved in dry NO_2Ph- d_5 (0.4 mL). The internal standard, 4-fluoroanisole was added (50 µL of a stock solution in dry DCE, 0.0198 mmol, 1 equiv), and the tube was sealed with a Teflon®-lined cap. The tube was immediately placed in an NMR spectrometer with the temperature pre-equilibrated at 60 ºC, and the reaction was allowed to equilibrate for three minutes. The rate of reductive elimination was studied using ^{19}F NMR spectroscopy by monitoring the appearance of product **2a** (1-fluoro-4-benzotrifluoride). The data was fit to a first order kinetic plot using Sigma Plot 10. A representative reaction profile is shown in **Figure S1**.

Figure S1. Representative Kinetics for the Reductive Elimination from **4** to Form **2a** at 60 °C

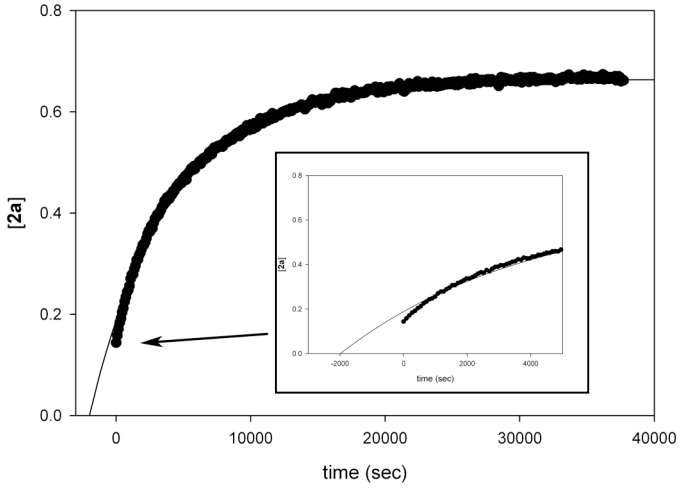
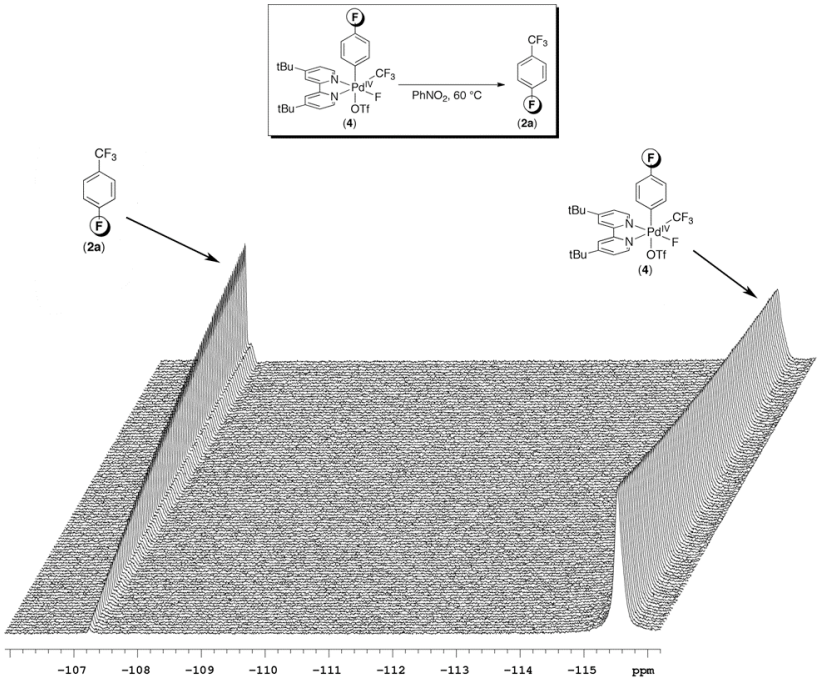


Figure S2. Array Spectrum Demonstrating the Reductive Elimination of **4** to **2a** in NO_2Ph-d_5 at 60 °C



As seen in Figure S1, the rate of product-formation changes as the reaction progresses. This is clearly seen at the beginning of the reaction (highlighted in the box). To confirm that this was the case, we plotted the rate data as function of percent conversion. As shown in Table S1, the initial rate of product formation decreased upon higher conversion. This suggests the possibility of inhibition by one of the products of this transformation. On the basis of this observation, we used initial rates (monitoring the 1st 10% of the reaction progress) for all subsequent rate experiments.

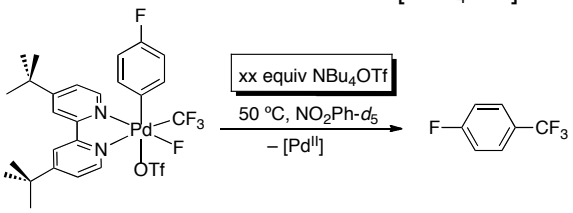
Table S1. Rate versus percent conversion of the **4** to **2a** in NO_2Ph-d_5 at 60 °C

Conversion	Rate (M s^{-1})
0-10%	2.20 x 10^{-4}
10-20%	1.91 x 10^{-4}
20-30%	1.66 x 10^{-4}
40-50%	1.64 x 10^{-4}
50-60%	1.31 x 10^{-4}
60-70%	1.11 x 10^{-4}
70-80%	1.16 x 10^{-4}
80-90%	1.18 x 10^{-4}
90-100%	1.34 x 10^{-4}

Determining Order in Triflate with 4 at 50 °C in NO_2Ph-d_5

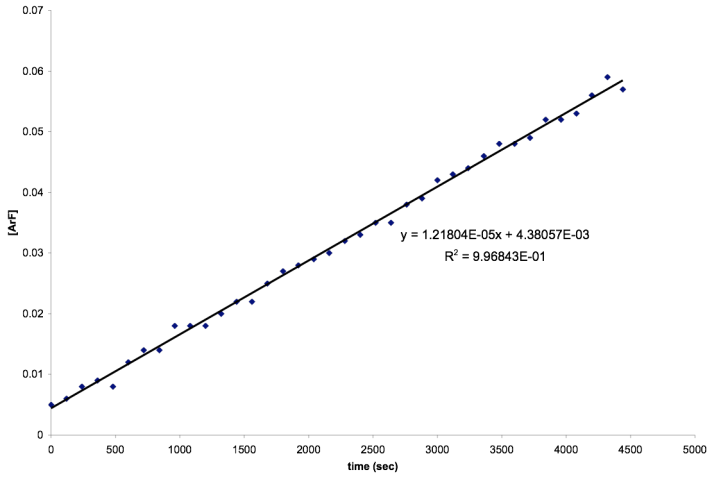
In a N_2-filled drybox, complex **4** (14 mg, 0.0198 mmol, 1.0 equiv) and NBu_4OTf (0.004 to 0.04 mmol, 0.01M to 0.1M) were combined in a screw-cap NMR tube and dissolved in dry NO_2Ph-d_5 (0.4 mL). An internal standard (4-fluoroanisole) was added (50 µL of a stock solution in dry NO_2Ph-d_5, 0.0198 mmol, 1 equiv), and the tube was sealed with a Teflon®-lined cap. The tube was immediately placed in an NMR spectrometer with the temperature pre-equilibrated at 50 ºC, and the reaction was allowed to equilibrate for three minutes. The rate of reductive elimination was studied using ^{19}F NMR spectroscopy by monitoring the appearance of the product signal. The reaction was followed to 10% conversion of **4** to 1-fluoro-4-benzotrifluoride (**2a**). The data was plotted as [**2a**] versus time and fit to a linear regression where m = initial rate. Each experiment was carried out in duplicate, and the initial rates reported in **Table S2** represent an average of two runs.

Table S2. Initial Rate as a Function of [NBu_4OTf] at 50 ºC.



equiv	[OTf^-]	1/[OTf^-]	Initial rate (M s^{-1})	Error in initial rate (M s^{-1})
0.20	0.01	100	2.91×10^{-5}	$\pm 3.4 \times 10^{-7}$
0.60	0.03	33.3	1.68×10^{-5}	$\pm 4.4 \times 10^{-7}$
1.0	0.05	20.0	1.35×10^{-5}	$\pm 8.4 \times 10^{-8}$
1.4	0.07	14.3	1.25×10^{-5}	$\pm 9.1 \times 10^{-8}$
2.0	0.1	10.0	1.18×10^{-5}	$\pm 5.6 \times 10^{-8}$

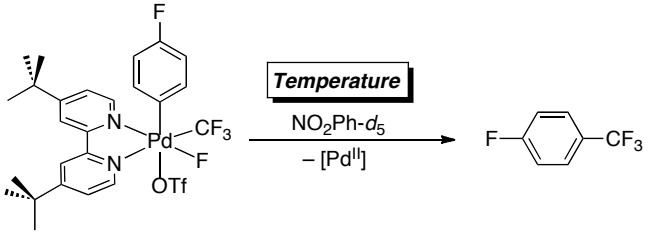
Figure S3. Representative Initial Rate Data (Reductive Elimination from **4** in the Presence of 0.07 M NBu_4OTf)



Activation Parameters for Reductive Elimination from 4

In a N_2-filled drybox, complex **4** (14 mg, 0.0198 mmol, 1.0 equiv) was added to a screw-cap NMR tube and dissolved in dry NO_2Ph-d_5 (0.4 mL). An internal standard (4-fluoroanisole) was added (50 µL of a stock solution in dry NO_2Ph-d_5, 0.0198 mmol, 1 equiv), and the tube was sealed with a Teflon®-lined cap. The tube was immediately placed in an NMR spectrometer with the temperature pre-equilibrated, and the reaction was allowed to equilibrate for three minutes. The rate of reductive elimination was studied using ^{19}F NMR spectroscopy by monitoring the appearance of the product signal. The rate was followed to 10% conversion of **4** to 1-fluoro-4-benzotrifluoride (**2a**) at 30 °C, 40 °C, 50 °C and, 60 °C. The rate data reported in **Table S3** represent an average of two runs.

Table S3. Initial Rate as a Function of Temperature



Temperature (K)	Initial Rate (M s^{-1})	Error in initial rate (M s^{-1})	ln(*k*/T)	1/T
303.2	1.15×10^{-6}	2.1×10^{-8}	–19.39	0.0033
313.2	5.15×10^{-6}	5.4×10^{-8}	–17.92	0.0032
323.2	2.21×10^{-5}	7.5×10^{-7}	–16.50	0.0031
333.2	9.59×10^{-5}	1.0×10^{-6}	–15.06	0.0030

Figure S4. Representative Initial Rate Data (Reductive Elimination from **4** at 50 ºC)

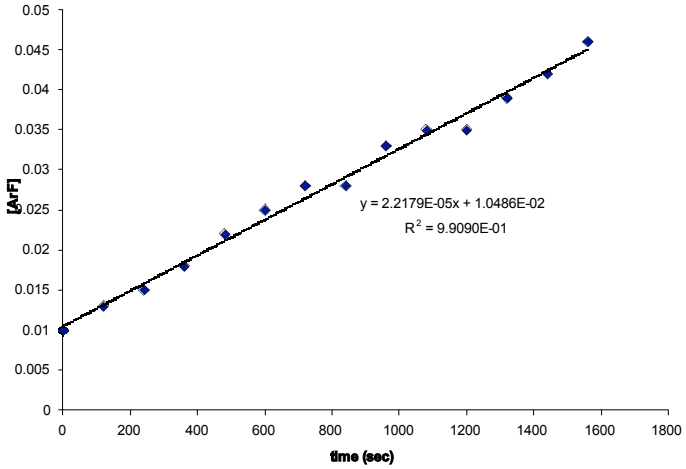
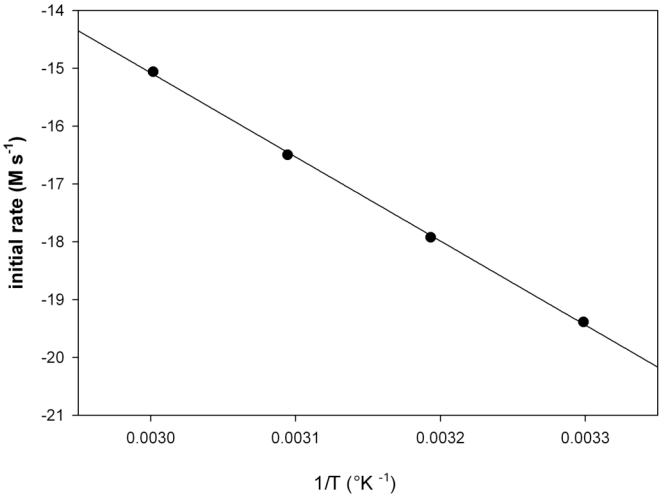


Figure S5. Eyring Plot for the Reductive Elimination of **4** in NO_2Ph-d_5



$\Delta H^{\ddagger}$ = +29.1 ± 0.2 kcal/mol, $\Delta S^{\ddagger}$ = +9.48 ± 0.8 eu

Determining Initial Rate of Reductive Elimination from Complexes 5 and 6 at 50 °C in NO_2Ph-d_5

In a N_2-filled drybox, complex **5** or **6** (14 mg, 1.0 equiv) was dissolved in dry NO_2Ph-d_5 (0.4 mL). An internal standard (4-fluoroanisole) was added (50 µL of a stock solution in dry in NO_2Ph-d_5, 0.0198 mmol, 1 equiv), and the tube was sealed with a Teflon®-lined cap. The tube was immediately placed in an NMR spectrometer with the temperature pre-equilibrated at 50 ºC, and the reaction was allowed to equilibrate for three minutes. The rate of reductive elimination was studied using ^{19}F NMR spectroscopy by monitoring the appearance of the product signal. The reaction was followed to 10% conversion of Pd^{IV} complex to product. The data was plotted as [**product**] versus time and fit to a linear regression where m

= initial rate. Each experiment was carried out in duplicate, and the initial rates reported in **Table S4** represent an average of two runs.

Table S4. Initial Rate for Aryl–CF_3 Reductive Elimination from Complexes **5** and **6** at 50 ºC in NO_2Ph-d_5

Compound	Initial rate (M s^{-1})	Error initial rate (M s^{-1})
5	4.58×10^{-4}	1.6×10^{-6}
6	1.43×10^{-5}	2.0×10^{-8}

Figure S6. Representative Initial Rate Data (Reductive Elimination from **5** at 50 ºC in NO_2Ph-d_5)

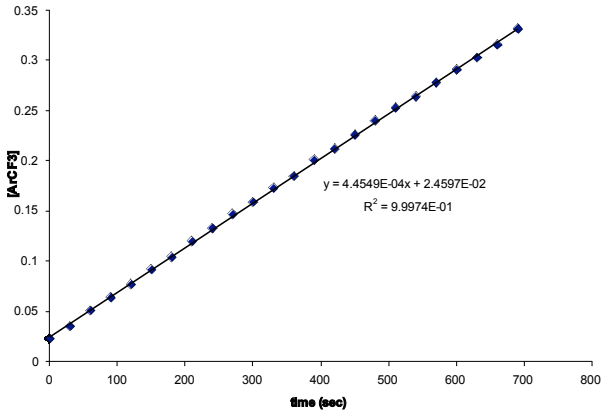
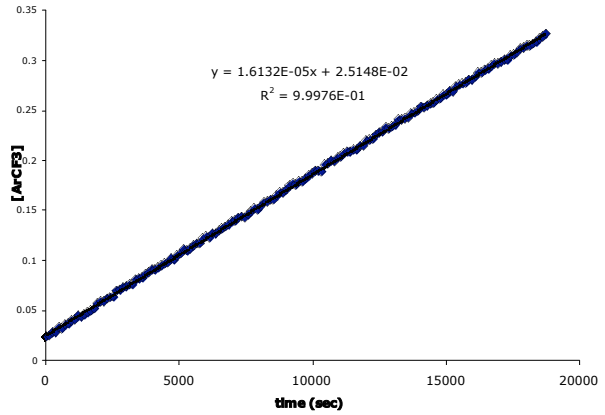


Figure S7. Representative Initial Rate Data (Reductive Elimination from **6** at 50 ºC in NO_2Ph-d_5)



Computational Methods

Using Gaussian 09 suite of programs,[9] all density functional theory (DFT) calculations were performed with the M06 functional[10] along with the Stevens (CEP-31G) valence basis sets with effective core potentials.[11,12] The CEP-31G basis set are triple-ξ for Pd and double-ξ for all main group elements. A d-polarization function (see 6-31G*)[13,14] was added to all non-hydrogen main group elements: ξ_d = 0.8 for carbon, nitrogen, oxygen, and fluorine and ξ_d = 0.65 for sulfur (referred to as CEP-31G(d) level of theory). All geometries were optimized using CEP-31G(d)/M06 without symmetry constraints using the restricted Kohn-Sham formalism for all complexes. All minima were confirmed by the absence of imaginary frequencies and all transitions states were verified by visual inspection of the single imaginary frequency vibration. Transition states for Ph-CF_3 and Ph-F reductive elimination from **8** and Ph-CF_3 reductive elimination from $[(tmeda)Pd(Ph)(CF_3)(F)]^+$ were optimized along the reaction coordinate in each direction. Thermochemical data was calculated using unscaled vibrational frequencies and default parameters at 298.15 K and 1 atm. Solvent corrections were performed as single point calculations using the SMD model[15] with default settings. Single point energy calculations (using CEP-31G(d)/M06 optimized geometries) were performed to distinguish between Aryl-CF_3 versus Aryl-F reductive elimination transition states using the related triple-ξ basis set for main group elements CEP-121G.[11,12] These calculations were also augmented with d-polarization function (f-polarization for Pd)[16] added to all atoms (see 6-311G**++)[13,14]: ξ_d = 0.626 for carbon, ξ_d = 0.913 for nitrogen, ξ_d = 1.750 for fluorine, ξ_s = 0.036 for hydrogen, and ξ_f = 1.472 for palladium and p-diffuse function were added to all main group elements: ξ_{sp} = 0.0438 for carbon, ξ_{sp} = 0.0639 for nitrogen, ξ_{sp} = 0.1076 for fluorine and ξ_s = 0.036 for hydrogen (referred to as CEP-121G(d,p). NBO analysis[17] was used to determine relevant charge distribution in transition states. All rate constants for Hammett analysis are calculated using transition state theory based on gas phase $\Delta H^{\ddagger}_{298}$ with the assumption of similar entropy components to all transition states at 298 K.

Table S5. Transition State and Solvent Correction Data

Transition state	Basis Set	Gas/Solvent	$\Delta SCF^{\ddagger}$	$\Delta(SCF+ZPE\ corr)^{\ddagger}$	$\Delta H^{\ddagger}_{298}$	$\Delta G^{\ddagger}_{298}$
Aryl-CF_3	CEP-31G(d)	Gas	10.15	9.93	9.41	10.85
Aryl-F	CEP-31G(d)	Gas	11.62	10.84	10.66	10.91
Aryl-CF_3	CEP-31G(d)	Nitrobenzene	13.69	13.74	13.72	13.55
Aryl-F	CEP-31G(d)	Nitrobenzene	15.01	14.48	14.75	13.79
Aryl-CF_3	CEP-121G(d,p)	Gas	9.41	9.42	8.88	10.17
Aryl-F	CEP-121G(d,p)	Gas	11.87	10.99	10.82	11.03
Aryl-CF_3	CEP-121G(d,p)	Nitrobenzene	13.12	13.39	12.76	14.67
Aryl-F	CEP-121G(d,p)	Nitrobenzene	15.38	14.77	14.47	15.50

$\Delta SCF^{\ddagger}$ = electronic transition state energy; $\Delta(SCF+ZPE\ corr)^{\ddagger}$ = zero point energy corrected electronic transition state energy; $\Delta H^{\ddagger}_{298}$ = thermally corrected transition state enthalpy; $\Delta G^{\ddagger}_{298}$ = thermally corrected transition state Gibbs energy. All energies are reported in kcal/mol.

Table S6. NBO Analysis Charges

Complex	Ipso-Ph	CF_3 carbon
$[(bpy)Pd^{IV}(Ph)(CF_3)(F)]^+$ intermediate	+0.07	+1.18
$[(bpy)Pd^{IV}(Ph)(\mathbf{C}H_3)(F)]^+$ intermediate	+0.06	-0.58 ($\mathbf{C}H_3$)
$[(bpy)Pd^{IV}(Ph)(CF_3)(F)]^+$ Ph-CF_3 ts	-0.11	+1.24

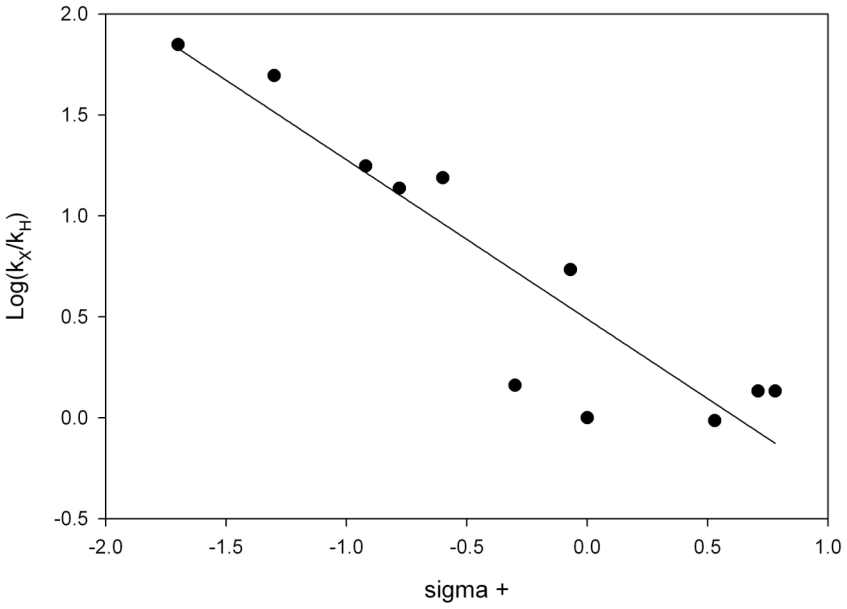
Calculations run using CEP-31G(d)/M06 in the gas phase.

Table S7. Electronic Substituent Analysis

X	$\Delta SCF^{\ddagger}$	$\Delta(SCF+ZPE\ corr)^{\ddagger}$	$\Delta H^{\ddagger}_{298}$	$\Delta G^{\ddagger}_{298}$	σ^+
NMe_2	7.08	7.57	6.89	9.05	-1.70
NH_2	7.82	7.49	7.10	8.03	-1.30
OH	8.40	8.11	7.70	8.30	-0.92
OMe	8.45	8.26	7.86	8.66	-0.78
SMe	8.61	8.05	7.79	7.93	-0.60
Me	9.74	9.76	9.19	10.95	-0.30
F	9.06	8.87	8.41	9.46	-0.07
H	10.15	9.93	9.41	10.85	0
CF_3	9.78	10.05	9.43	11.73	0.53
CN	9.83	9.72	9.23	10.66	0.71
NO_2	10.06	9.63	9.23	10.09	0.78

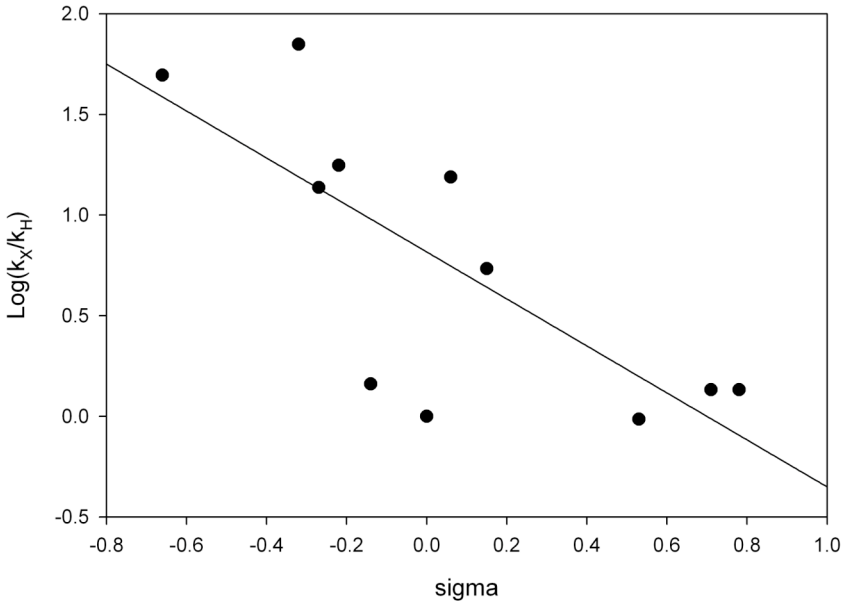
$\Delta SCF^{\ddagger}$ = electronic transition state energy; $\Delta(SCF+ZPE\ corr)^{\ddagger}$ = zero point energy corrected electronic transition state energy; $\Delta H^{\ddagger}_{298}$ = thermally corrected transition state enthalpy; $\Delta G^{\ddagger}_{298}$ = thermally corrected transition state Gibbs energy. All energies are reported in kcal/mol.

Figure S8. Hammett Plot (versus σ^+) for Aryl-CF_3 Reductive Elimination from [(bpy)Pd^{IV}(*p*-XC_6H_4)(CF_3)(F)]$^+$



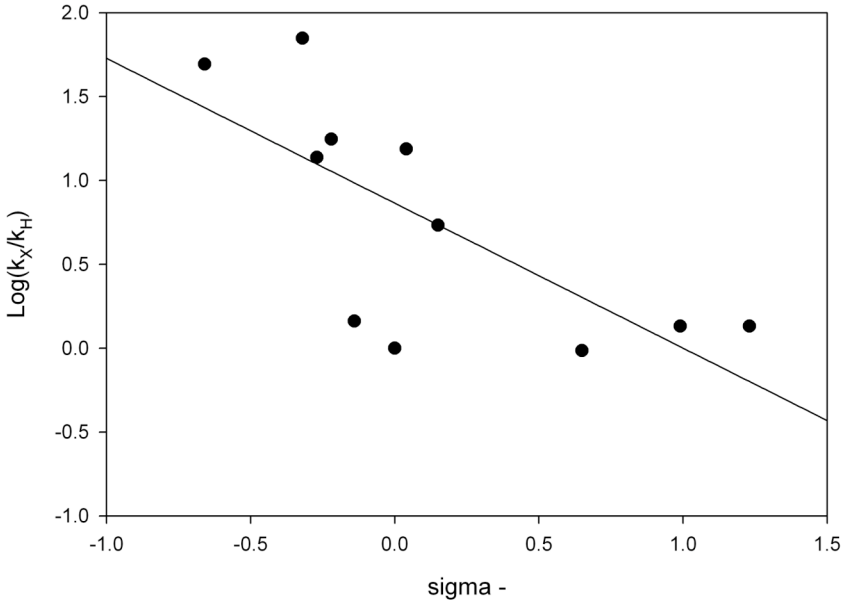
$\rho^+ = -0.79$; $R^2 = 0.84$

Figure S9. Hammett Plot (versus σ) for Aryl-CF_3 Reductive Elimination from [(bpy)Pd^{IV}(*p*-XC_6H_4)(CF_3)(F)]$^+$



$\rho = -1.17$; $R^2 = 0.57$

Figure S10. Hammett Plot (versus σ^-) for Aryl-CF_3 Reductive Elimination from [(bpy)Pd^{IV}(*p*-XC_6H_4)(CF_3)(F)]$^+$



$\rho^- = -0.86$; $R^2 = 0.52$

Calculations – Optimized Atomic Coordinates

Complex formulas along with element symbol followed by x, y, z Cartesian coordinates (Å). Complexes are tabulated in the order that the complexes appear in the paper.

$[Pd(bpy)(C_6H_5)(CF_3)(F)(OTf)]$

Pd	-0.65671900	-0.57900800	-0.34736500
C	-2.66727700	-0.19917500	-0.28954000
C	-3.35603400	-0.24579700	-1.51922500
C	-3.30110400	0.16403200	0.91798300
C	-4.73465100	0.08857500	-1.53041300
H	-2.83499000	-0.55174100	-2.43121900
C	-4.68163800	0.49343200	0.88248600
H	-2.77122100	0.17344900	1.87638200
C	-5.39715800	0.45997500	-0.33663600
H	-5.28300300	0.05015300	-2.47916500
H	-5.18753100	0.76787200	1.81593300
C	-0.09132200	-0.50882100	2.65486800
C	-0.06615900	1.57440100	1.55877500
C	0.29937900	0.07270900	3.87781500
H	-0.24477000	-1.58752900	2.56197900
C	0.29079700	2.22849400	2.75795600
C	0.47237600	1.47218300	3.93169900
H	0.46354400	-0.56586300	4.74943200
H	0.46846200	3.30738400	2.75987600
H	0.76839100	1.96402800	4.86382300
C	-0.30246100	1.96157600	-2.07722100
C	-0.12152500	2.28559200	0.24827400
C	-0.06581400	3.33081400	-2.33266000
H	-0.45011800	1.20979500	-2.86450200
C	0.12092600	3.66691400	0.08077000
C	0.14442500	4.18893500	-1.23169100
H	-0.03238900	3.69950200	-3.36112500
H	0.30459200	4.31965000	0.93943200
H	0.34048100	5.25465600	-1.38999400
C	-1.09729500	-2.53527300	0.14138200
F	-1.77458300	-2.61923800	1.31946900
F	0.03204600	-3.23220300	0.29706400
F	-1.84334400	-3.13815800	-0.77899400
F	-0.78702300	-1.08208400	-2.22653900
O	1.55596100	-0.98157700	-0.37796900
S	2.55479800	0.14573100	-0.34667500
O	2.62763100	0.81673000	0.96097500
O	2.53269100	1.01050900	-1.52827600
C	4.14638100	-0.82648700	-0.47706300
F	4.18231700	-1.52700100	-1.61107600
F	5.18486100	0.01810500	-0.46236500
F	4.27014100	-1.66852100	0.55445900
N	-0.33141400	1.48633400	-0.82425500
N	-0.29821000	0.22652600	1.54252200
H	-6.46282400	0.71542200	-0.35448700

$[Pd(bpy)(C_6H_5)(CF_3)F]^+$ intermediate

Pd	-0.38557800	0.02778500	-0.81707600
C	1.52717000	-2.39595700	-1.14119500
C	2.44289100	-0.51188000	-0.05698600
C	2.73187000	-3.12232400	-0.99440700
H	0.63372800	-2.80339500	-1.63322600
C	3.67968400	-1.17013400	0.13091000
C	3.81866800	-2.49363600	-0.34783500
H	2.80629900	-4.14352800	-1.37700100
H	4.51598100	-0.67802100	0.63662700
H	4.76716200	-3.02348600	-0.21422400
C	0.57106200	2.62431200	0.56408300
C	2.15898800	0.88544600	0.39317800
C	1.50501200	3.48682500	1.17553500
H	-0.45649500	2.94911200	0.37846100

C	3.14163300	1.69748300	1.00275300
C	2.81399500	3.01166800	1.40032200
H	1.19867700	4.49625000	1.46113900
H	4.15259000	1.30963800	1.15757100
H	3.56824300	3.64938500	1.87150900
C	-1.31695900	-0.76204800	0.85090500
C	-0.72461800	-0.51901500	2.09964900
C	-2.46455400	-1.52799800	0.60634300
C	-1.36722300	-1.12012300	3.21727100
H	0.17122300	0.09055100	2.24328600
C	-3.07312700	-2.10378200	1.75536800
H	-2.86490500	-1.68418500	-0.39837300
C	-2.53121800	-1.90283100	3.04578300
H	-0.94095800	-0.95870900	4.21386500
H	-3.97458100	-2.71039300	1.61491800
H	-3.01620500	-2.35567300	3.91664600
C	-2.00898000	1.26004800	-1.06687000
F	-1.22437300	-1.31108500	-1.93600800
F	-3.08995400	0.65078500	-1.52033500
F	-2.34982900	1.94533500	0.04218800
F	-1.59423700	2.15709300	-1.98631900
N	0.88616800	1.36367200	0.18452500
N	1.41034700	-1.13669300	-0.68313300

$[OTf]^-$

O	-1.24327900	-0.83281900	-1.17477400
S	-0.93688400	-0.00001500	-0.00006600
O	-1.24345800	-0.60094100	1.30852000
O	-1.24298300	1.43379900	-0.13401800
C	0.94594400	-0.00017900	0.00001400
F	1.45030200	0.51978900	-1.13921400
F	1.44963100	0.72692500	1.01992200
F	1.45031500	-1.24660300	0.11964200

$[Pd(bpy)(C_6H_5)(CF_3)F]^+$ transition state Ar-CF_3

Pd	-0.11014700	-0.46962200	-0.33367800
C	2.09787900	-2.50969300	-0.08351500
C	2.72251000	-0.27256100	0.37589600
C	3.38728000	-2.98013900	0.25534000
H	1.27347300	-3.15710200	-0.41093400
C	4.02750100	-0.67206000	0.73724500
C	4.35854300	-2.04542600	0.67554200
H	3.60895600	-4.04855700	0.19327500
H	4.76885100	0.06228300	1.06675700
H	5.36368600	-2.37666700	0.95476000
C	0.44474500	2.57950000	-0.09925800
C	2.24396800	1.13660300	0.35091500
C	1.24211800	3.72403300	0.10858400
H	-0.60350600	2.67952100	-0.40055900
C	3.09893700	2.23572700	0.59178000
C	2.59294700	3.54710200	0.47793400
H	0.80320800	4.71662000	-0.02104400
H	4.14964600	2.06785200	0.84611400
H	3.24332100	4.40847800	0.65784200
C	-2.05971200	-0.17180400	0.45838700
C	-2.88819100	-1.31238000	0.49660000
C	-2.14719800	0.88275900	1.39453000
C	-3.83218500	-1.39911600	1.54926300
H	-2.79494100	-2.10726700	-0.24655900
C	-3.09085200	0.76325600	2.44255300
H	-1.51949100	1.77682300	1.34010600
C	-3.93391600	-0.37185600	2.51700100
H	-4.48280200	-2.27859800	1.60052400
H	-3.16689600	1.56403500	3.18597200
H	-4.67150300	-0.45218000	3.32235700
C	-1.78486400	0.42959400	-1.56778400
F	-0.65719400	-2.26941300	-0.83552900
F	-2.64136800	-0.41905600	-2.09216500

F	-2.38147800	1.60342600	-1.32556900
F	-0.85612300	0.69688100	-2.51925500
N	0.91946200	1.32033800	0.03746400
N	1.80099000	-1.19753500	-0.01929700

$[Pd(bpy)(C_6H_5)(CF_3)F]^+$ transition state Ar-F

Pd	-0.28555600	0.12941600	-0.68415500
C	1.42526700	-2.45390800	-1.09618400
C	2.48906300	-0.67480100	0.02433500
C	2.61311000	-3.21914300	-1.11566900
H	0.48247000	-2.80925100	-1.53382500
C	3.71764600	-1.37588000	0.04469400
C	3.77422400	-2.66461700	-0.53250300
H	2.61983000	-4.21038600	-1.57644800
H	4.61686700	-0.93491500	0.48481900
H	4.71535100	-3.22358600	-0.53042100
C	0.83867300	2.51094400	0.93323900
C	2.30110100	0.69451500	0.59721700
C	1.81396600	3.23193800	1.65365100
H	-0.15956400	2.92893300	0.77516000
C	3.32607100	1.36344100	1.30399400
C	3.08473400	2.64828200	1.83522400
H	1.56869100	4.22032500	2.05018200
H	4.29998200	0.88674400	1.44727200
H	3.87262300	3.17525300	2.38216800
C	-1.82123100	-1.01096700	0.45910900
C	-3.17094900	-0.66976000	0.39819900
C	-1.16707000	-1.83644700	1.37581400
C	-3.93018000	-1.08999900	1.52296700
H	-3.61777400	-0.13025100	-0.43920900
C	-1.97653300	-2.23196700	2.47946100
H	-0.11586000	-2.12396000	1.30417800
C	-3.33954000	-1.86429600	2.55123100
H	-4.99345600	-0.82891700	1.55577800
H	-1.51476400	-2.83661900	3.26797100
H	-3.94758300	-2.19719700	3.39821000
C	-1.56844300	1.64839700	-1.13340600
F	-1.40690900	-1.26159000	-1.56069500
F	-2.55284300	1.28557100	-1.95593000
F	-2.13157200	2.24165800	-0.05643500
F	-0.83407000	2.58984800	-1.76462600
N	1.07417800	1.28582900	0.40952900
N	1.37980300	-1.22912500	-0.53578600

$[Pd(bpy)(C_6H_4NH_2)(CF_3)F]^+$ intermediate

Pd	-0.03065900	-0.47313800	-0.87725200
C	-1.30506300	2.22270000	-1.74485100
C	-2.35300800	1.13681400	0.07009700
C	-2.22177500	3.29855400	-1.69190300
H	-0.49757000	2.16515900	-2.47933100
C	-3.30667100	2.17617700	0.18839600
C	-3.23448700	3.26982900	-0.70605900
H	-2.13668400	4.12265700	-2.40171400
H	-4.08578300	2.14764900	0.95029700
H	-3.96023600	4.08307900	-0.63146400
C	-1.22705200	-2.10910800	1.46618500
C	-2.32263300	-0.08297200	0.93865500
C	-2.17342900	-2.42176200	2.46531400
H	-0.39112900	-2.77381100	1.26026800
C	-3.30083300	-0.33566200	1.92915200
C	-3.22928300	-1.51500300	2.70200000
H	-2.07080600	-3.34985500	3.02921900
H	-4.11418100	0.37140300	2.09034000
H	-3.98316400	-1.71857800	3.46589300
C	1.47376900	0.43330300	0.22892400
C	1.28011300	0.64851100	1.60302000
C	2.62909500	0.80408700	-0.47867100
C	2.31652100	1.30775000	2.30954400

H	0.38676000	0.33755100	2.14093400
C	3.64915600	1.45833300	0.25196200
H	2.74531900	0.60650000	-1.54226800
C	3.51352200	1.71879900	1.64957900
H	2.18208900	1.49799400	3.37848000
H	4.55408200	1.76608900	-0.28026400
C	1.09711900	-2.17784500	-0.98153400
F	0.76591300	0.12429900	-2.52865600
F	2.19205200	-2.07623100	-1.74448100
F	1.48568000	-2.68678600	0.22553100
F	0.26234100	-3.10378800	-1.55066700
N	-1.29602000	-0.97617100	0.72549300
N	-1.38419100	1.18934900	-0.88424300
N	4.50331400	2.42614500	2.34183600
H	4.52323000	2.30131400	3.35216400
H	5.43241500	2.41947300	1.92506500

$[Pd(bpy)(C_6H_4NH_2)(CF_3)F]^+$ transition state

Pd	-0.12901300	-0.49480100	0.34689800
C	-2.37553600	-2.50152900	-0.13217800
C	-2.90038200	-0.25035300	-0.63210800
C	-3.62536900	-2.94695600	-0.62045800
H	-1.61400100	-3.17193400	0.27430700
C	-4.16444600	-0.62346300	-1.14709400
C	-4.52748000	-1.99028200	-1.13954500
H	-3.87021600	-4.00971400	-0.59328700
H	-4.85064600	0.12183500	-1.54995600
H	-5.49859600	-2.29855900	-1.53391100
C	-0.64611200	2.56758300	0.12903300
C	-2.40351000	1.15394600	-0.53621000
C	-1.40323400	3.72709800	-0.13910600
H	0.35552100	2.65063400	0.54769000
C	-3.21464700	2.27279800	-0.84422900
C	-2.70970300	3.57603900	-0.65380800
H	-0.97056800	4.70880400	0.05852900
H	-4.23243800	2.12861500	-1.20613200
H	-3.32806700	4.44692500	-0.88258100
C	1.88568800	-0.14524900	-0.11802900
C	2.76979000	-1.25262700	-0.03026800
C	2.19538700	0.96926500	-0.94116200
C	3.92900100	-1.27220200	-0.82339100
H	2.54630800	-2.09000900	0.62701300
C	3.35017200	0.94131000	-1.74230400
H	1.55323900	1.84588200	-1.00331000
C	4.24315700	-0.17902400	-1.69445800
H	4.59405000	-2.13891900	-0.77203900
H	3.56229700	1.78363400	-2.40686300
C	1.27148600	0.34687700	1.91830100
F	0.36317400	-2.31245100	0.81929500
F	2.04972300	-0.53444300	2.54862400
F	1.89325000	1.55363100	1.86649700
F	0.18537200	0.55961000	2.73604800
N	-1.11358100	1.31501500	-0.08570100
N	-2.04494400	-1.19377300	-0.14287000
N	5.36420900	-0.22175700	-2.50480600
H	5.69289600	0.64003000	-2.93332700
H	6.08580600	-0.90930000	-2.30187800

$[Pd(bpy)(C_6H_4NMe_2)(CF_3)F]^+$ intermediate

Pd	-0.78882800	-0.74045000	-0.73998500
C	-1.44469400	1.89969500	-2.23883500
C	-2.29694900	1.73526000	-0.04409800
C	-1.99513500	3.19174000	-2.40658500
H	-0.87724500	1.38846000	-3.02086800
C	-2.87612800	3.02399300	-0.13340300
C	-2.71871500	3.75794000	-1.33235000
H	-1.85688600	3.72527800	-3.34811600
H	-3.43338500	3.45456900	0.69868600

H	-3.15725700	4.75458200	-1.42216600
C	-1.79998300	-1.21219000	2.15054700
C	-2.39802100	0.84640500	1.15750700
C	-2.53240600	-0.92013400	3.32098300
H	-1.24828200	-2.14515400	2.05598500
C	-3.14730500	1.20055100	2.30428400
C	-3.21772600	0.31157400	3.39882900
H	-2.55425200	-1.64637500	4.13461100
H	-3.67737700	2.15190400	2.34103600
H	-3.79700200	0.57650200	4.28627700
C	1.12362900	-0.12526200	-0.20833600
C	1.32666500	0.49791300	1.03224000
C	2.14217800	-0.37767000	-1.14007300
C	2.63985600	0.92837600	1.34128300
H	0.53429300	0.66263300	1.75970900
C	3.44633800	0.05675300	-0.80934000
H	1.95068200	-0.88134900	-2.08527600
C	3.73346700	0.72594100	0.43068700
H	2.79281800	1.41708600	2.30323400
H	4.23378500	-0.13763700	-1.53704900
C	-0.23399800	-2.68539200	-0.43913800
F	-0.26357200	-0.89161200	-2.59062800
F	0.60867900	-3.17641200	-1.35603300
F	0.30126100	-2.94769800	0.79055900
F	-1.40720400	-3.39237900	-0.51677600
N	-1.73272400	-0.35797300	1.10042100
N	-1.59993900	1.21382900	-1.08994600
N	5.01173100	1.16167200	0.73288900
C	5.29471200	1.72447900	2.05912600
H	4.68922200	2.62962900	2.24635100
H	5.09732300	0.99754500	2.87087900
H	6.35235500	2.01550000	2.11012600
C	6.12747600	0.82333100	-0.16205700
H	6.26851100	-0.27061000	-0.25476400
H	5.96907800	1.24184400	-1.17174300
H	7.05419400	1.25668200	0.23711200

$[Pd(bpy)(C_6H_4NMe_2)(CF_3)F]^+$ transition state

Pd	-0.60431200	-0.53209300	0.34056400
C	-2.80650600	-2.47516000	-0.51958600
C	-3.24904400	-0.19190900	-0.93818700
C	-3.98949100	-2.87194200	-1.18420800
H	-2.10519600	-3.18088000	-0.06709300
C	-4.44186400	-0.51360100	-1.62904700
C	-4.81323100	-1.87246200	-1.75114700
H	-4.24407000	-3.93059400	-1.25255200
H	-5.06671600	0.26488200	-2.06741000
H	-5.72989700	-2.14193200	-2.28101300
C	-1.09712400	2.54616100	0.27700600
C	-2.76120000	1.19726100	-0.69055200
C	-1.81428800	3.72838700	-0.00106600
H	-0.15480100	2.59123500	0.82011400
C	-3.52714800	2.34235500	-1.01865200
C	-3.04802500	3.62505800	-0.68069300
H	-1.40810600	4.69020900	0.31507400
H	-4.49361200	2.23208500	-1.50997500
H	-3.63292400	4.51510700	-0.92335600
C	1.43900300	-0.15040100	0.25365800
C	2.32693700	-1.24278200	0.44815100
C	1.88952400	1.02265600	-0.40996000
C	3.62133300	-1.19508600	-0.08938300
H	2.00037300	-2.12871400	0.98838100
C	3.18013800	1.06800900	-0.96053900
H	1.24960400	1.89143900	-0.55472200
C	4.09218500	-0.04158900	-0.81647800
H	4.26589500	-2.06107600	0.05700900
H	3.47469300	1.96461000	-1.50512900
C	0.45376100	0.17953200	2.21304300
F	-0.17075500	-2.38810200	0.71029600

F	1.10582900	-0.76299900	2.89768700
F	1.07942000	1.37503500	2.37269500
F	-0.76083400	0.34428900	2.83689900
N	-1.53469500	1.31510800	-0.07852000
N	-2.46705000	-1.17450400	-0.40660100
N	5.35860900	0.00125000	-1.34681700
C	6.27861500	-1.13373500	-1.15809700
H	6.49911300	-1.30239500	-0.08865800
H	5.85702900	-2.06204700	-1.58165600
H	7.22349700	-0.92186200	-1.67473700
C	5.83134000	1.20918800	-2.04221600
H	5.20062000	1.43782300	-2.91972400
H	5.83524400	2.08742200	-1.37146800
H	6.85713600	1.04434000	-2.39593200

$[Pd(bpy)(C_6H_4OMe)(CF_3)F]^+$ intermediate

Pd	-0.43061300	-0.59384100	-0.83999700
C	-1.22557700	2.20545000	-1.91872800
C	-2.29225500	1.54340500	0.08076300
C	-1.91185200	3.44203300	-1.93118600
H	-0.51362600	1.91094000	-2.69406700
C	-3.01561100	2.75874500	0.13966400
C	-2.81796100	3.71744400	-0.88167800
H	-1.73611000	4.15497600	-2.73805100
H	-3.71320100	2.96537500	0.95148400
H	-3.36593800	4.66223700	-0.85477000
C	-1.67175400	-1.69506700	1.77813900
C	-2.41173600	0.43994600	1.08652100
C	-2.55200800	-1.70005300	2.88131600
H	-1.00227300	-2.53292900	1.59582200
C	-3.31415200	0.49744000	2.17445100
C	-3.38810800	-0.58071400	3.08319200
H	-2.56764800	-2.56155700	3.55023800
H	-3.95657000	1.36737400	2.30802300
H	-4.08382000	-0.54419500	3.92457100
C	1.32893800	0.07746600	0.02879200
C	1.29667100	0.54543800	1.35611400
C	2.46852400	0.06209600	-0.78414900
C	2.50884000	1.03570100	1.89284900
H	0.40162900	0.54110200	1.97454000
C	3.67754800	0.55579400	-0.22302500
H	2.44296000	-0.30558900	-1.80785000
C	3.70283900	1.04262900	1.11395100
H	2.54142000	1.40880200	2.91898200
H	4.57182200	0.54620700	-0.84641900
C	0.30203400	-2.50516600	-0.83811800
F	0.30764300	-0.34092500	-2.60272500
F	1.29340400	-2.72439400	-1.71048700
F	0.71881300	-2.96393100	0.37813400
F	-0.77062500	-3.27422600	-1.20701200
N	-1.60189100	-0.65980400	0.90602000
N	-1.42174000	1.30329800	-0.93752800
O	4.80662500	1.53442600	1.74237500
C	6.05371100	1.55117100	1.01947800
H	6.79225500	1.97188000	1.71350200
H	6.35626600	0.52905500	0.73135900
H	5.98177300	2.19187600	0.12280300

$[Pd(bpy)(C_6H_4OMe)(CF_3)F]^+$ transition state

Pd	-0.36955500	-0.39942400	0.50659900
C	-2.38126700	-2.63002500	0.03397900
C	-3.00571300	-0.50320600	-0.79490000
C	-3.53414100	-3.23209700	-0.52029100
H	-1.62559600	-3.18242800	0.59814700
C	-4.17409200	-1.03933400	-1.38564100
C	-4.43768100	-2.42167500	-1.24468100
H	-3.70484300	-4.30101400	-0.38471100
H	-4.86291000	-0.40587600	-1.94492300

H	-5.33466100	-2.85410800	-1.69416500
C	-1.06733000	2.56315800	-0.13612500
C	-2.62560100	0.93973900	-0.82076900
C	-1.86393900	3.61634200	-0.63257700
H	-0.13267800	2.77695500	0.37999300
C	-3.46679700	1.94306500	-1.35882600
C	-3.08107700	3.29745000	-1.27396800
H	-1.52847700	4.64714800	-0.51052000
H	-4.41747100	1.67335100	-1.81844300
H	-3.72384900	4.08113800	-1.68116500
C	1.66851100	0.04357500	0.15956100
C	2.58535900	-1.00112000	0.41445000
C	1.95438700	1.06891800	-0.78064900
C	3.78789100	-1.06146900	-0.32455900
H	2.36591900	-1.76419000	1.15806200
C	3.14556400	1.00117400	-1.52162500
H	1.27742400	1.90032200	-0.96662800
C	4.07570600	-0.06175400	-1.30009100
H	4.47870600	-1.88149800	-0.12834900
H	3.37993600	1.76067200	-2.27036300
C	0.88009700	0.72348300	2.04104100
F	0.18758400	-2.10303000	1.25214000
F	1.66756300	-0.00970900	2.82905300
F	1.41146300	1.96221400	1.88068700
F	-0.27949000	0.94128400	2.75058700
N	-1.41734800	1.25988300	-0.24622900
N	-2.14512700	-1.30928100	-0.10755000
O	5.19633100	-0.02101700	-2.06114800
C	6.19647500	-1.04674700	-1.87803900
H	6.99844800	-0.80502500	-2.58653600
H	6.59160000	-1.02859500	-0.84786300
H	5.78244300	-2.04310400	-2.11037800

$[Pd(bpy)(C_6H_4OH)(CF_3)F]^+$ intermediate

Pd	-0.01093700	-0.45472000	-0.87507200
C	-1.33108400	2.22423200	-1.72407600
C	-2.37700600	1.09252200	0.06481500
C	-2.27891600	3.27295900	-1.67708000
H	-0.51127200	2.19573200	-2.44649600
C	-3.36185400	2.10319200	0.17545000
C	-3.30637000	3.20640000	-0.70843800
H	-2.20609700	4.10529200	-2.37859300
H	-4.15303400	2.04550000	0.92314400
H	-4.05654100	3.99765500	-0.63927000
C	-1.18014000	-2.13194200	1.45294900
C	-2.32482400	-0.13253000	0.92485800
C	-2.12489400	-2.47238800	2.44455900
H	-0.32537500	-2.77377400	1.25182000
C	-3.30358900	-0.41507700	1.90646000
C	-3.20650200	-1.59515900	2.67577200
H	-2.00080100	-3.39845200	3.00746900
H	-4.13569600	0.27037000	2.06503000
H	-3.95999800	-1.82104700	3.43373300
C	1.47596400	0.45336400	0.24636500
C	1.23234500	0.72545400	1.60453400
C	2.65538700	0.78617500	-0.43626700
C	2.25462400	1.38829600	2.32619300
H	0.31286900	0.44989300	2.11677500
C	3.66690600	1.44666600	0.30792700
H	2.79893900	0.55782200	-1.49032200
C	3.46965800	1.74656300	1.68252900
H	2.11668400	1.62159200	3.38422400
H	4.59927800	1.71804100	-0.19732600
C	1.13417600	-2.14828000	-0.99913100
F	0.79319000	0.18280900	-2.50642400
F	2.22088700	-2.03138100	-1.77175800
F	1.53742500	-2.66138500	0.19983500
F	0.30029800	-3.07396300	-1.56848300
N	-1.27444700	-0.99905600	0.71488300

N	-1.39417500	1.18158700	-0.87292700
O	4.40855700	2.38230500	2.45284700
H	5.20652200	2.56494000	1.92358600

$[Pd(bpy)(C_6H_4OH)(CF_3)F]^+$ transition state

Pd	-0.12709800	-0.46596000	0.41468300
C	-2.30853500	-2.52694000	-0.05487700
C	-2.87242000	-0.29994000	-0.62481900
C	-3.54481600	-3.00983900	-0.54192500
H	-1.53938100	-3.17013600	0.37996400
C	-4.12379800	-0.71302500	-1.13925100
C	-4.46002600	-2.08619600	-1.09627500
H	-3.76916900	-4.07597600	-0.48623400
H	-4.82100400	0.00750300	-1.56736000
H	-5.42132800	-2.42452200	-1.48999300
C	-0.68020700	2.57704300	0.08948200
C	-2.40333400	1.11532800	-0.56425300
C	-1.44917000	3.71513900	-0.23216500
H	0.31245500	2.68938600	0.52286000
C	-3.22492400	2.21029800	-0.92443100
C	-2.74282700	3.52679600	-0.76662900
H	-1.03476500	4.70946300	-0.06017400
H	-4.23252600	2.03894100	-1.30280500
H	-3.36889200	4.38019300	-1.03655500
C	1.89812600	-0.11965200	-0.09351800
C	2.76080900	-1.23831100	-0.01141100
C	2.15781300	0.95601400	-0.98103400
C	3.87355500	-1.30631600	-0.87580600
H	2.56505200	-2.04467900	0.69186200
C	3.26234000	0.87875900	-1.85005600
H	1.52506000	1.83983400	-1.03132900
C	4.12691000	-0.25214000	-1.79800600
H	4.53668200	-2.17572600	-0.82749700
H	3.47143800	1.68093600	-2.56059900
C	1.34105800	0.44712800	1.89920000
F	0.38614300	-2.25526700	0.96648100
F	2.13489300	-0.40301900	2.55033200
F	1.95098300	1.65365400	1.78375900
F	0.26801600	0.68729300	2.72702500
N	-1.12613200	1.31153300	-0.09237900
N	-2.00349600	-1.21365500	-0.10202900
O	5.18577100	-0.25436300	-2.65865400
H	5.72048000	-1.06014500	-2.53118400

$[Pd(bpy)(C_6H_4Me)(CF_3)F]^+$ intermediate

Pd	-0.04997600	-0.47836800	-0.86953600
C	-1.30776500	2.21804800	-1.75406000
C	-2.35068500	1.15785300	0.07979500
C	-2.22365200	3.29503000	-1.71303800
H	-0.50383100	2.14889700	-2.49142800
C	-3.30358900	2.19920600	0.18584400
C	-3.23351300	3.28035700	-0.72389700
H	-2.14064100	4.10889500	-2.43480100
H	-4.08140000	2.18083400	0.94933200
H	-3.95913600	4.09453100	-0.65883400
C	-1.22630300	-2.07244600	1.51344100
C	-2.31864500	-0.04956200	0.96560300
C	-2.16274300	-2.36421200	2.52824000
H	-0.39592100	-2.74463300	1.30926600
C	-3.28728400	-0.28211700	1.97012600
C	-3.21224500	-1.44927000	2.76119900
H	-2.05743000	-3.28305800	3.10660000
H	-4.09545300	0.43129000	2.12948200
H	-3.95846500	-1.63698800	3.53657400
C	1.48999000	0.41464200	0.20216600
C	1.28611600	0.70253200	1.55861900
C	2.65312200	0.71670400	-0.52139000
C	2.35306700	1.35584700	2.23703400

H	0.37667300	0.45043300	2.10008800
C	3.69130800	1.36508000	0.19799100
H	2.76147800	0.47505700	-1.57668100
C	3.56329200	1.69154500	1.57648000
H	2.22095300	1.59214800	3.29660100
H	4.61021900	1.61205300	-0.34144700
C	1.04284400	-2.20716700	-0.97172000
F	0.73376300	0.09475100	-2.53578500
F	2.10895300	-2.14709900	-1.77823600
F	1.46684500	-2.69061800	0.23329700
F	0.16865400	-3.12962600	-1.48415700
N	-1.29889200	-0.95152000	0.75512700
N	-1.38415500	1.19711100	-0.87808600
C	4.70835100	2.37314700	2.32174300
H	5.56451400	1.68516100	2.43311200
H	5.06650500	3.25952900	1.77228000
H	4.39825400	2.69368000	3.32808900

$[Pd(bpy)(C_6H_4Me)(CF_3)F]^+$ transition state

Pd	-0.14498700	-0.43978300	0.46939700
C	-2.27127700	-2.54429300	-0.00601100
C	-2.85515200	-0.34249300	-0.65217600
C	-3.48927200	-3.05918600	-0.50620000
H	-1.50318500	-3.16251000	0.46540100
C	-4.08870600	-0.78931000	-1.18096400
C	-4.40547700	-2.16576000	-1.10632000
H	-3.69904600	-4.12662200	-0.42469100
H	-4.78712000	-0.09132200	-1.64306600
H	-5.35298200	-2.52971600	-1.51047700
C	-0.71985000	2.58287100	0.03221700
C	-2.40800200	1.08061200	-0.62156500
C	-1.49402100	3.70086200	-0.34361200
H	0.26070000	2.71996900	0.48585500
C	-3.23326800	2.15332900	-1.03580100
C	-2.77114000	3.47998200	-0.90478500
H	-1.09627500	4.70522300	-0.19175200
H	-4.22830000	1.95800900	-1.43539200
H	-3.40016500	4.31694200	-1.21613500
C	1.90190100	-0.10052100	-0.03837400
C	2.74756100	-1.22858700	0.06423300
C	2.13992300	0.93548800	-0.96874400
C	3.83301900	-1.33031900	-0.83411200
H	2.56123300	-2.00617600	0.80162300
C	3.22809200	0.80106700	-1.86298500
H	1.51895000	1.82707600	-1.03021200
C	4.09456900	-0.32555200	-1.80933300
H	4.48335600	-2.20669100	-0.76657400
H	3.40337600	1.59095500	-2.59801200
C	1.34720200	0.53646100	1.90946900
F	0.37004200	-2.20039300	1.10346400
F	2.15361500	-0.27596400	2.59196400
F	1.93777500	1.74825000	1.75136900
F	0.26989300	0.79003000	2.72971400
N	-1.14693600	1.30743500	-0.12170100
N	-1.98459400	-1.22837900	-0.08526700
C	5.28568800	-0.45208400	-2.75153900
H	5.28765100	0.34522000	-3.51004700
H	6.23364000	-0.39085800	-2.18868500
H	5.27561400	-1.42558300	-3.27030800

$[Pd(bpy)(C_6H_4F)(CF_3)F]^+$ intermediate

Pd	0.00202300	-0.43313200	-0.87629600
C	-1.33793500	2.24757800	-1.68725000
C	-2.38625400	1.07278700	0.07305800
C	-2.29741300	3.28514900	-1.62933500
H	-0.51269600	2.24086800	-2.40400000
C	-3.38269100	2.07080600	0.19309300
C	-3.33172200	3.19035400	-0.67046700
H	-2.22786300	4.13050700	-2.31543700

H	-4.17972000	1.99140800	0.93258200
H	-4.09091900	3.97221700	-0.59345000
C	-1.16715500	-2.16505000	1.41164000
C	-2.32847700	-0.16738500	0.91057400
C	-2.11810700	-2.53468900	2.38659000
H	-0.30389700	-2.79445900	1.20708800
C	-3.31369100	-0.47967800	1.87664800
C	-3.21147300	-1.67360600	2.62372900
H	-1.98985200	-3.47036200	2.93245500
H	-4.15490000	0.19349800	2.03960600
H	-3.97014500	-1.92245300	3.36924400
C	1.48077200	0.45999400	0.26288900
C	1.22849000	0.70006400	1.62482500
C	2.65850800	0.81691900	-0.41597400
C	2.24391200	1.35971400	2.36635500
H	0.30963400	0.40442700	2.12636200
C	3.66486000	1.47219800	0.34002600
H	2.80149700	0.60936000	-1.47429500
C	3.43705200	1.72937900	1.70933400
H	2.11006100	1.57441200	3.42860700
H	4.60374700	1.77360600	-0.12920700
C	1.16003000	-2.11737200	-1.02658900
F	0.80903100	0.24095800	-2.48974100
F	2.24667500	-1.97865600	-1.79441200
F	1.56308600	-2.64693800	0.16459900
F	0.33126500	-3.03511600	-1.61349200
N	-1.26648000	-1.01867100	0.69467300
N	-1.39637600	1.18934000	-0.85476700
F	4.40102600	2.35568300	2.42369600

$[Pd(bpy)(C_6H_4F)(CF_3)F]^+$ transition state

Pd	-0.12467300	-0.44264100	0.45725500
C	-2.26264600	-2.53876600	0.00789800
C	-2.85314100	-0.33099200	-0.61385900
C	-3.48973400	-3.04787500	-0.47574400
H	-1.48853700	-3.16225700	0.46201300
C	-4.09572900	-0.77226100	-1.12533200
C	-4.41376600	-2.14878000	-1.05489200
H	-3.69994700	-4.11550600	-0.39814500
H	-4.80024000	-0.07004100	-1.57148300
H	-5.36824700	-2.50835000	-1.44631800
C	-0.70240100	2.58562700	0.05940600
C	-2.40302900	1.09083000	-0.58029700
C	-1.48065400	3.70776900	-0.29454100
H	0.28477100	2.71837300	0.49998200
C	-3.23294200	2.16829700	-0.97222600
C	-2.76670400	3.49319100	-0.83771300
H	-1.07930300	4.71029000	-0.14002400
H	-4.23458900	1.97777000	-1.35732200
H	-3.39922500	4.33357900	-1.13224800
C	1.91017000	-0.10785900	-0.08227900
C	2.75082000	-1.24385300	-0.00504800
C	2.13828000	0.94210700	-1.00423200
C	3.82530800	-1.35483600	-0.91599400
H	2.56900900	-2.02704100	0.72746000
C	3.20535500	0.82647300	-1.92254900
H	1.51994500	1.83653700	-1.03959700
C	4.02854100	-0.32154000	-1.85820700
H	4.49102600	-2.21988700	-0.89729000
H	3.40449200	1.60482600	-2.66157100
C	1.39816200	0.51473400	1.88125700
F	0.39920500	-2.20898300	1.06710700
F	2.21342800	-0.30842000	2.53803700
F	1.98987500	1.72409900	1.71961900
F	0.33684700	0.76312500	2.72001300
N	-1.13331500	1.31180900	-0.09940400
N	-1.97495400	-1.22265500	-0.06725500
F	5.05601800	-0.42698500	-2.72771700

$[Pd(bpy)(C_6H_4CF_3)(CF_3)F]^+$ intermediate

Pd	-1.00473200	-0.70707400	-0.75209200
C	-1.60134800	1.99439100	-2.16193300
C	-2.40682700	1.79464400	0.04966800
C	-2.12174700	3.30386800	-2.28324300
H	-1.06803200	1.49005700	-2.97187200
C	-2.95432300	3.09905400	0.00554600
C	-2.80509900	3.86005900	-1.17789400
H	-1.99146100	3.85769800	-3.21410300
H	-3.48260900	3.52153000	0.86032600
H	-3.21953900	4.86946600	-1.23180800
C	-1.94592400	-1.22655000	2.15344600
C	-2.50428800	0.87807600	1.23024000
C	-2.63327000	-0.94099400	3.35229900
H	-1.42961200	-2.17492500	2.01982700
C	-3.20761200	1.22491100	2.40765500
C	-3.27490400	0.30997300	3.48116600
H	-2.65452200	-1.68663000	4.14819900
H	-3.70376000	2.19194800	2.48553000
H	-3.81800000	0.57060300	4.39241600
C	0.94649700	-0.22249900	-0.26688300
C	1.19014800	0.42705000	0.95441900
C	1.92432900	-0.53440700	-1.22409800
C	2.53358200	0.79435800	1.23010700
H	0.41300900	0.65154900	1.68120700
C	3.25879300	-0.15845900	-0.91799500
H	1.68340900	-1.03238400	-2.16075800
C	3.55678200	0.50249500	0.29770200
H	2.76379200	1.30513100	2.16713100
H	4.04844800	-0.38059800	-1.63854900
C	-0.54580600	-2.69227900	-0.52659000
F	-0.52321500	-0.81854900	-2.61500400
F	0.21063800	-3.20149000	-1.50451600
F	0.04243800	-3.01275500	0.66136300
F	-1.76413900	-3.31607700	-0.55386400
N	-1.88161900	-0.34680800	1.12348200
N	-1.74620500	1.28318700	-1.02611600
C	5.00585400	0.86087600	0.63106700
F	5.62884200	-0.15833100	1.28296200
F	5.72690800	1.12388500	-0.48844300
F	5.07656000	1.95441300	1.43628400

$[Pd(bpy)(C_6H_4CF_3)(CF_3)F]^+$ transition state

Pd	-0.85109900	-0.27022300	0.70207800
C	-2.66603000	-2.63605400	0.22395800
C	-3.18780500	-0.68159100	-1.01075000
C	-3.69014500	-3.36673700	-0.42125600
H	-2.00999300	-3.06323100	0.98633200
C	-4.22275000	-1.35470800	-1.70013000
C	-4.47274800	-2.71438500	-1.40055000
H	-3.85555000	-4.41224000	-0.15746400
H	-4.82032300	-0.84190600	-2.45417200
H	-5.26717000	-3.25071800	-1.92472100
C	-1.45668600	2.52983900	-0.49373900
C	-2.84158500	0.75808100	-1.18849500
C	-2.17010500	3.46444900	-1.27345100
H	-0.63055300	2.85594400	0.13732900
C	-3.59033200	1.63515600	-2.00880700
C	-3.24858100	3.00332400	-2.06063200
H	-1.87943400	4.51566000	-1.25188200
H	-4.43825700	1.26103000	-2.58240900
H	-3.82165800	3.69173500	-2.68573500
C	1.24961200	0.14955100	0.57921600
C	2.08301500	-0.87382700	1.08015400
C	1.63533200	0.98983900	-0.49001200
C	3.33061900	-1.09006100	0.44835000
H	1.77139600	-1.49315500	1.91808000
C	2.87976100	0.75497900	-1.11750200

H	1.01376600	1.80607300	-0.85170000
C	3.72188700	-0.28352300	-0.64792700
H	3.98274000	-1.88625600	0.81164300
H	3.18531000	1.37866200	-1.95939200
C	0.27363900	1.11336600	2.17420200
F	-0.41882600	-1.79956100	1.81508800
F	0.93464100	0.52239800	3.16710900
F	0.84088500	2.30899000	1.88387100
F	-0.96966600	1.43257700	2.66543100
N	-1.76238400	1.21113600	-0.46624800
N	-2.44004200	-1.33966600	-0.07530000
C	5.09218400	-0.48955900	-1.29684600
F	5.51047100	-1.77561900	-1.18803200
F	5.06940400	-0.17127800	-2.61841400
F	6.03548900	0.29577600	-0.71009400

$[Pd(bpy)(C_6H_4CN)(CF_3)F]^+$ intermediate

Pd	-0.31907200	-0.60818400	-0.81710900
C	-1.27790200	2.10965500	-1.96900000
C	-2.26556500	1.46184600	0.07679400
C	-2.02853400	3.30765200	-2.00623800
H	-0.57022500	1.82685600	-2.75250800
C	-3.05035700	2.63911100	0.11119600
C	-2.92481800	3.57163100	-0.94553000
H	-1.90807200	4.00021600	-2.84051800
H	-3.74142300	2.83671000	0.93077100
H	-3.52095900	4.48711900	-0.93715700
C	-1.44801900	-1.68677800	1.86058900
C	-2.30781600	0.38787000	1.11940800
C	-2.30449100	-1.69973000	2.98193200
H	-0.74306700	-2.49763000	1.69005800
C	-3.18941700	0.43459300	2.22475900
C	-3.19078800	-0.61664200	3.16759000
H	-2.26423200	-2.53966900	3.67678800
H	-3.87185800	1.27538900	2.34567900
H	-3.87009700	-0.58769800	4.02255000
C	1.43351900	0.14630900	-0.02520800
C	1.41882300	0.64528600	1.28879800
C	2.54866600	0.15459500	-0.87904200
C	2.62669600	1.20202200	1.78055700
H	0.54136800	0.61863000	1.93086800
C	3.74607200	0.71307600	-0.36442000
H	2.50506000	-0.24148900	-1.89141400
C	3.78520900	1.23552800	0.95763200
H	2.66159600	1.60039800	2.79656700
H	4.63817000	0.73875100	-0.99352600
C	0.49428500	-2.49070100	-0.77442700
F	0.37050400	-0.37476500	-2.60111500
F	1.46266100	-2.69724700	-1.67285800
F	0.96901600	-2.88371000	0.44209800
F	-0.56060100	-3.30624300	-1.07938200
N	-1.44705200	-0.67630300	0.95588000
N	-1.40411400	1.23275400	-0.95303000
C	5.01839600	1.81120600	1.47623800
N	6.01446100	2.28031700	1.90006900

$[Pd(bpy)(C_6H_4CN)(CF_3)F]^+$ transition state

Pd	-0.30222200	-0.38448200	0.57372400
C	-2.30879800	-2.57852100	0.04516100
C	-2.87801700	-0.44459100	-0.81477100
C	-3.45675600	-3.16451500	-0.53591700
H	-1.57900000	-3.13936300	0.63414200
C	-4.03883300	-0.96705900	-1.43051800
C	-4.32774700	-2.34455400	-1.28839900
H	-3.64751500	-4.22970300	-0.39802300
H	-4.70355700	-0.32562900	-2.00953700
H	-5.21965300	-2.76557400	-1.75824700
C	-0.90550900	2.58626900	-0.10659900

C	-2.47318700	0.99056200	-0.83835600
C	-1.66207300	3.65215700	-0.63756500
H	0.01524000	2.78458700	0.44098800
C	-3.27336300	2.00698400	-1.41233400
C	-2.86191600	3.35364700	-1.32071400
H	-1.31042100	4.67687500	-0.50984400
H	-4.21168000	1.75415800	-1.90587100
H	-3.47260700	4.14794800	-1.75571800
C	1.77944800	-0.03379100	0.20205700
C	2.61246900	-1.15648600	0.41023400
C	2.06610000	0.95605500	-0.76660400
C	3.74358800	-1.31652800	-0.42093500
H	2.38375500	-1.89096200	1.17918800
C	3.19264600	0.78382000	-1.59963200
H	1.45182400	1.84416700	-0.89674800
C	4.03177200	-0.35338500	-1.42831200
H	4.39554000	-2.18165200	-0.28693900
H	3.42357700	1.52550600	-2.36635800
C	1.10408700	0.70893300	2.05173800
F	0.19593100	-2.08050500	1.37123800
F	1.89181400	-0.03647100	2.82370300
F	1.66339700	1.92659300	1.85170000
F	-0.03082500	0.96371500	2.78143600
N	-1.28038300	1.29022900	-0.22218900
N	-2.04824400	-1.26237700	-0.10085300
C	5.19598600	-0.52255900	-2.28485600
N	6.13640700	-0.65825200	-2.98454000

$[Pd(bpy)(C_6H_4NO_2)(CF_3)F]^+$ intermediate

Pd	-0.67915900	-0.70513400	-0.76201400
C	-1.38433100	1.97144100	-2.16929600
C	-2.28773200	1.68298000	-0.00545600
C	-1.98490100	3.24510400	-2.30128300
H	-0.77776200	1.51701600	-2.95687300
C	-2.91908600	2.94828400	-0.06220700
C	-2.76064900	3.73648500	-1.22661000
H	-1.84427400	3.82118500	-3.21700700
H	-3.51804300	3.32088300	0.76881300
H	-3.23912100	4.71661000	-1.28961300
C	-1.73328400	-1.33475800	2.08129000
C	-2.38421000	0.74287200	1.15620800
C	-2.50322700	-1.11715500	3.24354200
H	-1.14619700	-2.24307900	1.96368600
C	-3.17219700	1.02097300	2.29762800
C	-3.23491000	0.08530700	3.35346900
H	-2.51680200	-1.87622900	4.02681000
H	-3.73759700	1.95035900	2.36057000
H	-3.84343900	0.29288300	4.23656300
C	1.20332800	-0.10250400	-0.16867000
C	1.34178200	0.53368000	1.07862600
C	2.24685400	-0.32934800	-1.08246400
C	2.63817800	0.98488000	1.43376700
H	0.51572500	0.68576500	1.76930700
C	3.53758900	0.12540100	-0.70907100
H	2.08184800	-0.82531600	-2.03643400
C	3.70524000	0.77201400	0.53480400
H	2.81366700	1.48515300	2.38655300
H	4.39012400	-0.02077700	-1.37320500
C	-0.09478100	-2.65994300	-0.54394800
F	-0.09934600	-0.75622100	-2.59963500
F	0.76759700	-3.08722600	-1.47164300
F	0.42542500	-2.96855900	0.67817600
F	-1.25975400	-3.36363100	-0.67759700
N	-1.67341800	-0.43502300	1.06821200
N	-1.53926100	1.23404700	-1.05144800
N	5.06397500	1.25234500	0.91823200
O	5.98810700	1.05632100	0.10678200
O	5.17649900	1.81849800	2.02356500

[Pd(bpy)($C_6H_4NO_2$)(CF_3)F]$^+$ transition state

Pd	-0.57368700	-0.35706600	0.63794300
C	-2.45044300	-2.63012600	-0.00656400
C	-3.01294500	-0.53655100	-0.96560000
C	-3.52545000	-3.26771700	-0.66733300
H	-1.75663100	-3.15239400	0.65664500
C	-4.10005900	-1.11218000	-1.66293900
C	-4.35520900	-2.49533500	-1.51118500
H	-3.69280400	-4.33541600	-0.51887300
H	-4.73383500	-0.50661700	-2.31112200
H	-5.18977300	-2.95724000	-2.04377000
C	-1.20396000	2.57411000	-0.17352500
C	-2.65417600	0.91056100	-0.99178200
C	-1.94595400	3.60162700	-0.79316400
H	-0.33812000	2.81609500	0.44209000
C	-3.43490600	1.88625600	-1.65604000
C	-3.07496000	3.24769600	-1.56490500
H	-1.63782700	4.64007800	-0.66394300
H	-4.32013400	1.59111500	-2.21924800
H	-3.67176200	4.01111300	-2.06897800
C	1.52438600	0.05001500	0.44192100
C	2.36618400	-1.04071500	0.75671300
C	1.85917500	1.01682300	-0.53540500
C	3.56729700	-1.19554500	0.02612700
H	2.09438200	-1.75633600	1.52921100
C	3.05365800	0.85384800	-1.27122100
H	1.23177500	1.88045900	-0.74303400
C	3.88304300	-0.25141700	-0.97570400
H	4.24110500	-2.02843500	0.22790200
H	3.34133700	1.56493000	-2.04556400
C	0.67365300	0.82366300	2.19763300
F	-0.09993900	-2.01226100	1.52884500
F	1.39067500	0.11234100	3.06377400
F	1.23513300	2.04228600	2.01480800
F	-0.53095900	1.08310500	2.80215400
N	-1.52789700	1.26410000	-0.28575700
N	-2.22048100	-1.30950500	-0.16423400
N	5.14752800	-0.41905100	-1.74998100
O	5.86562000	-1.39547100	-1.46385800
O	5.39158500	0.42916900	-2.63055200

[Pd(tmeda)(C_6H_5)(CF_3)(F)(OTf)]

Pd	-0.54426500	-0.00588600	0.00700900
C	-2.54260300	-0.16710700	-0.53001100
C	-2.82169800	-0.96097300	-1.66526200
C	-3.57316400	0.54051100	0.12239400
C	-4.16053400	-1.06705100	-2.11898300
H	-2.02001300	-1.47263500	-2.20141900
C	-4.90871600	0.43339900	-0.34851400
H	-3.38619300	1.19699000	0.97356900
C	-5.20789200	-0.37770700	-1.46499800
H	-4.37164800	-1.69142800	-2.99495200
H	-5.70065300	0.98934700	0.16770300
C	-0.68012500	-2.01783400	0.49183900
F	-1.71381200	-2.23123300	1.34786000
F	0.42531300	-2.41771300	1.12905800
F	-0.85526400	-2.80246900	-0.56173100
F	-0.19373000	-0.35193600	-1.87530600
O	1.64791300	0.15751600	0.32355600
S	2.77155700	-0.83393200	0.06141700
O	2.43317900	-1.89574600	-0.87235600
O	3.48345800	-1.15464200	1.29757700
C	3.94245700	0.28670000	-0.87646700
F	4.21972800	1.38942100	-0.15790800
F	5.08698300	-0.34787100	-1.13236200
F	3.40107300	0.67566800	-2.03804200
H	-6.23907800	-0.46451200	-1.82540200
C	-0.72223600	2.84938200	0.87543400

H	-0.35763400	3.89870100	0.89125900
H	-1.81968000	2.88710400	1.01702000
C	-0.05437600	2.05823600	2.00607200
H	1.03129900	1.97532400	1.82904500
H	-0.20612700	2.56732700	2.98015400
C	-1.88536900	0.66377400	2.85833500
H	-2.41361000	-0.29067700	2.70805400
H	-1.67491600	0.80328700	3.93636200
H	-2.52178200	1.49996700	2.53684800
C	0.35740500	-0.13910100	2.96928700
H	0.48966300	0.40240600	3.92721200
H	-0.07974900	-1.12821800	3.17286200
H	1.32681900	-0.25474400	2.46775700
C	-1.42595300	2.65612000	-1.46776500
H	-1.32344800	3.74506300	-1.65843500
H	-1.22528100	2.09538000	-2.39588900
H	-2.45535900	2.43772500	-1.14172600
C	0.90614000	2.60106700	-0.94237000
H	0.91090500	3.68143700	-1.19913900
H	1.67947300	2.39137600	-0.18994800
H	1.13290300	1.99766400	-1.83534100
N	-0.59444000	0.65219600	2.11140100
N	-0.44465300	2.22043700	-0.44268300

$[Pd(tmeda)(C_6H_5)(CF_3)F]^+$ intermediate

Pd	0.38464400	0.19848000	-0.44272200
C	-1.52133900	-0.38077800	0.15413100
C	-1.68176200	-0.85514900	1.46308300
C	-2.52580800	-0.32588800	-0.82295200
C	-2.97890500	-1.31637300	1.82000300
H	-0.87953900	-0.89758600	2.20520600
C	-3.80825600	-0.79247900	-0.42410500
H	-2.34111500	0.04396700	-1.83317100
C	-4.03523200	-1.28077900	0.88272300
H	-3.13872700	-1.69482600	2.83583100
H	-4.62048400	-0.76207500	-1.15878000
H	-5.03123300	-1.63210500	1.17077800
C	-0.39383200	2.11156900	-0.39809300
F	-0.19265000	0.00611800	-2.28853300
F	-1.31087900	2.34360100	-1.31874800
F	-0.88588400	2.47806400	0.79625200
F	0.67815400	2.89447300	-0.65680500
N	1.56456500	0.36844600	1.34534800
N	1.44226400	-1.76806700	-0.61311000
C	2.44680200	-1.82527200	0.48967800
H	2.64744800	-2.87500200	0.78134300
H	3.40234200	-1.41270300	0.12129900
C	1.95470800	-1.04167700	1.70837600
H	2.74323700	-1.00312500	2.48682400
H	1.06943800	-1.52774900	2.15668600
C	1.08347500	1.07223300	2.57290400
H	1.85707400	0.99680000	3.36111400
H	0.89781300	2.13026400	2.34259300
H	0.14761100	0.62310700	2.93599500
C	2.76494100	1.11489600	0.83845400
H	2.51879300	2.18259200	0.74663200
H	3.60897000	0.99022500	1.54429500
H	3.07754600	0.74386900	-0.15374700
C	2.11134700	-1.86961600	-1.94186400
H	2.66063900	-2.82893300	-2.02170400
H	1.34756800	-1.80216800	-2.73098300
H	2.82067100	-1.03284600	-2.06932300
C	0.45805100	-2.87798400	-0.49001100
H	0.00385200	-2.88062400	0.51511500
H	-0.33858100	-2.73954800	-1.23945300
H	0.96143700	-3.85079000	-0.66046900

$[Pd(tmeda)(C_6H_5)(CF_3)F]^+$ transition state

Pd	-0.41478000	-0.21983500	-0.16144100
C	1.69566200	-0.01297600	-0.23297200
C	2.13831500	-0.74710200	-1.36175800
C	2.49114800	0.98512300	0.37394900
C	3.37136800	-0.38170700	-1.95659100
H	1.54071400	-1.57177600	-1.76029400
C	3.72772600	1.32094600	-0.22768600
H	2.20657700	1.47399000	1.31009300
C	4.16221200	0.64862300	-1.39591000
H	3.71129700	-0.92349000	-2.84572800
H	4.35328800	2.09210000	0.23489100
H	5.12429700	0.90913000	-1.84956600
C	0.82708000	-1.11192400	1.49131100
F	-0.28236700	-2.07059300	-0.79935800
F	1.72826000	-2.04956100	1.32240700
F	1.21318000	-0.24500500	2.42914300
F	-0.28751000	-1.70323100	1.96283400
C	-3.17979800	0.84221100	-0.21947100
H	-4.11199500	1.01902300	-0.79163500
H	-3.47060500	0.65754600	0.82975900
C	-2.25020100	2.04143700	-0.33139800
H	-2.72111100	2.95298700	0.08734800
H	-2.01373300	2.25014500	-1.39065900
C	-0.02303900	2.89326200	-0.07389300
H	0.88703000	2.90807100	0.53888000
H	0.25516400	2.73284900	-1.12834500
H	-0.53985900	3.86685100	0.03438500
C	-1.12019400	1.90441600	1.85674700
H	-0.14450800	1.76838100	2.34854300
H	-1.52577800	2.90190000	2.11684200
H	-1.80479000	1.12241600	2.22496900
C	-3.08805300	-1.60322100	-0.13553000
H	-2.54984600	-2.48525000	-0.51045500
H	-2.99498700	-1.56361300	0.96271500
H	-4.15814100	-1.65566300	-0.41859800
C	-2.53976300	-0.47488100	-2.21750000
H	-2.11935800	0.43078600	-2.68610800
H	-1.94623300	-1.34903000	-2.52669500
H	-3.59157000	-0.59939700	-2.54210400
N	-2.47985000	-0.37377800	-0.72883900
N	-0.93798200	1.79730700	0.37698600

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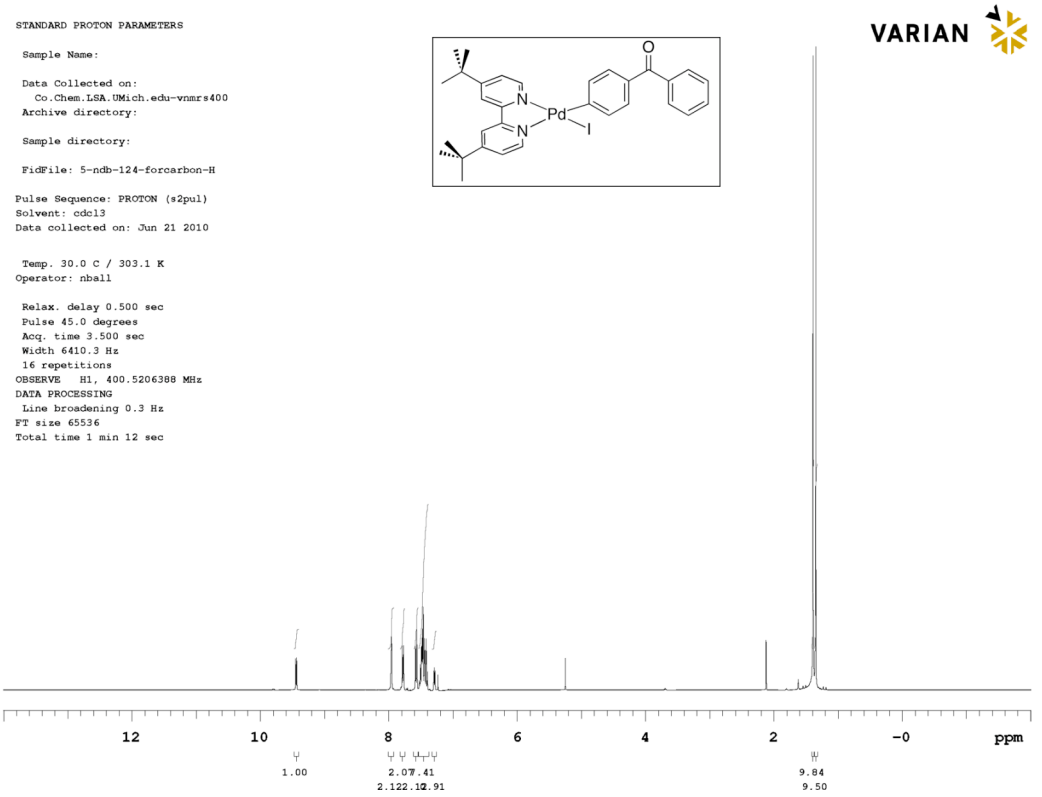
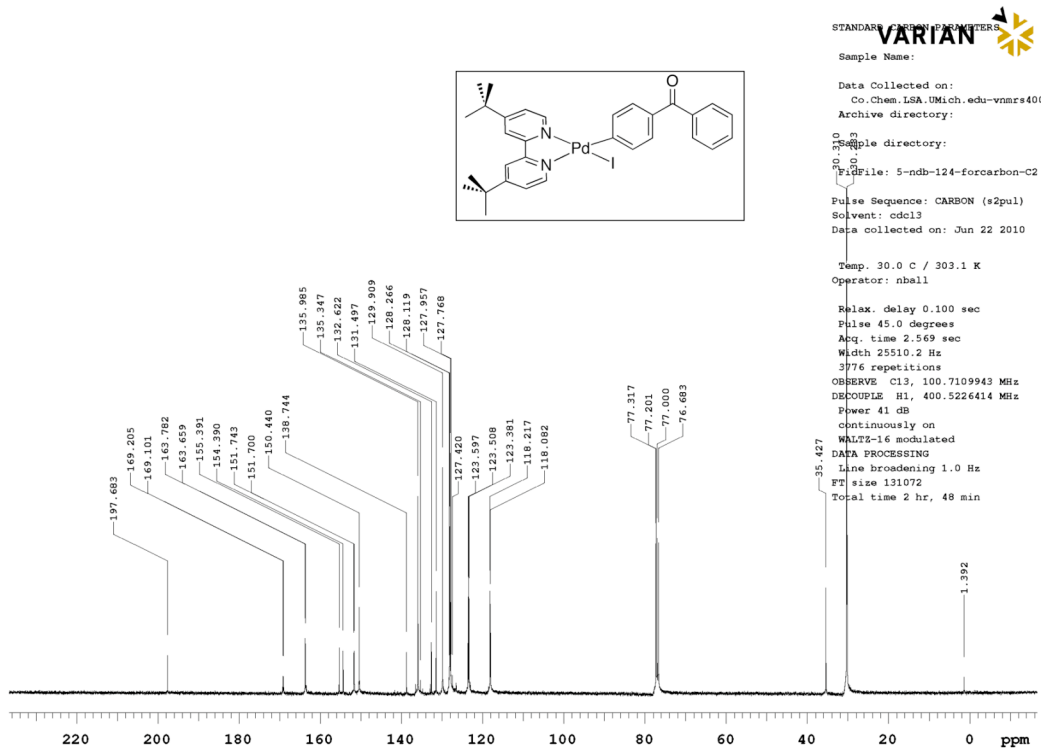
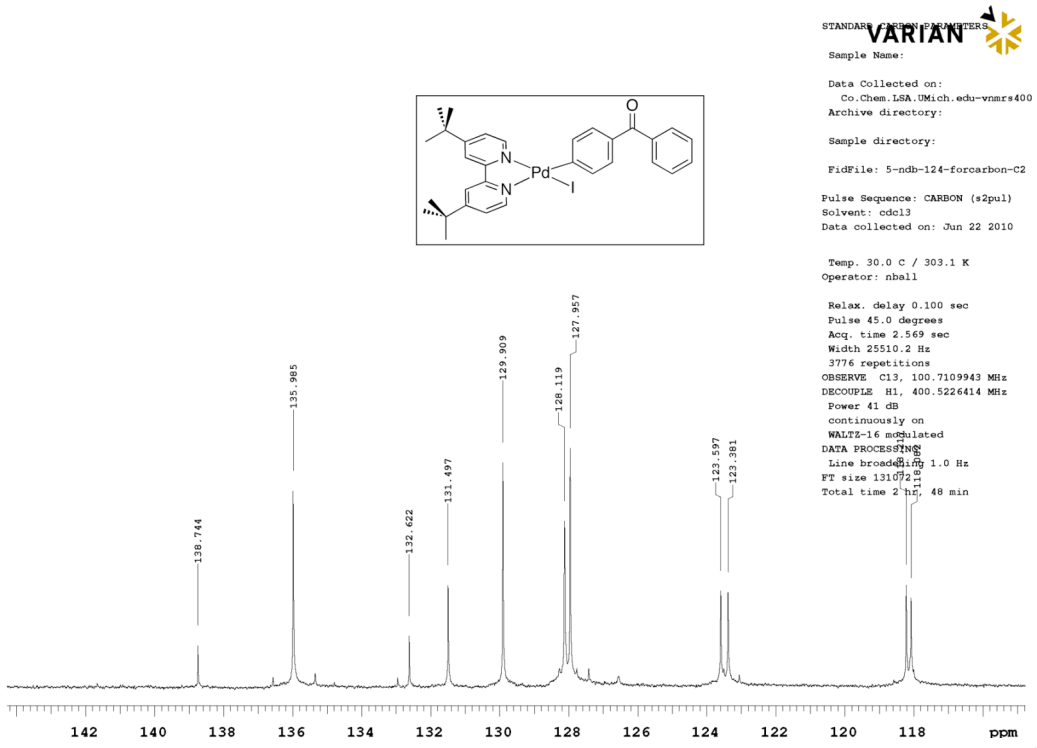
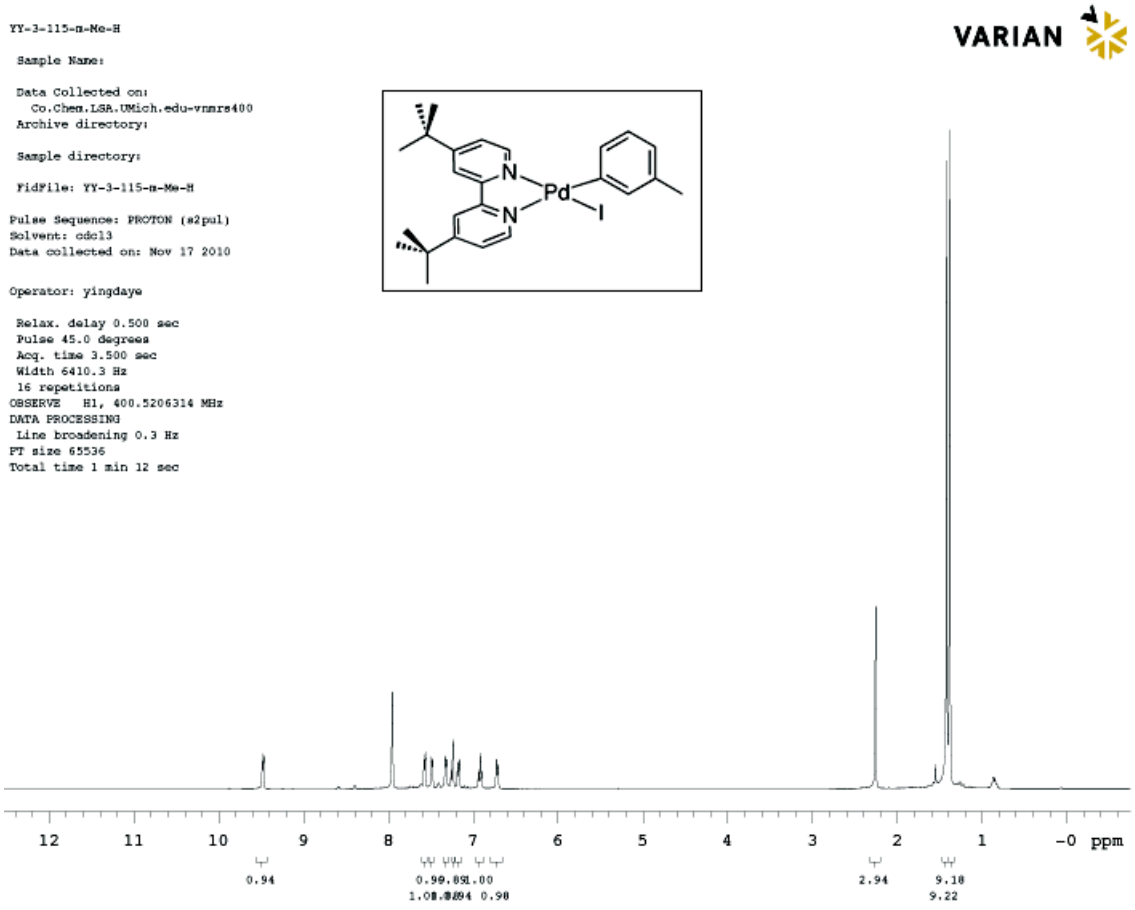
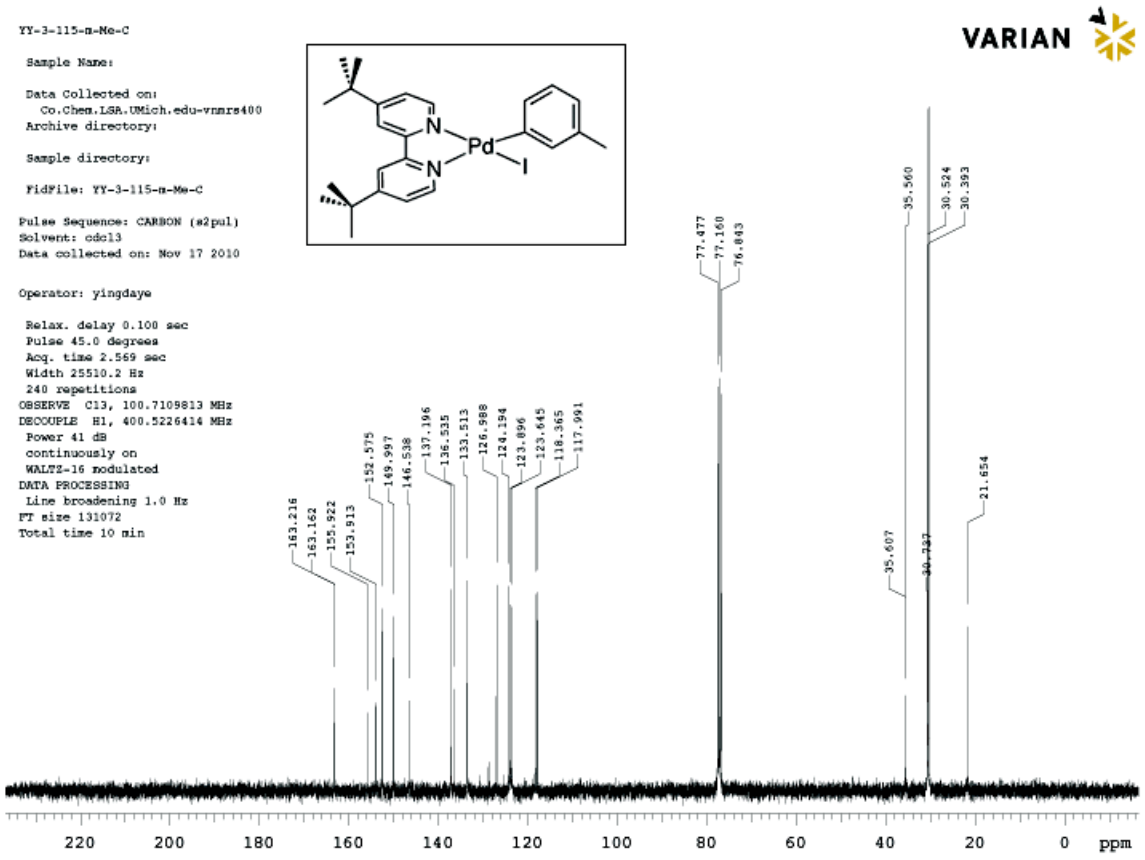
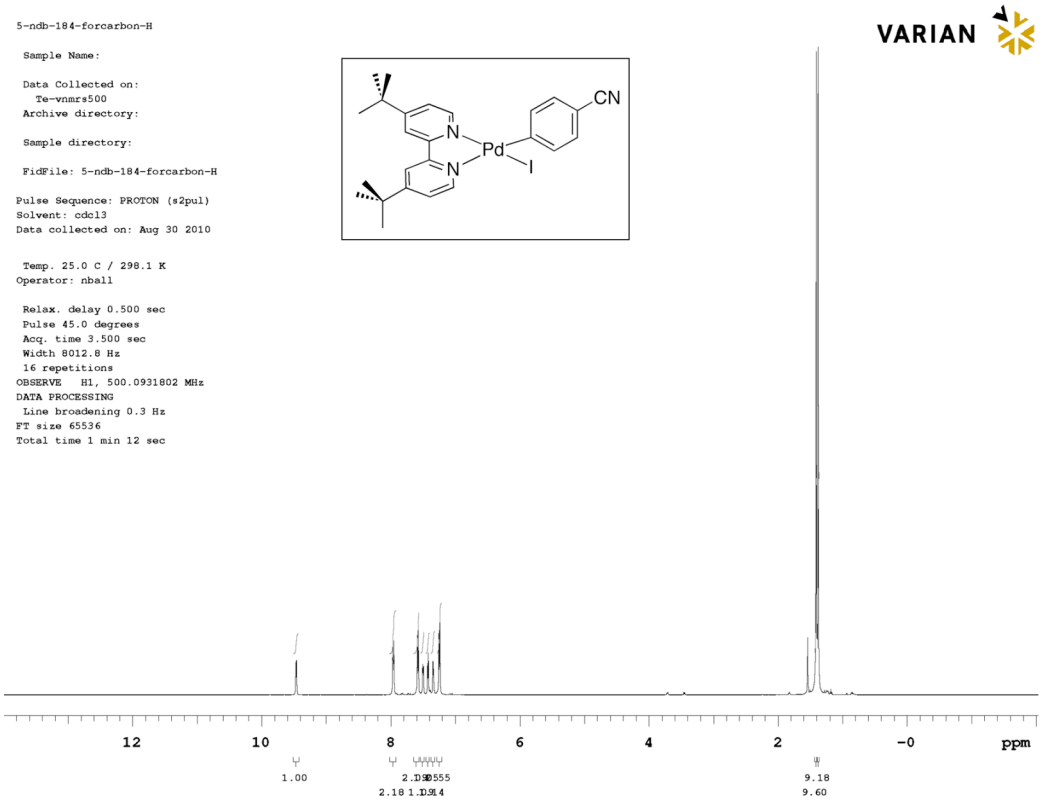

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-124-forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2010
Temp. 30.0 C / 303.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206388 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Pd
I
N
O
12
10
8
6
4
2
-0
ppm
1.00
2.07
7.41
2.12
2.12
2.91
9.84
9.50

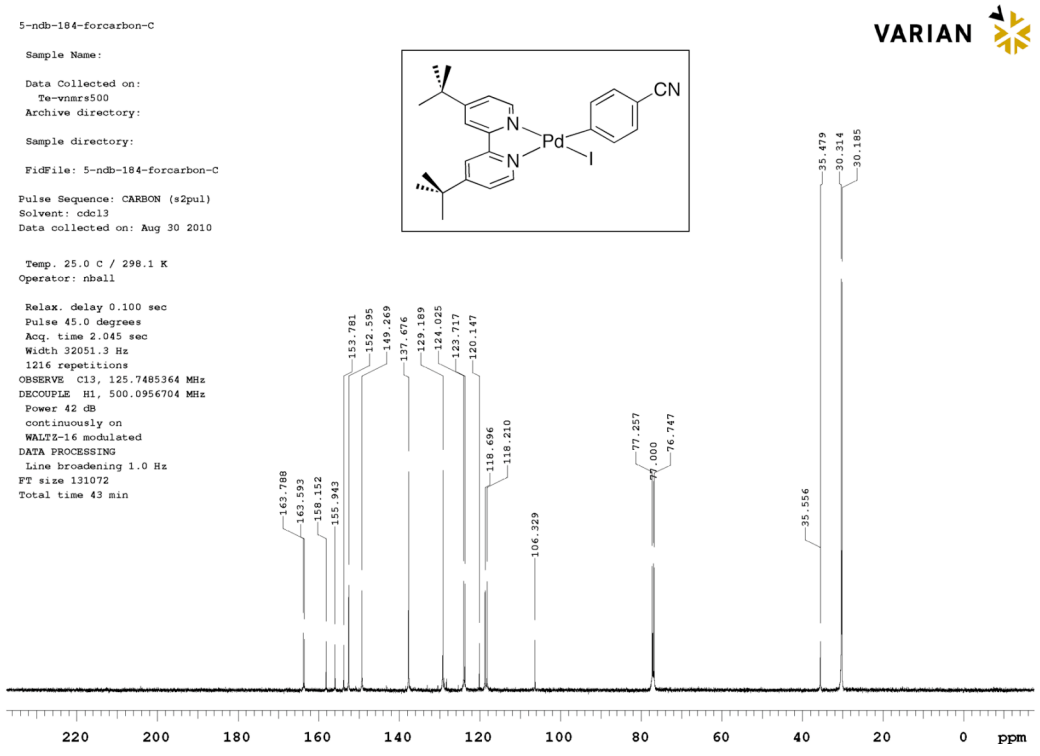

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs40
Archive directory:
Sample directory:
FidFile: 5-ndb-124-forcarbon-C2
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 30.0 C / 303.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3776 repetitions
OBSERVE C13, 100.7109943 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 48 min
VARIAN
Pd
I
N
O
197.683
169.205
169.101
163.782
163.659
155.391
154.390
151.743
151.700
150.440
138.744
135.985
135.347
132.622
131.497
129.909
128.266
128.119
127.957
127.768
127.420
123.597
123.508
123.381
118.217
118.082
77.317
77.201
77.000
76.683
35.427
30.310
30.203
1.392
220
200
180
160
140
120
100
80
60
40
20
0
ppm

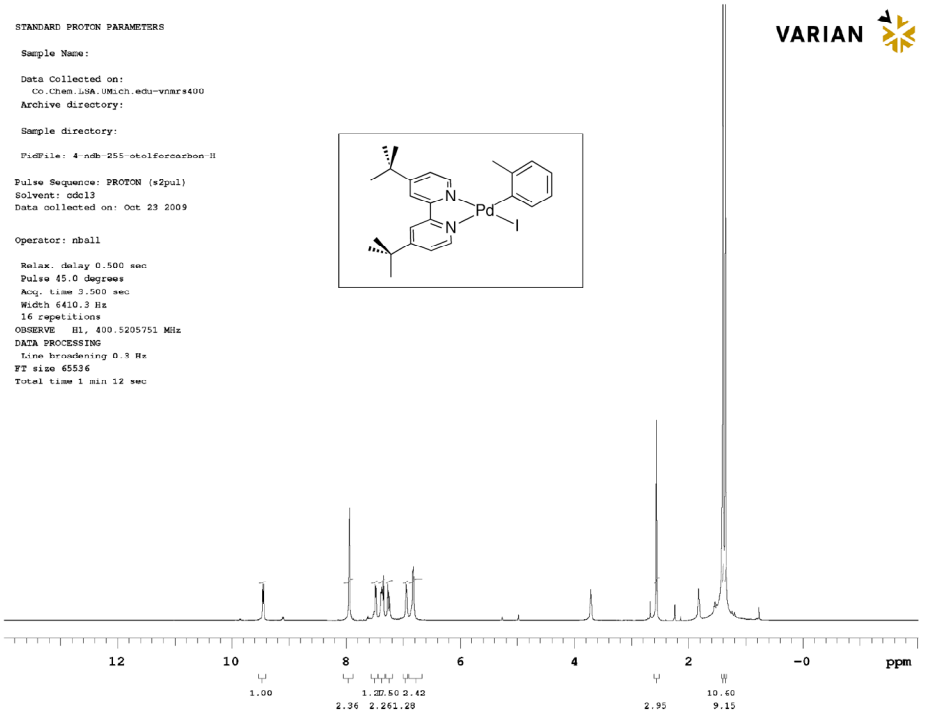

STANDARD CARBON PARAMETERS
VARIAN
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-124-forcarbon-C2
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 30.0 C / 303.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3776 repetitions
OBSERVE C13, 100.7109943 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 48 min
O
N
Pd
N
I
138.744
135.985
132.622
131.497
129.909
128.119
127.957
123.597
123.381
118.141
118.028
142
140
138
136
134
132
130
128
126
124
122
120
118
ppm

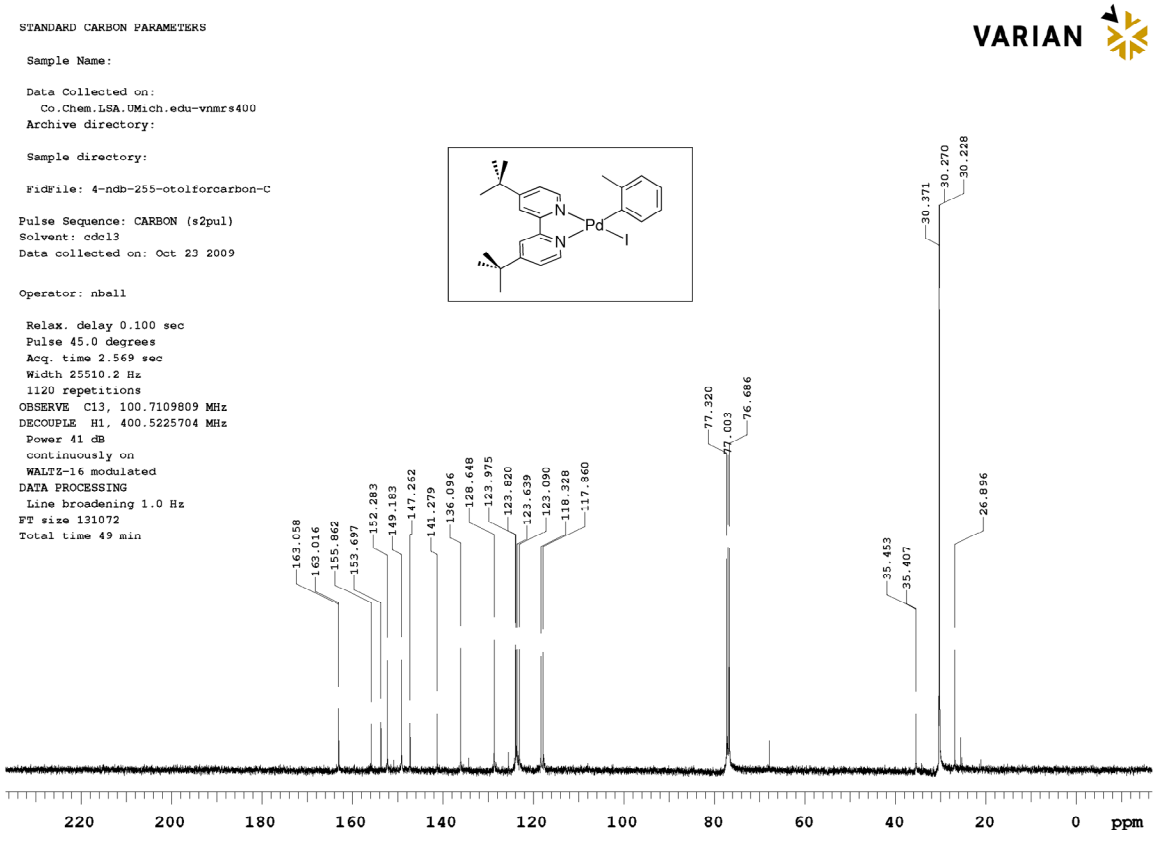

YY-3-115-m-Me-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-115-m-Me-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 17 2010
Operator: yingdaye
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206314 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
N
Pd
N
I
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.94
2.94
9.18
9.22


YY-3-115-n-Me-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-115-n-Me-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 17 2010
Operator: yingdaye
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
240 repetitions
OBSERVE C13, 100.7109813 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 10 min
VARIAN
N
Pd
I
163.216
163.162
155.922
153.913
152.575
149.997
146.538
137.196
136.535
133.513
126.988
124.194
123.096
123.645
118.365
117.991
77.477
77.160
76.843
35.560
30.524
30.393
35.607
30.247
21.654
220
200
180
160
140
120
100
80
60
40
20
0
ppm


5-ndb-184-forcarbon-H
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-184-forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 30 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 500.0931802 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
CN
N
Pd
N
I
12
10
8
6
4
2
-0
ppm
1.00
9.18
9.60


5-ndb-184-forcarbon-C
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-184-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 30 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 32051.3 Hz
1216 repetitions
OBSERVE C13, 125.7485364 MHz
DECOUPLE H1, 500.0956704 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 43 min
VARIAN
CN
N
Pd
N
I
163.788
163.593
158.152
155.943
153.781
152.595
149.269
137.676
129.189
124.025
123.717
120.147
118.696
118.210
106.329
77.257
77.000
76.747
35.556
35.479
30.314
30.185
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-255-otolforcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2009
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5205751 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
N
Pd
I
12
10
8
6
4
2
-0
ppm
1.00
2.36
1.27
2.26
0.50
1.28
2.42
2.95
10.60
9.15


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-255-otolforcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2009
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1120 repetitions
OBSERVE C13, 100.7109809 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 49 min
VARIAN
N
Pd
I
163.058
163.016
155.862
153.697
152.283
149.183
147.262
141.279
136.096
128.648
123.975
123.820
123.639
123.090
118.328
117.360
77.320
77.003
76.686
35.453
35.407
30.371
30.270
30.228
26.856
220
200
180
160
140
120
100
80
60
40
20
0
ppm

5-ndb-134forcarbon1132010-H

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

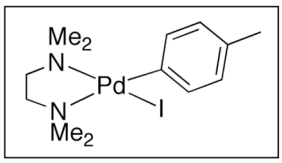
Sample directory:

FidFile: 5-ndb-134forcarbon1132010-H

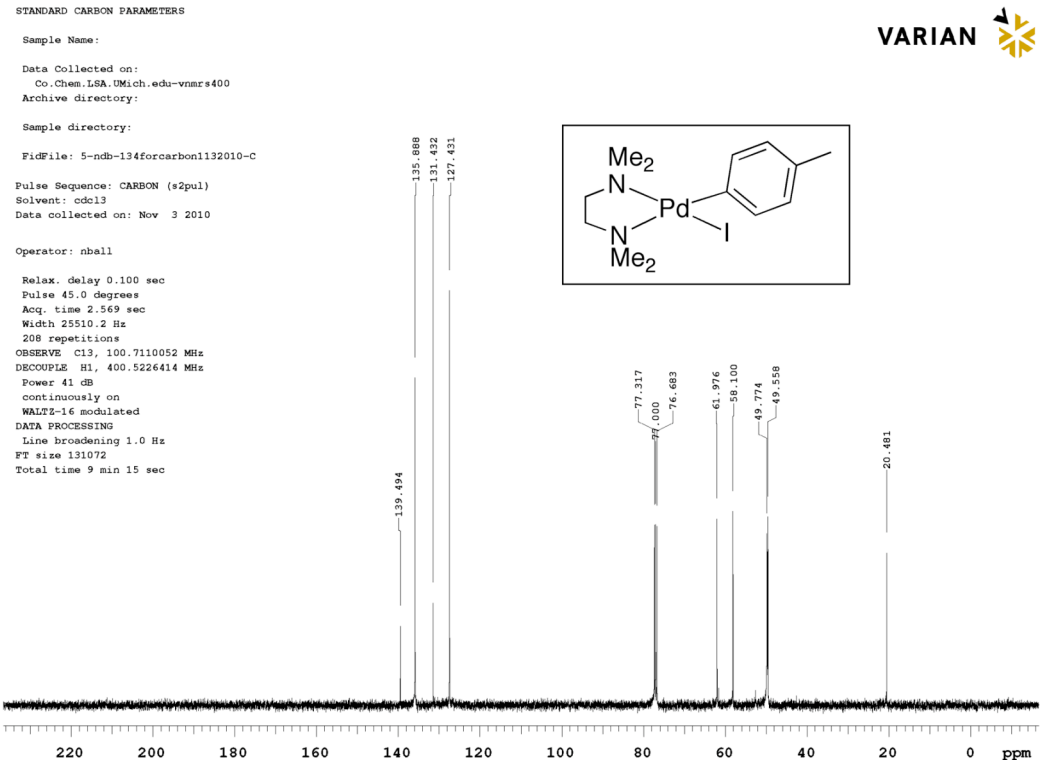
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2010

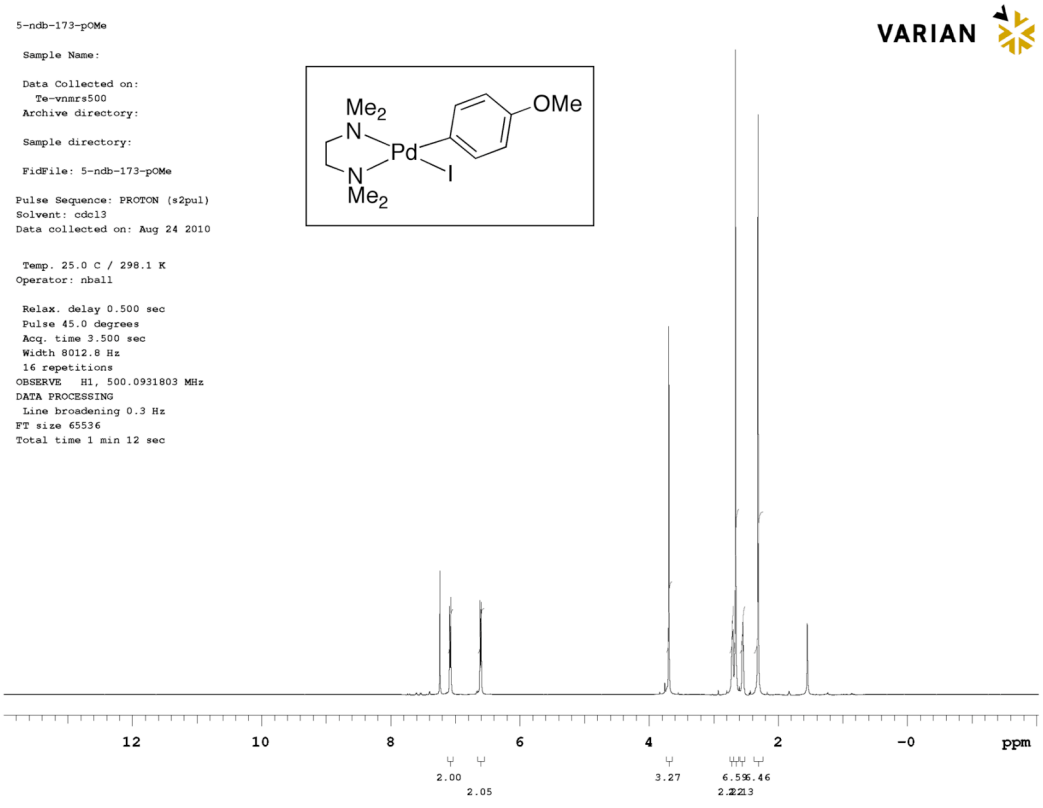
Operator: nball

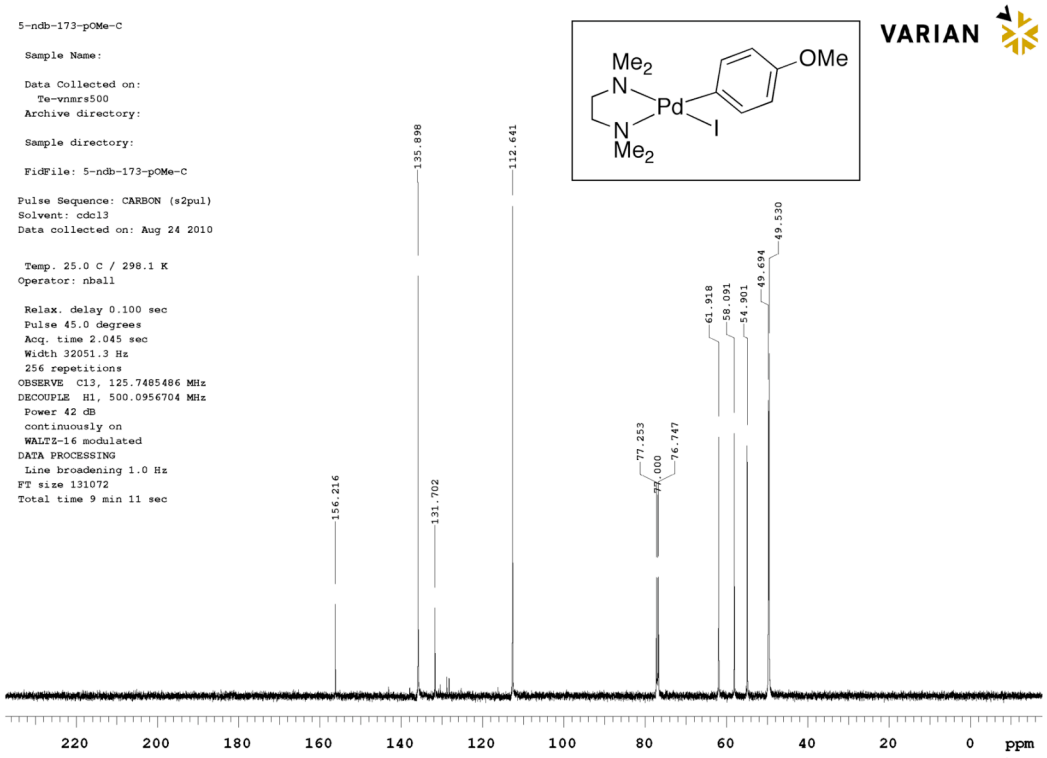
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206396 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec

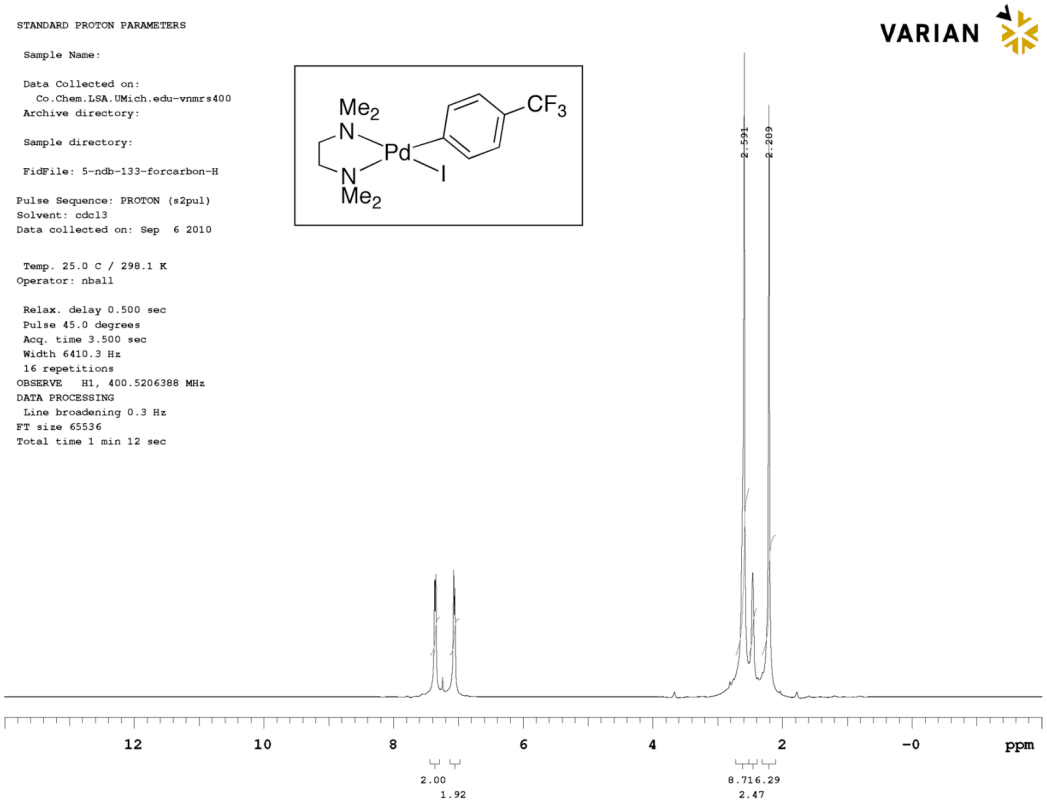


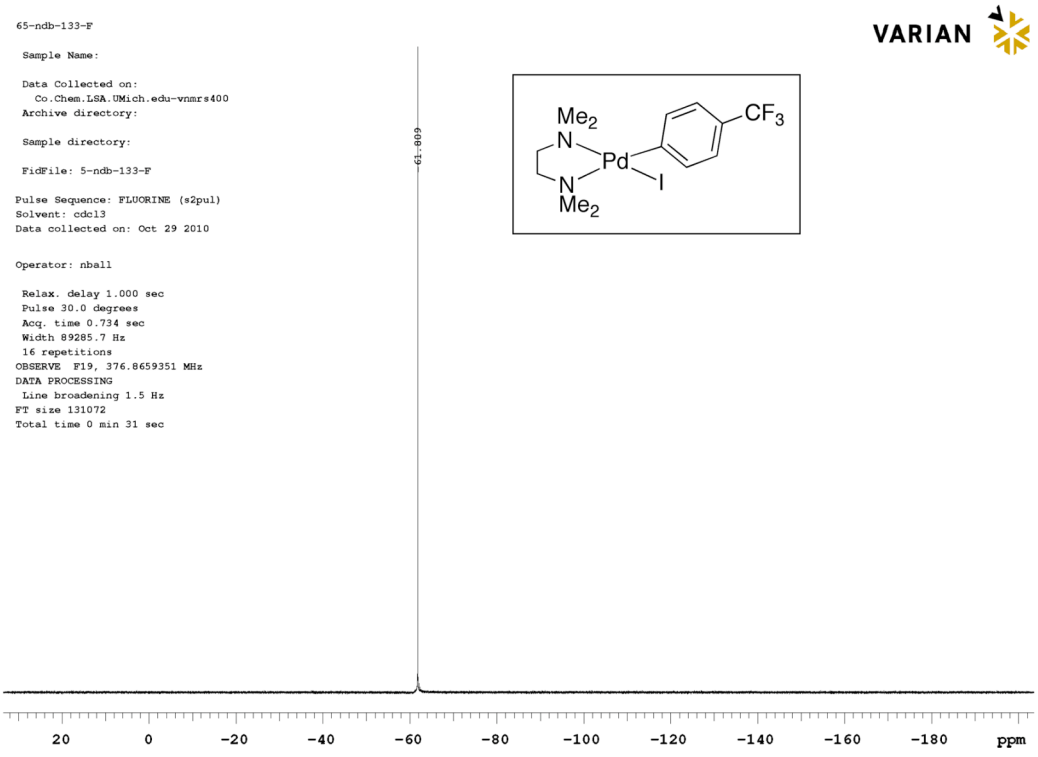
VARIAN

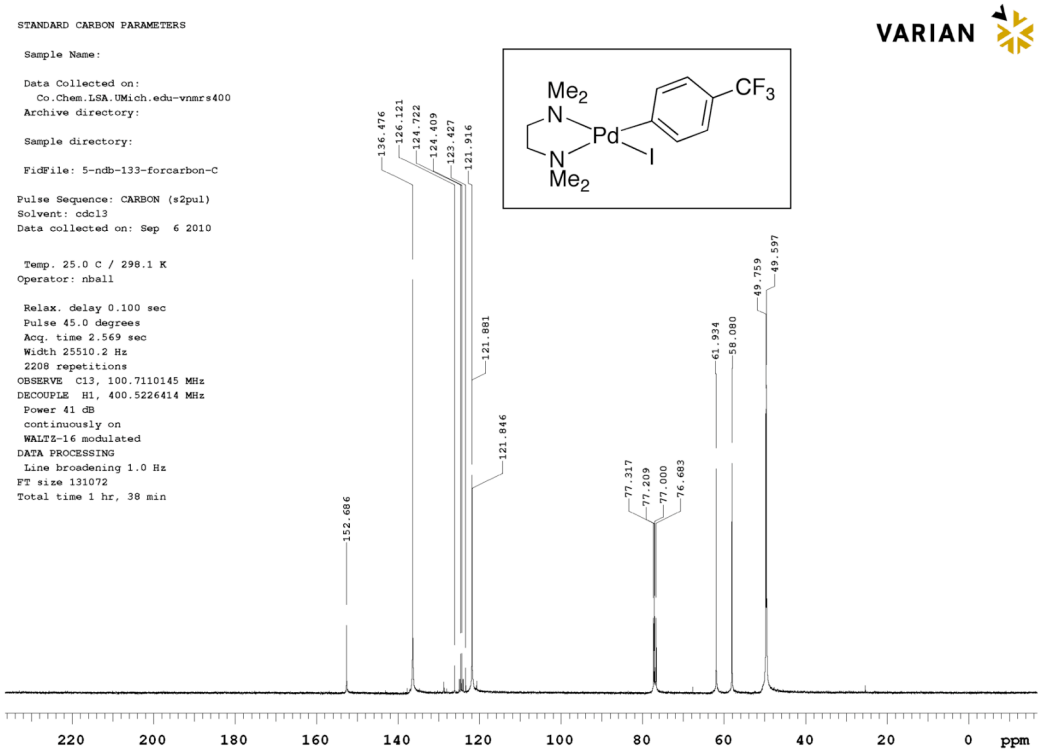

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-134forcarbon1132010-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
208 repetitions
OBSERVE C13, 100.7110052 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min 15 sec
VARIAN
Me2
N
Pd
I
N
Me2
135.888
131.432
127.431
139.494
77.317
77.000
76.683
61.976
58.100
49.774
49.558
20.481
220
200
180
160
140
120
100
80
60
40
20
0
ppm


5-ndb-173-pOMe
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-173-pOMe
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 24 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 500.0931803 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Me2
N
Pd
I
N
Me2
OMe
12
10
8
6
4
2
-0
ppm
2.00
2.05
3.27
6.59
6.46


5-ndb-173-pOMe-C
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-173-pOMe-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 24 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 32051.3 Hz
256 repetitions
OBSERVE C13, 125.7485486 MHz
DECOUPLE H1, 500.0956704 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min 11 sec
Me2
N
Pd
I
N
Me2
OMe
VARIAN
156.216
135.898
131.702
112.641
77.253
77.000
76.747
61.918
58.091
54.901
49.694
49.530
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-133-forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 6 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206388 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
Me2
N
Pd
I
N
Me2
CF3
VARIAN
2.591
2.209
12
10
8
6
4
2
−0
ppm
2.00
1.92
8.716.29
2.47


65-ndb-133-F
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-133-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 29 2010
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8659351 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 31 sec
VARIAN
61.809
Me2
N
Pd
I
N
Me2
CF3
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-133-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 6 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2208 repetitions
OBSERVE C13, 100.7110145 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 38 min
VARIAN
136.476
126.121
124.722
124.409
123.427
121.916
121.881
121.846
152.686
77.317
77.209
77.000
76.683
61.934
58.080
49.759
49.597
Me2
N
Pd
I
N
Me2
CF3
220
200
180
160
140
120
100
80
60
40
20
0
ppm

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

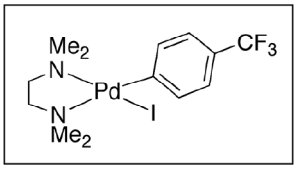
Sample directory:

FidFile: 5-ndb-133-forcarbon-C

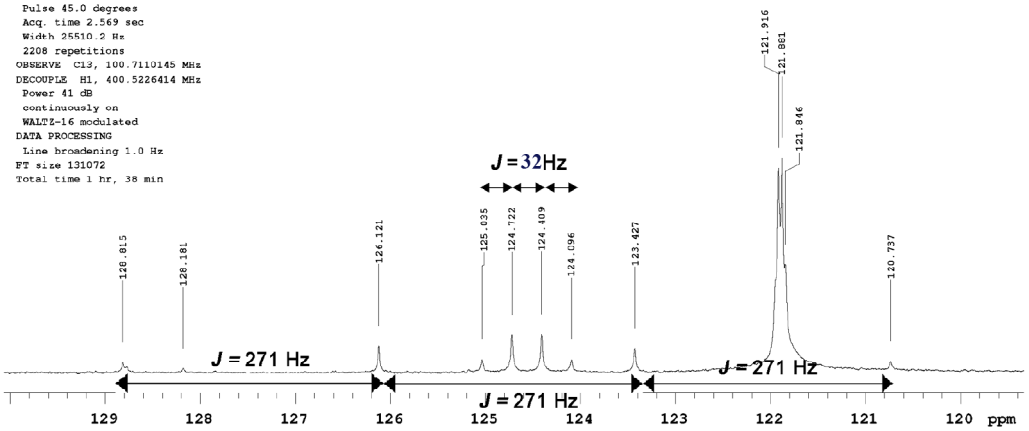
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 6 2010

Temp. 25.0 C / 298.1 K
Operator: nball

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2208 repetitions
OBSERVE C13, 100.7110145 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 38 min



VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

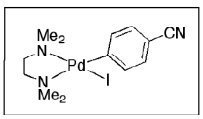
Sample directory:

FidFile: 5-ndb-203forcarbon-H

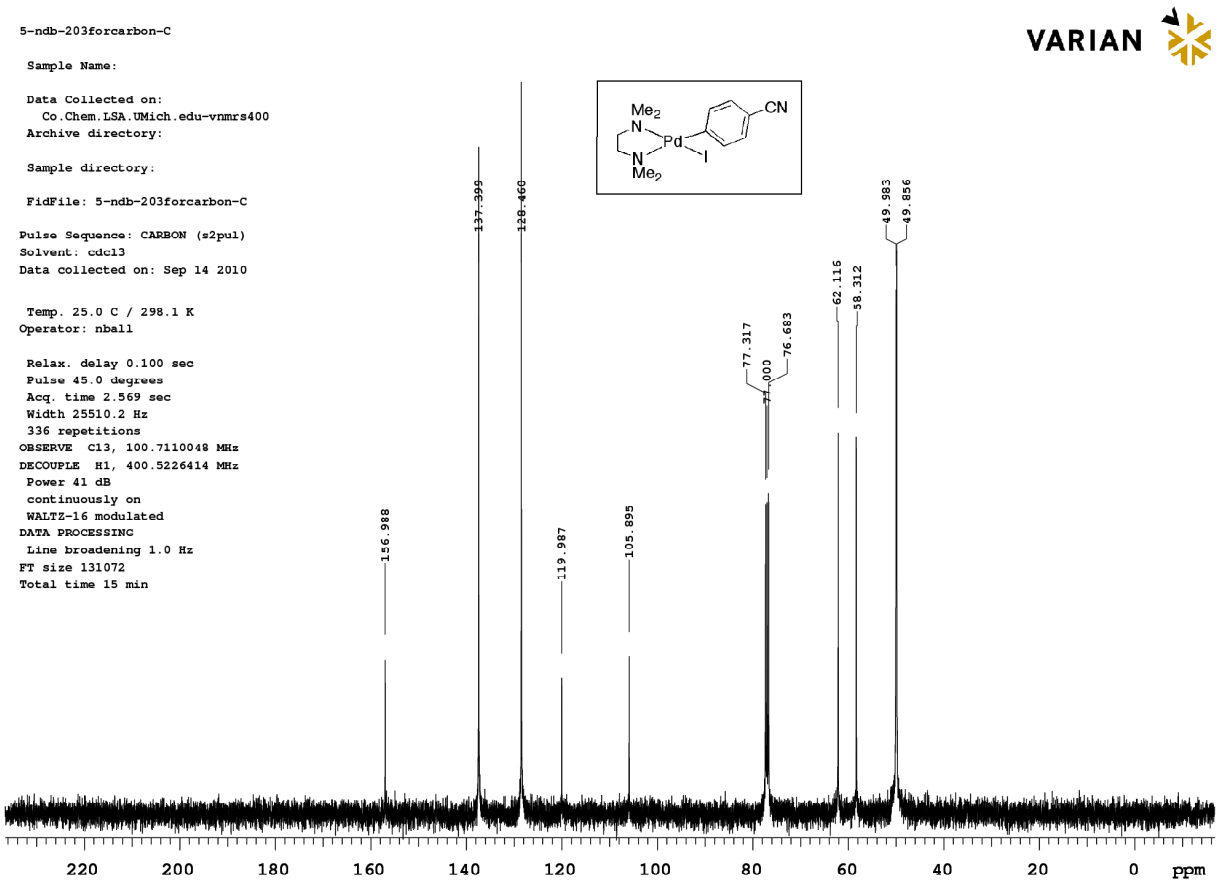
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 14 2010

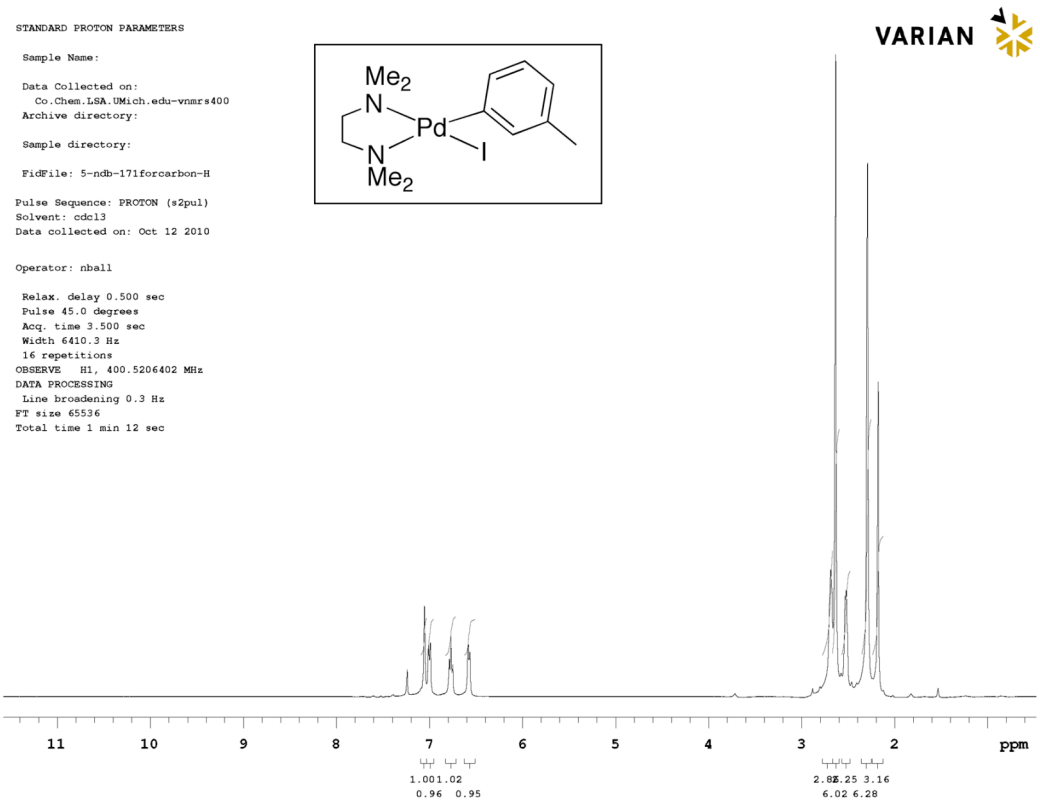
Temp. 25.0 C / 298.1 K
Operator: nball

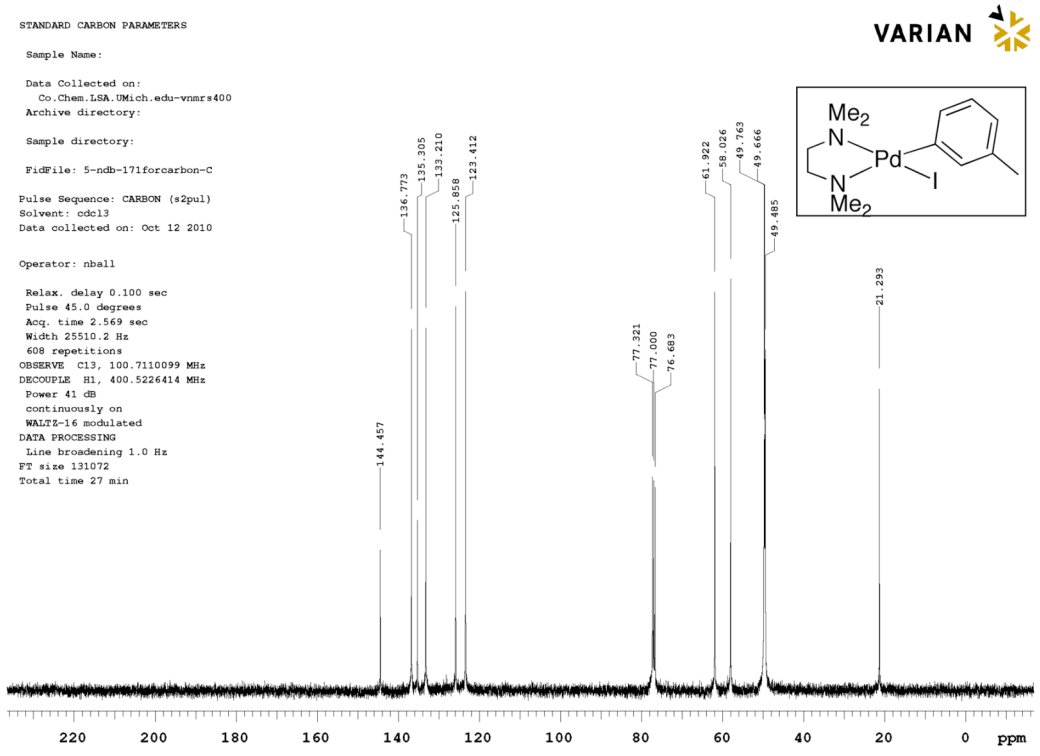
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206320 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec

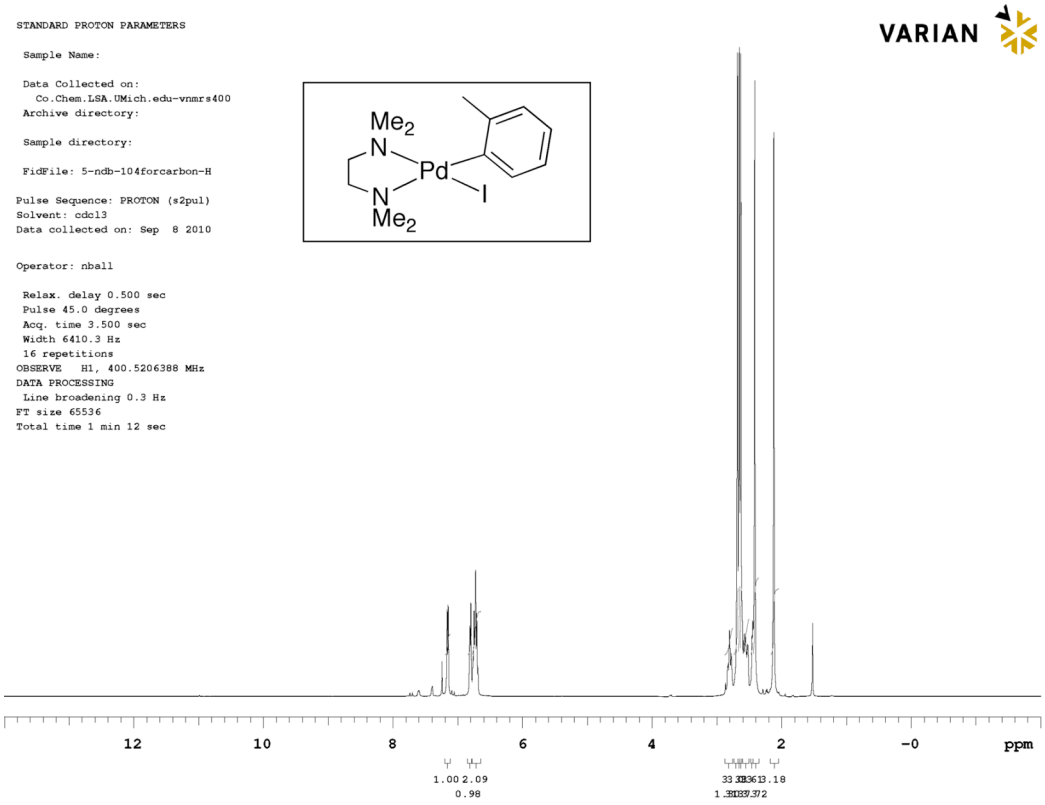


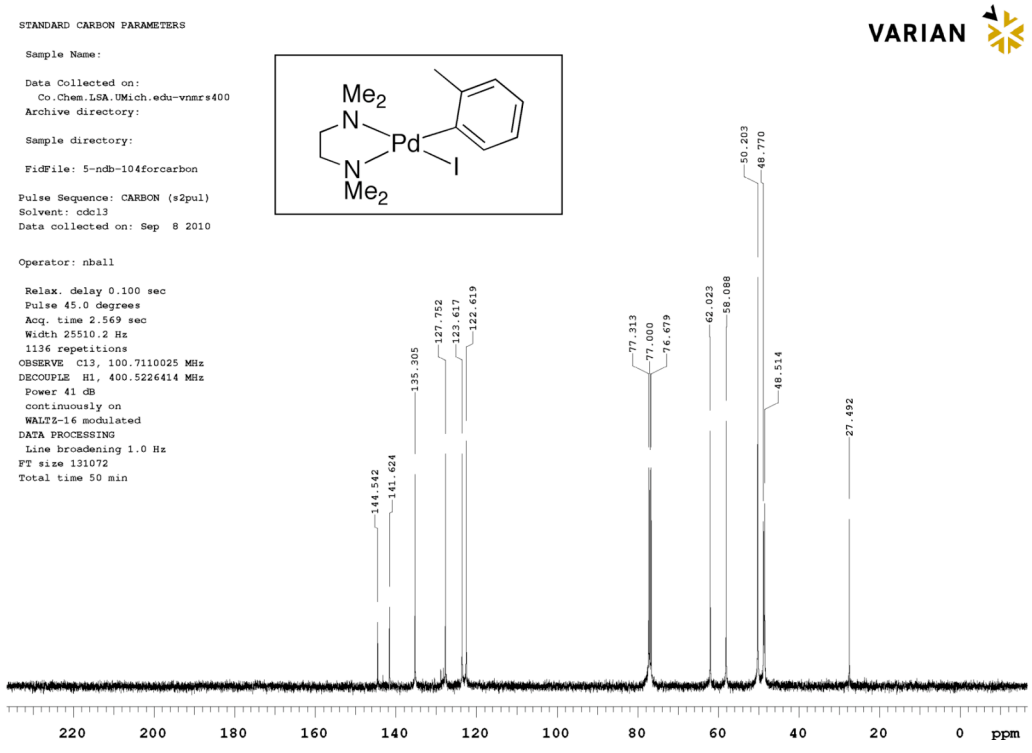
VARIAN

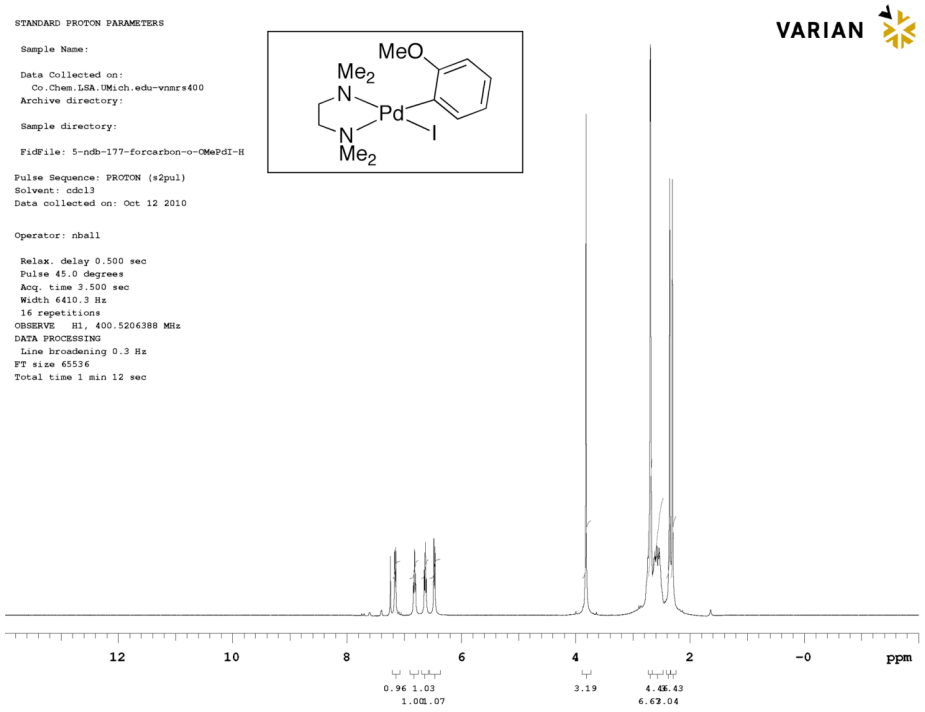

5-ndb-203forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-203forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 14 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
336 repetitions
OBSERVE C13, 100.7110048 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 15 min
Me2
N
Pd
I
N
Me2
CN
156.988
137.399
128.460
119.987
105.895
77.317
77.000
76.683
62.116
58.312
49.983
49.856
220
200
180
160
140
120
100
80
60
40
20
0
ppm

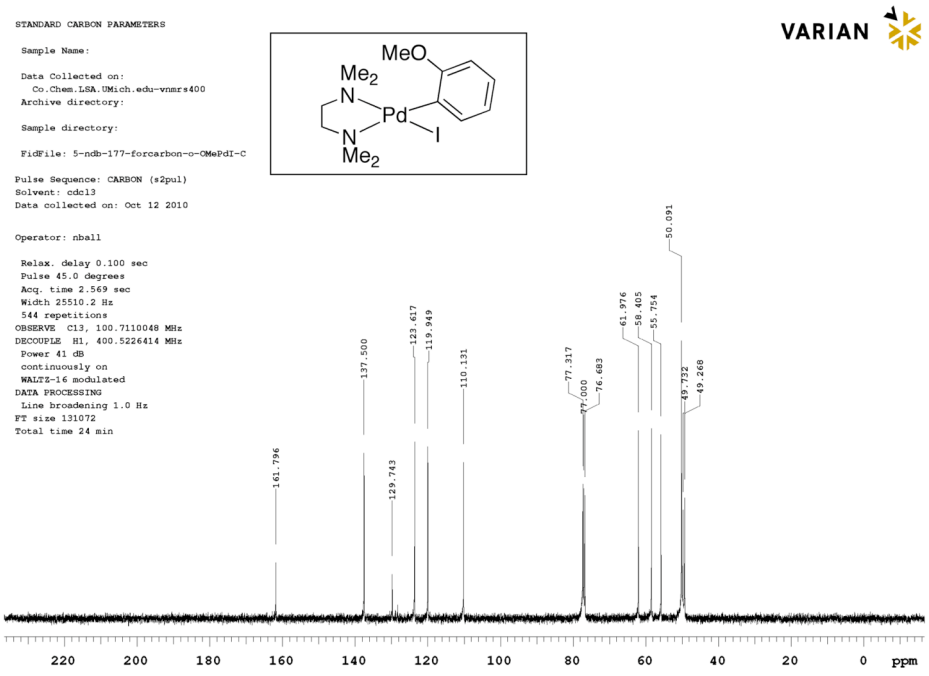

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-171forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206402 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Me2
N
Pd
I
N
Me2
11
10
9
8
7
6
5
4
3
2
ppm
1.00
1.02
0.96
0.95
2.82
3.25
3.16
6.02
6.28

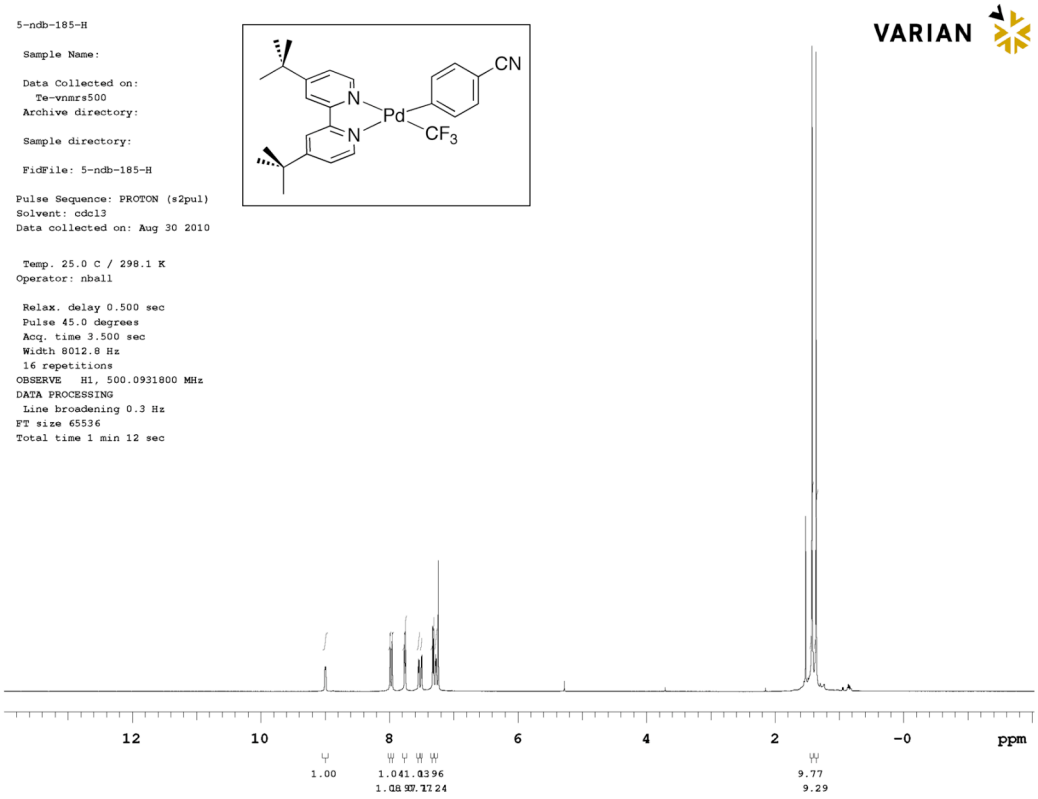

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-171forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
608 repetitions
OBSERVE C13, 100.7110099 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 27 min
VARIAN
Me2
N
Pd
I
N
Me2
144.457
136.773
135.305
133.210
125.858
123.412
77.321
77.000
76.683
61.922
58.026
49.763
49.666
49.485
21.293
220
200
180
160
140
120
100
80
60
40
20
0
ppm

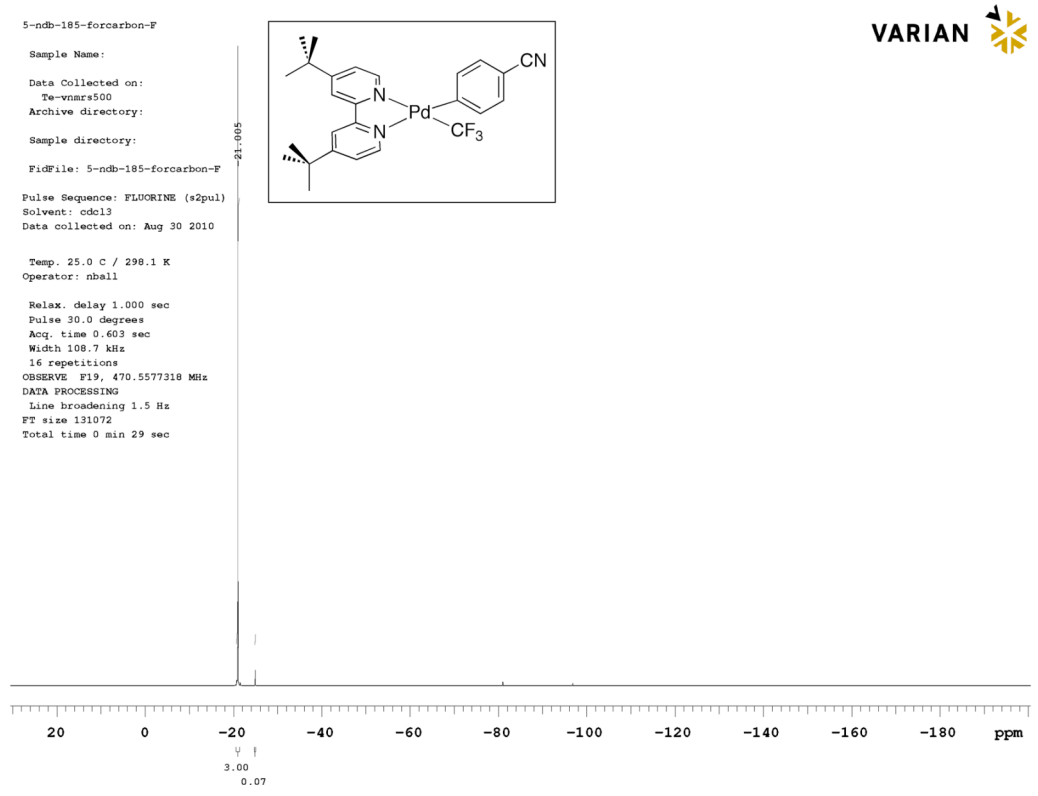

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-104forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206388 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Me2
N
Pd
I
N
Me2
12
10
8
6
4
2
-0
ppm
1.00
2.09
0.98

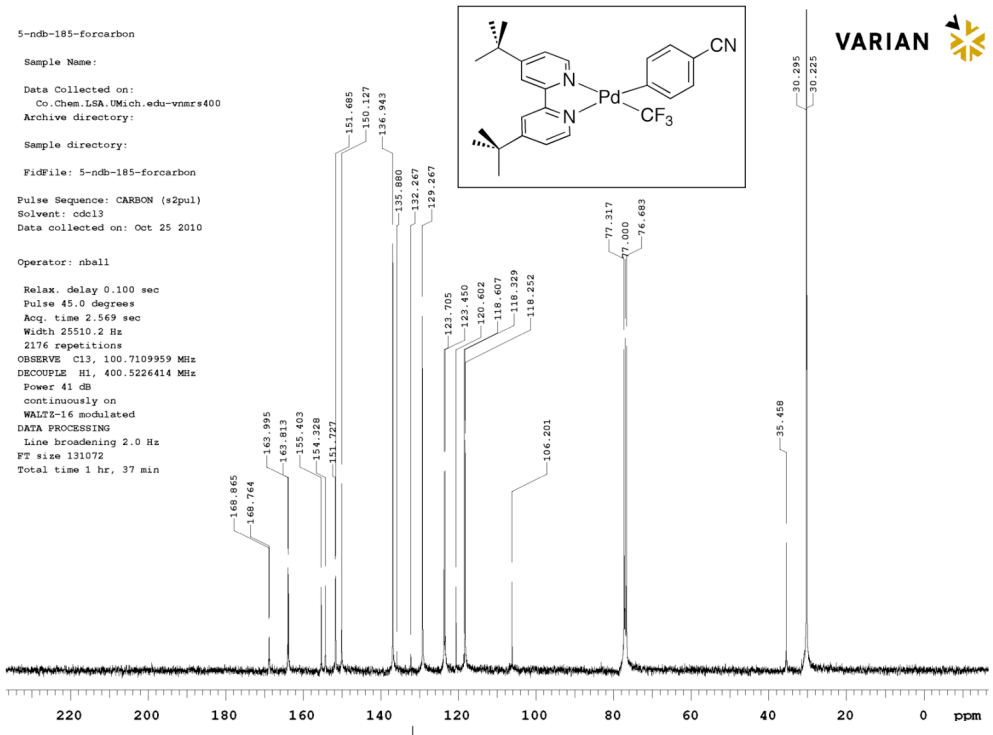

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-104forcarbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1136 repetitions
OBSERVE C13, 100.7110025 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 50 min
VARIAN
Me2
N
Pd
I
N
Me2
144.542
141.624
135.305
127.752
123.617
122.619
77.313
77.000
76.679
62.023
58.088
50.203
48.770
48.514
27.492
220
200
180
160
140
120
100
80
60
40
20
0
ppm

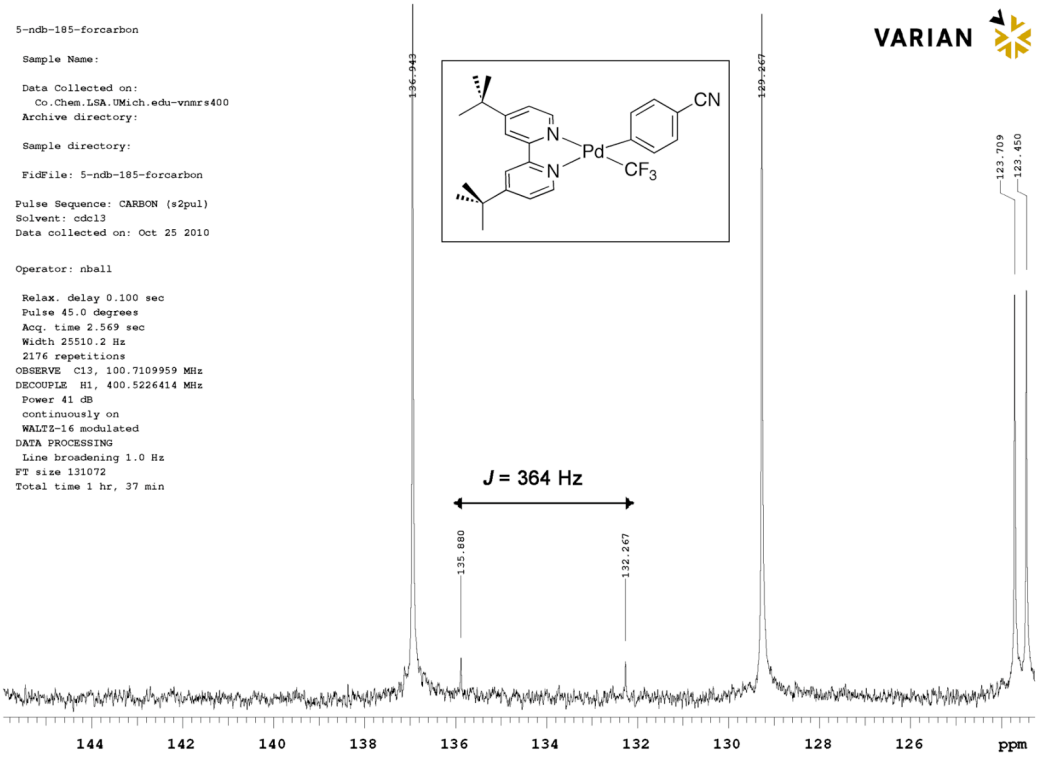

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-177-forcarbon-o-OMePdI-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206388 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
MeO
Me2
N
Pd
I
N
Me2
VARIAN
12
10
8
6
4
2
−0
ppm
0.96 1.03
1.00 1.07
3.19
4.43
6.63 3.04

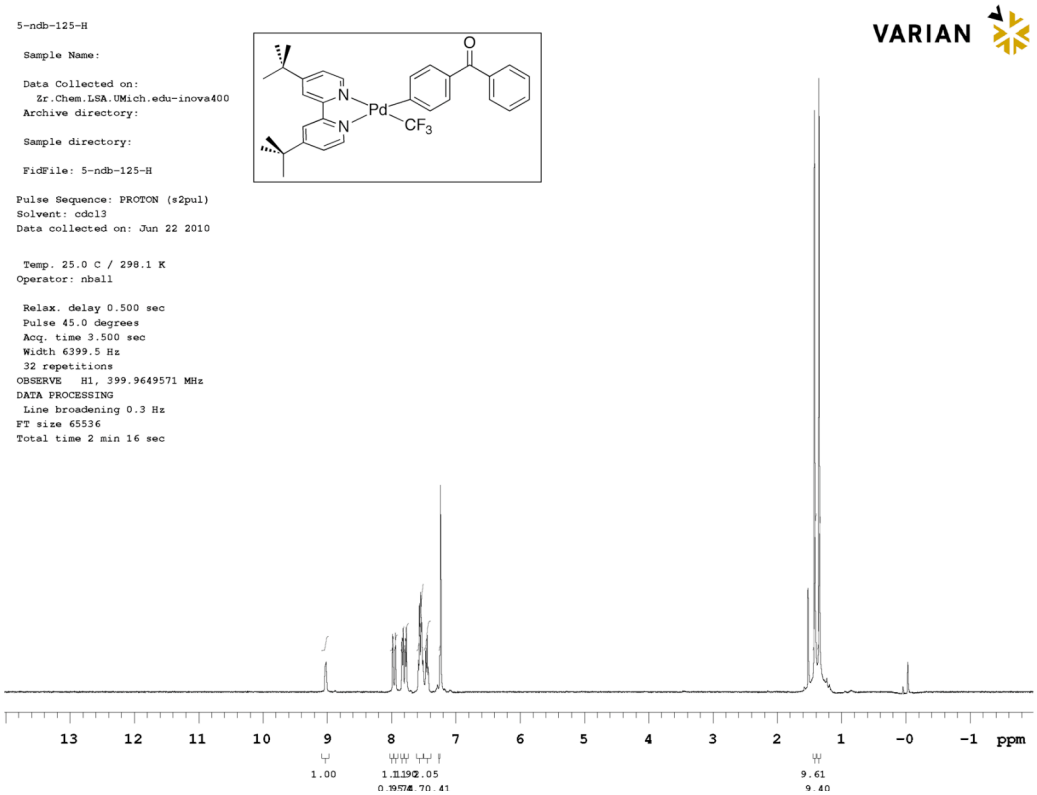

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-177-forcarbon-o-OMePdI-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
544 repetitions
OBSERVE C13, 100.7110048 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 24 min
MeO
Me2
N
Pd
I
N
Me2
VARIAN
161.796
137.500
129.743
123.617
119.949
110.131
77.317
77.000
76.683
61.976
58.405
55.754
50.091
49.732
49.268
220
200
180
160
140
120
100
80
60
40
20
0
ppm

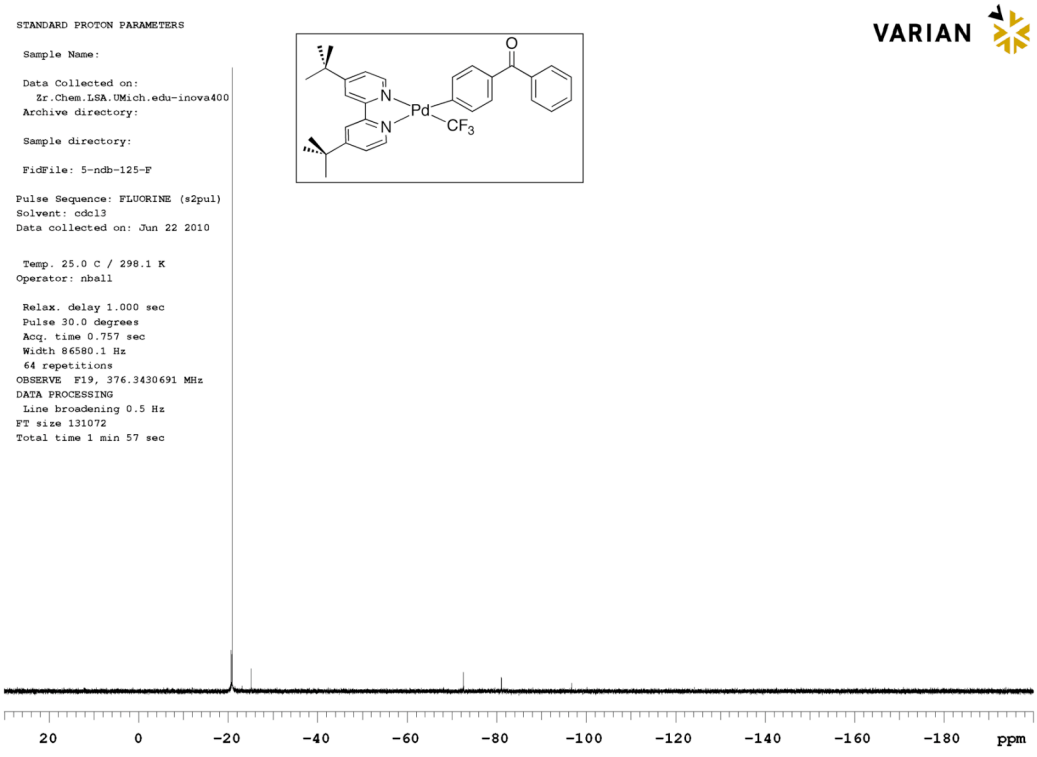

5-ndb-185-H
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-185-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 30 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 500.0931800 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
CN
N
Pd
N
CF3
12
10
8
6
4
2
-0
ppm
1.00
1.04
1.03
1.00
9.77
9.29

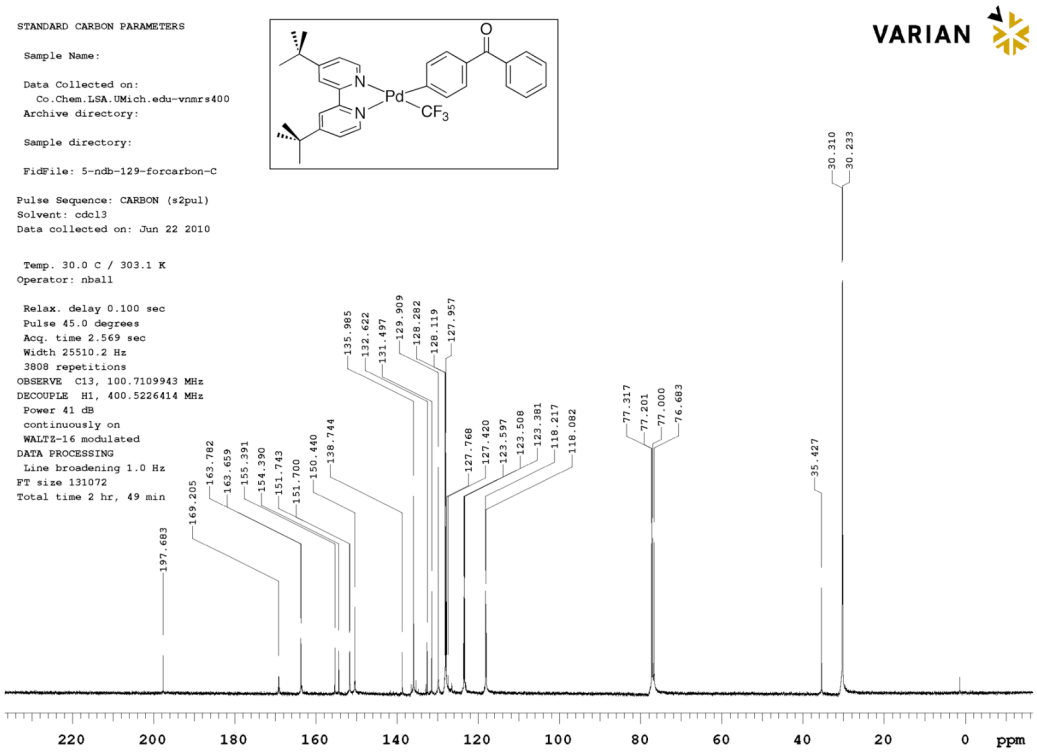

5-ndb-185-forcarbon-F
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-185-forcarbon-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Aug 30 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
16 repetitions
OBSERVE F19, 470.5577318 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 29 sec
21.005
VARIAN
CN
N
Pd
N
CF3
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
3.00
0.07

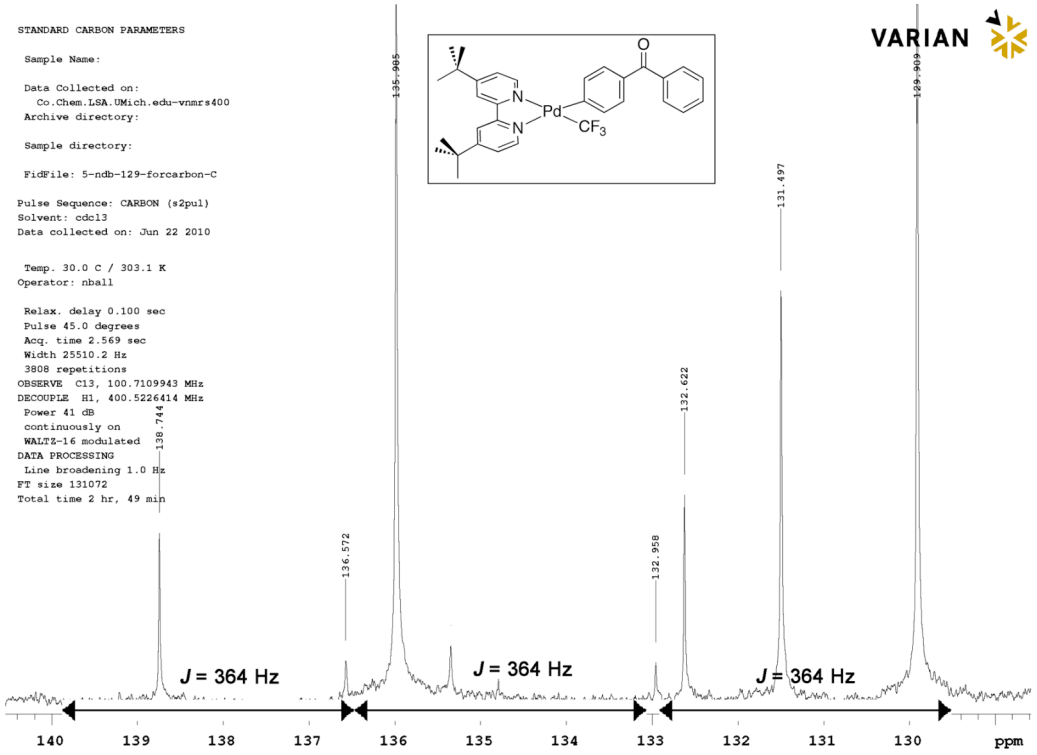

5-ndb-185-forcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-185-forcarbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2176 repetitions
OBSERVE C13, 100.7109959 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 1 hr, 37 min
VARIAN
CN
N
Pd
N
CF3
168.865
168.764
163.995
163.813
155.403
154.328
151.722
151.685
150.127
136.943
135.880
132.267
129.267
123.705
123.450
120.602
118.607
118.329
118.252
106.201
77.317
77.000
76.683
35.458
30.295
30.225
220
200
180
160
140
120
100
80
60
40
20
0
ppm


5-ndb-185-forcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-185-forcarbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2176 repetitions
OBSERVE C13, 100.7109959 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 37 min
VARIAN
CN
N
Pd
N
CF3
136.943
129.267
123.709
123.450
J = 364 Hz
135.880
132.267
144
142
140
138
136
134
132
130
128
126
ppm


5-ndb-125-H
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-125-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
32 repetitions
OBSERVE H1, 399.9649571 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 2 min 16 sec
VARIAN
O
N
Pd
N
CF3
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
1.00
9.61


STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-125-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
64 repetitions
OBSERVE F19, 376.3430691 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 1 min 57 sec
VARIAN
O
N
Pd
N
CF3
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-129-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 30.0 C / 303.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3808 repetitions
OBSERVE C13, 100.7109943 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 49 min
VARIAN
Pd
CF3
197.683
169.205
163.782
163.659
155.391
154.390
151.743
151.700
150.440
138.744
135.985
132.622
131.497
129.909
128.282
128.119
127.957
127.768
127.420
123.597
123.508
123.381
118.217
118.082
77.317
77.201
77.000
76.683
35.427
30.310
30.233
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-129-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2010
Temp. 30.0 C / 303.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3808 repetitions
OBSERVE C13, 100.7109943 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 49 min
VARIAN
Pd
CF3
138.744
136.572
135.985
132.958
132.622
131.497
129.909
J = 364 Hz
J = 364 Hz
J = 364 Hz
140
139
138
137
136
135
134
133
132
131
130
ppm

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

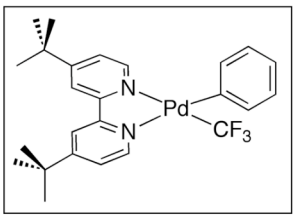
Sample directory:

FidFile: 5-ndb-51-forcarbon-H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2010

Operator: nball

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5205678 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec



VARIAN

5-ndb-51-forcarbon-F

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

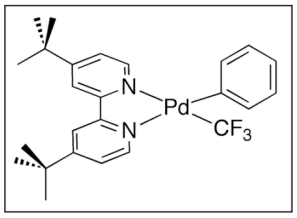
Sample directory:

FidFile: 5-ndb-51-forcarbon-F

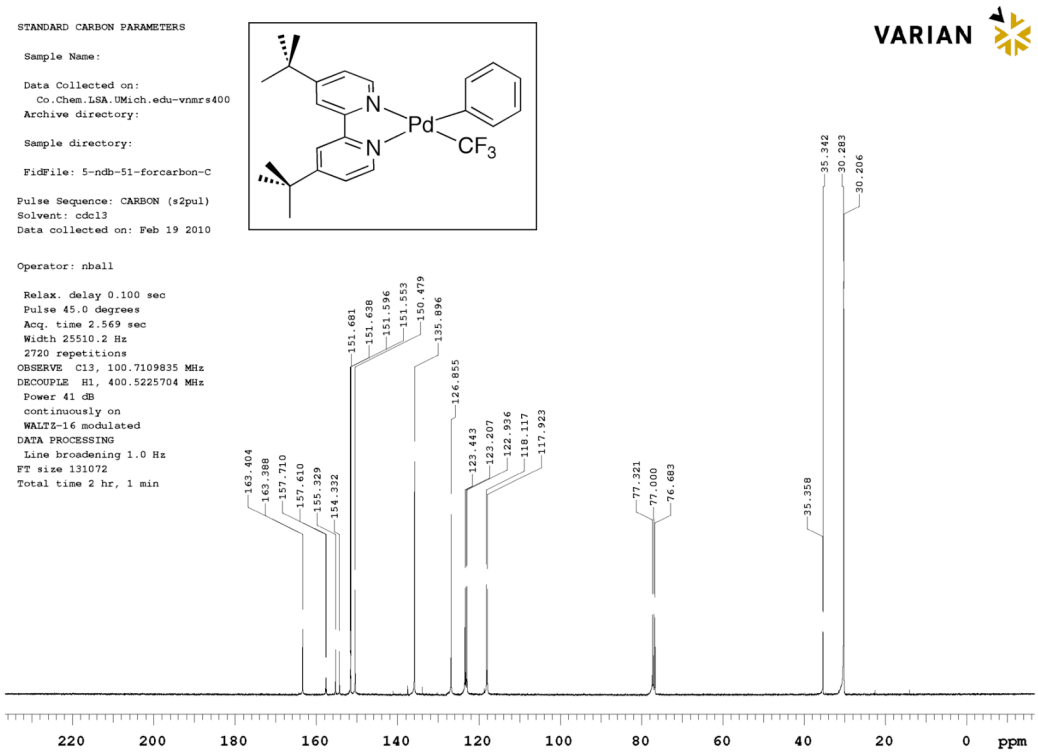
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2010

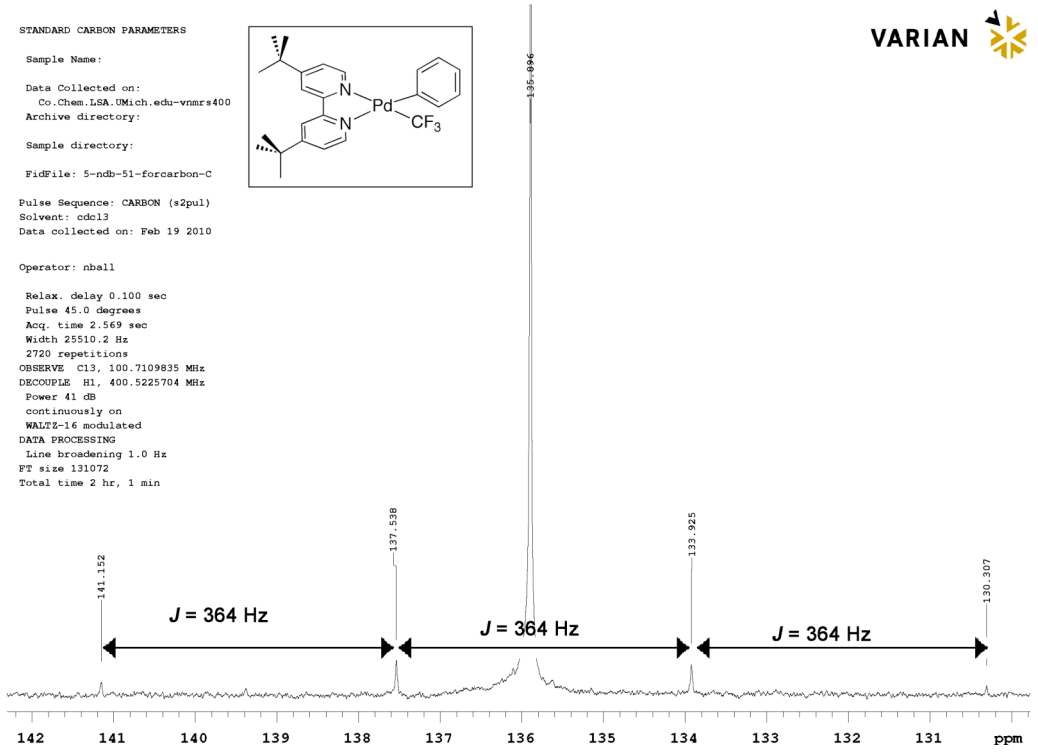
Operator: nball

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8658920 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 31 sec



VARIAN


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-51-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2720 repetitions
OBSERVE C13, 100.7109835 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 1 min
VARIAN
N
Pd
N
CF3
163.404
163.388
157.710
157.610
155.329
154.332
151.681
151.638
151.596
151.553
150.479
135.896
126.855
123.443
123.207
122.936
118.117
117.923
77.321
77.000
76.683
35.358
35.342
30.283
30.206
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-51-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
2720 repetitions
OBSERVE C13, 100.7109835 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 1 min
VARIAN
N
Pd
N
CF3
135.896
141.152
137.538
133.925
130.307
J = 364 Hz
J = 364 Hz
J = 364 Hz
142
141
140
139
138
137
136
135
134
133
132
131
ppm

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

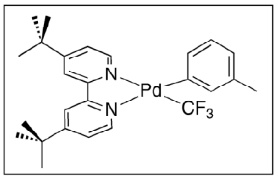
Sample directory:

FidFile: 5-ndb-56forcarbon-H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2010

Operator: nball

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5205979 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

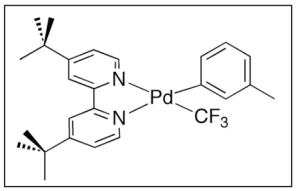
Sample directory:

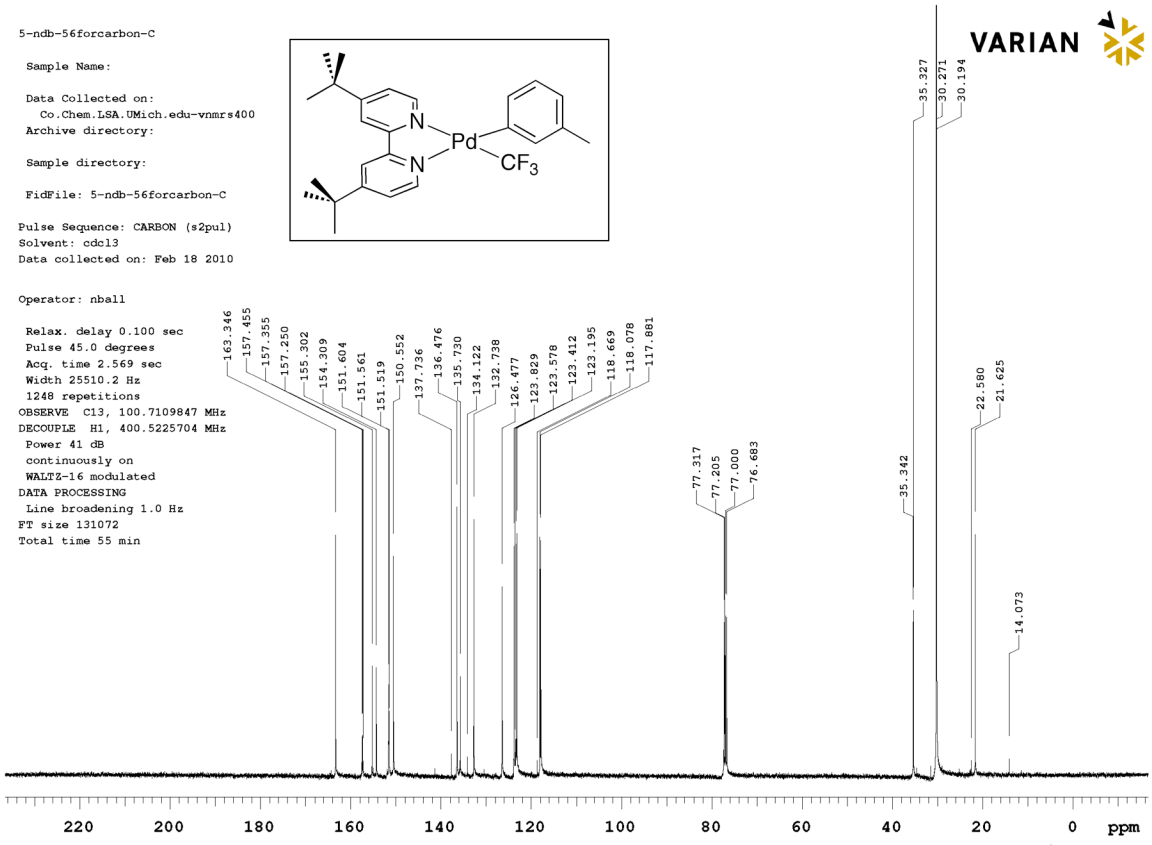
FidFile: 5-ndb-56forcarbon-F

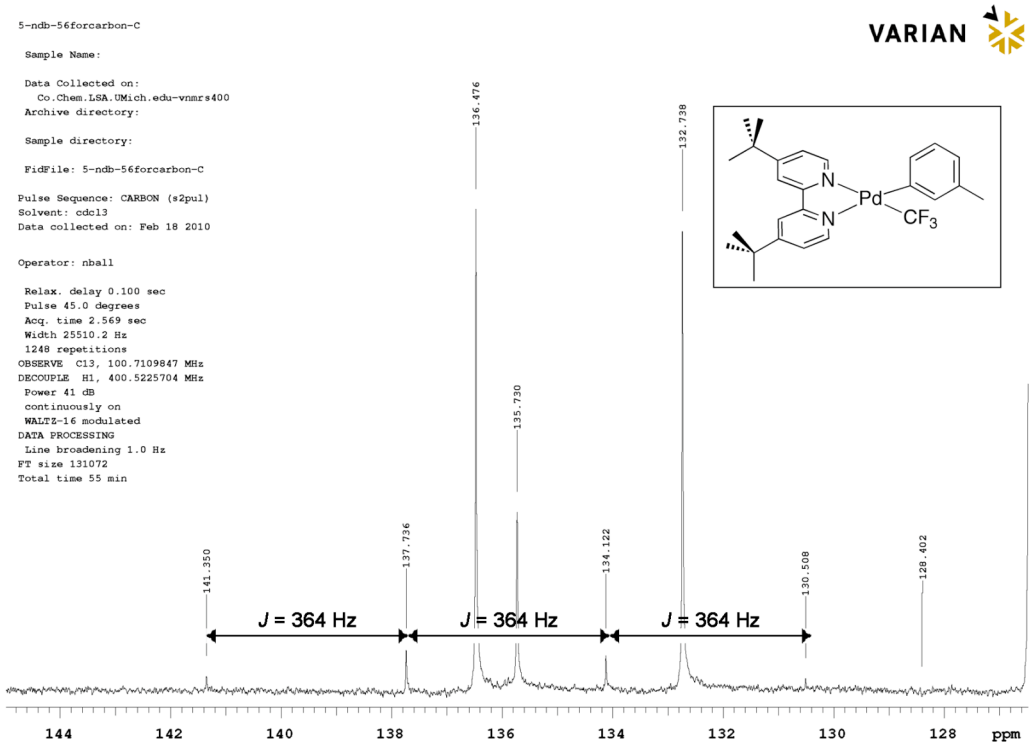
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2010

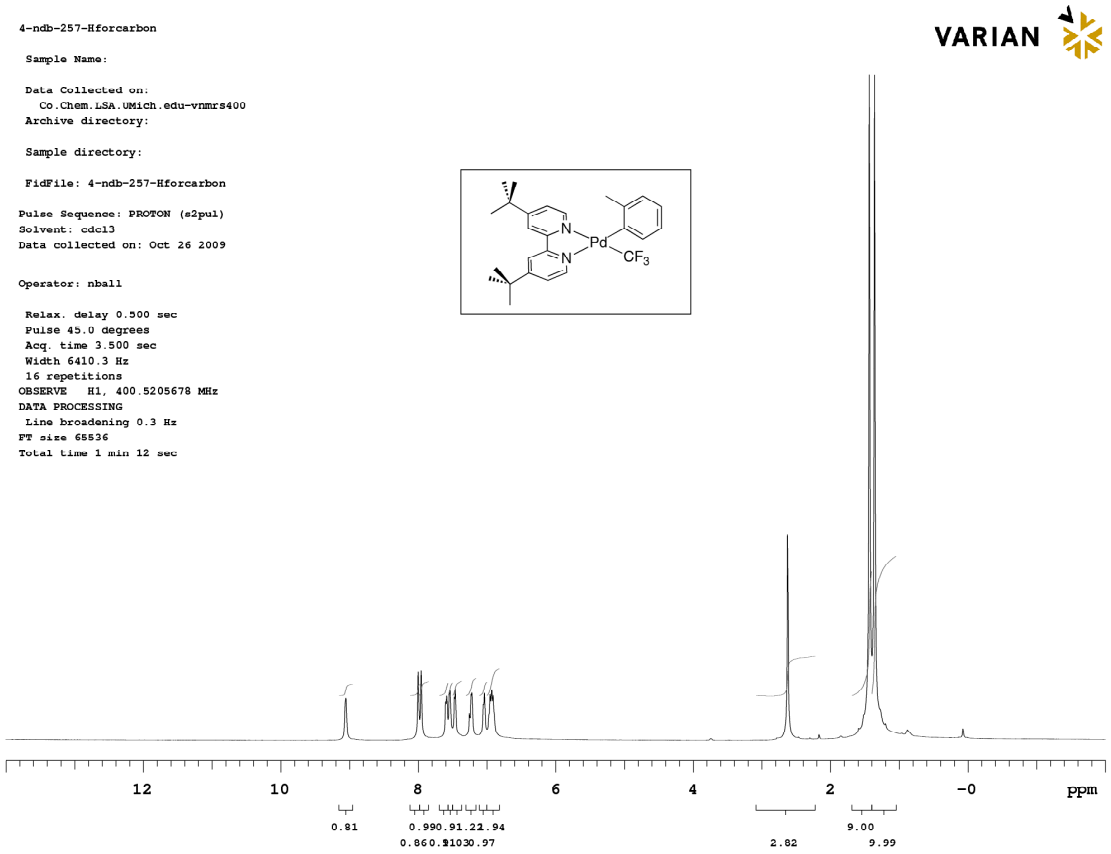
Operator: nball

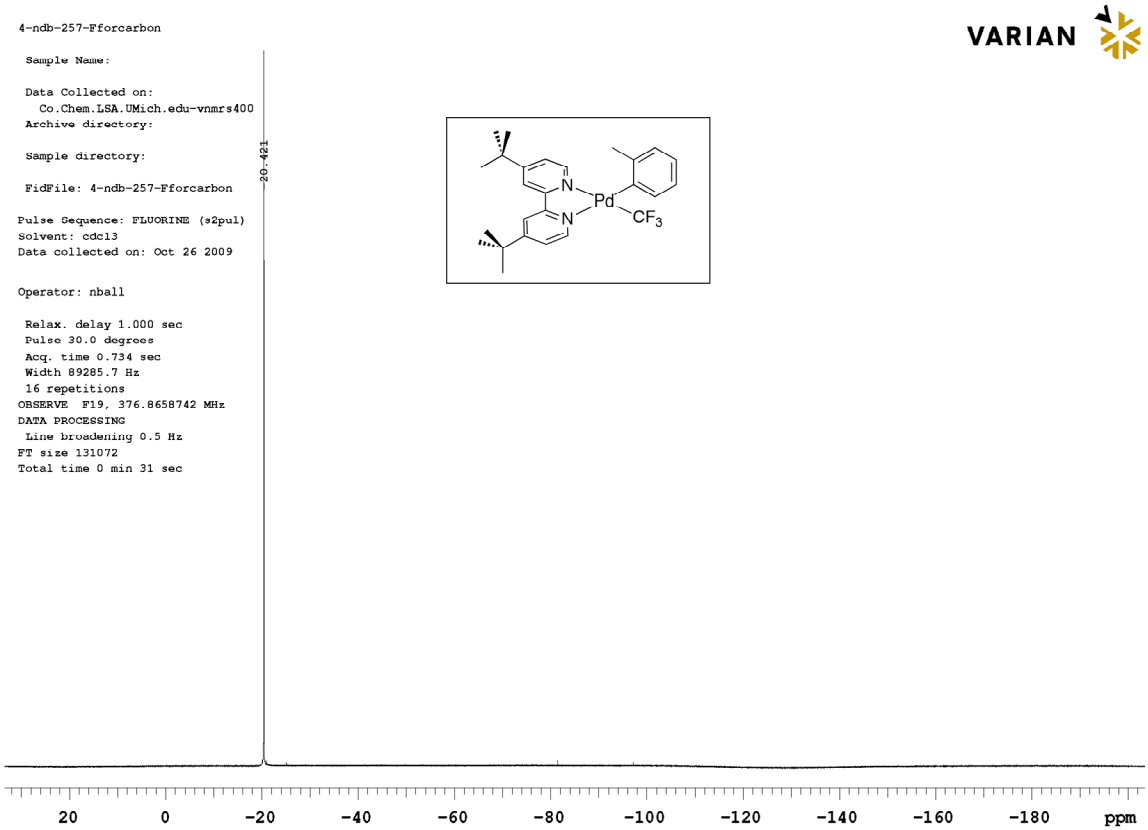
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8658963 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 31 sec

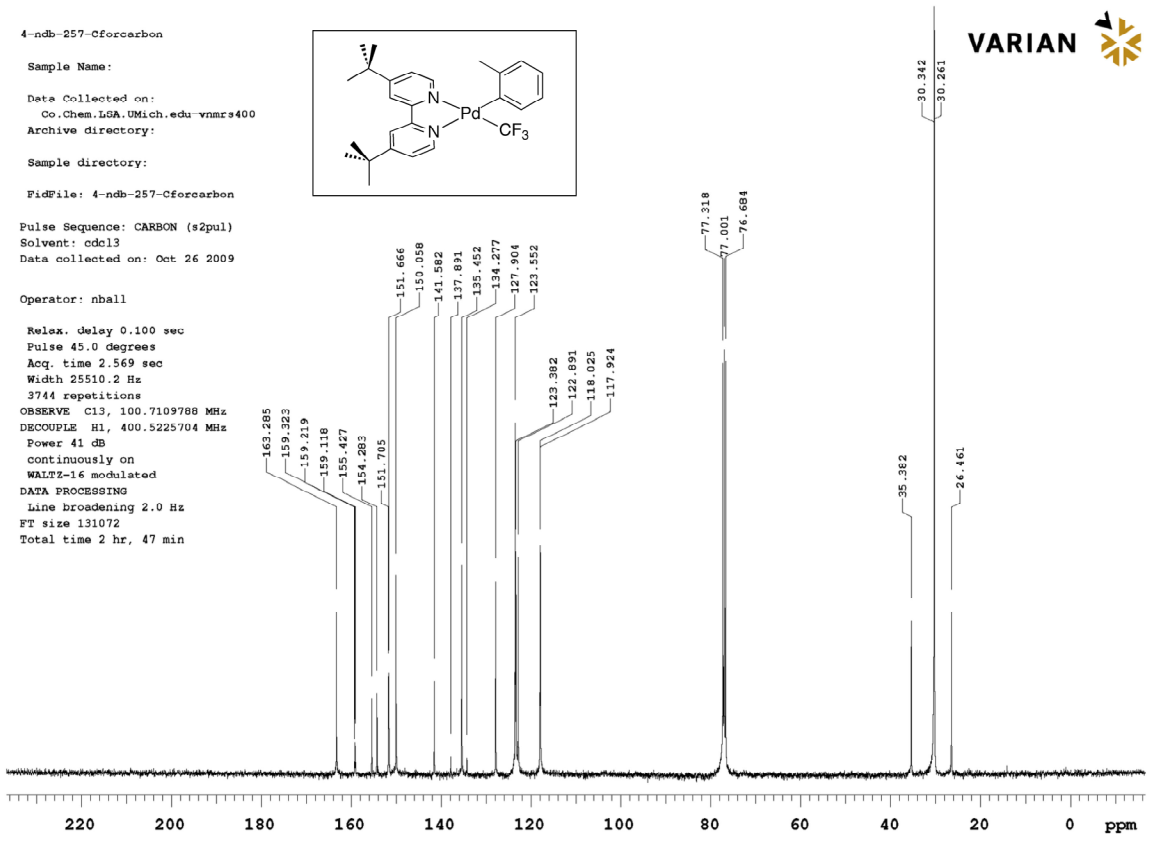


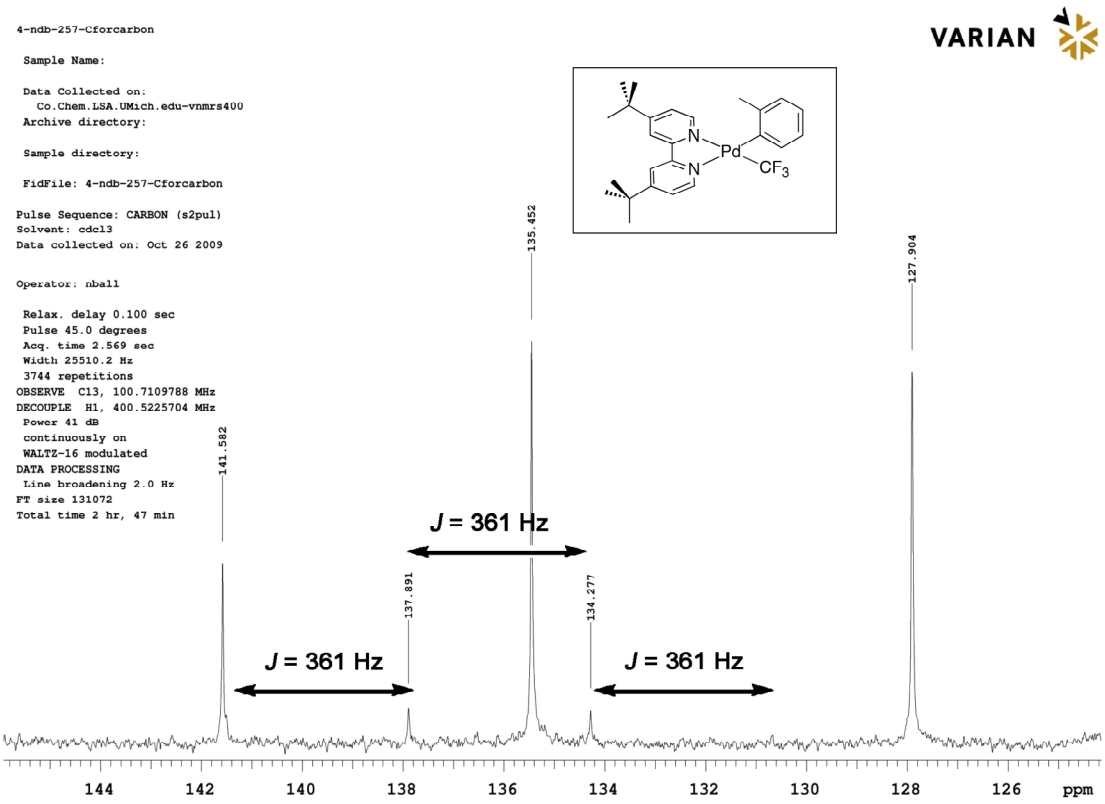

5-ndb-56forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-56forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1248 repetitions
OBSERVE C13, 100.7109847 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 55 min
VARIAN
N
Pd
CF3
163.346
157.455
157.355
157.250
155.302
154.309
151.604
151.561
151.519
150.552
137.736
136.476
135.730
134.122
132.738
126.477
123.829
123.578
123.412
123.195
118.669
118.078
117.881
77.317
77.205
77.000
76.683
35.342
35.327
30.271
30.194
22.580
21.625
14.073
220
200
180
160
140
120
100
80
60
40
20
0
ppm

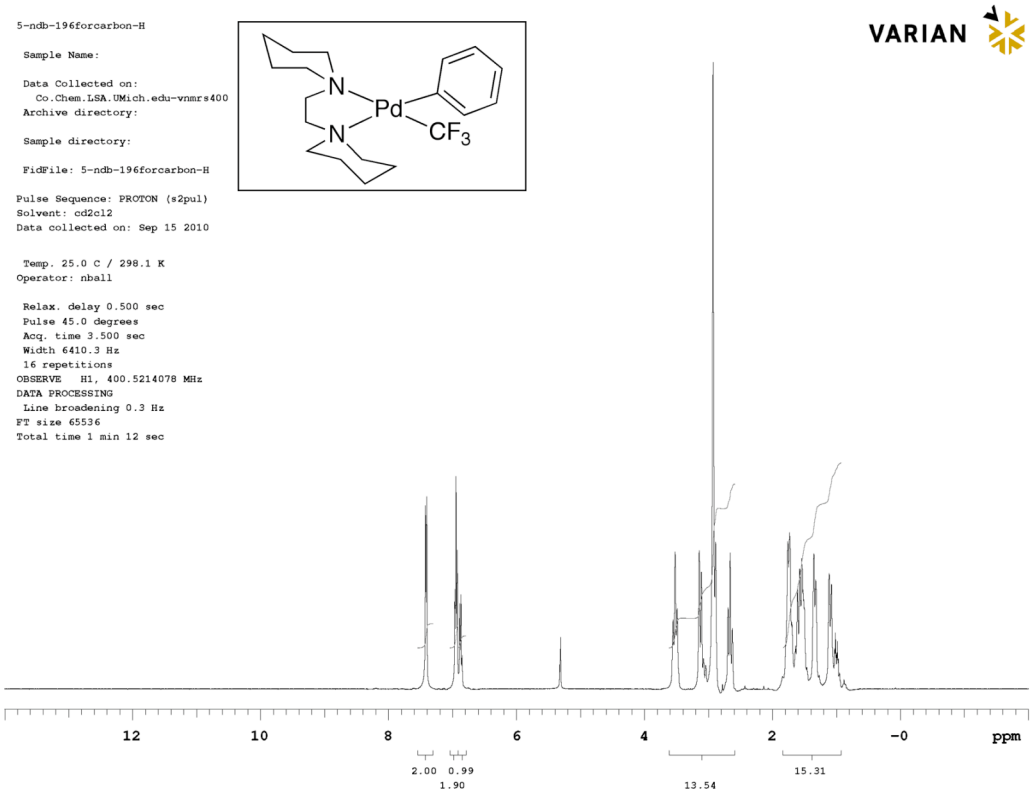

5-ndb-56forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-56forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1248 repetitions
OBSERVE C13, 100.7109847 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 55 min
VARIAN
N
Pd
CF3
136.476
132.738
135.730
141.350
137.736
134.122
130.508
128.402
J = 364 Hz
J = 364 Hz
J = 364 Hz
144
142
140
138
136
134
132
130
128
ppm

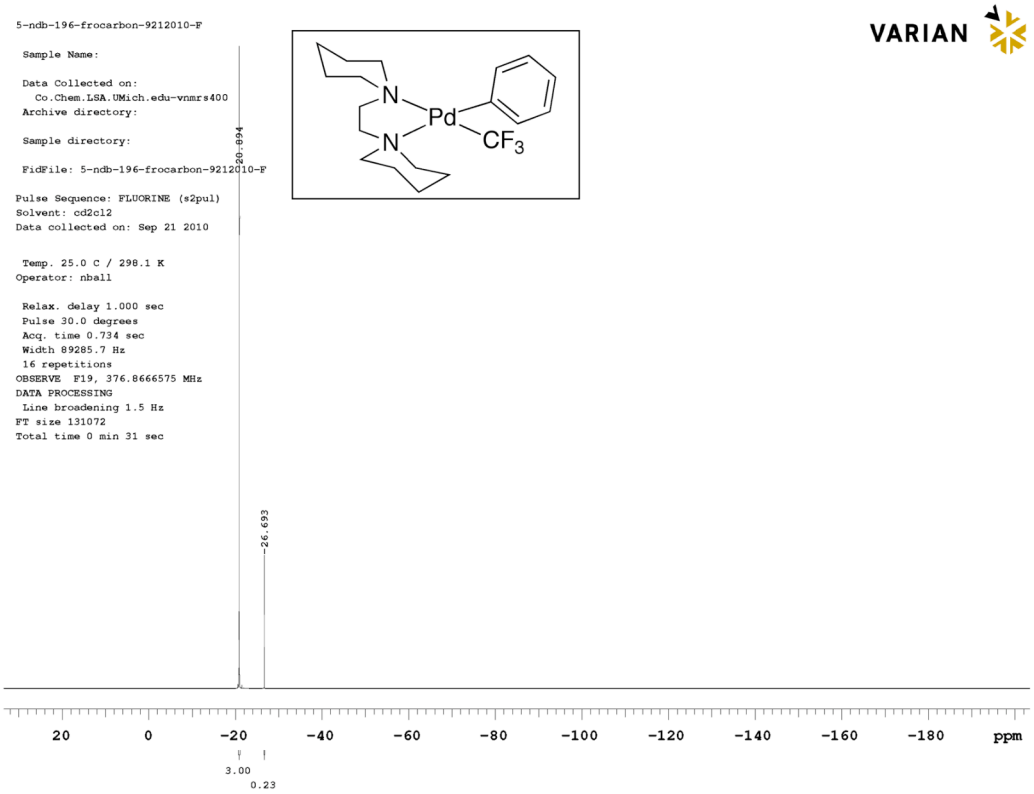

4-ndb-257-Hforcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-257-Hforcarbon
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2009
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5205678 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
N
Pd
N
CF3
12
10
8
6
4
2
-0
ppm
0.81
0.99
0.91
2.94
0.86
1.03
0.97
2.82
9.00
9.99

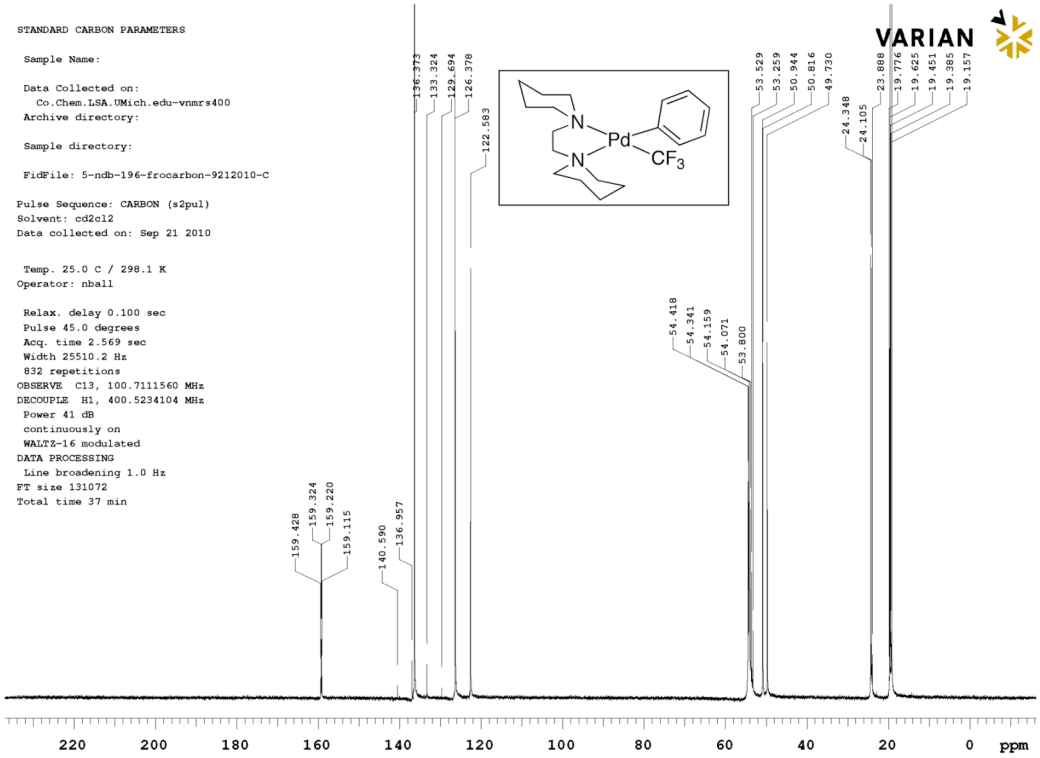

4-ndb-257-Fforcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-257-Fforcarbon
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2009
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8658742 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 31 sec
-20.421
VARIAN
N
Pd
N
CF3
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

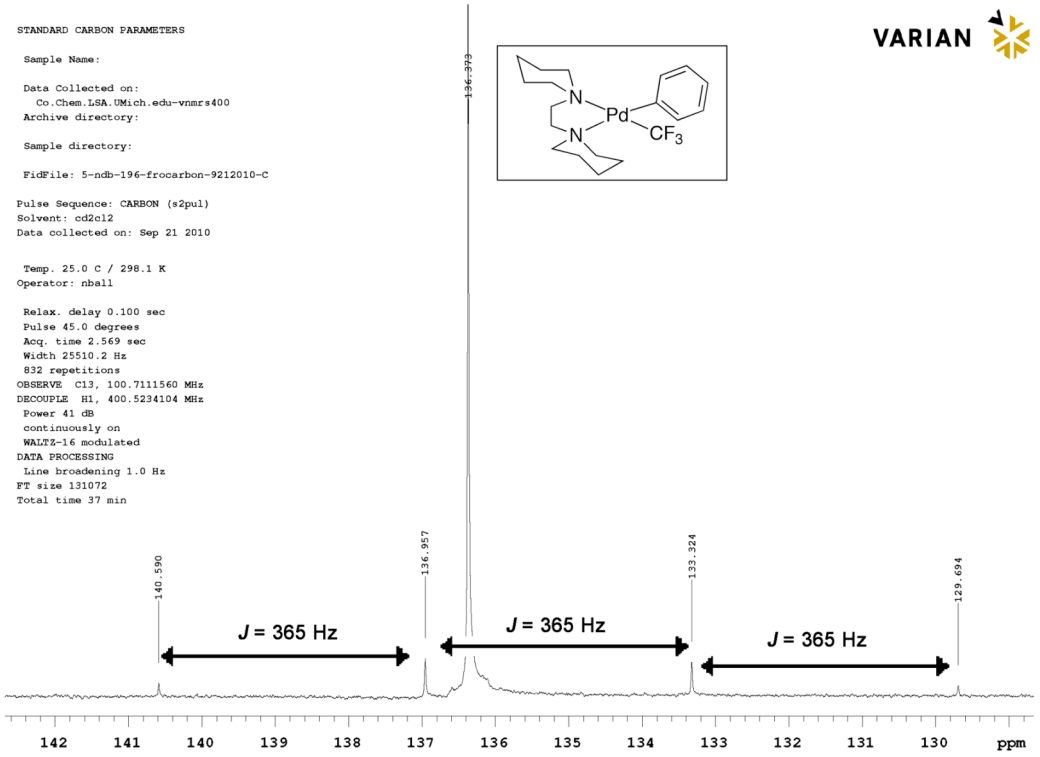

4-ndb-257-Cforcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-257-Cforcarbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2009
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3744 repetitions
OBSERVE C13, 100.7109788 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 47 min
VARIAN
Pd
CF3
163.285
159.323
159.219
159.118
155.427
154.283
151.705
151.666
150.058
141.582
137.891
135.452
134.277
127.904
123.552
123.382
122.891
118.025
117.924
77.318
77.001
76.684
35.362
30.342
30.261
26.461
220
200
180
160
140
120
100
80
60
40
20
0
ppm

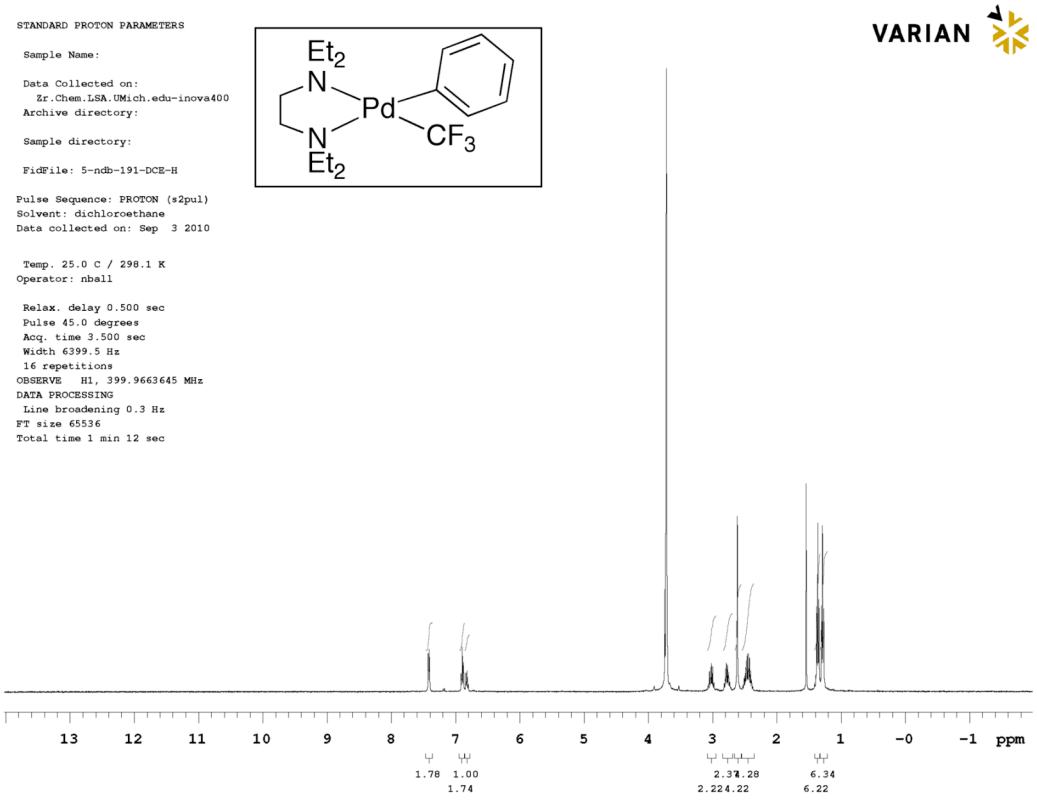

4-ndb-257-Cforcarbon
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 4-ndb-257-Cforcarbon
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2009
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3744 repetitions
OBSERVE C13, 100.7109788 MHz
DECOUPLE H1, 400.5225704 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 47 min
VARIAN
Pd
CF3
141.582
137.891
135.452
134.277
127.904
J = 361 Hz
J = 361 Hz
J = 361 Hz
144
142
140
138
136
134
132
130
128
126
ppm

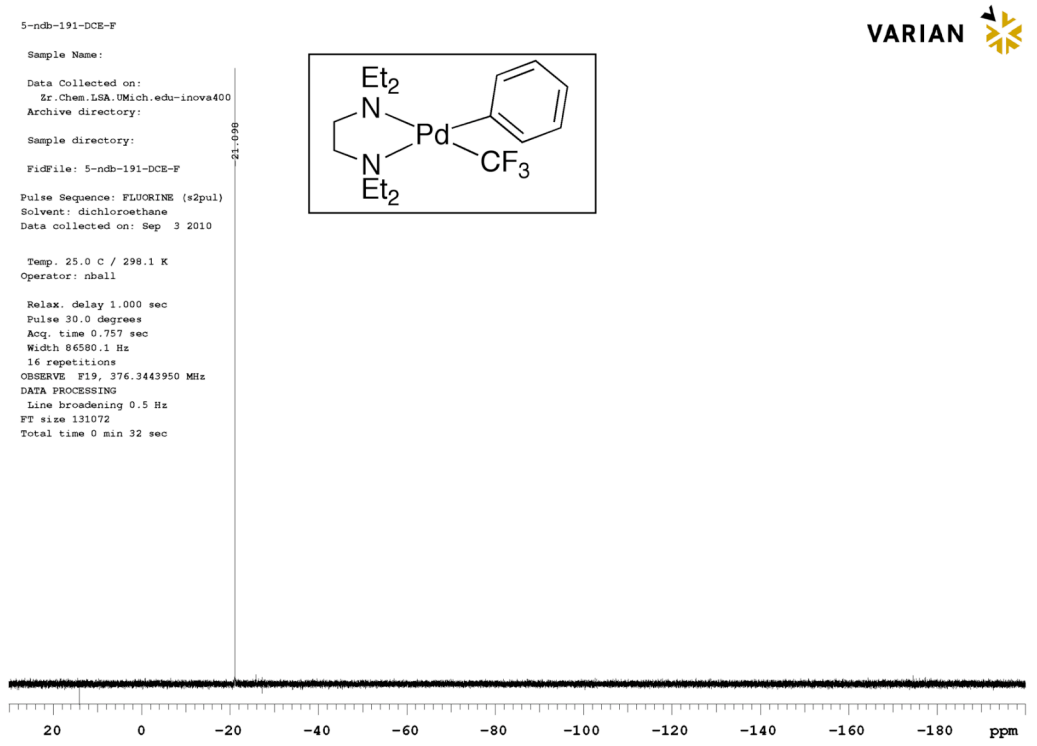

5-ndb-196forcarbon-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-196forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 15 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5214078 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
N
Pd
N
CF3
VARIAN
12
10
8
6
4
2
-0
ppm
2.00
0.99
1.90
13.54
15.31

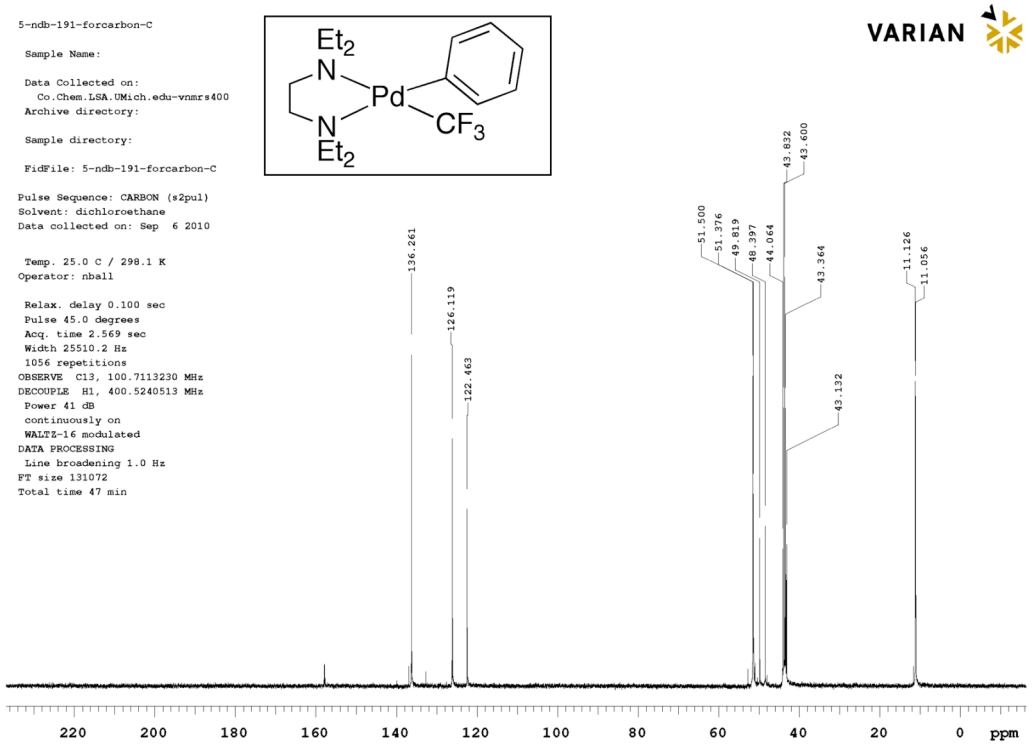

5-ndb-196-frocarbon-9212010-F
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-196-frocarbon-9212010-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cd2cl2
Data collected on: Sep 21 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8666575 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 31 sec
-20.894
-26.693
N
Pd
N
CF3
VARIAN
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
3.00
0.23

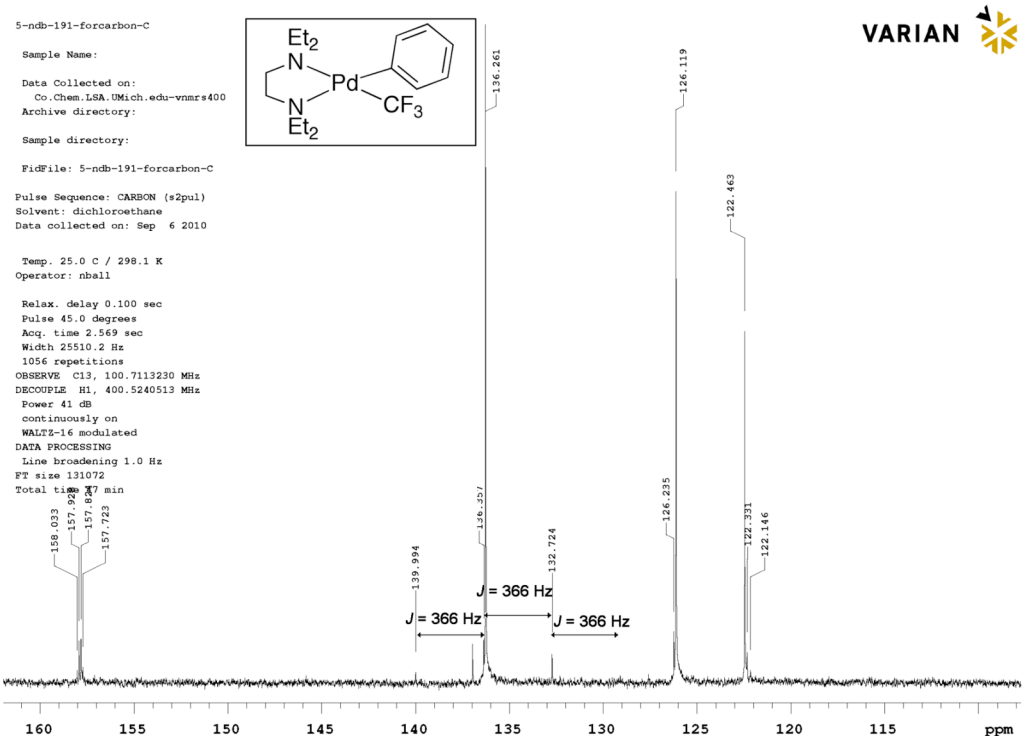

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-196-frocarbon-9212010-C
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 21 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
832 repetitions
OBSERVE C13, 100.7111560 MHz
DECOUPLE H1, 400.5234104 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 37 min
VARIAN
136.373
133.324
129.694
126.378
122.583
53.529
53.259
50.944
50.816
49.730
24.348
24.105
23.888
19.776
19.625
19.451
19.385
19.157
54.418
54.341
54.159
54.071
53.800
159.428
159.324
159.220
159.115
140.590
136.957
N
Pd
CF3
220
200
180
160
140
120
100
80
60
40
20
0
ppm

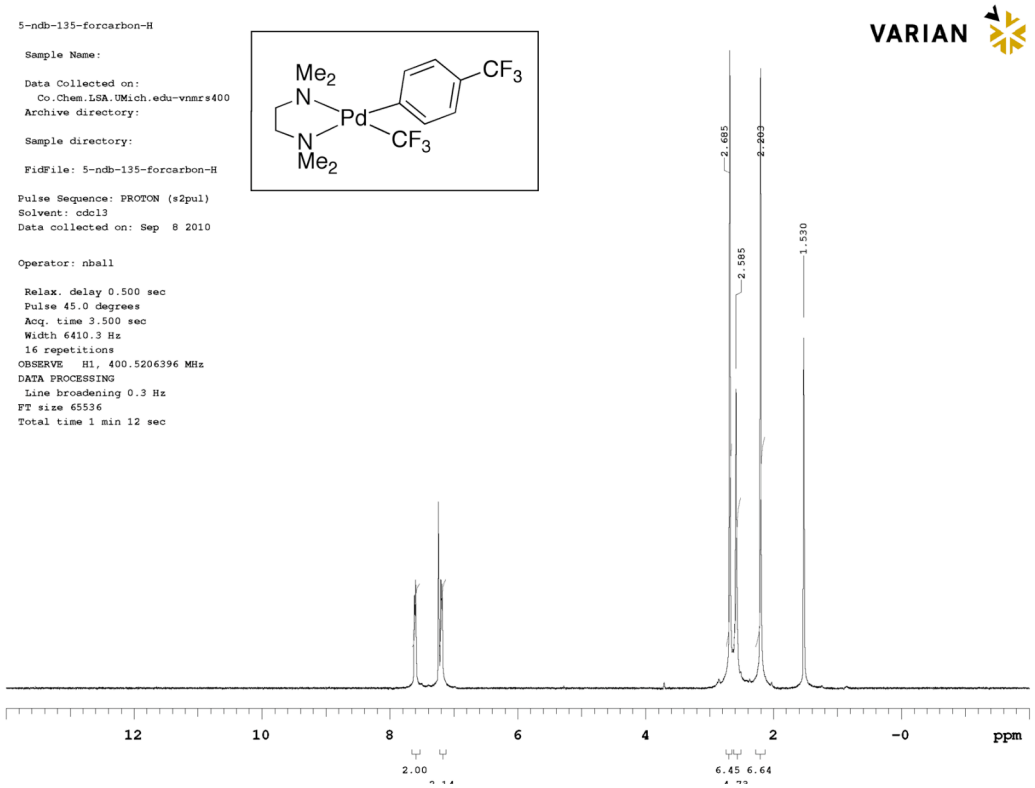

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-196-frocarbon-9212010-C
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 21 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
832 repetitions
OBSERVE C13, 100.7111560 MHz
DECOUPLE H1, 400.5234104 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 37 min
VARIAN
136.373
140.590
136.957
133.324
129.694
J = 365 Hz
J = 365 Hz
J = 365 Hz
N
Pd
CF3
142
141
140
139
138
137
136
135
134
133
132
131
130
ppm

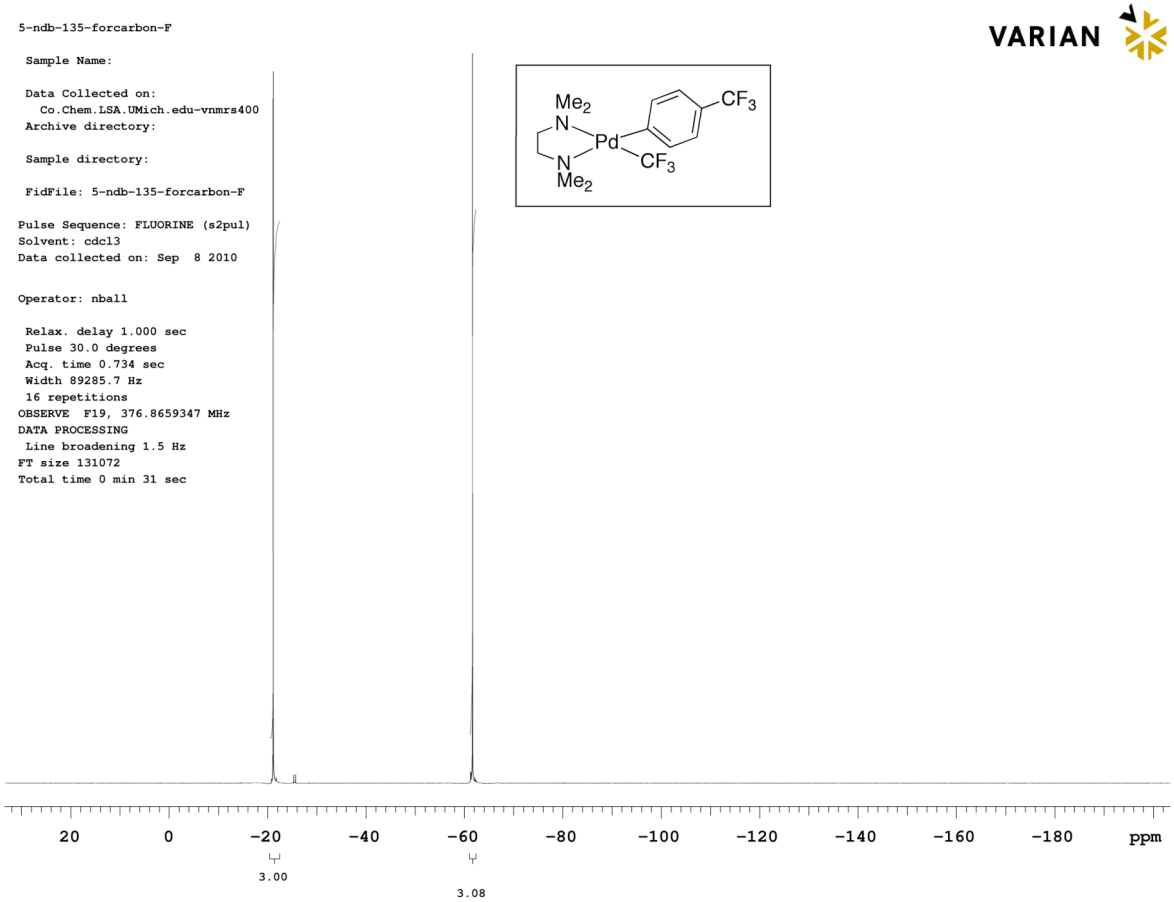

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-191-DCE-H
Pulse Sequence: PROTON (s2pul)
Solvent: dichloroethane
Data collected on: Sep 3 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9663645 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Et2
N
Pd
CF3
N
Et2
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
1.78 1.00
1.74
2.37 1.28
2.22 4.22
6.34
6.22

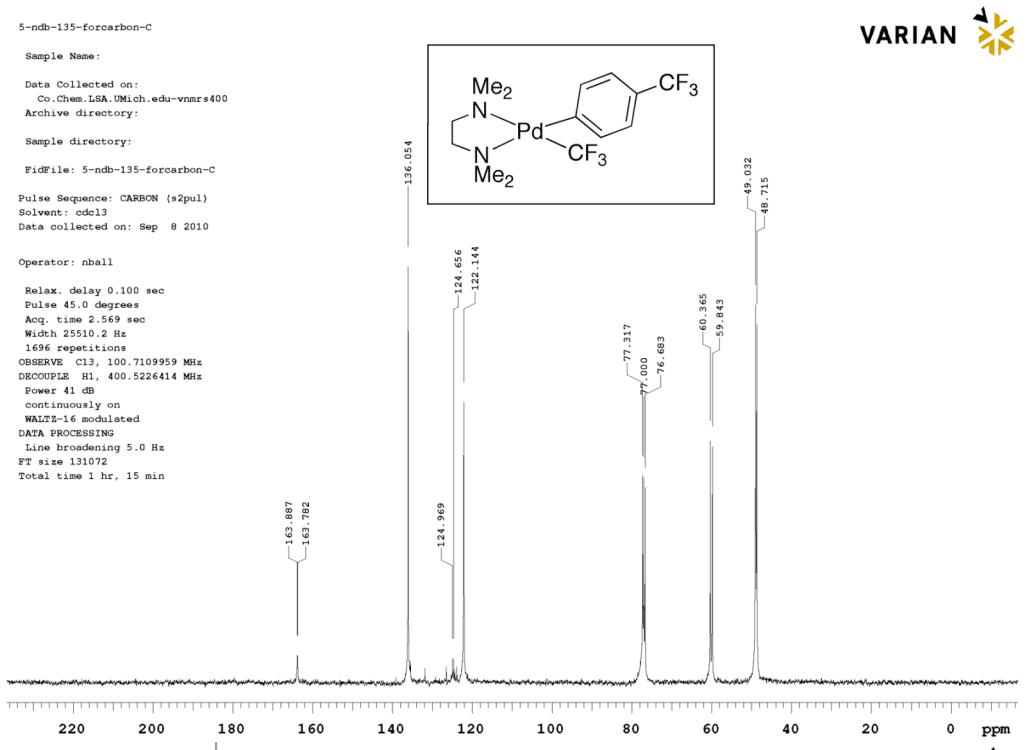

5-ndb-191-DCE-F
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-191-DCE-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: dichloroethane
Data collected on: Sep 3 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
16 repetitions
OBSERVE F19, 376.3443950 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 32 sec
21.096
VARIAN
Et2
N
Pd
CF3
N
Et2
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

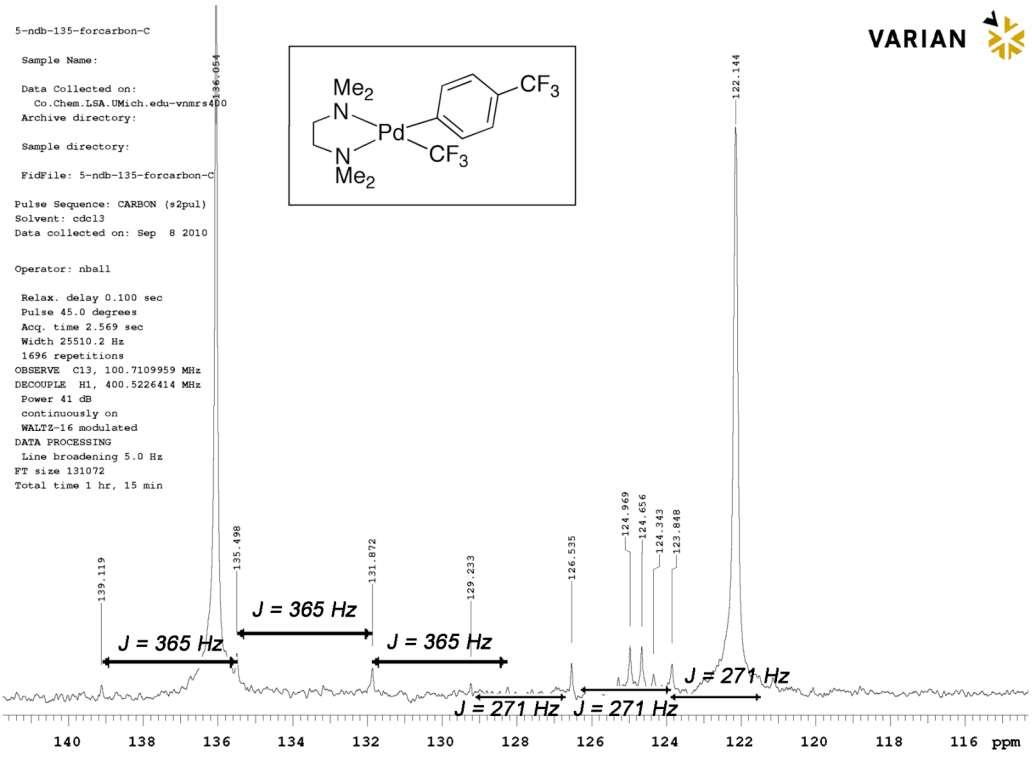

5-ndb-191-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-191-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: dichloroethane
Data collected on: Sep 6 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1056 repetitions
OBSERVE C13, 100.7113230 MHz
DECOUPLE H1, 400.5240513 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 47 min
Et2
N
Pd
CF3
N
Et2
VARIAN
136.261
126.119
122.463
51.500
51.376
49.819
48.397
44.064
43.832
43.600
43.364
43.132
11.126
11.056
220
200
180
160
140
120
100
80
60
40
20
0
ppm

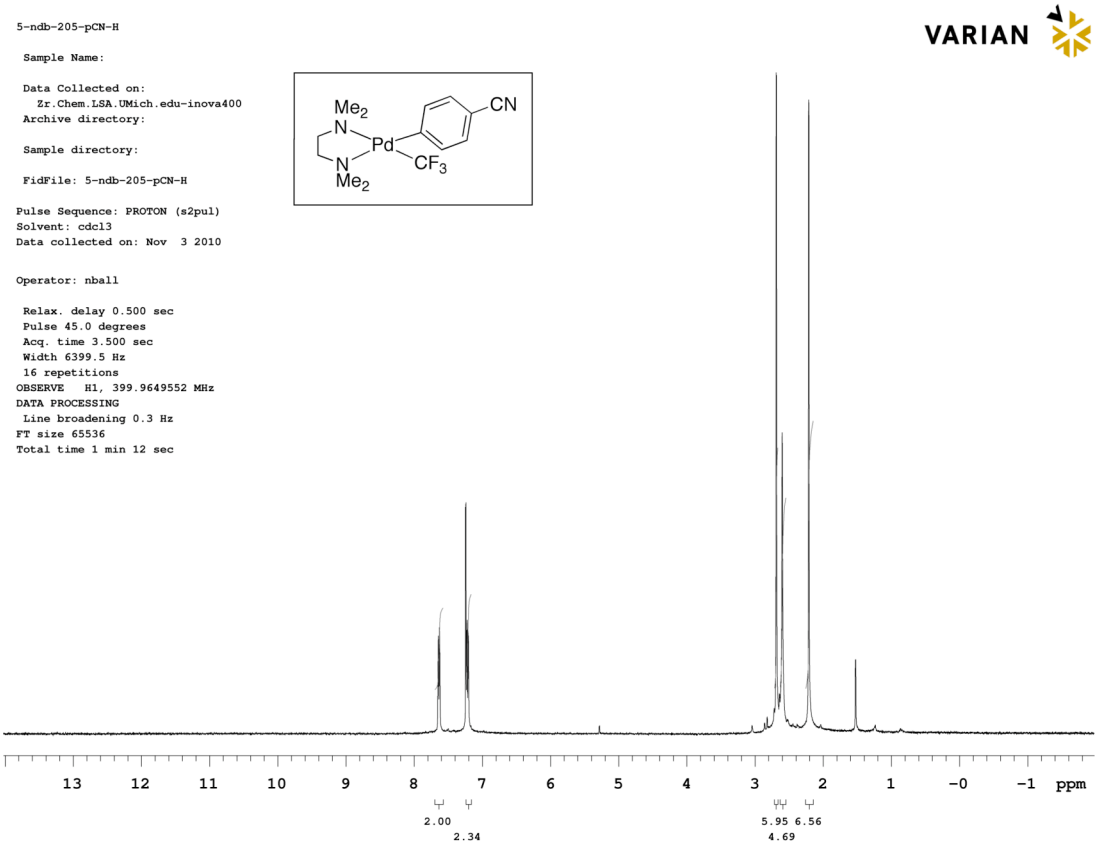

5-ndb-191-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-191-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: dichloroethane
Data collected on: Sep 6 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1056 repetitions
OBSERVE C13, 100.7113230 MHz
DECOUPLE H1, 400.5240513 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Et2
N
Pd
CF3
N
Et2
VARIAN
136.261
126.119
122.463
158.033
157.723
139.994
132.724
126.235
122.331
122.146
J = 366 Hz
J = 366 Hz
J = 366 Hz
160
155
150
145
140
135
130
125
120
115
ppm

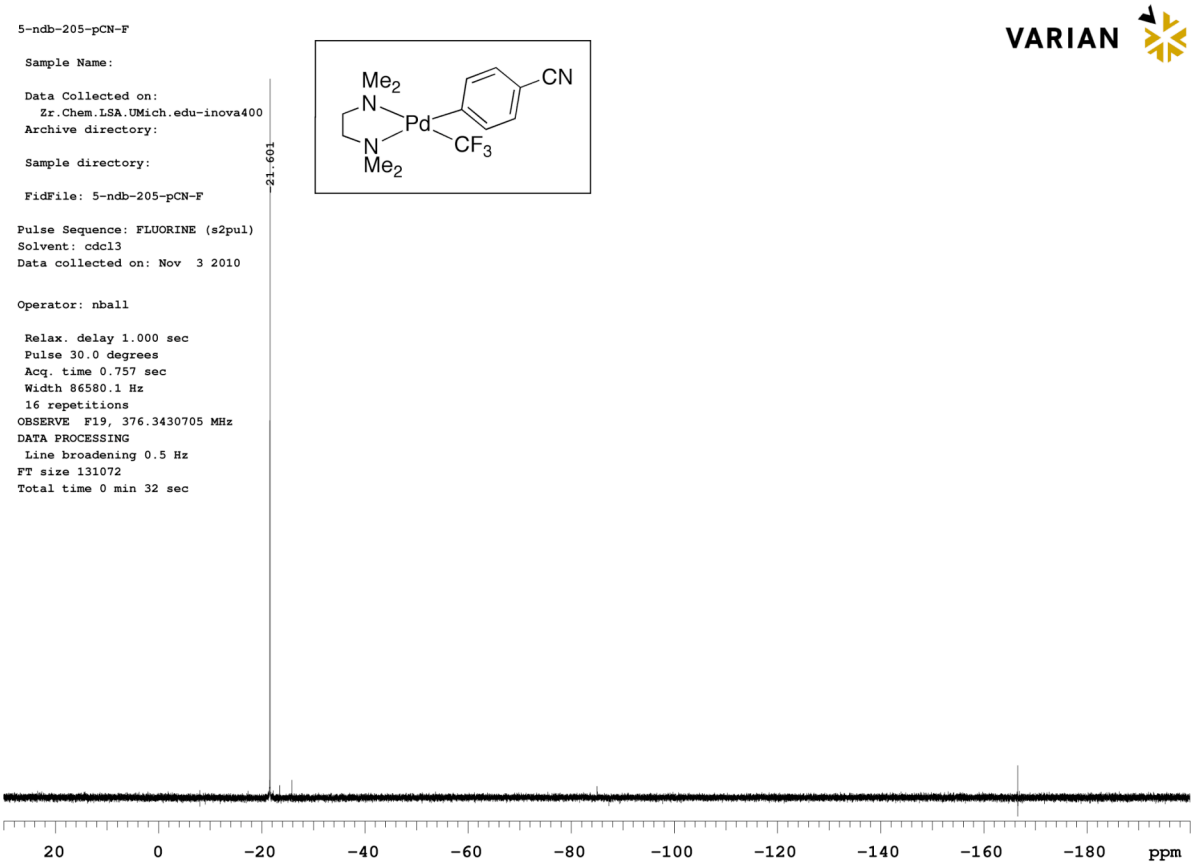

5-ndb-135-forcarbon-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-135-forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206396 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
Me2
N
Pd
CF3
N
Me2
CF3
2.685
2.203
2.585
1.530
12
10
8
6
4
2
−0
ppm
2.00
6.45
6.64

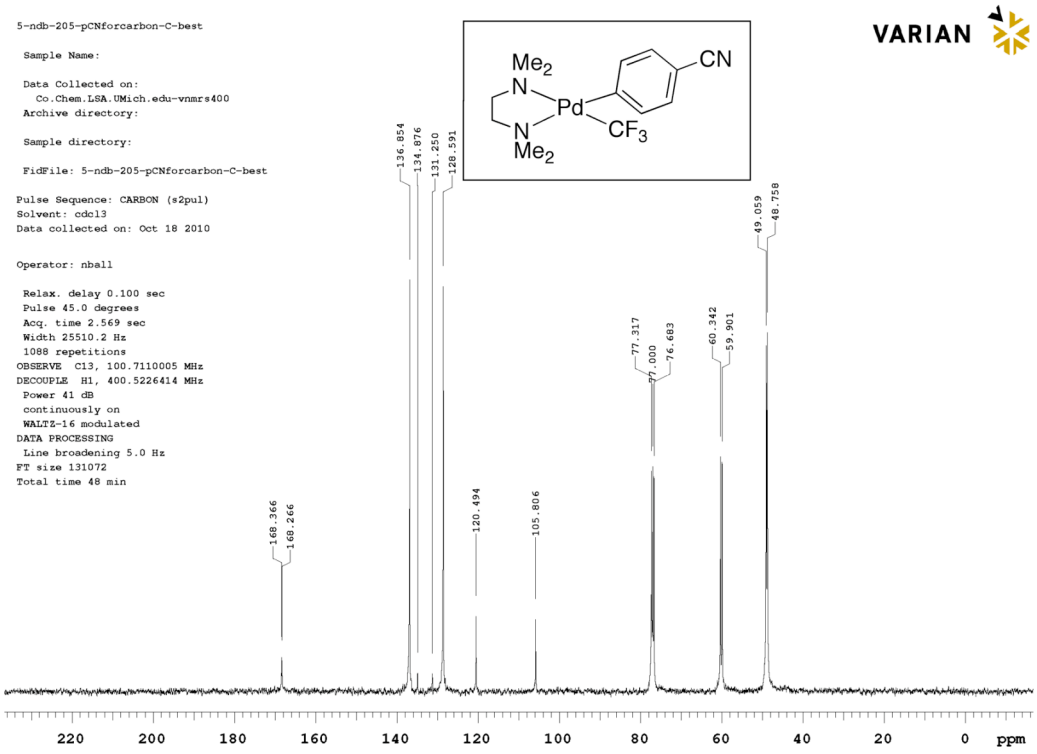

5-ndb-135-forcarbon-F
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-135-forcarbon-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8659347 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 31 sec
Me2
N
Pd
CF3
N
Me2
CF3
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
ppm
3.00
3.08

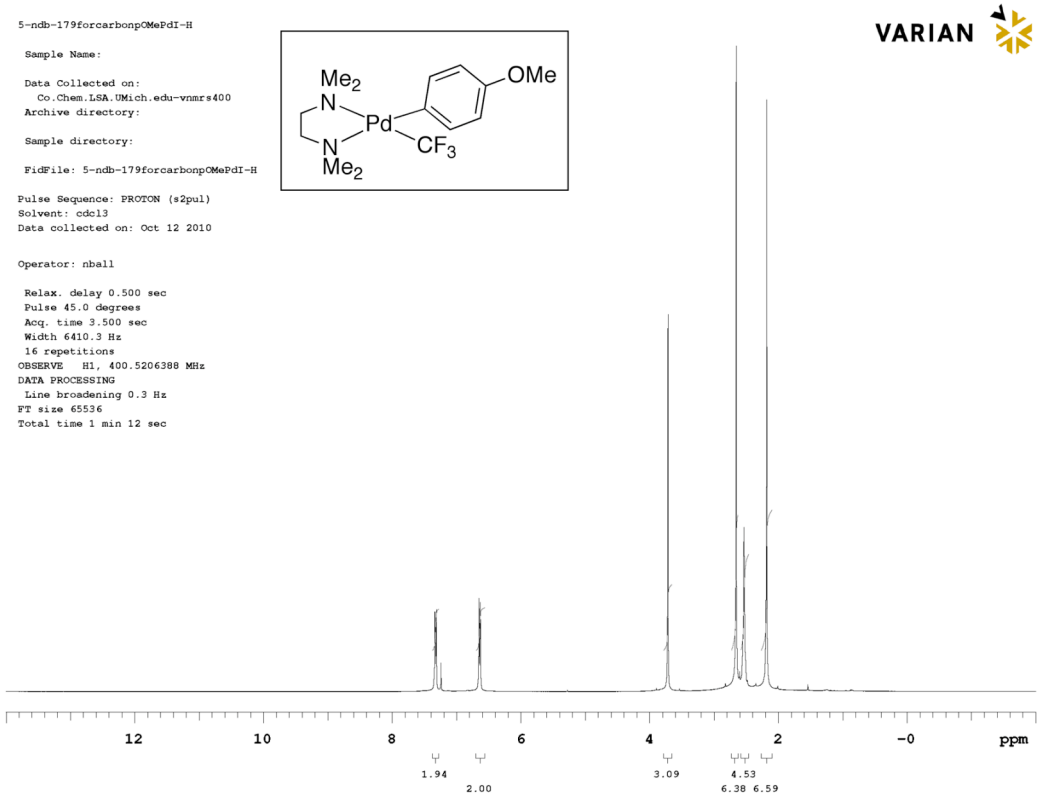

5-ndb-135-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-135-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1696 repetitions
OBSERVE C13, 100.7109959 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 131072
Total time 1 hr, 15 min
VARIAN
Me2
N
Pd
CF3
CF3
N
Me2
136.054
124.656
122.144
49.032
48.715
77.317
77.000
76.683
60.365
59.843
163.887
163.782
124.969
220
200
180
160
140
120
100
80
60
40
20
0
ppm

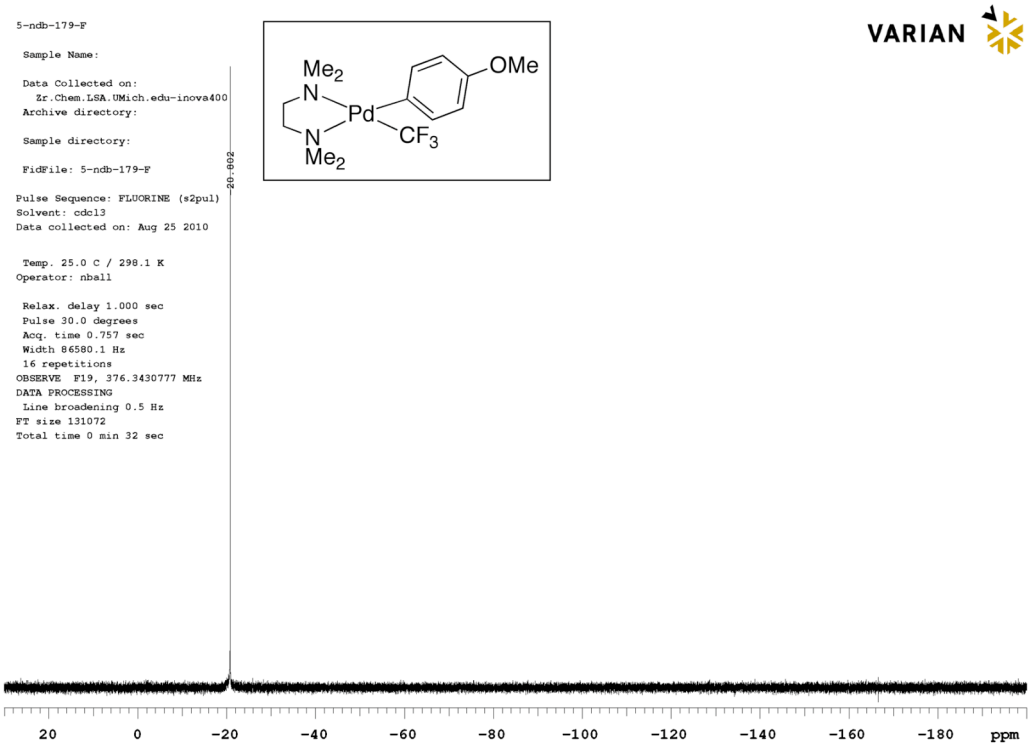

5-ndb-135-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-135-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1696 repetitions
OBSERVE C13, 100.7109959 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 131072
Total time 1 hr, 15 min
VARIAN
Me2
N
Pd
CF3
CF3
N
Me2
136.054
122.144
139.119
135.498
131.872
129.233
126.535
124.969
124.656
124.343
123.848
J = 365 Hz
J = 365 Hz
J = 365 Hz
J = 271 Hz
J = 271 Hz
J = 271 Hz
140
138
136
134
132
130
128
126
124
122
120
118
116
ppm

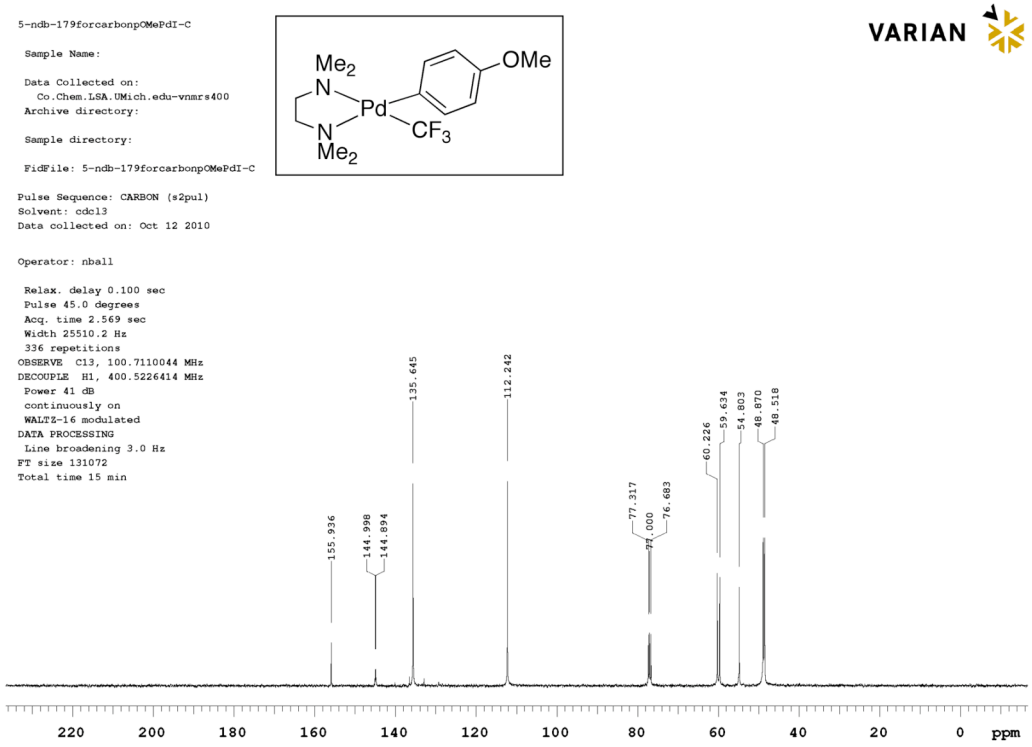

5-ndb-205-pCN-H
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-205-pCN-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9649552 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
Me2
N
Pd
CF3
CN
N
Me2
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
2.00
2.34
5.95
6.56
4.69

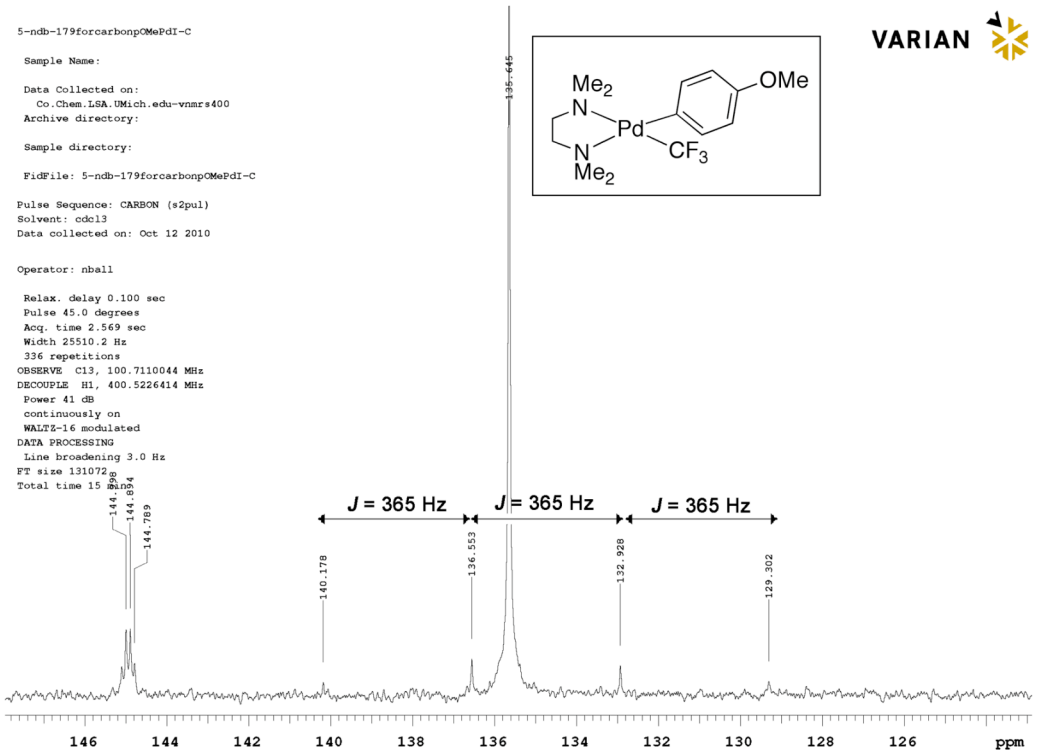

5-ndb-205-pCN-F
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-205-pCN-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2010
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
16 repetitions
OBSERVE F19, 376.3430705 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 32 sec
-21.601
Me2
N
Pd
CF3
CN
N
Me2
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

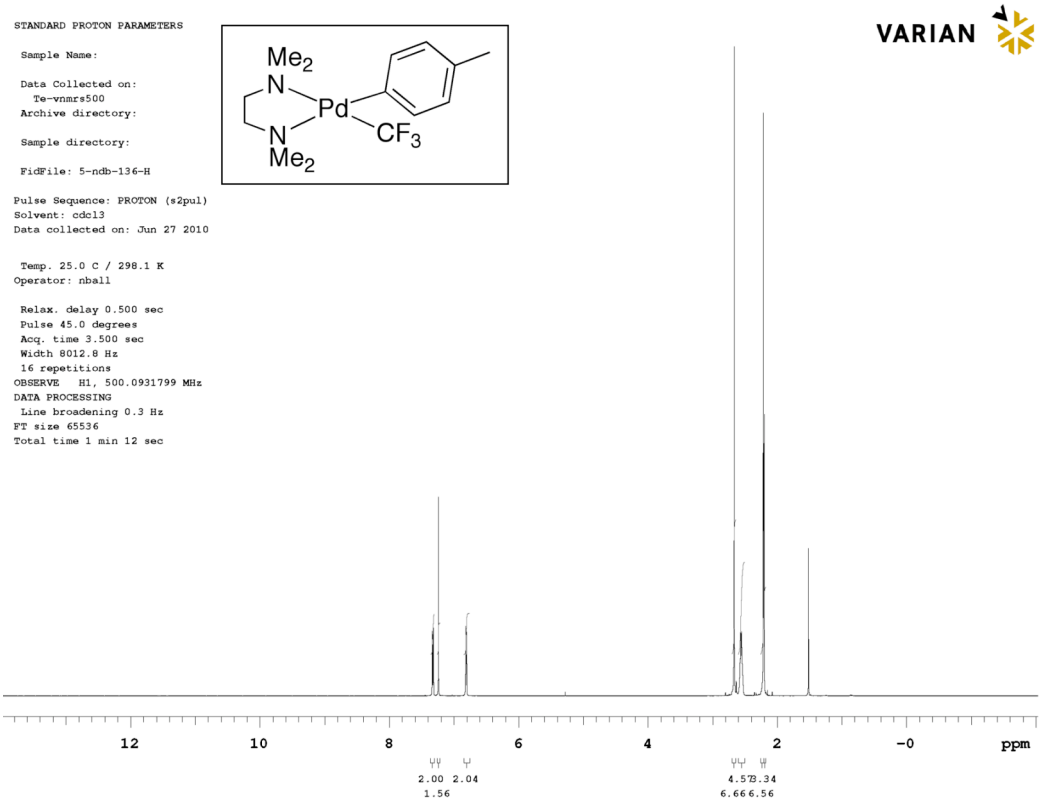

5-ndb-205-pCNforcarbon-C-best
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-205-pCNforcarbon-C-best
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 18 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1088 repetitions
OBSERVE C13, 100.7110005 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 131072
Total time 48 min
Me2
N
Pd
CF3
CN
N
Me2
136.854
134.876
131.250
128.591
120.494
105.806
168.366
168.266
77.317
77.000
76.683
60.342
59.901
49.059
48.758
220
200
180
160
140
120
100
80
60
40
20
0
ppm

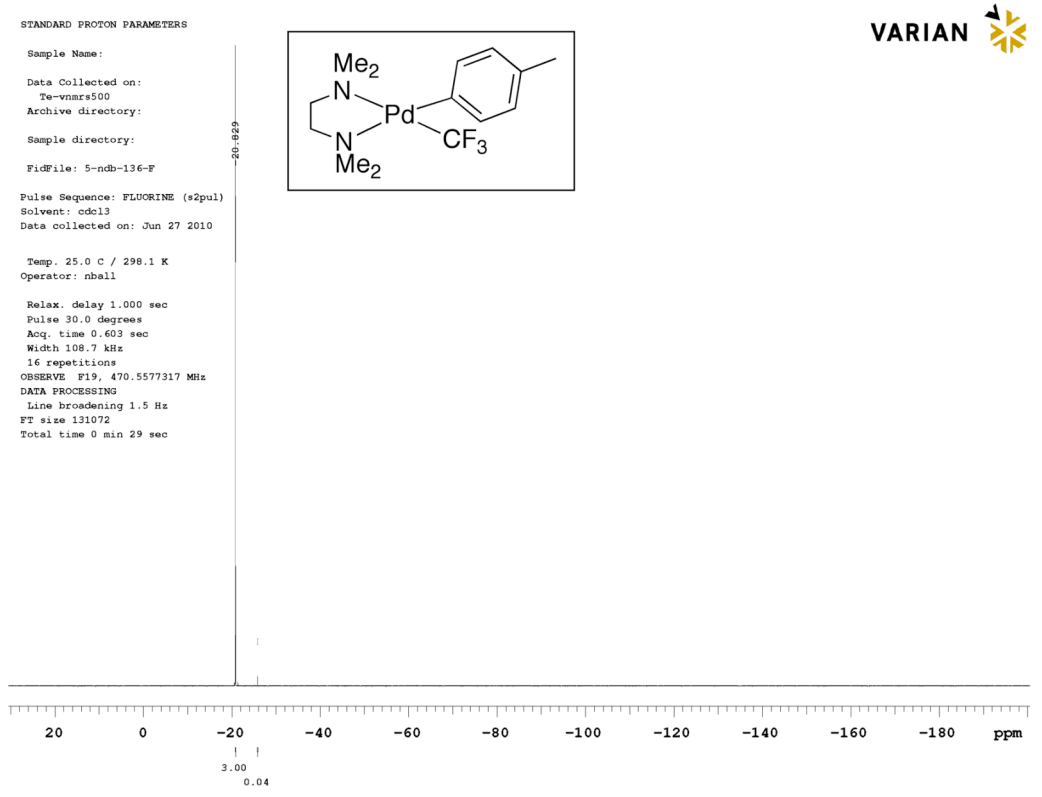

5-ndb-179forcarbonpOMePdI-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-179forcarbonpOMePdI-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206388 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
Me2
N
Pd
CF3
OMe
N
Me2
12
10
8
6
4
2
-0
ppm
1.94
2.00
3.09
4.53
6.38 6.59

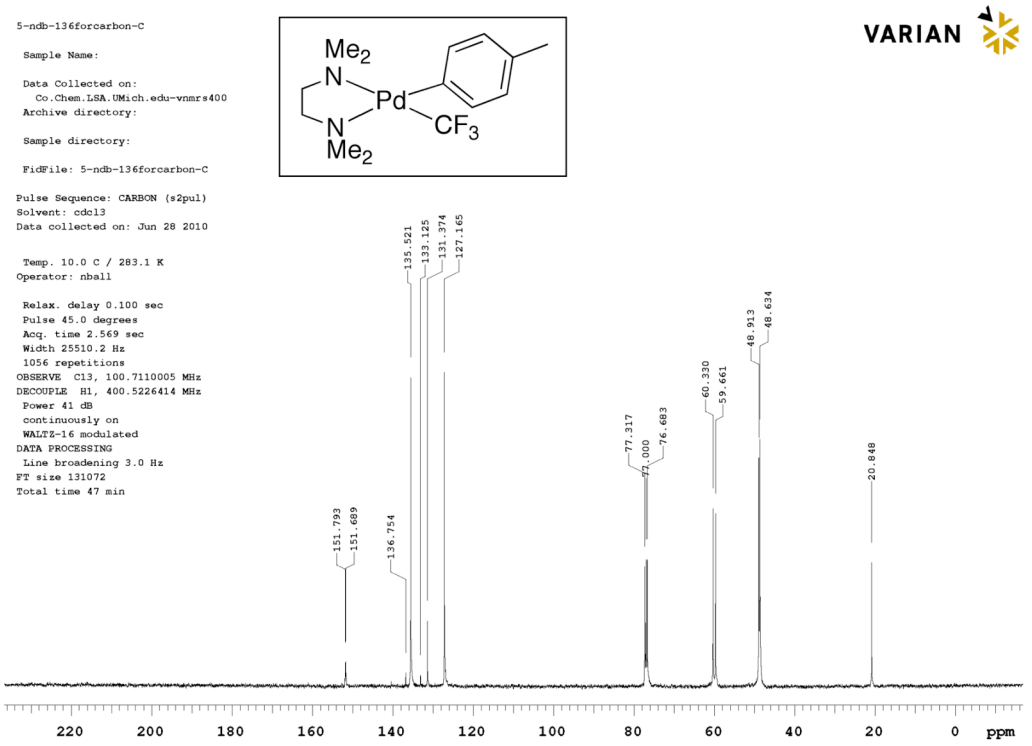

5-ndb-179-F
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-179-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Aug 25 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
16 repetitions
OBSERVE F19, 376.3430777 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 32 sec
-20.902
Me2
N
Pd
OMe
CF3
N
Me2
VARIAN
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

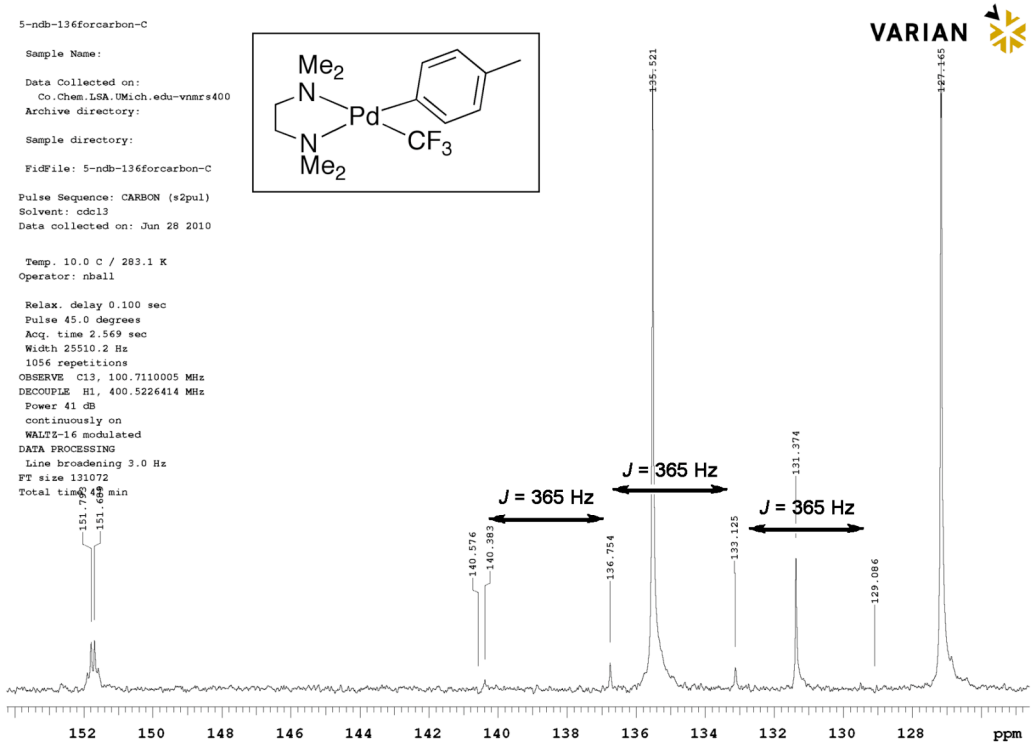

5-ndb-179forcarbonpOMePdI-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-179forcarbonpOMePdI-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
336 repetitions
OBSERVE C13, 100.7110044 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 15 min
155.936
144.998
144.894
135.645
112.242
77.317
77.000
76.683
60.226
59.634
54.803
48.870
48.518
Me2
N
Pd
OMe
CF3
N
Me2
VARIAN
220
200
180
160
140
120
100
80
60
40
20
0
ppm

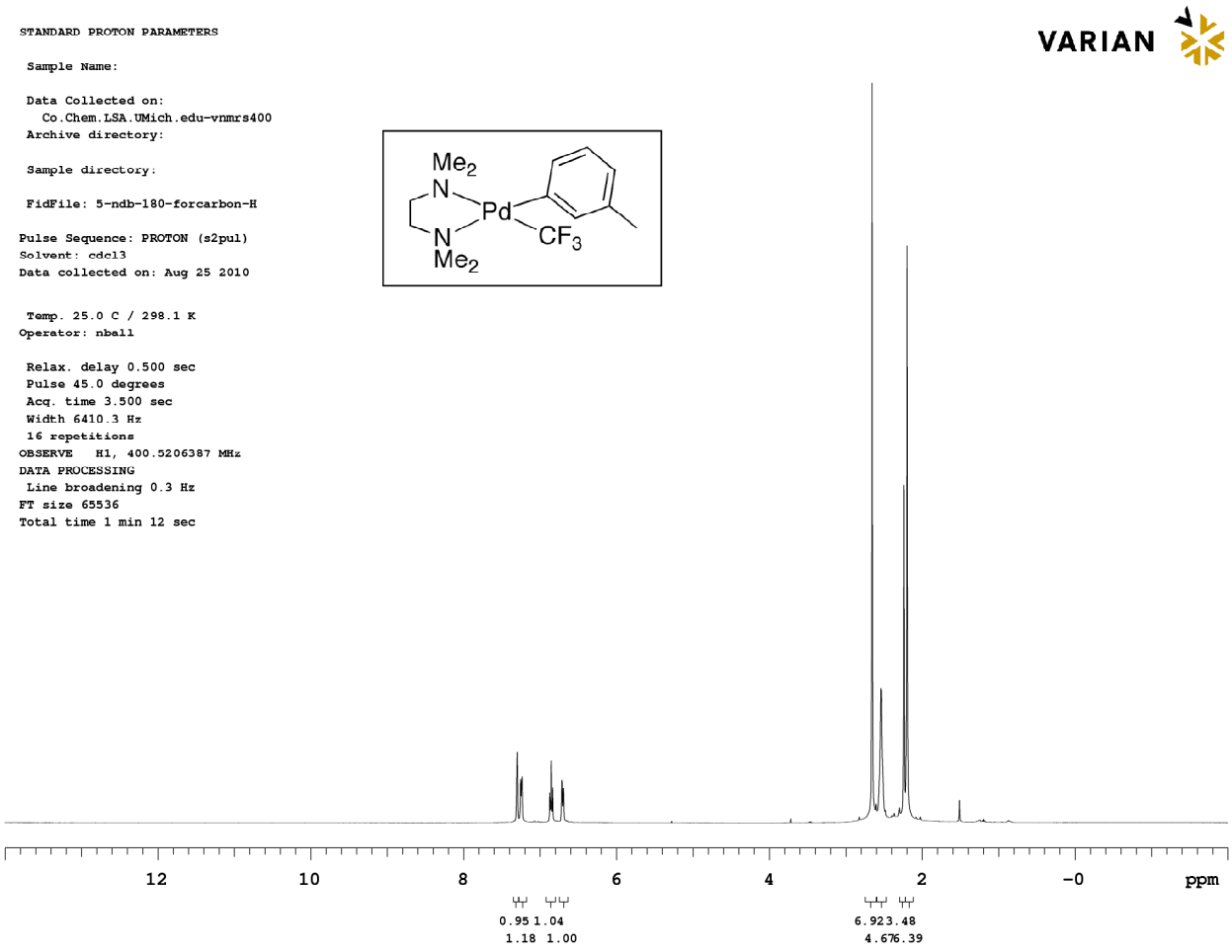

5-ndb-179forcarbonpOMePdI-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-179forcarbonpOMePdI-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 12 2010
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
336 repetitions
OBSERVE C13, 100.7110044 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 15 min
VARIAN
Me2
N
Pd
OMe
CF3
N
Me2
135.645
144.894
144.789
140.178
136.553
132.928
129.302
J = 365 Hz
J = 365 Hz
J = 365 Hz
146
144
142
140
138
136
134
132
130
128
126
ppm

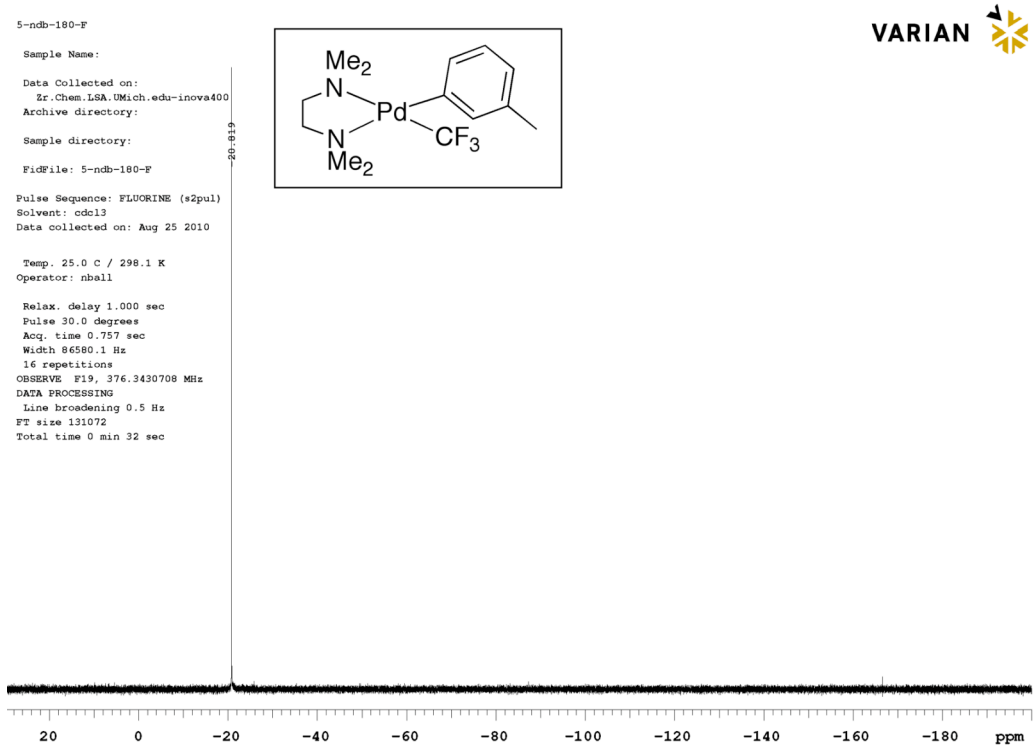

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-136-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 27 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 500.0931799 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
Me2
N
Pd
CF3
N
Me2
VARIAN
12
10
8
6
4
2
-0
ppm
2.00 2.04
1.56
4.57 3.34
6.66 6.56

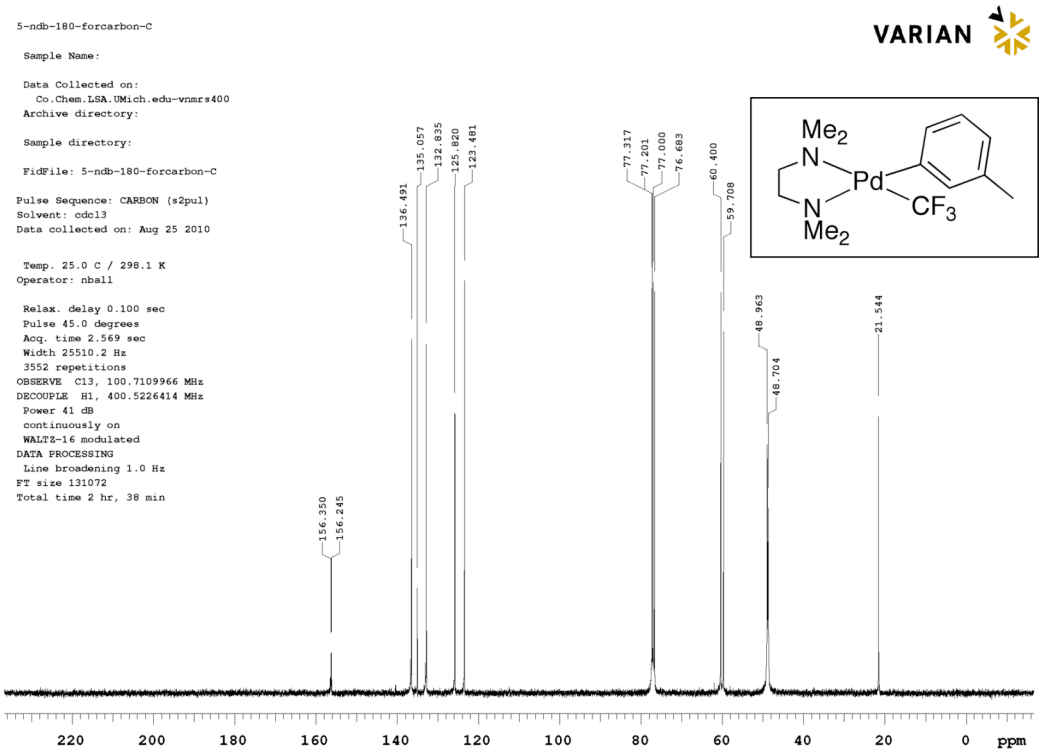

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Te-vnmrs500
Archive directory:
Sample directory:
FidFile: 5-ndb-136-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jun 27 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
16 repetitions
OBSERVE F19, 470.5577317 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 29 sec
-20.029
Me2
N
Pd
CF3
N
Me2
VARIAN
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
3.00
0.04

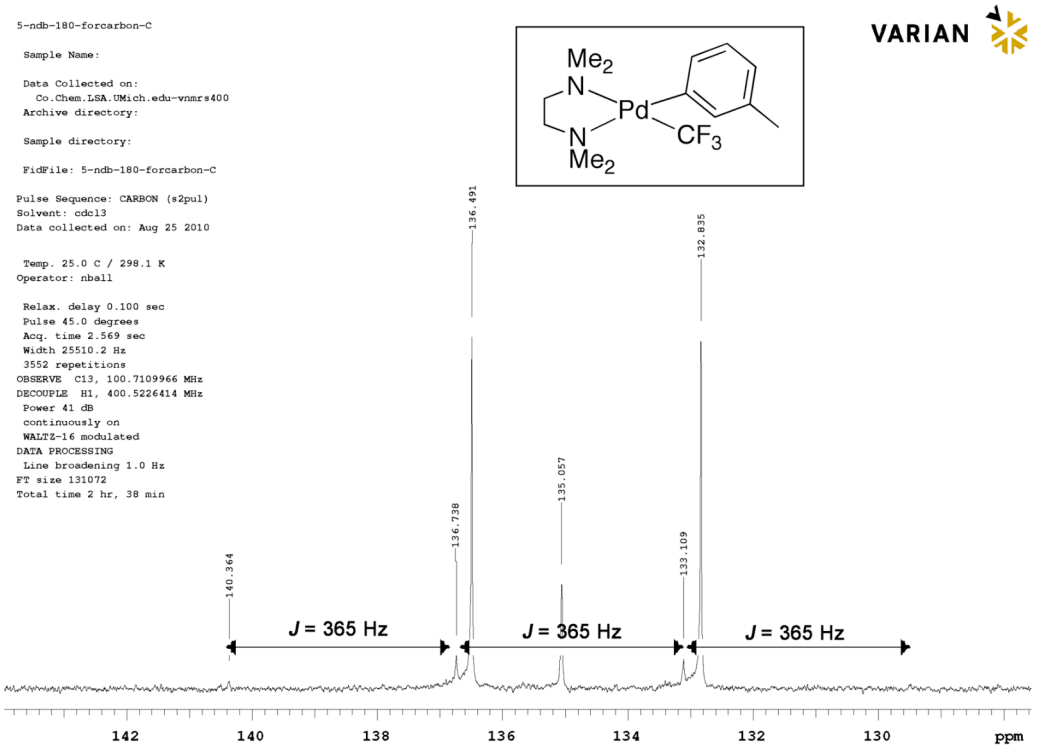

5-ndb-136forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-136forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2010
Temp. 10.0 C / 283.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1056 repetitions
OBSERVE C13, 100.7110005 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 47 min
Me2
N
Pd
CF3
N
Me2
VARIAN
135.521
133.125
131.374
127.165
77.317
77.000
76.683
60.330
59.661
48.913
48.634
20.848
151.793
151.689
136.754
220
200
180
160
140
120
100
80
60
40
20
0
ppm

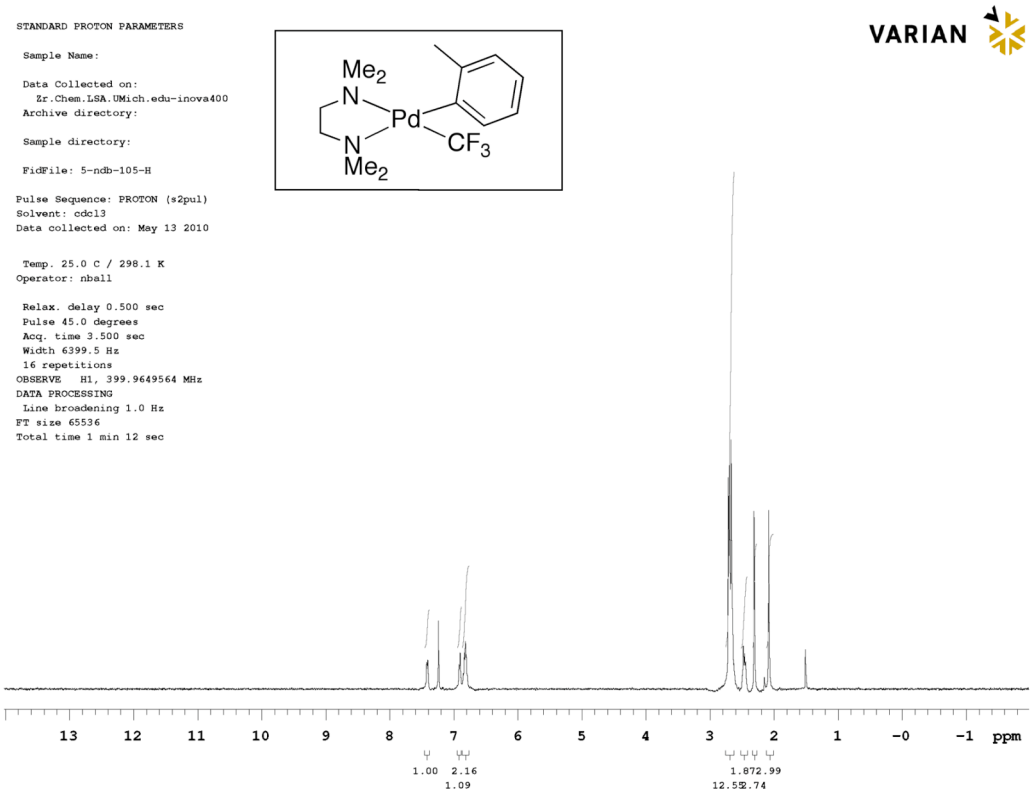

5-ndb-136forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-136forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2010
Temp. 10.0 C / 283.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1056 repetitions
OBSERVE C13, 100.7110005 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 47 min
Me2
N
Pd
CF3
N
Me2
VARIAN
135.521
127.165
131.374
J = 365 Hz
J = 365 Hz
J = 365 Hz
151.793
151.689
140.576
140.383
136.754
133.125
129.086
152
150
148
146
144
142
140
138
136
134
132
130
128
ppm

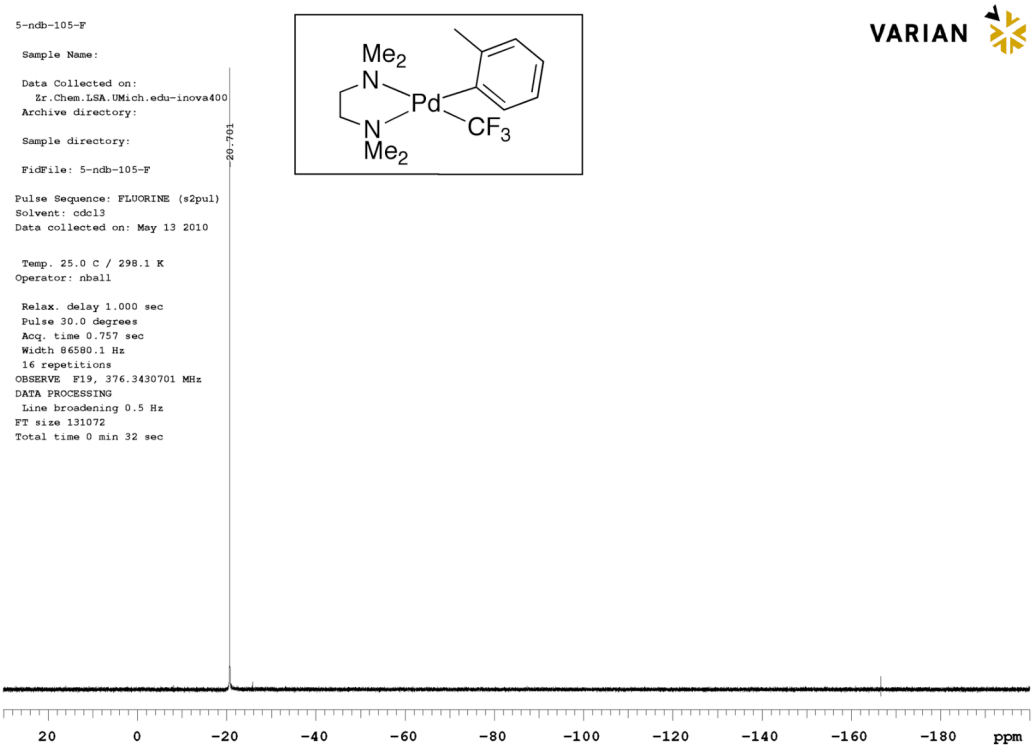

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-180-forcarbon-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 25 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206387 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Me2
N
Pd
CF3
N
Me2
12
10
8
6
4
2
-0
ppm
0.95 1.04
1.18 1.00
6.92 3.48
4.67 6.39

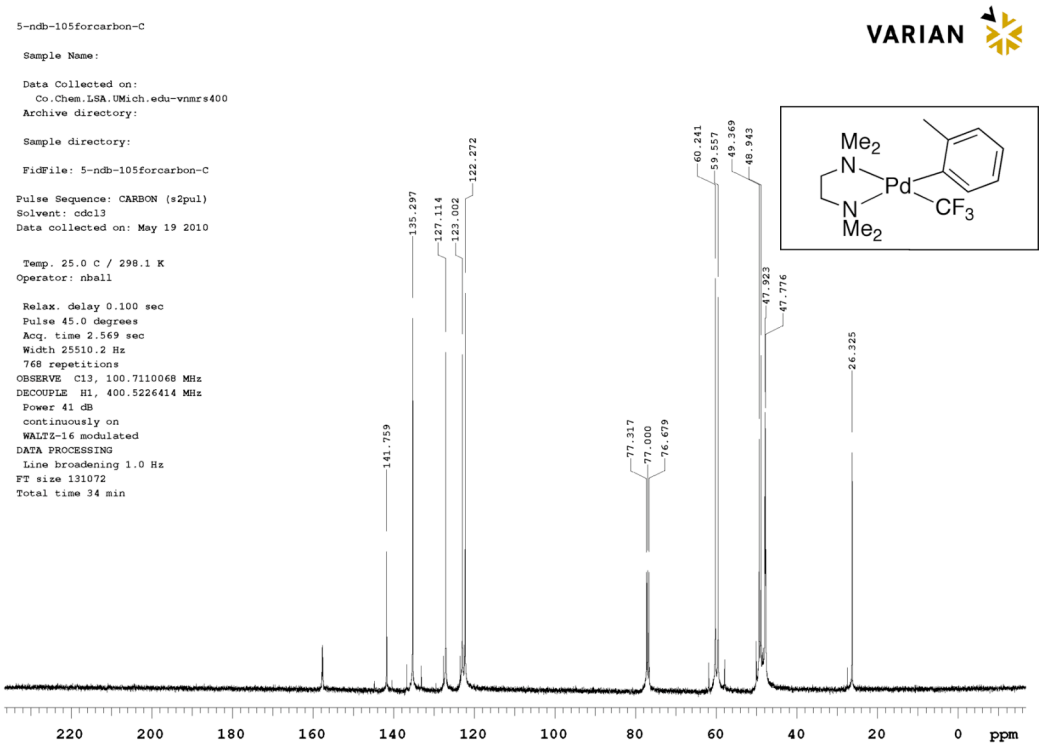

5-ndb-180-F
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-180-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Aug 25 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
16 repetitions
OBSERVE F19, 376.3430708 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 32 sec
-20.819
VARIAN
Me2
N
Pd
CF3
N
Me2
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

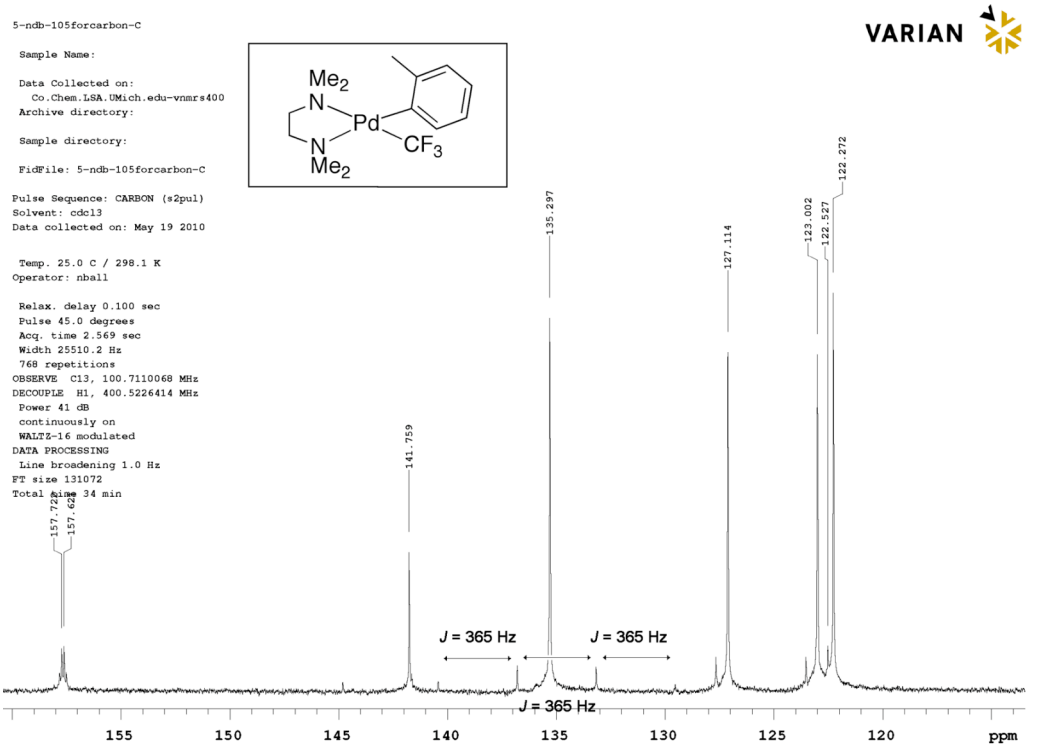

5-ndb-180-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-180-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 25 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3552 repetitions
OBSERVE C13, 100.7109966 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 38 min
VARIAN
Me2
N
Pd
CF3
N
Me2
156.350
156.245
136.491
135.057
132.835
125.820
123.481
77.317
77.201
77.000
76.683
60.400
59.708
48.963
48.704
21.544
220
200
180
160
140
120
100
80
60
40
20
0
ppm

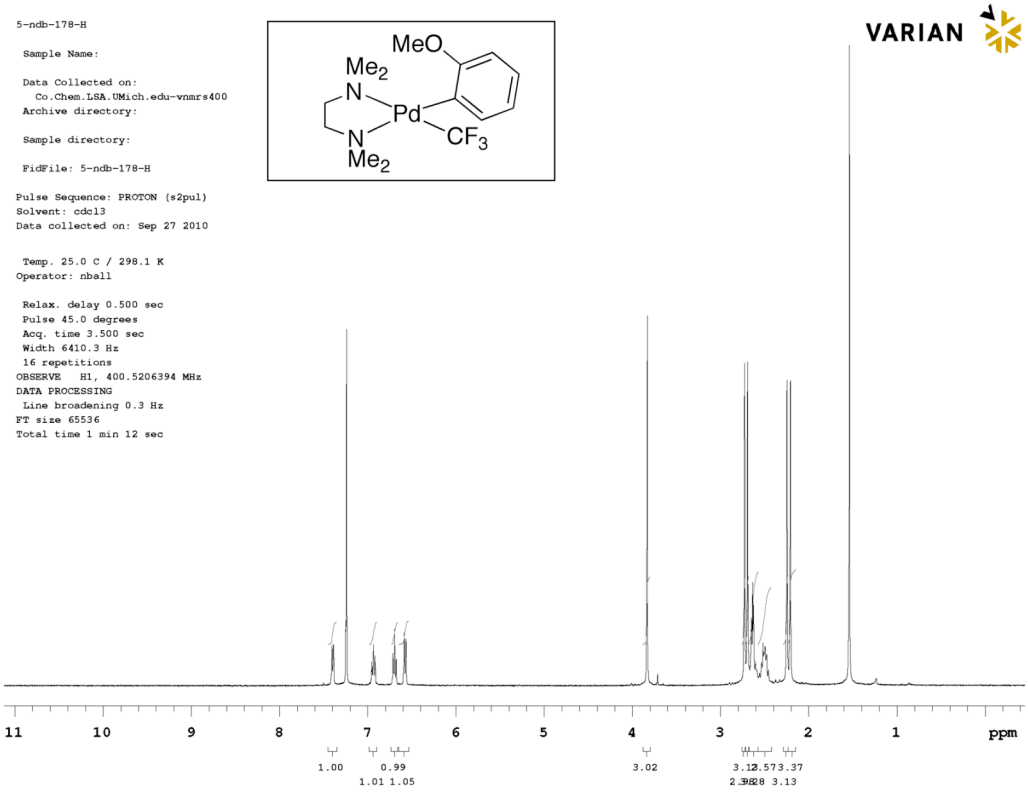

5-ndb-180-forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-180-forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 25 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
3552 repetitions
OBSERVE C13, 100.7109966 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 38 min
VARIAN
Me2
N
Pd
CF3
N
Me2
136.491
132.835
136.738
135.057
133.109
140.364
J = 365 Hz
J = 365 Hz
J = 365 Hz
142
140
138
136
134
132
130
ppm

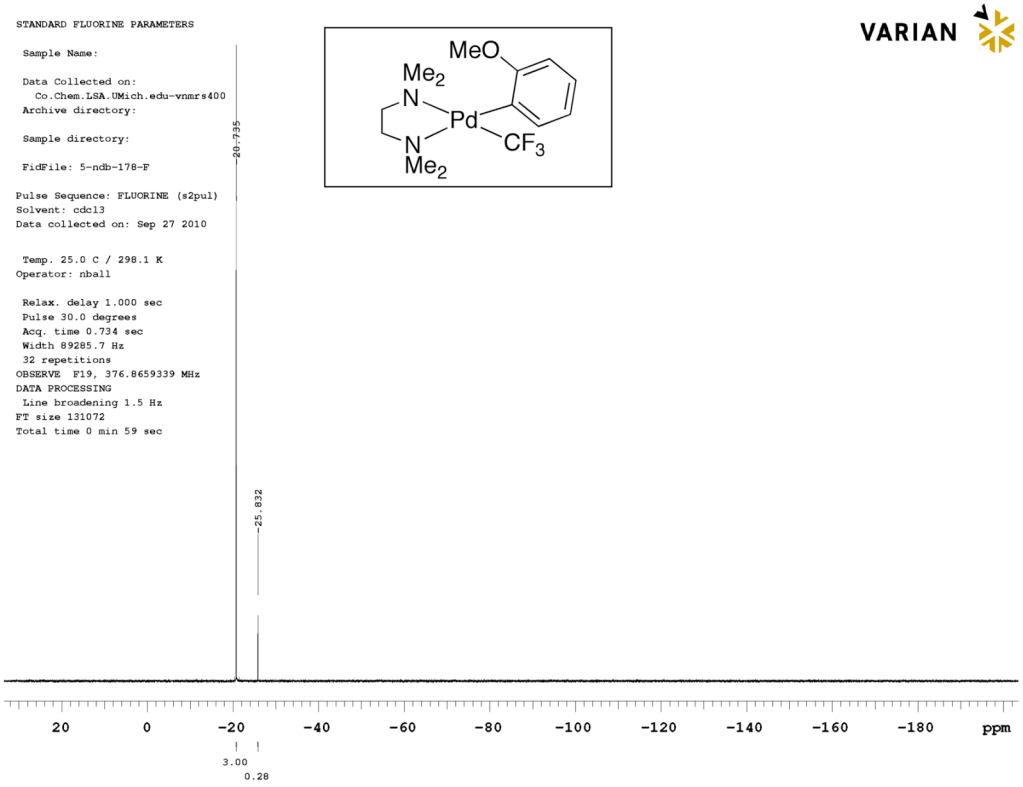

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-105-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 13 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9649564 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
Me2
N
Pd
CF3
N
Me2
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
1.00 2.16
1.09
1.87 2.99
12.55 2.74

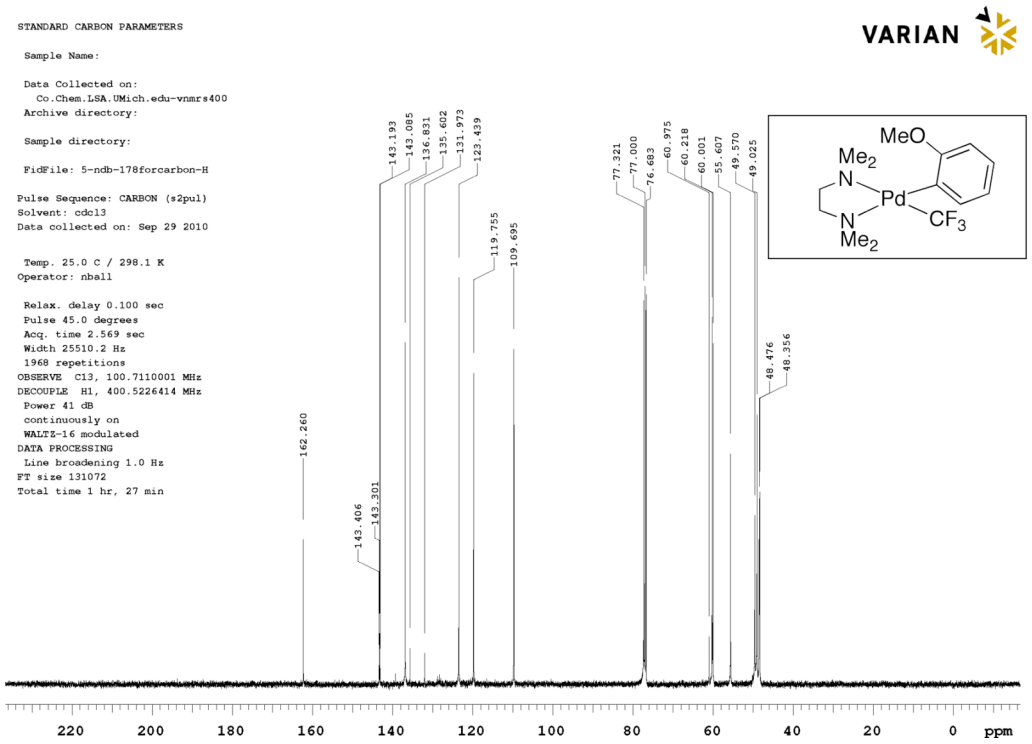

5-ndb-105-F
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-105-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: May 13 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.757 sec
Width 86580.1 Hz
16 repetitions
OBSERVE F19, 376.3430701 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 32 sec
-20.701
VARIAN
Me2
N
Pd
CF3
N
Me2
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

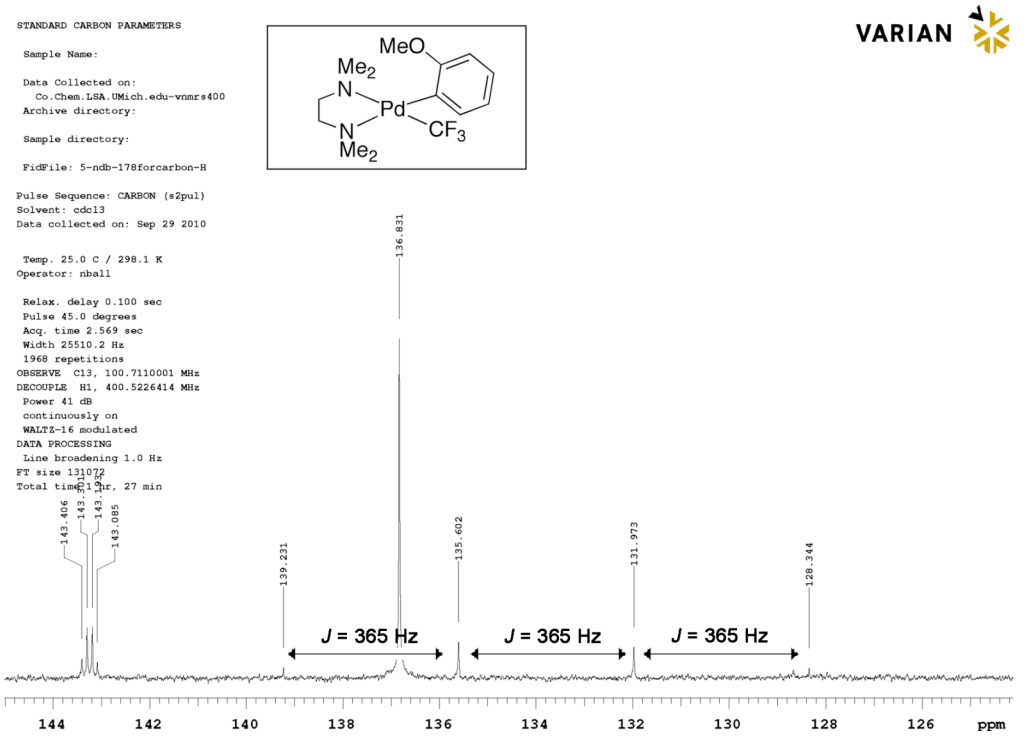

5-ndb-105forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-105forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 19 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
768 repetitions
OBSERVE C13, 100.7110068 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min
VARIAN
Me2
N
Pd
CF3
N
Me2
141.759
135.297
127.114
123.002
122.272
77.317
77.000
76.679
60.241
59.557
49.369
48.943
47.923
47.776
26.325
220
200
180
160
140
120
100
80
60
40
20
0
ppm

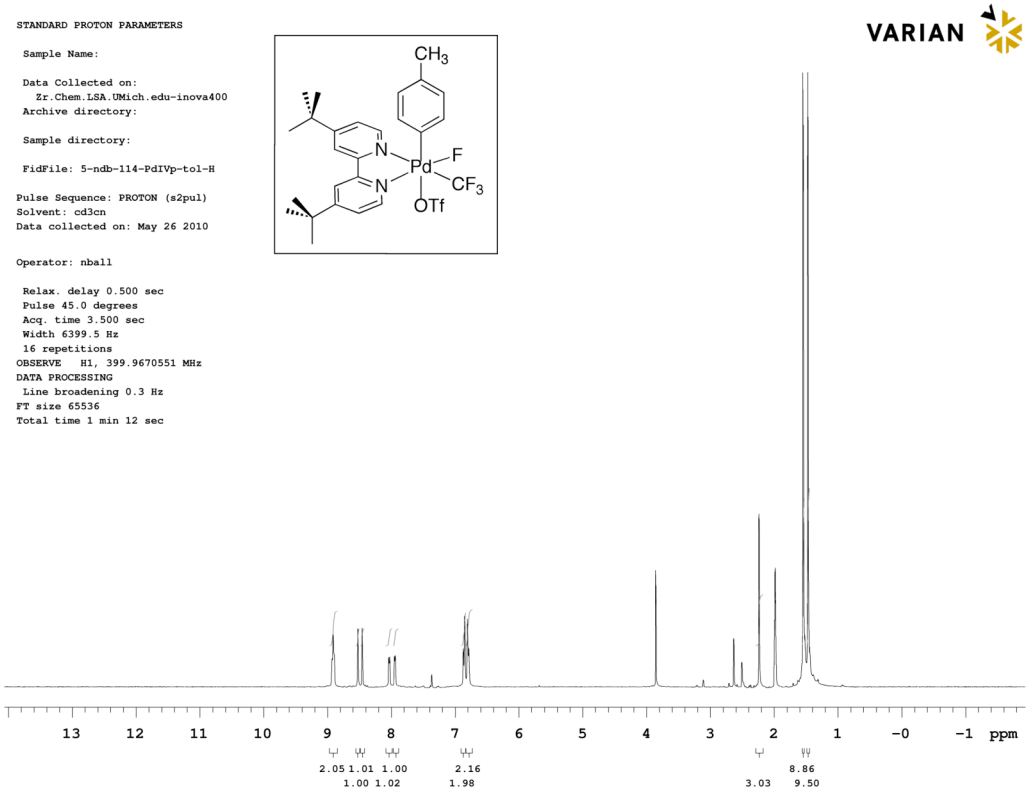

5-ndb-105forcarbon-C
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-105forcarbon-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 19 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
768 repetitions
OBSERVE C13, 100.7110068 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min
VARIAN
Me2
N
Pd
CF3
N
Me2
157.724
157.628
141.759
135.297
127.114
123.002
122.527
122.272
J = 365 Hz
J = 365 Hz
J = 365 Hz
155
150
145
140
135
130
125
120
ppm

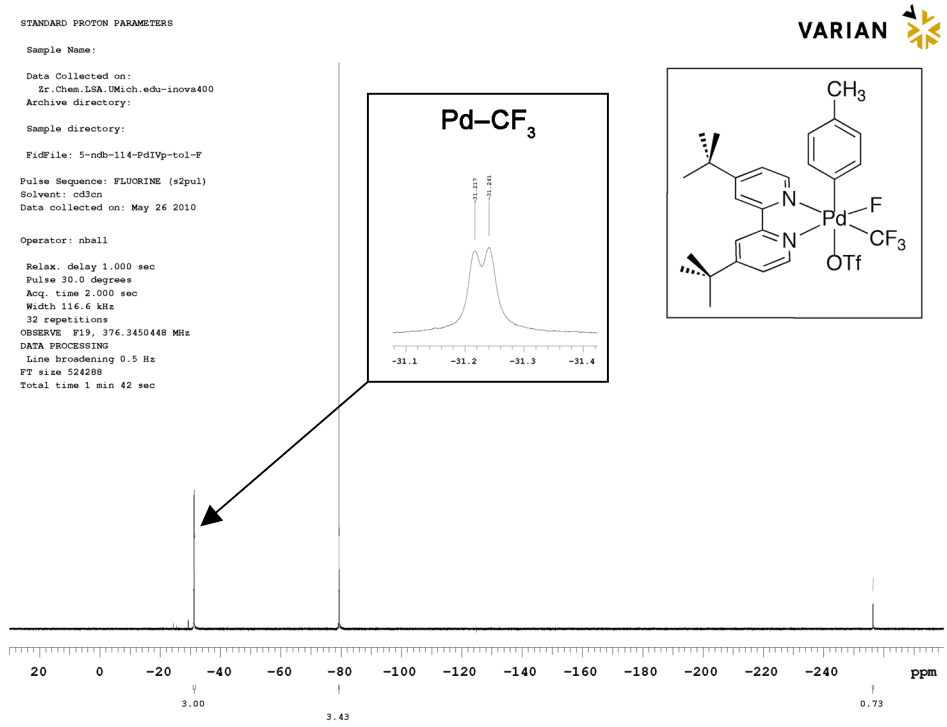

5-ndb-178-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-178-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 27 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 400.5206394 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
MeO
Me2
N
Pd
CF3
N
Me2
VARIAN
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.99
1.01 1.05
3.02
3.12
3.57
3.37
2.92
3.28
3.13

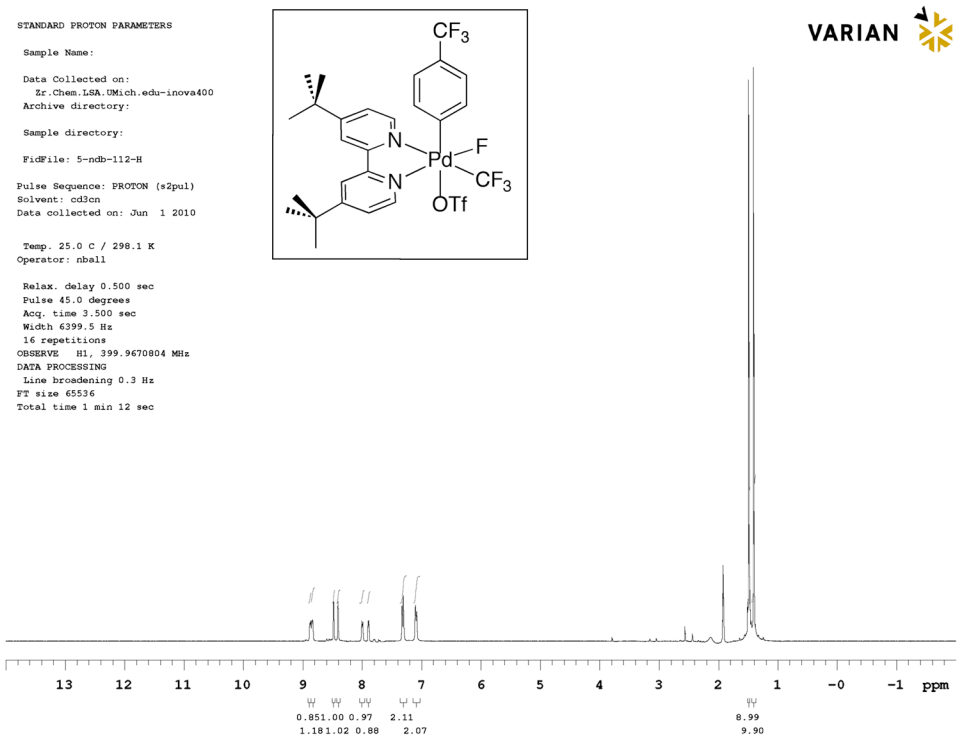

STANDARD FLUORINE PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-178-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Sep 27 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
32 repetitions
OBSERVE F19, 376.8659339 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 59 sec
MeO
Me2
N
Pd
CF3
N
Me2
VARIAN
-20.735
-25.832
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm
3.00
0.28

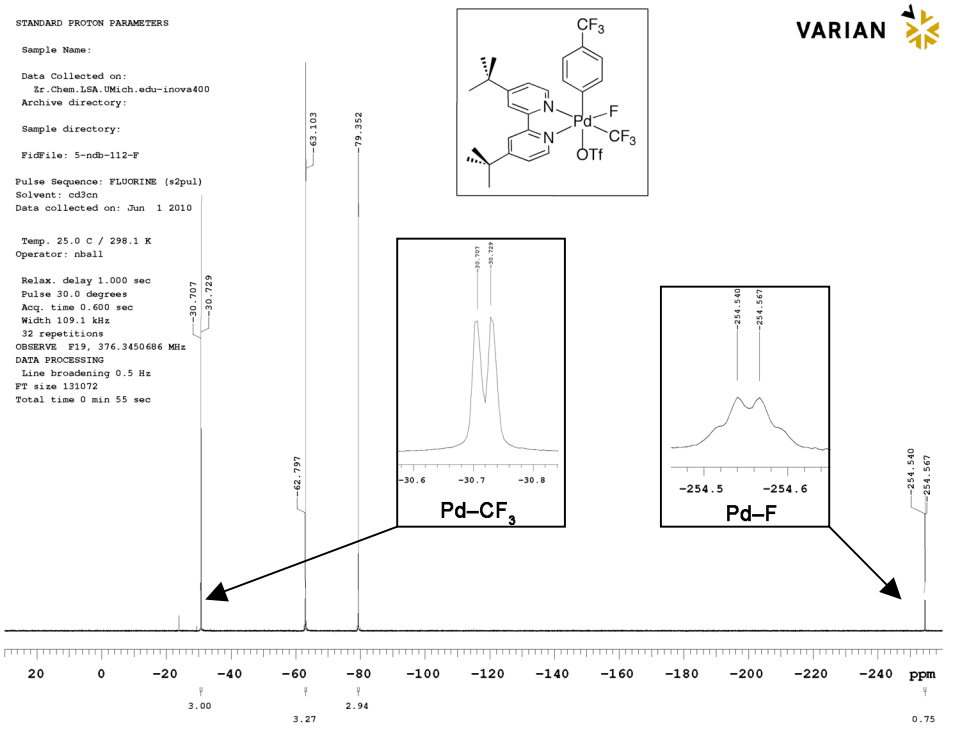

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-178forcarbon-H
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 29 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1968 repetitions
OBSERVE C13, 100.7110001 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 27 min
VARIAN
MeO
Me2
N
Pd
CF3
N
Me2
143.193
143.085
136.831
135.602
131.973
123.439
119.755
109.695
77.321
77.000
76.683
60.975
60.218
60.001
55.607
49.570
49.025
48.476
48.356
162.260
143.406
143.301
220
200
180
160
140
120
100
80
60
40
20
0
ppm

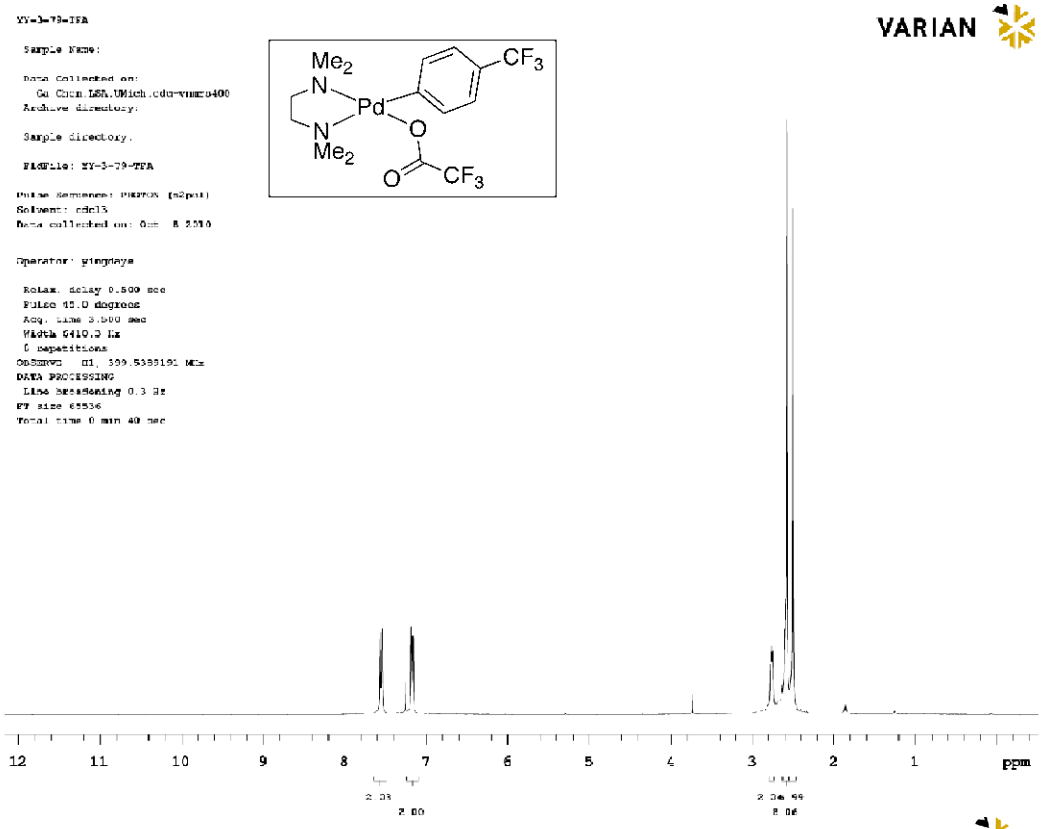

STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 5-ndb-178forcarbon-H
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 29 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1968 repetitions
OBSERVE C13, 100.7110001 MHz
DECOUPLE H1, 400.5226414 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 27 min
VARIAN
MeO
Me2
N
Pd
CF3
N
Me2
136.831
143.406
143.301
143.193
143.085
139.231
135.602
131.973
128.344
J = 365 Hz
J = 365 Hz
J = 365 Hz
144
142
140
138
136
134
132
130
128
126
ppm

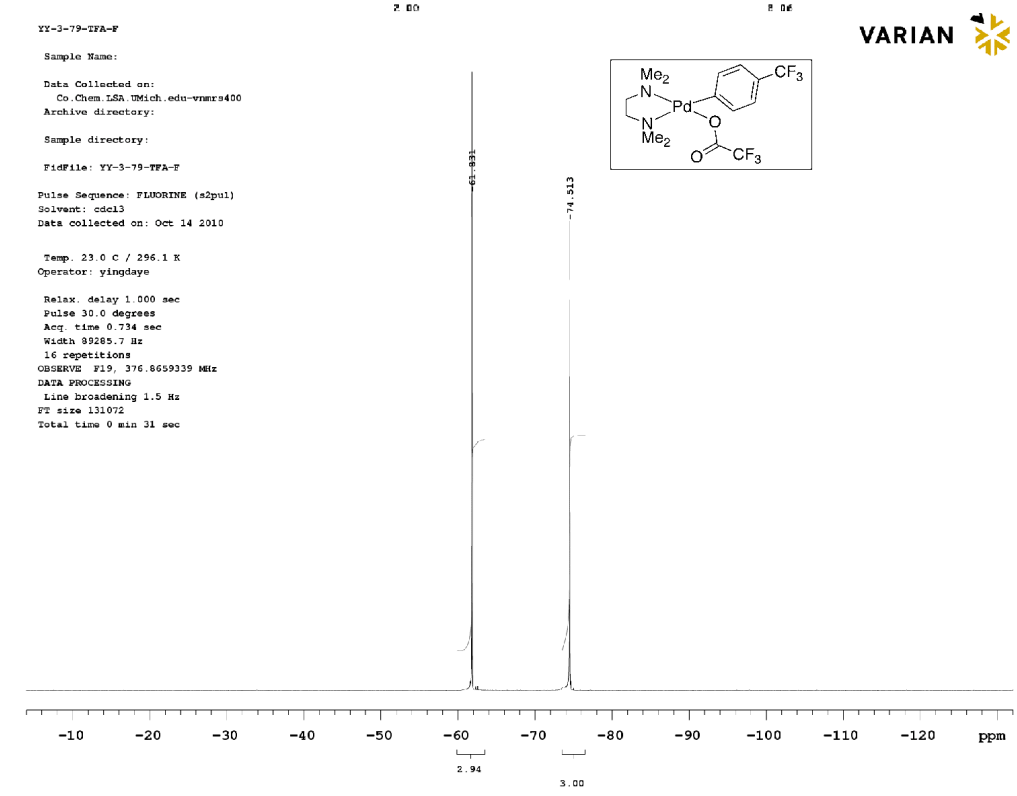

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-114-PdIVp-tol-H
Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: May 26 2010
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9670551 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
CH3
N
Pd
F
CF3
N
OTf
13 12 11 10 9 8 7 6 5 4 3 2 1 −0 −1 ppm
2.05 1.01 1.00 2.16
1.00 1.02 1.98
3.03 8.86
9.50

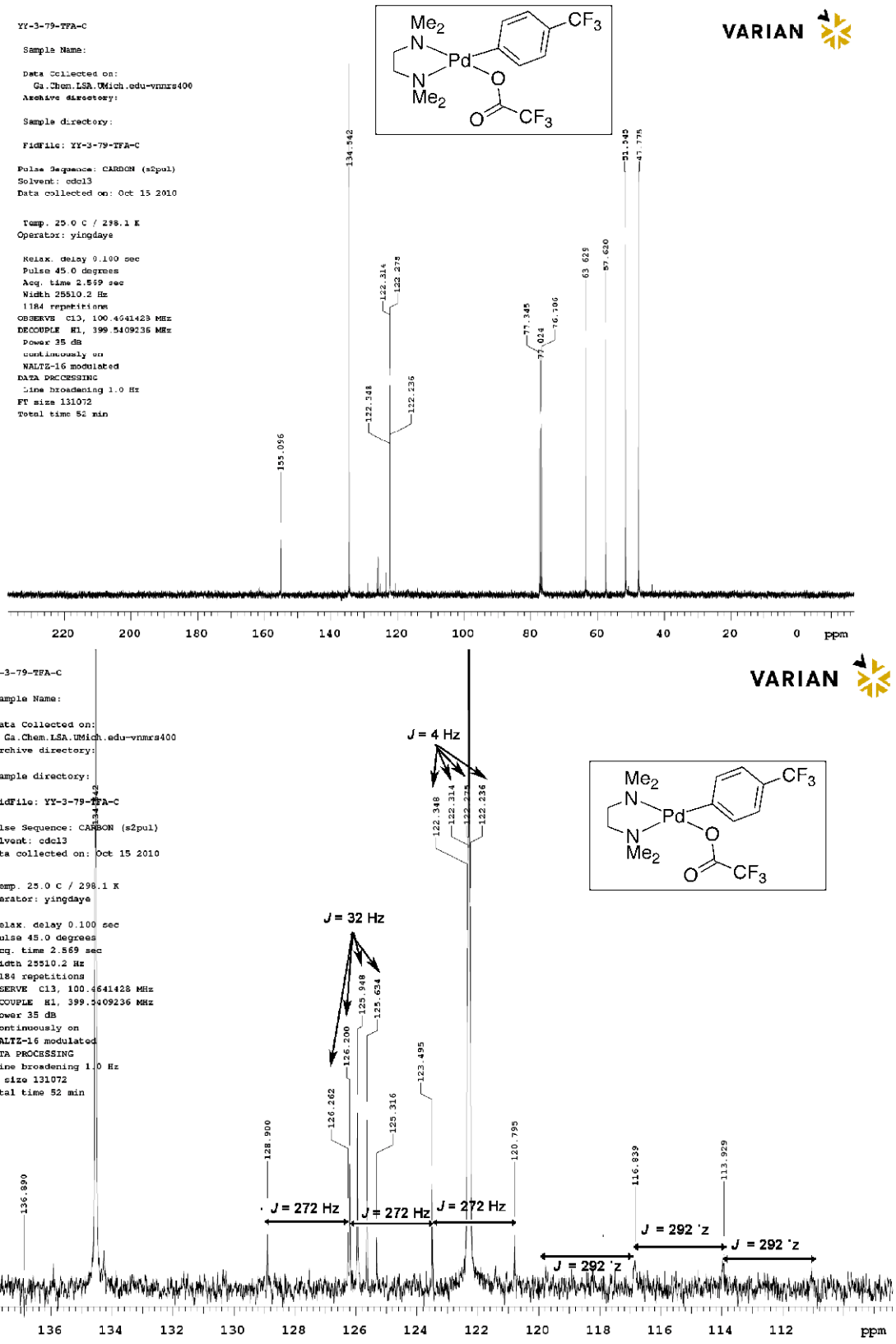

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-114-PdIVp-tol-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cd3cn
Data collected on: May 26 2010
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 2.000 sec
Width 116.6 kHz
32 repetitions
OBSERVE F19, 376.3450448 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 524288
Total time 1 min 42 sec
VARIAN
Pd–CF3
−31.217
−31.241
−31.1 −31.2 −31.3 −31.4
CH3
N
Pd
F
CF3
N
OTf
20 0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 −220 −240 ppm
3.00
3.43
0.73

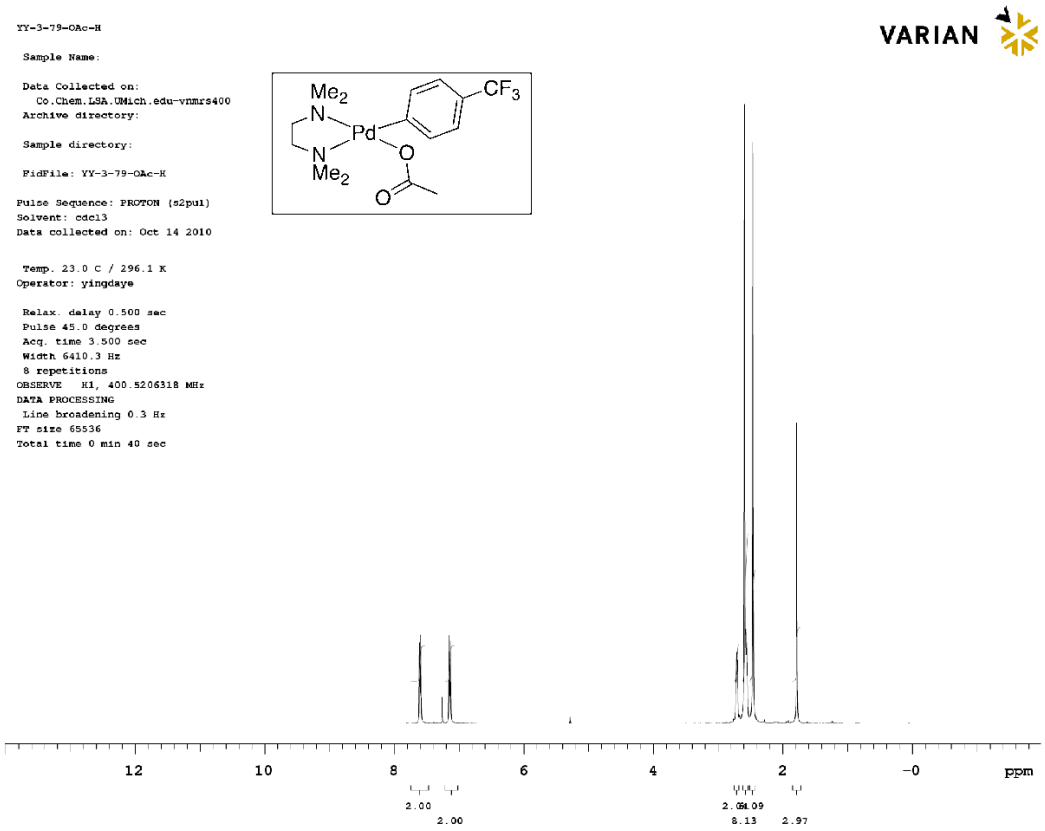

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-112-H
Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Jun 1 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9670804 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min 12 sec
VARIAN
CF3
N
Pd
F
CF3
N
OTf
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
0.85 1.00 0.97 2.11 8.99
1.18 1.02 0.88 2.07 9.90

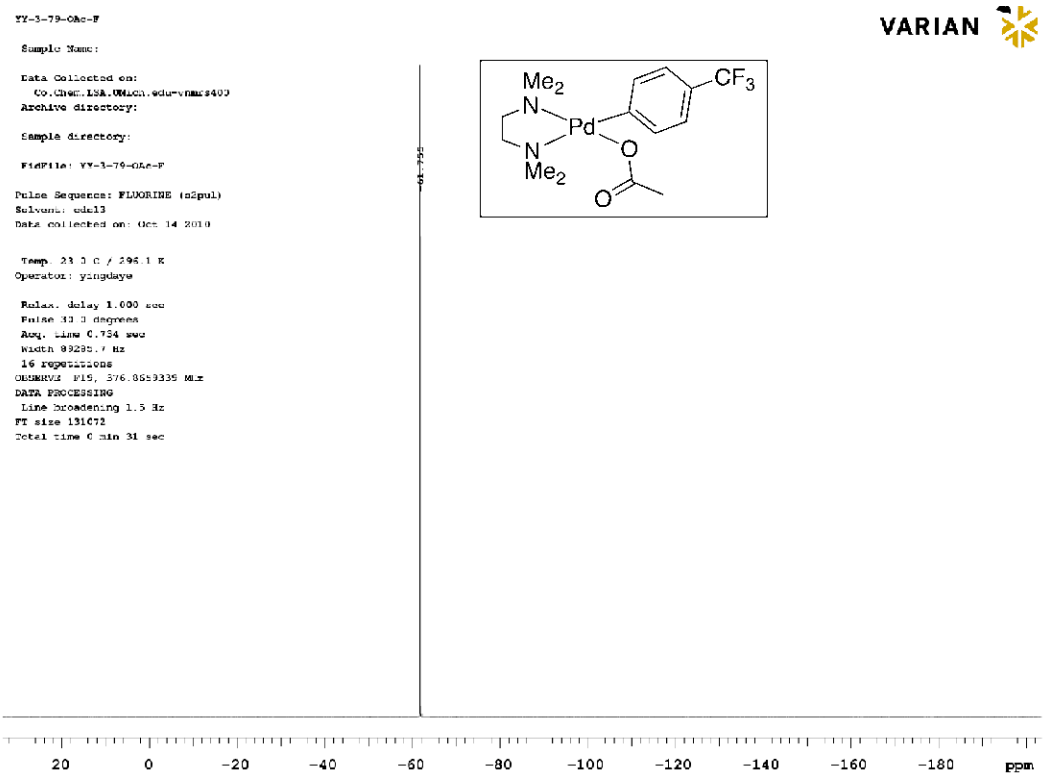

STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Zr.Chem.LSA.UMich.edu-inova400
Archive directory:
Sample directory:
FidFile: 5-ndb-112-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cd3cn
Data collected on: Jun 1 2010
Temp. 25.0 C / 298.1 K
Operator: nball
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.600 sec
Width 109.1 kHz
32 repetitions
OBSERVE F19, 376.3450686 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 0 min 55 sec
VARIAN
CF3
N
Pd
F
CF3
N
OTf
-30.707
-30.729
-62.797
-63.103
-79.352
-254.540
-254.567
Pd–CF3
Pd–F
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 ppm
3.00 3.27 2.94 0.75

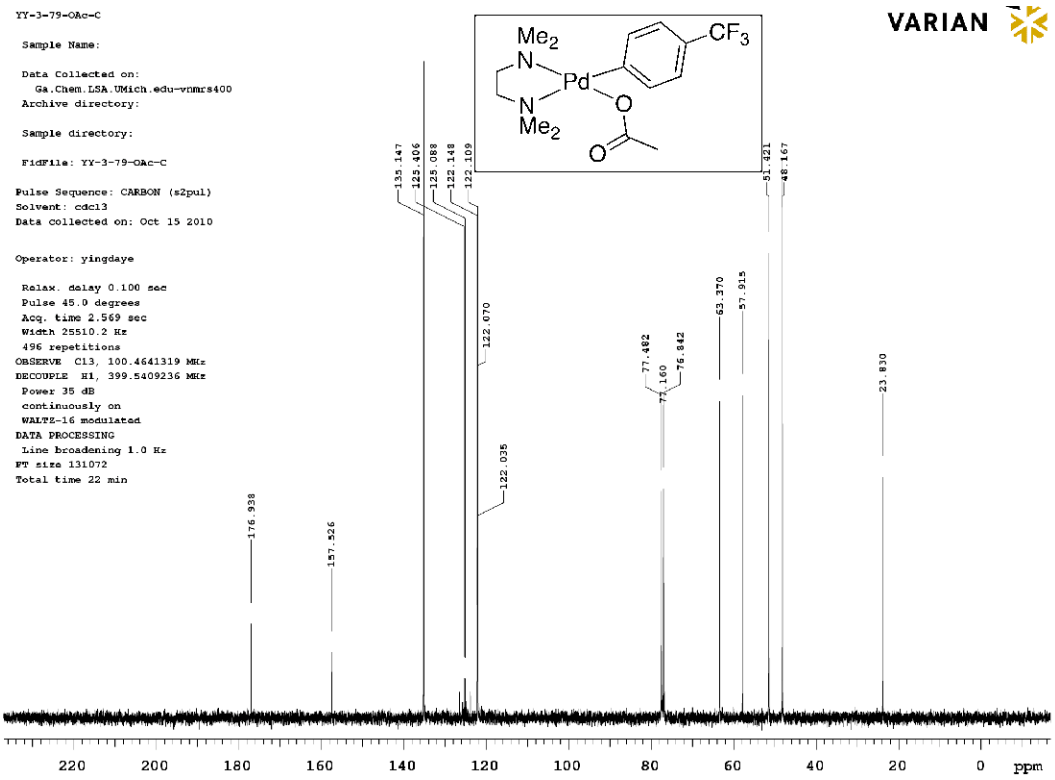

YY-3-79-TFA
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-TFA
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 14 2010
Operator: yingdaye
Relax. delay 0.500 sec
Pulse 15.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.5338191 MHz
DATA PROCESSING
Line Broadening 0.3 Hz
FT size 65536
Total time 0 min 40 sec
Me2
N
Pd
N
Me2
O
O
CF3
CF3
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.33
2.00
3.00
8.06

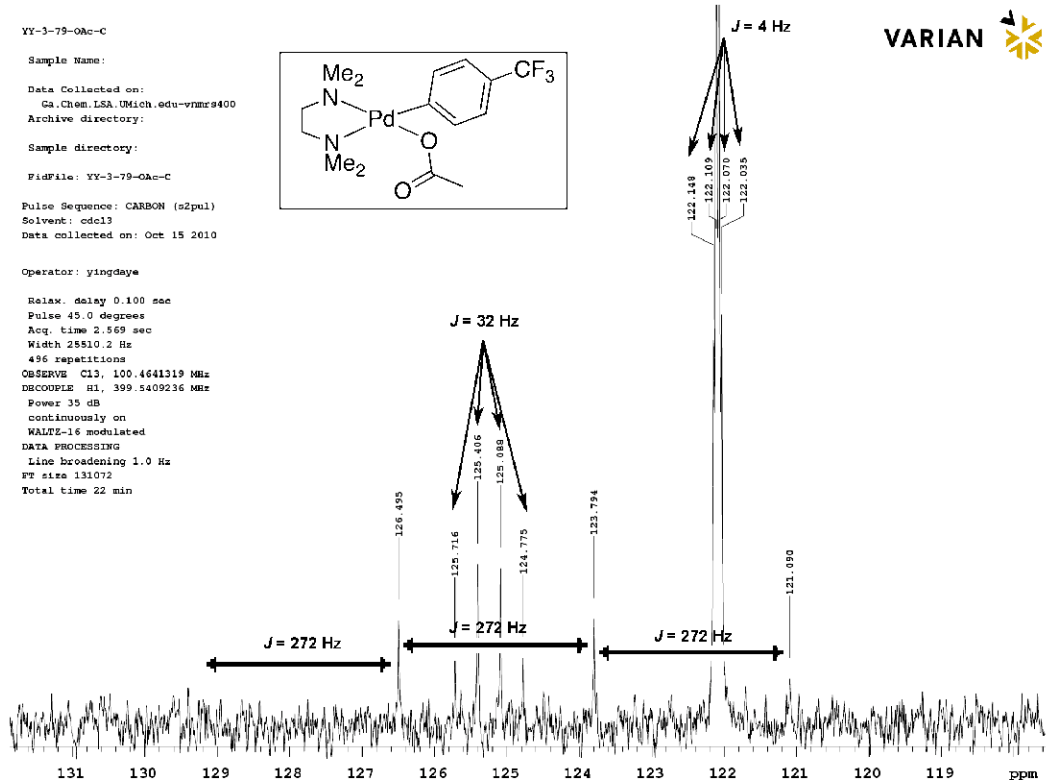

YY-3-79-TFA-F
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-TFA-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 14 2010
Temp. 23.0 C / 296.1 K
Operator: yingdaye
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8659339 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 31 sec
-61.831
-74.513
Me2
N
Pd
N
Me2
O
O
CF3
CF3
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
ppm
2.94
3.00


YY-3-79-TFA-C
Sample Name:
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-TFA-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 15 2010
Temp. 25.0 C / 298.1 K
Operator: yingdaye
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
1184 repetitions
OBSERVE C13, 100.4641428 MHz
DECOUPLE H1, 399.5409236 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 52 min
Me2
N
Pd
O
CF3
VARIAN
134.542
122.314
122.275
122.348
122.236
155.096
77.345
77.024
76.706
63.628
57.630
51.945
41.776
220
200
180
160
140
120
100
80
60
40
20
0
ppm
J = 4 Hz
J = 32 Hz
J = 272 Hz
J = 272 Hz
J = 272 Hz
J = 292 Hz
J = 292 Hz
J = 292 Hz
136.890
128.900
126.262
126.200
125.948
125.634
125.316
123.495
120.795
116.839
113.929
138
136
134
132
130
128
126
124
122
120
118
116
114
112
ppm


YY-3-79-OAc-H
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-OAc-H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 14 2010
Temp. 23.0 C / 296.1 K
Operator: yingdaye
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 400.5206318 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min 40 sec
VARIAN
Me2
N
Pd
N
Me2
O
O
CF3
12
10
8
6
4
2
0
ppm
2.00
2.00
2.06
8.13
2.09
2.97


YY-3-79-OAc-F
Sample Name:
Data Collected on:
Co.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-OAc-F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 14 2010
Temp. 23.0 C / 296.1 K
Operator: yingdaye
Relax. delay 1.000 sec
Pulse 33.1 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.8559335 MHz
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 0 min 31 sec
VARIAN
-61.755
Me2
N
Pd
N
Me2
O
O
CF3
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


YY-3-79-OAc-C
Sample Name:
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-OAc-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 15 2010
Operator: yingdaye
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
496 repetitions
OBSERVE C13, 100.4641319 MHz
DECOUPLE H1, 399.5409236 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 22 min
Me2
N
Pd
O
N
Me2
CF3
O
135.147
125.406
125.088
122.148
122.109
122.070
122.035
176.938
157.526
77.482
77.160
76.842
63.370
57.915
51.421
48.167
23.830
220
200
180
160
140
120
100
80
60
40
20
0
ppm


YY-3-79-OAc-C
Sample Name:
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: YY-3-79-OAc-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 15 2010
Operator: yingdaye
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
496 repetitions
OBSERVE C13, 100.4641319 MHz
DECOUPLE H1, 399.5409236 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 22 min
Me2
N
Pd
O
N
Me2
CF3
O
J = 4 Hz
122.148
122.109
122.070
122.035
J = 32 Hz
126.495
125.716
125.406
125.088
124.775
123.794
121.090
J = 272 Hz
J = 272 Hz
J = 272 Hz
131
130
129
128
127
126
125
124
123
122
121
120
119
ppm

1