Supporting information

Facile Buchwald-Hartwig coupling of sterically encumbered substrates effected by diphosphinoamine as ligands

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Content:

S1. Experimental Section:

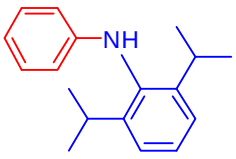
General: All manipulations were performed under a dry and oxygen free atmosphere (N_2) using standard Schleck techniques and glove box. All solvents were dried over activated molecular sieves after distillation. 200-300 mesh silica gel was employed for column chromatography. ^{1}H, ^{13}C, ^{19}F solution NMR spectra were recorded on Jeol and Bruker 400 MHz instrument. Fourier-transform infrared (FT-IR) spectra were taken on a PerkinElmer spectrophotometer.

Synthesis of ligand **1** and **2** is done as per the reported procedure.[S1]

Typical procedure for coupling reactions:

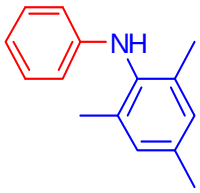
Method 1: NaO^{t}Bu (7 eq), Pd (dba)$_2$ (5 mol%), PNP ligand **1** (5 mol%) or **2** (5 mol%) was taken in 100 mL schlenk flask inside the glove box. To that flask toluene, aromatic amine (1 eq.) and aromatic bromide (1 eq.) was added, and the reaction mixture was subjected to conventional heating (110^{o}C for 5 d). Reaction completion monitored by TLC and NMR and purified using column chromatography using ethyl acetate and *n*-Hexane mixture (2% EA + 98% *n*-Hexane).

Method 2: Required amount of NaOtBu (7 eq), 5 mol% of Pd (dba)$_2$ and 5 mol% PNP ligand (**1** or **2)** was taken in microwave tube inside the glove box. 4 mL of toluene added to that tube and required amount of aromatic amine and aromatic bromide was added and subjected to microwave heating (184^{o}C for 15-30 min) reaction. Reaction completion monitored by TLC and NMR and some of the compounds purified using column chromatography using ethyl acetate and *n*-Hexane mixture (2% EA + 98% *n*-Hexane).

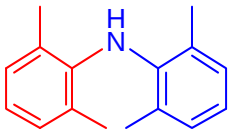


3a: Conventional heating method: 2,6-diisopropylaniline 1.88 mL (10 mmol) , bromobenzene 1.05 mL (10 mmol), Isolated Yield: **1** = 2.18 gm (86%), **2**= 2.34 gm (92%). Microwave heating method: Yield: **1** = 83%, **2** = 90%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 1.17 (*d,* 12H, J= 6.9 Hz, C*H*$_3$), 3.14-3.31 (*m*, 2H, (CH$_3$)$_2$C*H*), 5.14 (*s*, 1H, N*H*), 6.51 (*d*, J = 8.5 Hz, 2H, Ph), 6.74 (*t*, J = 7.3 Hz, 1H, Ph), 7.18 (*dd*, 3H, J=22.2 Hz, Ph), 7.31 (*dd*, *J* = 14.4, 7.7 Hz, 2H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) δ 148.1, 147.9, 147.6, 147.6, 135.2, 135.1, 129.2, 127.2, 123.8, 117.7, 113.0, 77.3, 77.0, 76.7,

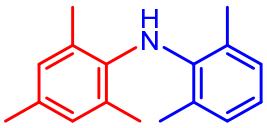
28.2, 23.8; IR (cm^{-1}) : 688.62, 742.28, 800.11, 1056.91, 1257.62, 1308.28, 1454.05, 1495.84, 1601.34, 2961.08, 3402.80; HRMS (positive ESI) : 254.1917 (100 % M^+ +H)



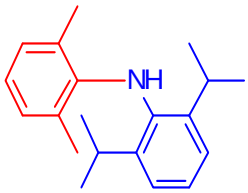
3b: Conventional heating method: 2,4,6-trimethylaniline 0.35 mL (2.5 mmol), bromobenzene 0.26 mL (2.5 mmol), Isolated Yield: **1** = 0.47 gm (90%), **2**= 0.48 gm (92%). Microwave heating method: Yield **1** = 91%, **2**= 90%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 2.24 (s, 6H, *o*-C*H*$_3$) 2.31 (s, 3H, *p*-C*H*$_3$), 5.10 (s, 1H, N*H*), 6.92 (d, J = 19.4 Hz, 7H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) δ 146.7, 136.1, 135.6, 135.5, 129.3, 118.0, 113.3, 77.5, 77.1, 76.8, 21.0, 18.4; IR (cm^{-1}) : 685.24, 738.33, 797.04, 1017.62, 1301.56, 1488.69, 1596.67, 2920.95, 3086.04 ; HRMS (positive ESI) : 212.1452 (100 % M^+ +H).



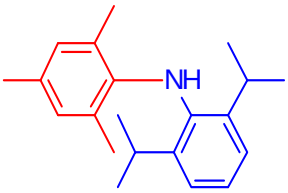
3c: Conventional heating method: NaOtBu, 2,6-dimethylaniline 0.31 mL (2.5 mmol), 2,6-dimethylbromobenzene 0.33 mL (2.5 mmol), Isolated Yield: **1** = 0.51 gm (91%), **2** = 0.55 gm (98%). Microwave heating method: Yield **1** = 88%, **2** = 92%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 2.02 (*s,* 12H, C*H*$_3$, Ph), 4.81 (*s*, 1H, N-*H*), 6.79-6.93 (*m*, 2H, Ph), 6.99 (*d*, J = 7.5 Hz, 4H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 141.8, 129.7, 128.8, 121.8, 77.5, 77.1, 76.8, 19.2; IR (cm^{-1}) : 791.48, 1011.91, 1087.26, 1259.16, 1433.55, 2922.27, 2961.26; HRMS (positive ESI) : 226.1599 (100 % M^++H).



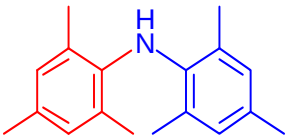
3d: Conventional heating method: 2,6-dimethylaniline 0.31 mL (2.5 mmol), 2,4,6-trimethyl-1-bromobenzene 0.38 mL (2.5 mmol), Isolated Yield **1** = 0.52 gm (87%), **2**= 0.56 gm (94%). Microwave heating method: Yield **1** = 90%, **2** = 95%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 2.02 (*d*, 12H, J= 2.2 Hz, C*H*$_3$-*o*Ph), 2.28 (*s*, 3H, C*H*$_3$-*p*Ph), 4.74 (*s*, 1H, N*H*), 6.83 (*s*, 3H, Ph), 6.99 (*d*, J = 7.5 Hz, 2H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm): δ 142.2, 139.0, 131.6, 130.5, 129.2, 128.8, 128.5, 121.0, 77.3, 77.0, 76.7, 20.6, 19.1, 19.0; IR (cm^{-1}):793.18, 1012.81, 1085.40, 1258.91, 1516.84, 2918.98, 2960.67, 3676.56; HRMS (positive ESI): 240.1760 (100 % M^++H).



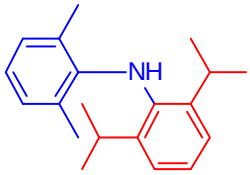
3e: Conventional heating method: 2,6-diisopropylaniline 0.47 mL (2.5 mmol), 2,6-dimethyl-1-bromobenzene 0.33 mL (2.5 mmol), Yield: **1** = 0.62 gm (88%), **2** = 0.66 gm (95%), Microwave heating method: Yield (%)**1** = 88%, **2** = 93%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 1.18 (*d*, J=6.9 Hz,12H, (C*H*$_3$)$_2$CH), 2.04 (*s*, 6H, C*H*$_3$-Ph), 3.22 (dt, 2H, J= 13.7, 6.9 Hz, C*H*(CH$_3$)$_2$), 4.88 (*d,* 1H, J= 20 Hz, N-*H*), 6.78 (*t,* J=7.4 Hz, 1H, Ph), 7.00 (*d*, 2H, J= 7.4 Hz, Ph), 7.15-7.22 (m, 3H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz): δ 144.3, 143.3, 138.9, 129.7, 125.8, 125.0, 123.4, 119.8, 77.5, 77.2, 76.9, 28.2, 23.6, 19.5; IR (cm^{-1}): 693.14, 930.35, 1427, 1461.85, 1548.47, 1946.42, 2561.63, 3304.84; HRMS (Positive ESI): 282.2229 (100% M^{+}+H).



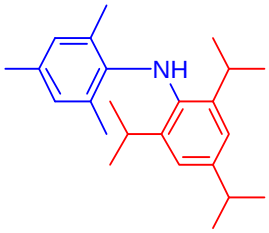
3f : Conventional heating method: 2,6-diisopropylaniline 0.94 mL (5 mmol), 2,4,6-trimethyl-1-bromobenzene 0.76 mL (5 mmol) , Isolated Yield (%):**1** = 1.37 gm (87%), **2** = 1.41 gm (89%), Microwave heating method: Yield **1** = 88%, **2** = 90%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 1.16 (*d*, 12H, J = 6.9 Hz,(C*H*$_3$)$_2$CH), 2.01 (*s*, 6H, C*H*$_3$-*o*Ph), 2.28 (*s*, 3H, CH3-*p*-Ph), 3.06-3.28 (*m*, 2H, C*H*(CH)$_3$), 4.72 (*s,* 1H, N*H*), 6.81 (s, 2H, Ph), 7.15 (*s*, 3H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 143.4, 140.5, 139.2, 130.1, 126.4, 124.2, 123.3, 77.4, 77.0, 76.7, 28.0, 23.5, 20.5, 19.3.; IR (cm^{-1}) 737.68, 787.59, 852.65, 1017.48, 1265.45, 1334.33, 1480.46, 2959.72 ; HRMS (Positive ESI) : 296.2384 (100% M^{+}+H).



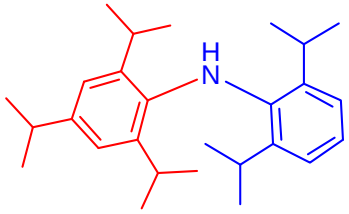
3g: Conventional heating method: 2,4,6-trimethylaniline 0.62 mL (5 mmol), 2,4,6-trimethyl-1-bromobenzene 0.77 mL (5 mmol), Isolated Yield: **2.1** = 1.12 gm (90%), **2.3** = 1.13 gm (90%). Microwave heating method: Yield **1** = 93%, **2** = 95%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 2.01 (*s*, 12H, C*H*$_3$-*o*-Ph), 2.27 (*s*, 12H, C*H*$_3$-*p*-Ph), 4.64 (*s*, 1H, N*H*), 6.82 (*s*, 4H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 139.5, 130.7, 129.4, 129.3, 77.3, 77.0, 76.7, 20.5, 19.0; IR (cm^{-1}) :650.56, 990.36, 1456.56, 1589.36, 1956.56, 2600.25, 3402.25; HRMS (Positive ESI) : 254.1914 (100% M^{+}+H).



3h: Conventional heating method: 2,6-dimethylaniline 1.23 mL (10 mmol), 2,6-diisopropyl-1-bromobenzene 2.06 mL (10 mmol), Isolated Yield : **1** = 2.32 gm (83%), **2**= 2.63 gm (94%). Microwave heating method: Yield **1** = 88%, **2** = 94%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 1.13 (d, 12H, J = 6.9 Hz,(CH_3)$_2$CH-*o*Ph), 1.99 (s, 6H, CH_3), 3.15 (*dd*, 2H, J = 13.7, 6.9 Hz, CH(CH_3)$_2$) 4.80 (s, 1H, N*H*), 6.73 (*t*, J = 7.4 Hz, 1H, Ph), 6.95 (*d*, 2H, J= 7.5 Hz, Ph), 7.13 (t, 3H, J = 4.8 Hz, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 144.3, 143.2, 138.9, 129.6, 125.7, 124.9, 123.3, 119.7, 28.2, 23.6, 19.5; IR (cm^{-1}) :693.14, 930.35, 142733, 1461.85, 1548.47, 1946.42, 2561, 3304.84; MALDI: 280.98 (M^+-H).

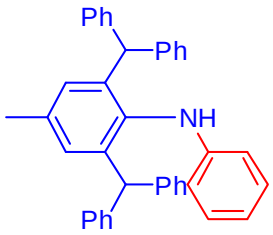


3i: Conventional heating method: 2,4,6-trimethylaniline 0.62 mL (5 mmol), 2,4,6-triisopropyl-1-bromobenzene 1.26 mL (5 mmol); Isolated Yield : **1** = 1.52 gm (90%), **2**= 1.48 (88%). Microwave heating method: Yield **1** = 93%, **2** = 95%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : δ 1.14 (*d*, J= 6.9 Hz, 12H, (CH_3)$_2$CH-*o*Ph), 1.28 (*d*, J = 6.9 Hz, 6H, (CH_3)$_2$CH-*o*Ph), 1.96 (*s*, 6H, CH_3-*o*Ph), 2.25 (*s*, 3H, CH_3-*p*Ph), 2.91 (*s*, 1H, (CH_3)$_2$C*H*-*p*Ph), 3.17 (*dt*, J= 13.7, 6.9 Hz, 1H, (CH_3)$_2$C*H*-*p*Ph), 4.63 (*s*, 1H, N*H*), 6.77 (*s*, 2H, Ph), 6.97 (*s*, 2H, Ph);^{13}C NMR ($CDCl_3$, 100.613MHz, ppm) : δ ^{13}C NMR (101 MHz, CDCl3) δ 144.96, 143.91, 140.89, 136.66, 130.08, 128.26, 125.35, 121.03, 34.05, 28.11, 24.24, 23.57, 20.40, 19.23; IR (cm^{-1}) : 642.38, 698.40, 739.08, 804.43, 853.54, 876.96, 943.02, 1057.25, 1100.89, 1314.17, 1459.07, 1605.03, 1717.71, 2958.62; HRMS (positive ESI) : 338.3423 (100% M^+).

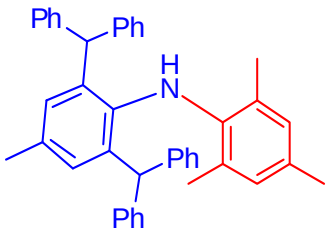


3j: Conventional heating method: 2,6-diisopropylaniline, 1.88 mL (10 mmol) 2,4,6-triisopropyl-1-bromobenzene 2.4 mL (10 mmol); Isolated Yield : **1** = 3.63 gm (96%), **2**= 3.71 gm (98%). Microwave heating method: Yield: **1** = 97%, **2** = 96%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) : 1.00-1.24 (*m*, 24H, (CH_3)$_2$CH-*o*Ph), 1.00-1.24 (*d*, 6H, J = 6.9 Hz,(CH_3)$_2$CH-*p*Ph), 1.29 (d, J = 6.9 Hz, 5H), 2.90 (*s*, 1H, (CH_3)$_2$C*H*-*p*Ph), 3.13 (*ddt*, J=25.9,

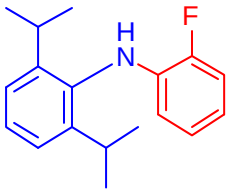
13.7, 6.8 Hz, 4H, $(CH_3)_2CH$-*o*Ph), 4.82 (*s*, 1H, N*H*), 6.90-7.17 (*m*, 5H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 142.57, 140.65, 139.93, 138.81, 137.00, 122.76, 120.88, 120.56, 32.93, 26.84, 26.63, 23.20, 22.56; IR (cm^{-1}) :729.22, 757.23, 1030.84, 1098.92, 1224.89, 1268.70, 1297.98, 1329.61, 1329.61, 1465.44, 2321.01, 2354.76, 2958.37, 3744.29; HRMS (positive ESI) : 380.3314 (95% M^++H).



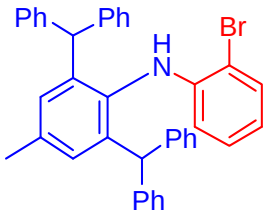
3k: Conventional heating method: 2,6-($CHPh_2$)-3-methyl-aniline 2.19 gm (5 mmol), bromobenzene 0.52 mL (5 mmol); Isolated Yield (%) : **1** = 2.03 gm (79%), **2** = 2.32 gm (90%). Microwave heating method: Yield: **1** = 88%, **2** = 94%; ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 2.20 (s, 3H, CH_3- *p*-Ph), 4.41 (s, 1H, N*H*), 5.65 (s, 2H, $CH(Ph)_2$), 6.49 (d, J = 8.5 Hz, 2H, Ph), 6.71 (s, 2H, Ph), 6.79 (s, 1H, Ph), 6.99 (d, J = 7.5 Hz, 8H, Ph), 7.17-7.30 (m,14H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm) : δ 147.28, 144.06, 143.53, 136.24, 135.18, 129.79, 129.37, 128.22, 126.19, 117.87, 112.79, 51.71, 21.67; IR (cm^{-1}) 531.47, 602.17, 996.83, 1218.41, 1442.46, 1722.25, 2311.69, 3396.24, 3850.31; HRMS (positive ESI) : 516.2690 (100% M^++H).



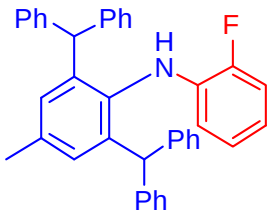
3l: Conventional heating method: 2,6-($CHPh_2$)-3-methyl-aniline 1.1 gm (2.5 mmol), 2,4,6-trimethyl-1-bromobenzene 0.38 mL (2.5 mmol), Isolated Yield : **1** = 1.29 gm (93%), **2** = 1.36 gm (98%), Microwave heating method: Yield: **1** = 97%, **2** = 96%. ^1H NMR ($CDCl_3$, 400 MHz, ppm) : 1.45 (s, 6H, CH_3- *o*-Ph),) 2.13 (s, 3H, CH_3- *p*-Ph), 2.25 (s, 3H, CH_3- *p*-Ph), 4.12 (s, 1H, N*H*), 5.53 (s, 2H, $CH(Ph)_2$), 6.49 (s, 2H, Ph), 6.72 (s, 2H, Ph), 6.85-6.97 (m, 8H, Ph), 7.23 (ddd, J = 8.5, 7.5, 6.0 Hz, 13H, Ph); ^{13}C NMR ($CDCl_3$, 100.61 MHz, ppm): δ 143.66, 138.79, 138.55, 137.58, 131.79, 129.60, 129.10, 128.27, 126.27, 125.95, 76.79, 52.30, 21.50, 20.55, 18.54; IR (cm^{-1}) : 650.52, 790.25, 905.32, 1056.26, 1300.02 1446.67, 2321.01, 2354.76, 2958.37; HRMS (positive ESI) : 557. 2483 (95% M^+).



3m: Conventional heating method: 2,6-diisopropylaniline 0.47 mL (2.5 mmol), 1-bromo-2-fluorobenzene 0.27 mL (2.5 mmol); Isolated Yield: **1** = 0.47 gm (70%), **2**: 0.53 gm (78%). Microwave heating method: Yield: **1** = 70%, **2** = 79%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 1.19 (d, J = 6.9 Hz, 12H, $(CH_3)_2CH$), 3.22 (m, 2H, $(CH_3)_2CH$), 5.35 (s, 1H, N*H*), 6.23 (t, J = 8.5 Hz, 1H, Ph), 6.67 (m, 1H, Ph), 6.88 (t, J = 7.6 Hz, 1H, Ph), 7.02-7.18 (m, 1H, Ph), 7.23-7.43 (m, 3H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz): δ 147.79, 127.64, 124.44, 123.95, 117.07, 114.61, 113.19, 28.25, 23.88 ppm; ^{19}F NMR : δ -137.33 (s) ppm; IR (cm^{-1}) : 729.22, 808.01, 1035.33, 1102.75, 1446.67, 2321.01, 2354.76, 2958.37; HRMS (positive ESI) : 272.1825 (100% M^{+}+H).

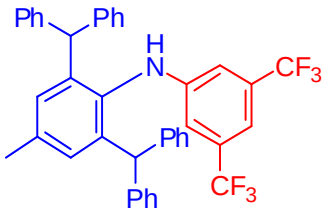


3n: Conventional heating method: 2,6-$(CHPh_2)$-3-methyl-aniline 1.1 gm (2.5 mmol), 1,2-dibromobenzene 0.3 mL (2.5 mmol); Isolated Yield: **1** = 1.34 gm (90%), **2**= 1.36 gm (92%). Microwave heating method: Yield: **1** = 91%, **2** = 90%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 2.23 (s, 3H, CH_3- *p*-Ph),), 5.08 (s, 1H, N*H*), 5.55 (s, 2H, $CH(Ph)_2$), 6.30 (s, 2H, Ph), 6.60 (m, 8H, Ph), 6.75-7.43 (m, 16H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm): δ 144.06, 143.73, 143.25, 143.04, 136.63, 134.21, 132.50, 129.69, 129.11, 128.24, 126.21, 118.39, 112.04, 108.73, 51.94, 21.70; IR (cm-1) : 694.11, 805.01, 1024.36, 1094.77, 1262.88, 1507.67, 1686.49, 2310.40, 2963.36, 3732.30; MALDI: 616.48 (M^{+}+Na)

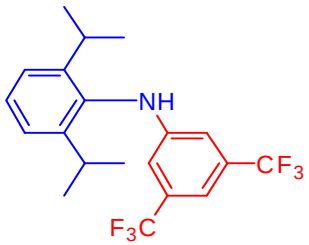


3o: Conventional heating method: 2,6-$(CHPh_2)$-3-methyl-aniline 2.2 gm (5 mmol), 1-bromo-2-fluorobenzene 0.54 mL (5 mmol); Isolated Yield (%) : **1** = 2.55 gm (95%), **2.3** = 2.36 gm (97%). Microwave heating method: Yield: **1** = 96%, **2.** = 95%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 2.19 (s, 3H, CH_3- *p*-Ph), 4.73 (s, 1H, N*H*), 5.61 (s, 2H, $CH(Ph)_2$), 6.29-6.39 (m, 1H, Ph), 6.73 (s, 9H, Ph), 6.84 (s, 15H, Ph), 6.97 (d, J = 7.1 Hz, 8H), 7.26–7.13 (m, 13H, Ph); ^{13}C NMR (101 MHz, $CDCl_3$, ppm) δ 144.15, 143.27, 136.55, 135.43, 134.07, 129.82, 129.26, 128.16, 127.79, 126.25, 124.51, 117.29, 114.77, 112.86, 51.77, 21.68; ^{19}F NMR : δ -136.85

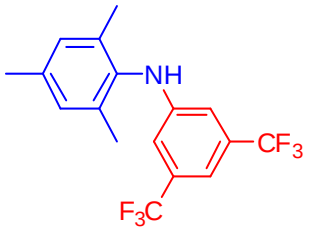
(s) ppm; IR (cm-1) : 565.86, 804.88, 872.06, 997.73, 1092.14, 1217.65, 1378.26, 1734.35, 2311.34, 3739.40; HRMS (positive ESI) : 532.2427 (100% M^++H).



3p: Conventional heating method: 2,6-($CHPh_2$)-3-methyl-aniline 1.1 gm (2.5 mmol), 3,4-trifluoromethyl-1-bromobenzene 0.43 mL (2.5 mmol); Isolated Yield: **1** = 1.38 gm (85%), **2** = 1.39 gm (86%). Microwave heating method: Yield: **1** = 86%, **2** = 88%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 2.21 (s, 3H, C*H*$_3$- *p*-Ph),), 4.83 (s, 1H, N*H*), 5.48 (s, 2H, C*H*$(Ph)_2$), 6.70 (d, J = 23.4 Hz, 4H, Ph), 6.93 (d, J = 7.5 Hz, 8H, Ph), 7.11-7.33 (m, 13H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm): δ 148.00, 143.96, 142.71, 137.68, 132.93, 132.63, 132.30, 130.18, 129.17, 128.45, 126.50, 124.82, 122.11, 110.92, 77.34, 77.03, 76.71, 52.13, 21.74; ^{19}F NMR : δ -63.06 (s) ppm; IR (cm^{-1}): 603.61, 894.42, 894.42, 1432.71, 1689.42, 2313.24, 3562.92, 3736.25; MALDI : 652.13 (M^+).



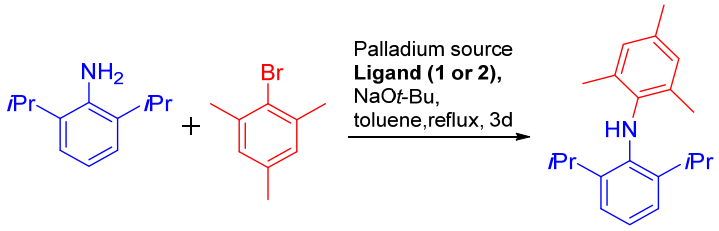
3q: Conventional heating method: 2,6-diisopropylaniline 0.47 mL (2.5 mmol), 3,4-trifluoromethyl-1-bromobenzene 0.43 mL (2.5 mmol); Isolated Yield: **1** = 0.86 gm (89%), **2** = 0.89 gm (92%). Microwave heating method: Yield: **1** = 92%, **2**= 91%; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 1.17 (d, J = 6.9 Hz, 12H, $(CH_3)_2$CH), 3.01-3.20 (m, 2H, $(CH_3)_2$C*H*), 5.54 (s, 1H, N*H*), 6.86 (s, 2H, Ph), 7.20 (s, 1H, Ph), 7.20 (s, 1H, Ph), 7.28 (d, J = 2.1 Hz, 1H, Ph), 7.39 (d, J = 7.8 Hz, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm): δ 148.95, 147.41, 133.01, 132.70, 132.36, 132.03, 128.50, 124.84, 124.40, 122.13, 112.01, 111.22–110.02 (m), 77.32, 77.01, 76.69, 28.36, 23.79; ^{19}F NMR : δ -63.22 (s) ppm; IR (cm^{-1}) : 535.03, 606.59, 740.76, 999.65, 1125.60, 1273.69, 1381.54, 1485.16, 1619.11, 2920.13, 3369.52; MALDI: 389.0893 (M^+).



3r: Conventional heating method: 2,4,6-trimethylaniline 0.31 mL (2.5 mmol), 3,4-trifluoromethyl-1-bromobenzene 0.43 mL (2.5 mmol); Yield: **1** = 0.78 gm (90%), **2** = 0.82 gm (94%). Microwave heating method: Yield: **1** = 93%, **2** = 95%. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 2.14 (s, 6H, C*H*$_3$- *o*-Ph), 2.32 (s, 3H, C*H*$_3$-*p*-Ph), 5.46 (s,

1H, N*H*), 6.80 (s, 2H, Ph), 6.97 (s, 2H, Ph), 7.16 (s, 1H, Ph); ^{13}C NMR ($CDCl_3$, 100.613 MHz, ppm): δ 147.66, 136.94, 136.03, 133.17, 132.73, 132.41, 129.65 , 124.86, 122.15, 112.11, 110.80 (m), 77.33, 20.95, 18.13; ^{19}F NMR : δ -63.16 (s) ppm; IR (cm^{-1}) : 729.22, 1446.67, 2321.01, 2354.76, 2958.37; HRMS (positive ESI) : 348.1191 (100% M+).

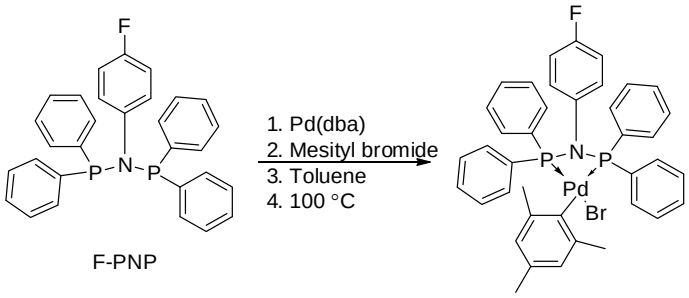
Optimization Table S[1]:



Entry	Palladium source	Ligand	Mol %	Yield[a] (%)
1	$Pd(dba)_2$	1	1	55
2	$Pd(dba)_2$	1	2.5	65
3	$Pd(dba)_2$	1	3	65
4	**$Pd(dba)_2$**	**1**	**5**	**88**
5	$Pd(OAc)_2$	1	5	75
6	$Pd_2(dba)_3$	1	5	93
7	$Pd(dba)_2$	2	1	60
8	$Pd(dba)_2$	2	2.5	65
9	**$Pd(dba)_2$**	**2**	**5**	**90**
8	$Pd(OAc)_2$	2	5	78
9	$Pd_2(dba)_3$	2	5	90
10	$Pd(dba)_2$	-	5	>10

Reaction conditions: Aryl amine = 2,6-diisopropyl aniline, (1 mmol), Aryl bromide = Mesityl bromide (1 mmol) sodium tert-butoxide (2.8 mmol). [a]Isolated yields (average of two runs) dba = dibenzylideneacetone, OAc = Acetate.*Blank reaction with only Pd source afforded <10% yield.

Reaction to support the mechanism:



Chemical Formula: $C_{39}H_{35}BrFNP_2Pd$
Exact Mass: 783.0447

Mass Spectrum:

M+H⁺ = 784.14

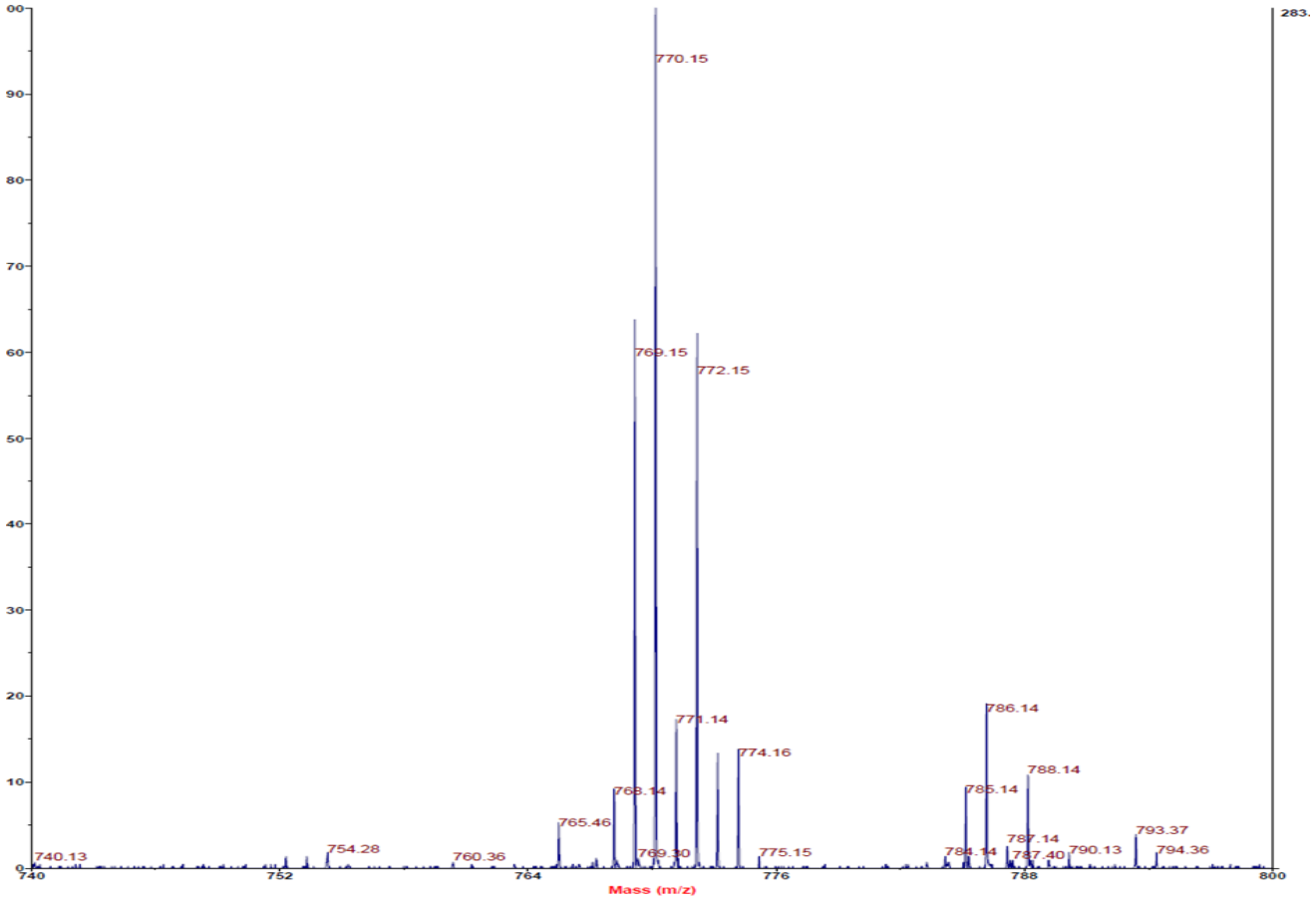
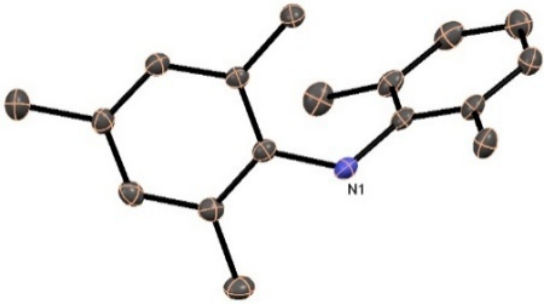


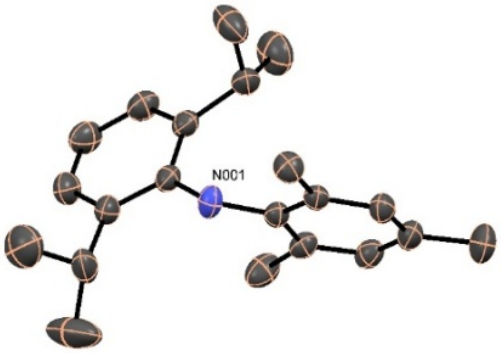
Table S^2: NMR data for mechanistic studies

Compound	NMR	
	^{31}P NMR (ppm)	**^{1}H NMR (ppm)**
F-PNP ligand	70	6.49-6.62 and 7.27-7.34 (24H, Ph)
F-PNP-Pd-complex	16.47	6.97-7.93 (24H, Ph)
F-PNP-Pd-ArBr complex	43.79	1.90 (3H, CH_3), 2.20(6H, CH_3), 6.54-7.76 (26, Ph)

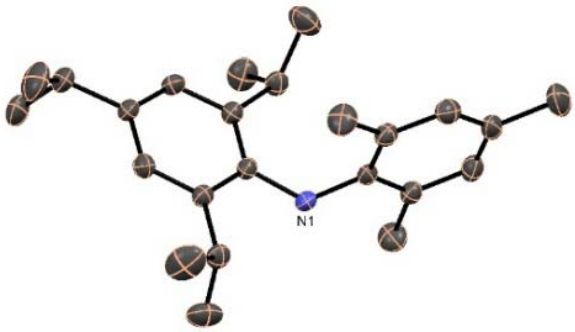
S2. Molecular structures of 3d, 3f, and 3i: Molecular structure of (a) **3d**, (b) **3f** and (c) **3i** at the ellipsoid probability level of 30 %. Hydrogen atoms are omitted for clarity.



(a)



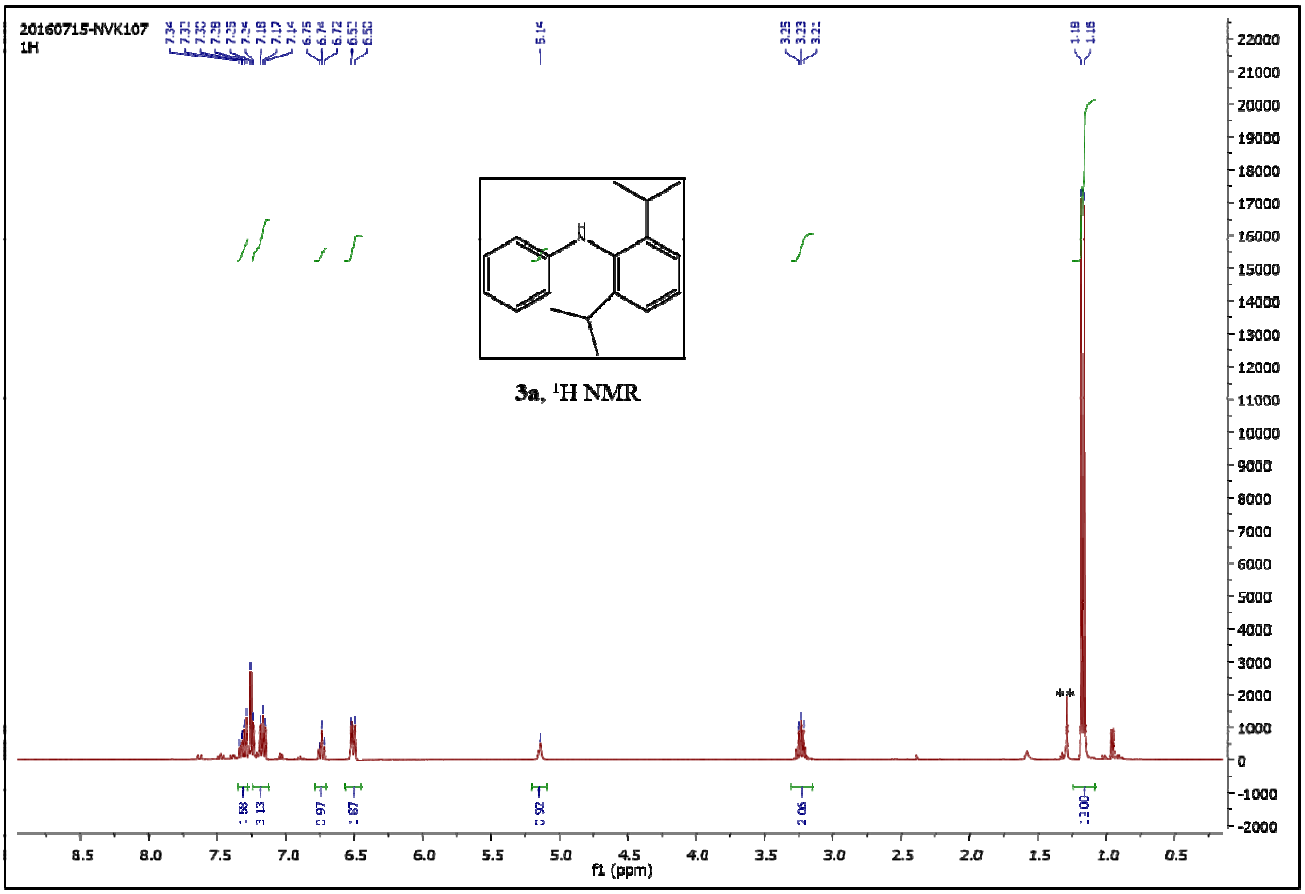
(b)

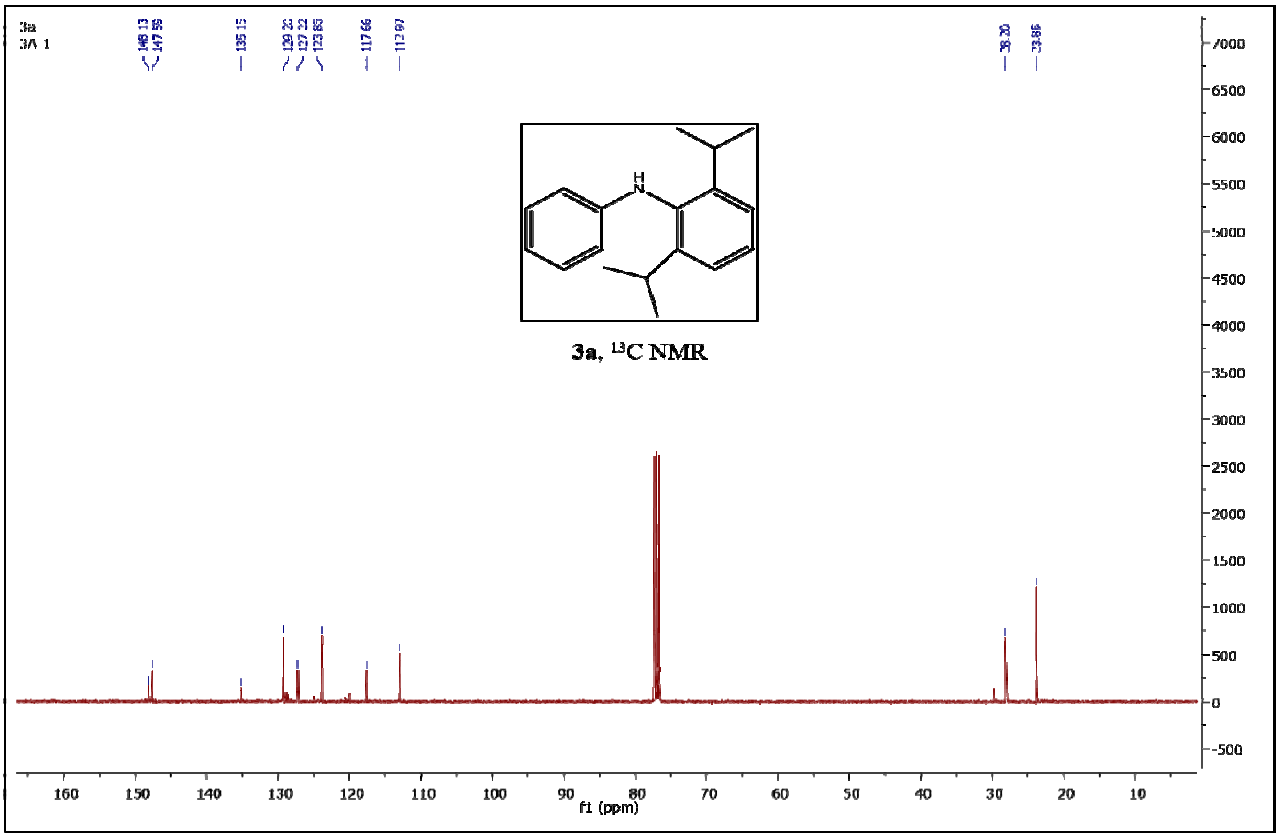


(c)

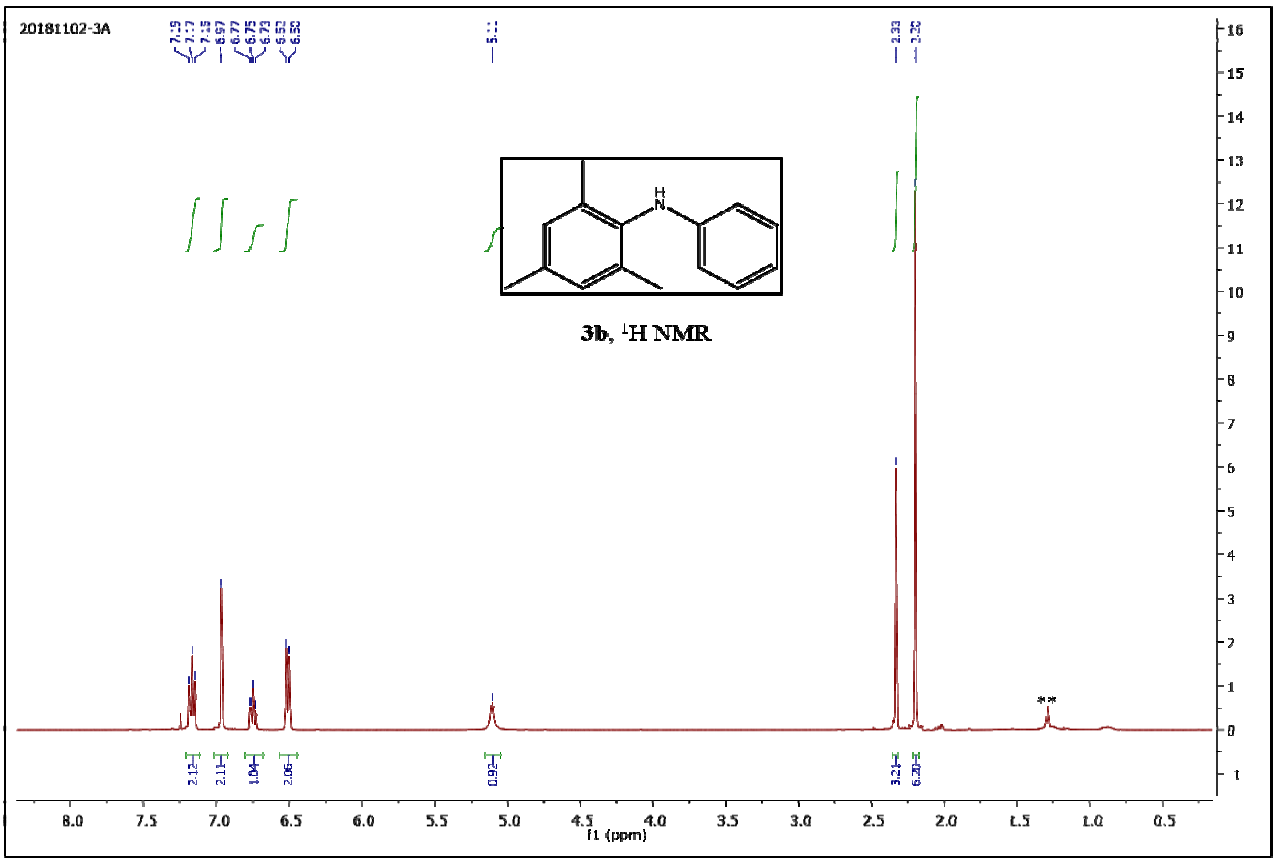
S3. NMR Data:

NMR solvent $CDCl_3$ *=Toluene; **=H-grease; #=H_2O.

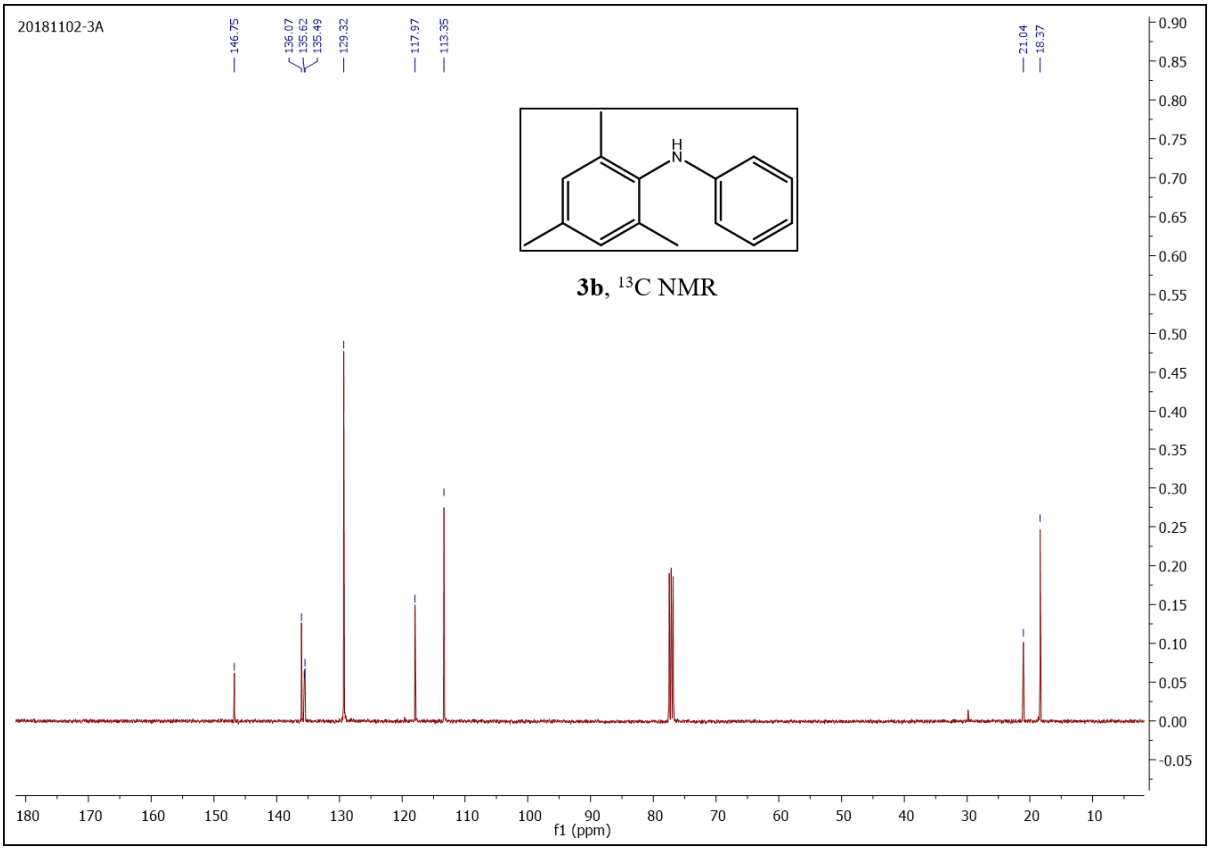




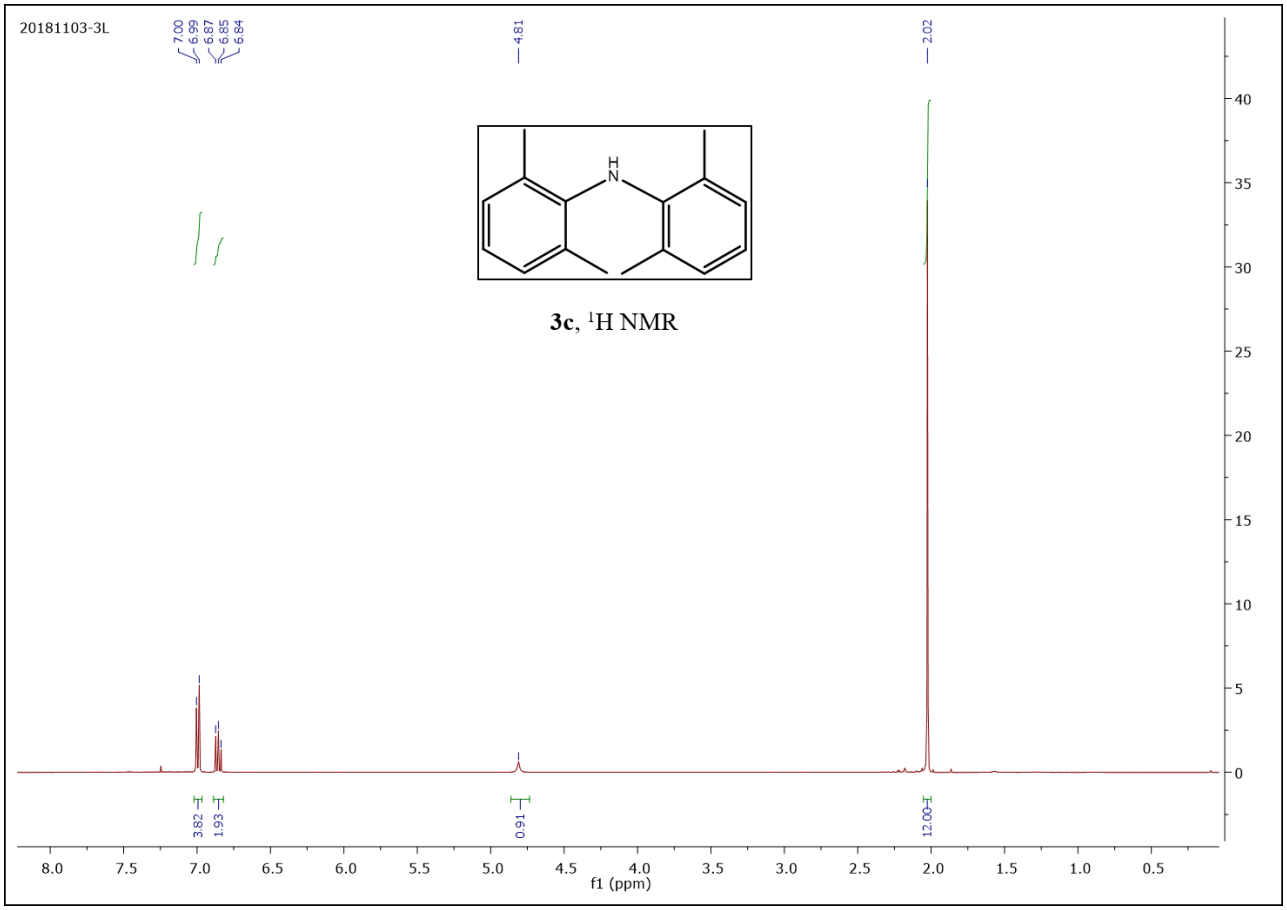
3a, ^{13}C NMR



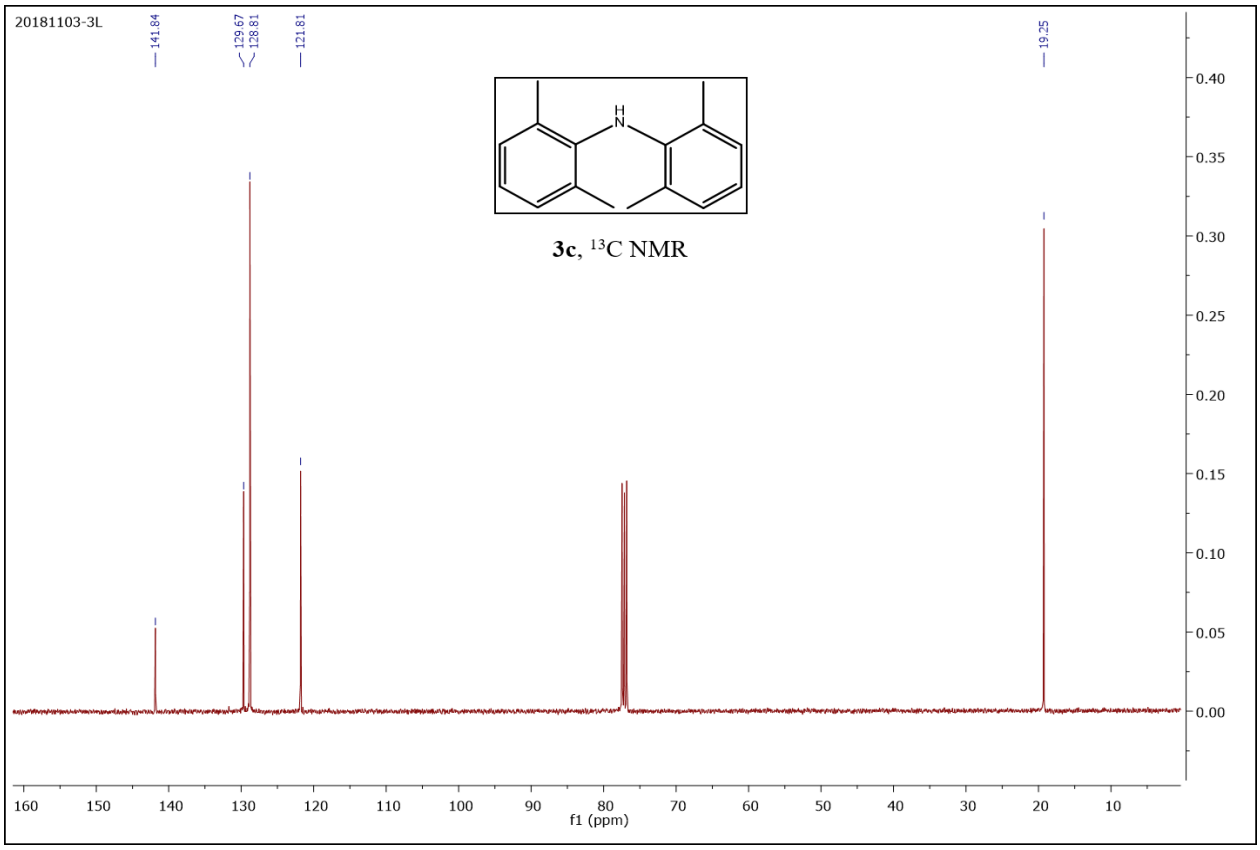
3b, ^{1}H NMR


20181102-3A
146.75
136.07
135.62
135.49
129.32
117.97
113.35
21.04
18.37
H
N
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

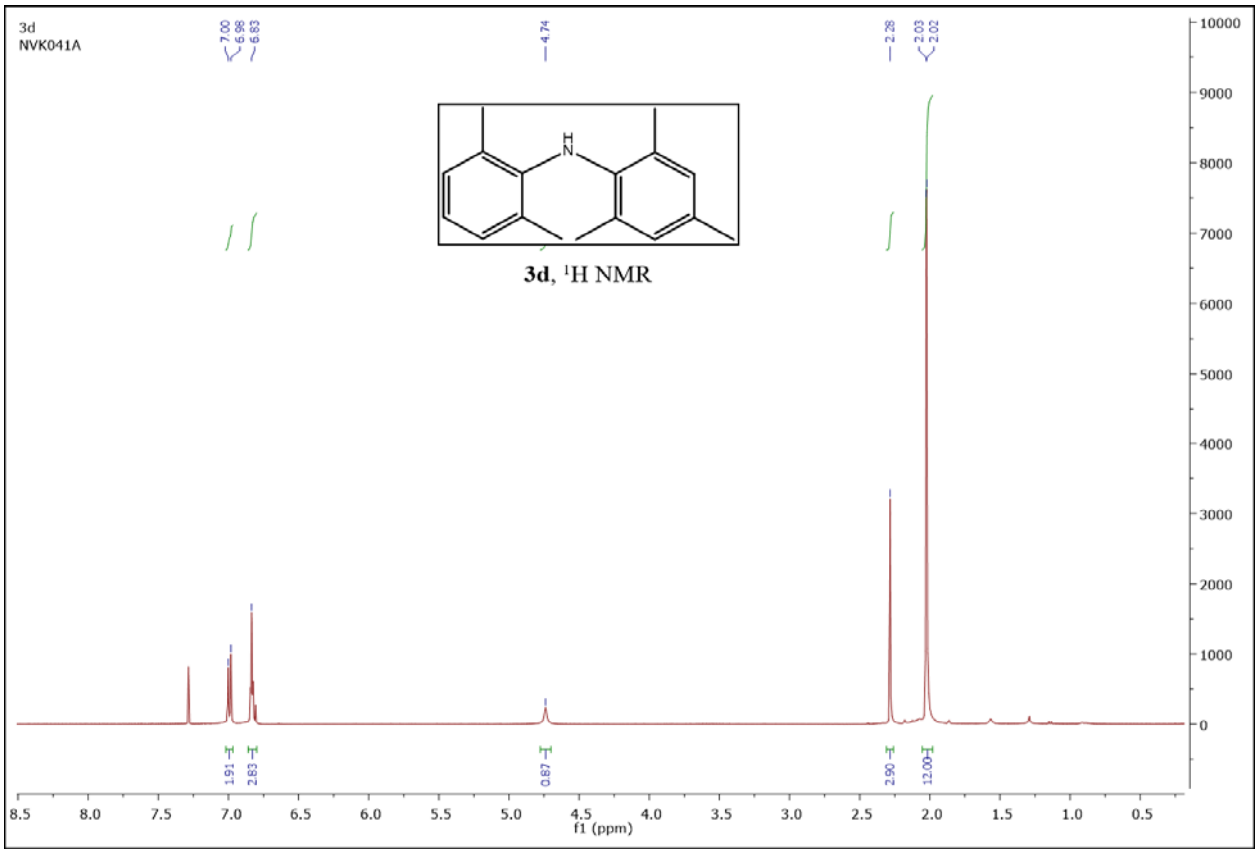
3b, ^{13}C NMR


20181103-3L
7.00
6.99
6.87
6.85
6.84
4.81
2.02
H
N
3.82
1.93
0.91
12.00
f1 (ppm)

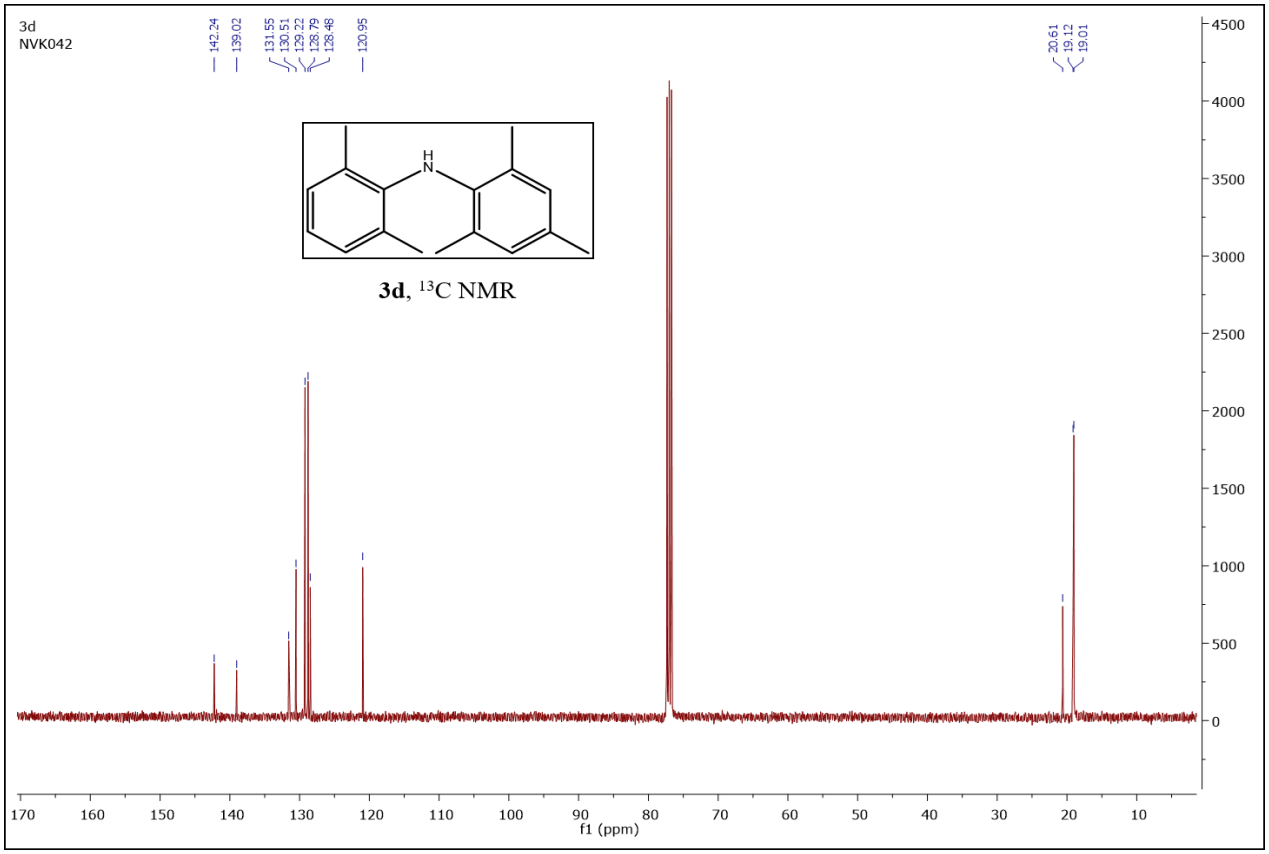
3c, ^{1}H NMR



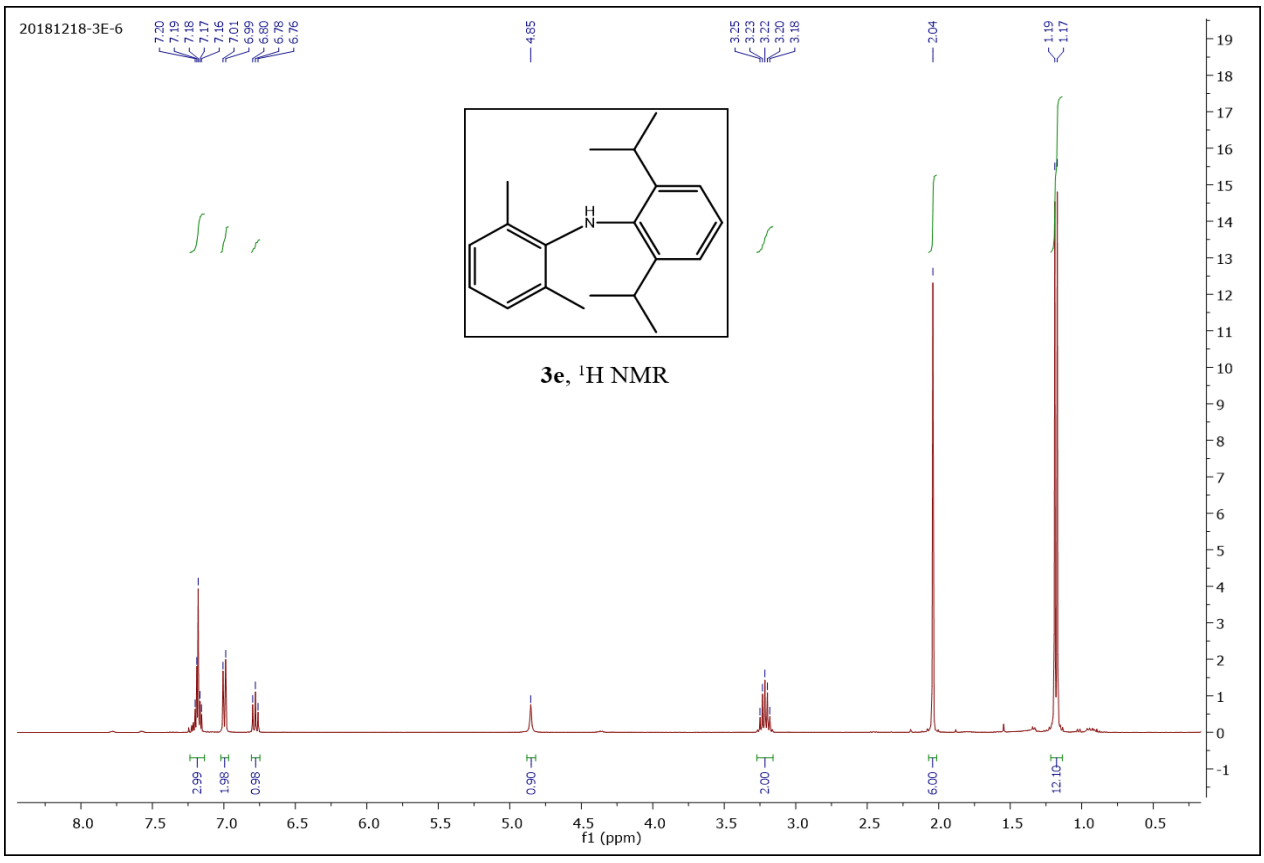
3c, ^{13}C NMR



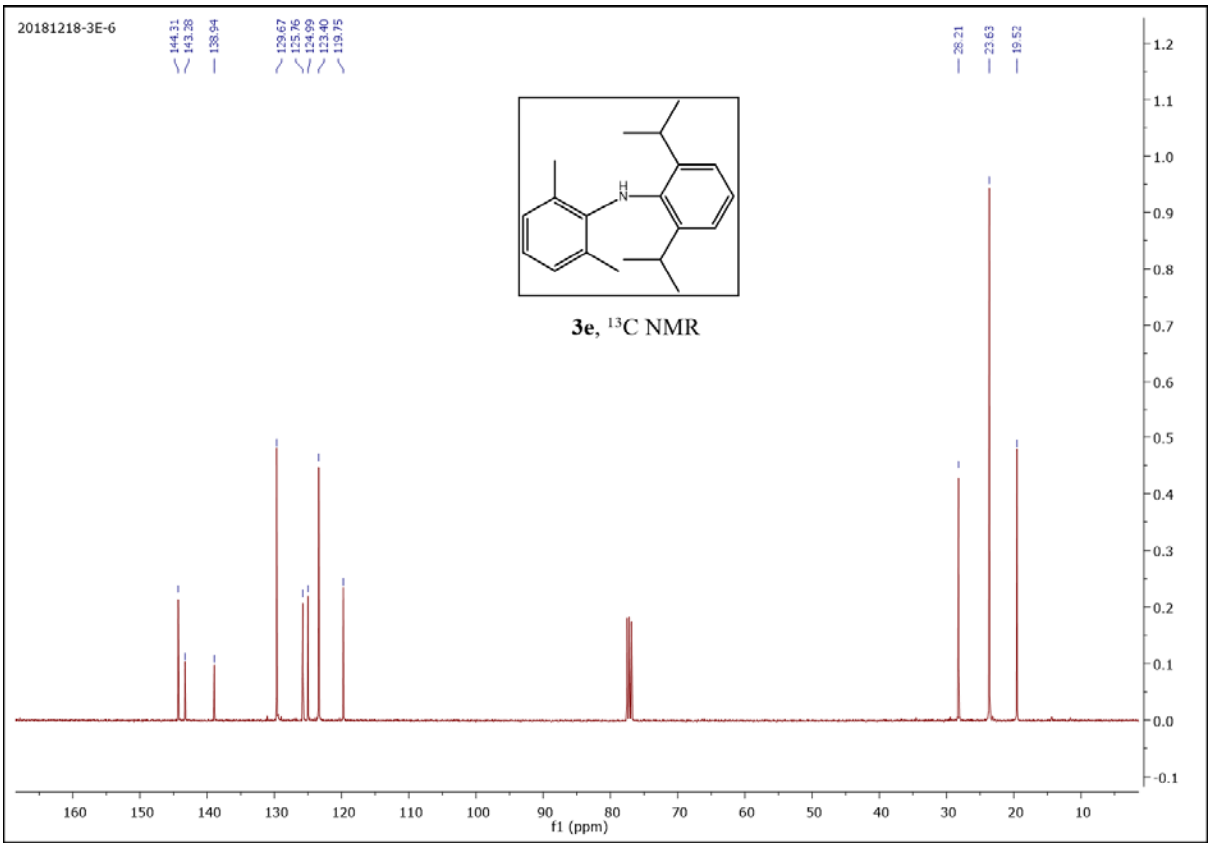
3d, ^{1}H NMR



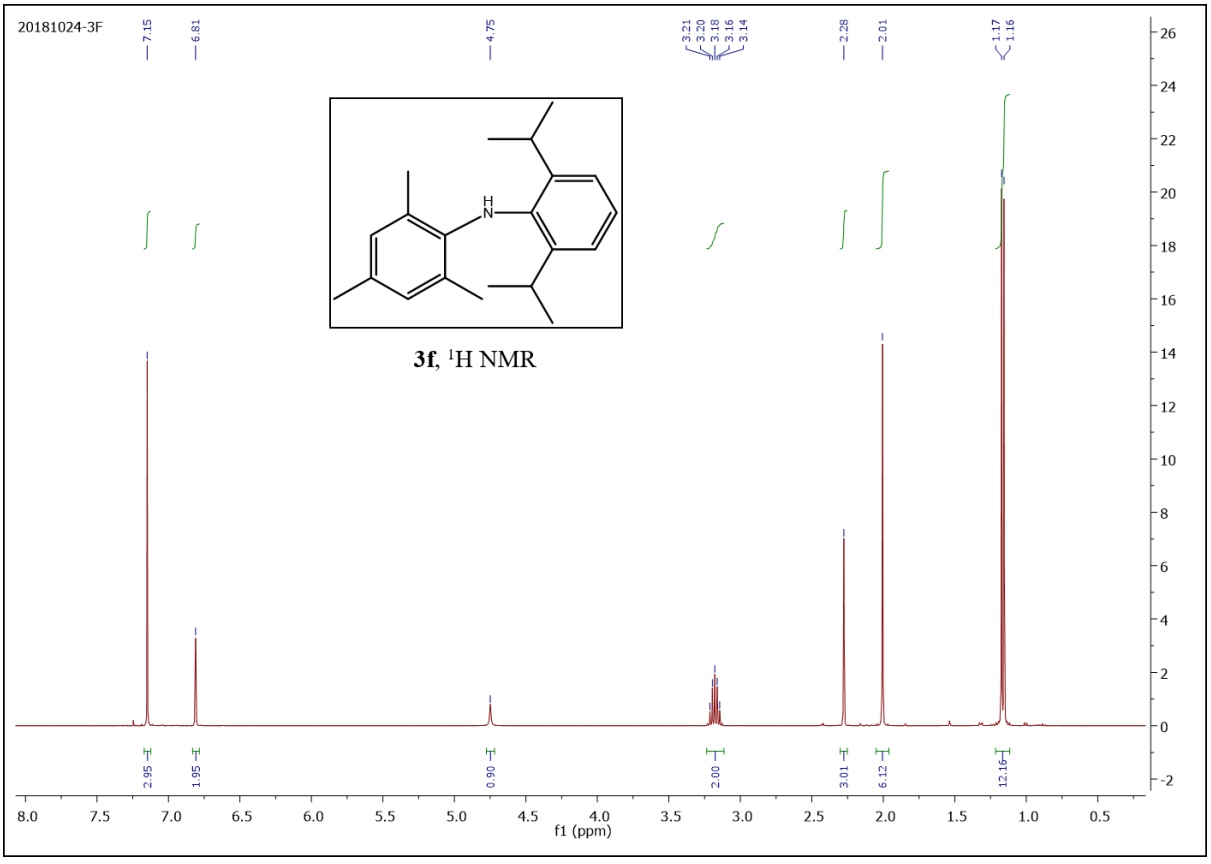
3d, ^{13}C NMR



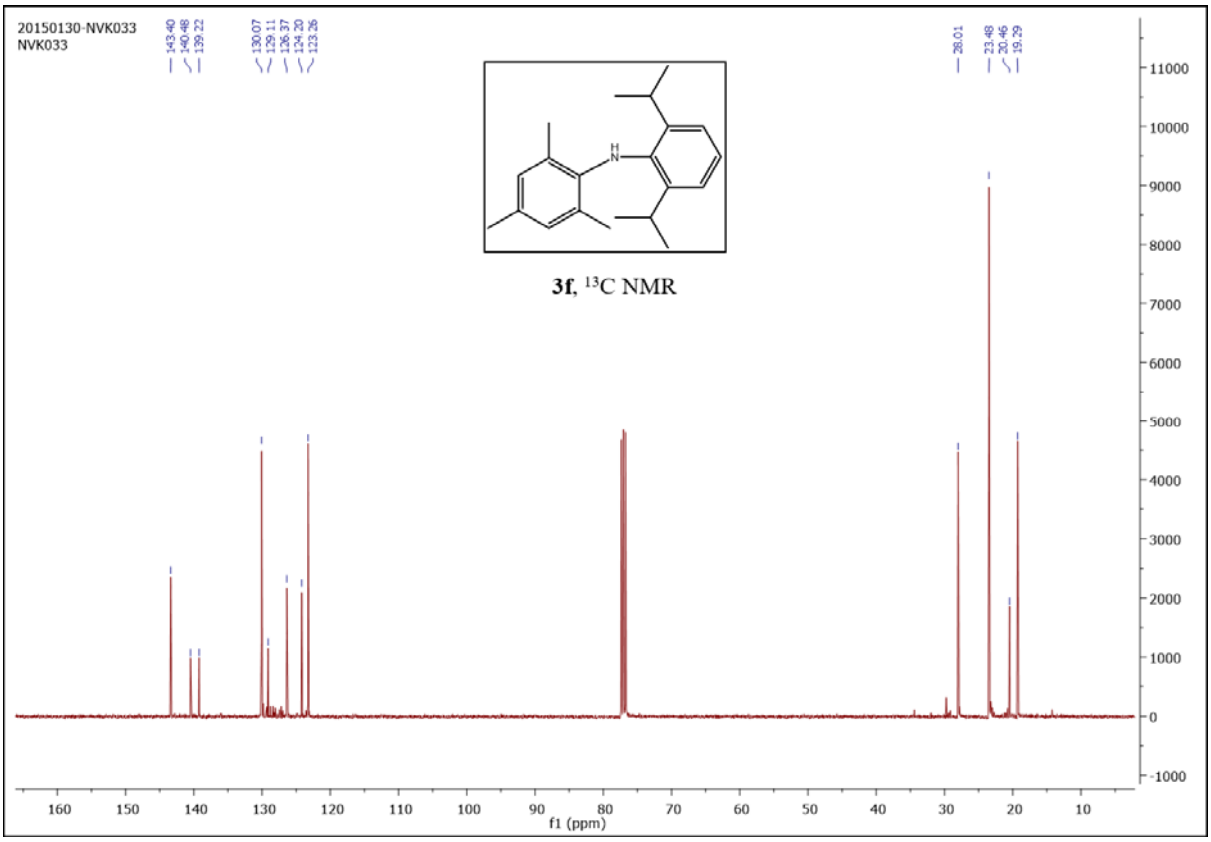
3e, ^{1}H NMR



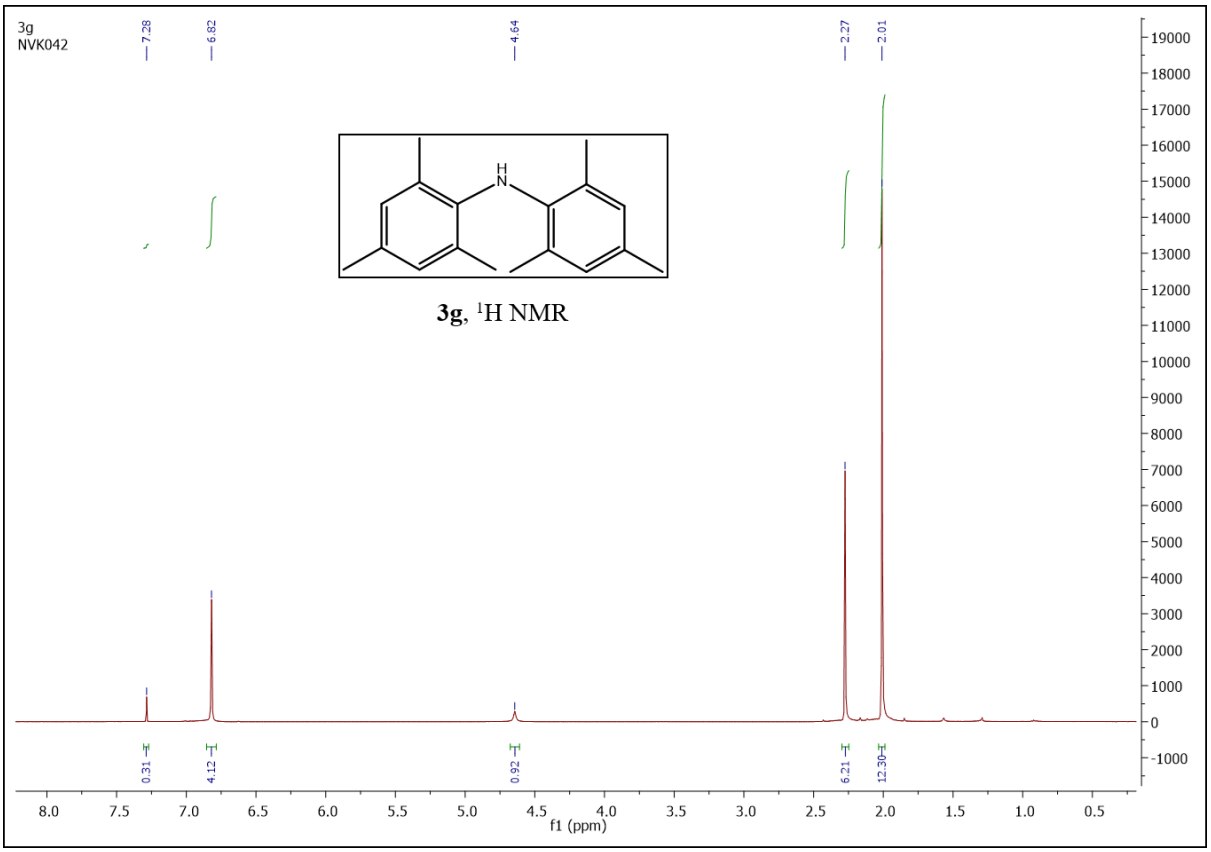
3e, ^{13}C NMR



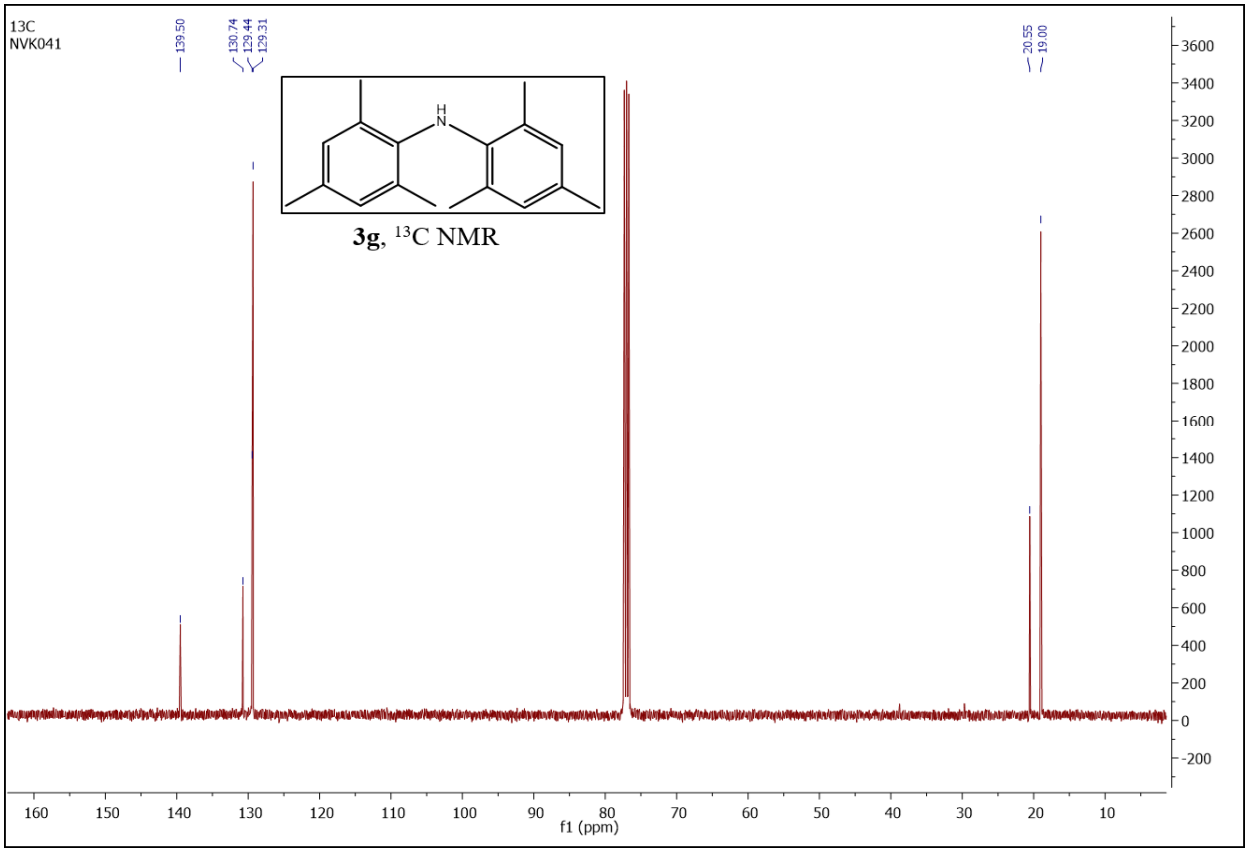
3f, ^{1}H NMR



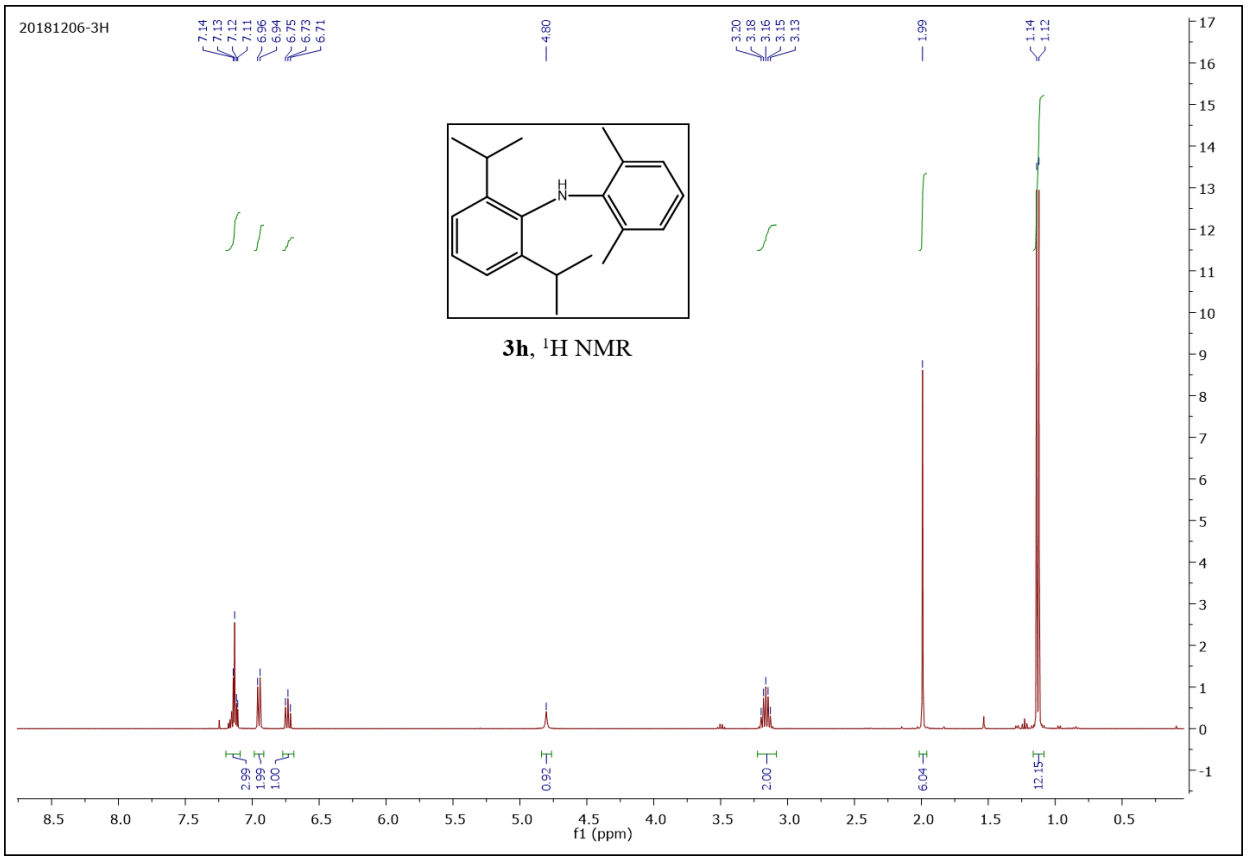
3f, ^{13}C NMR



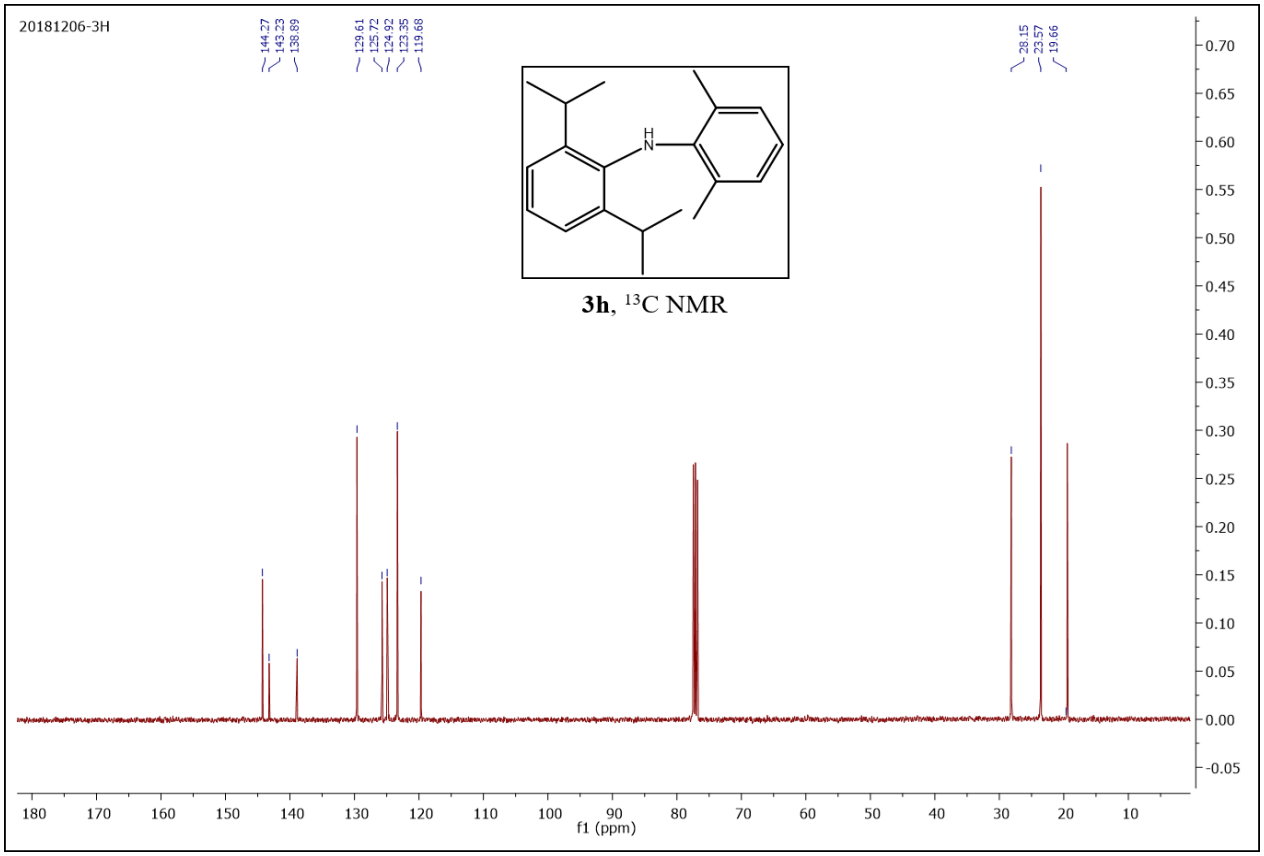
3g, ^{1}H NMR



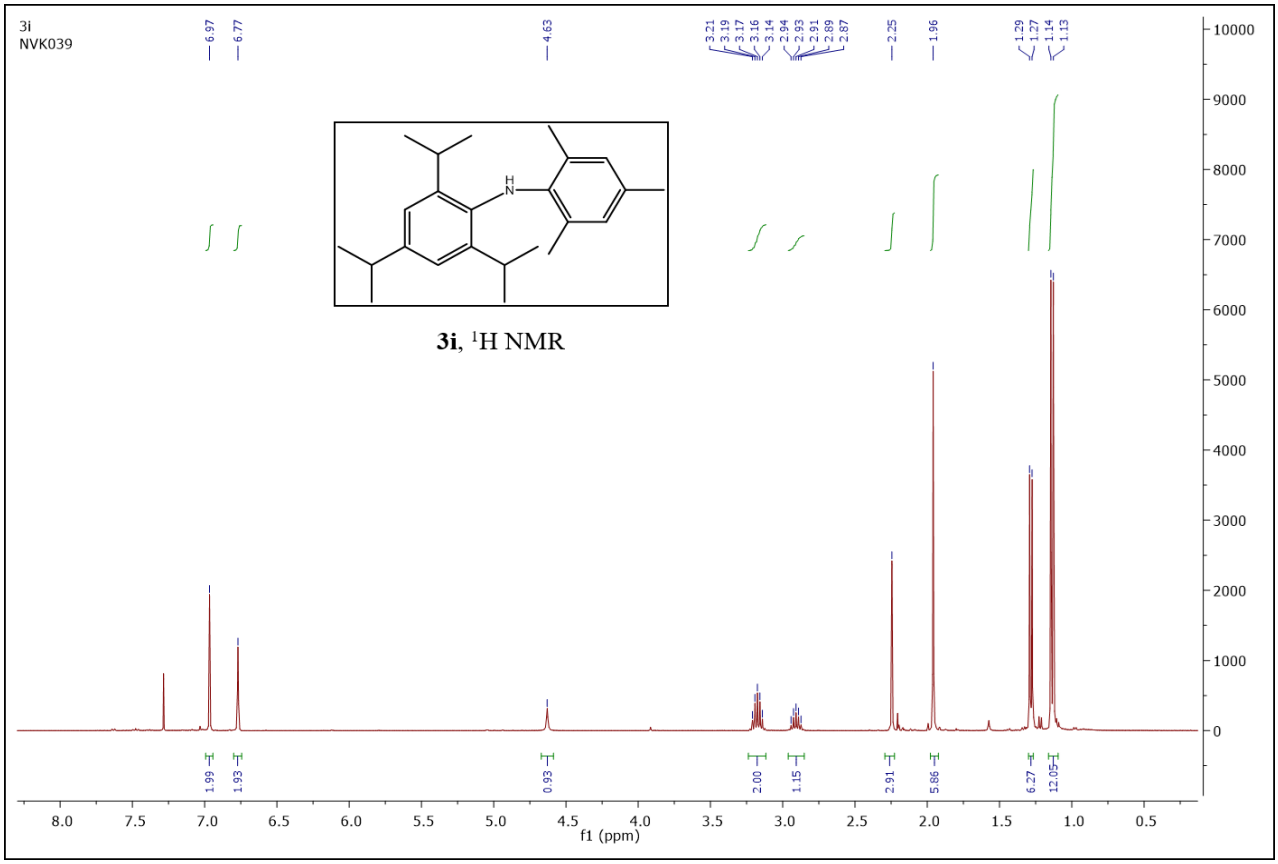
3g, ^{13}C NMR



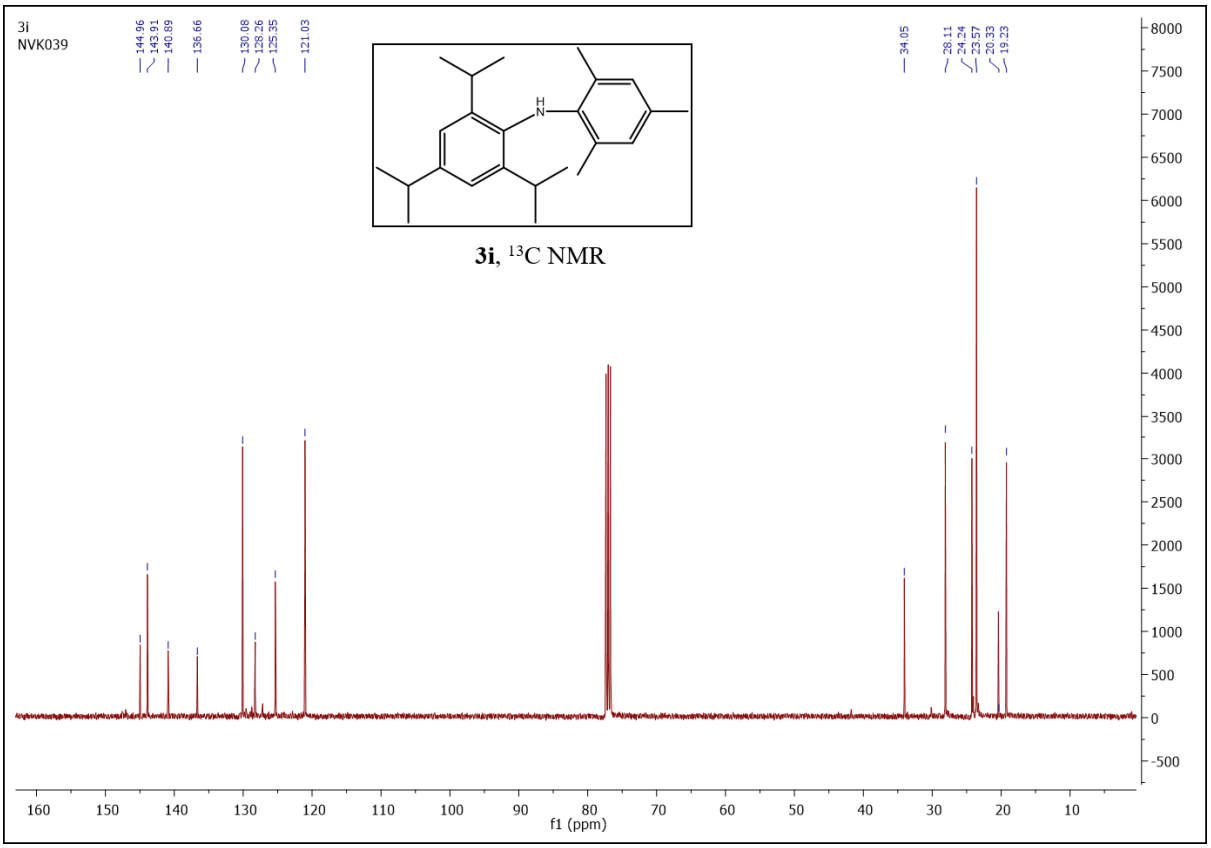
3h, ^{1}H NMR



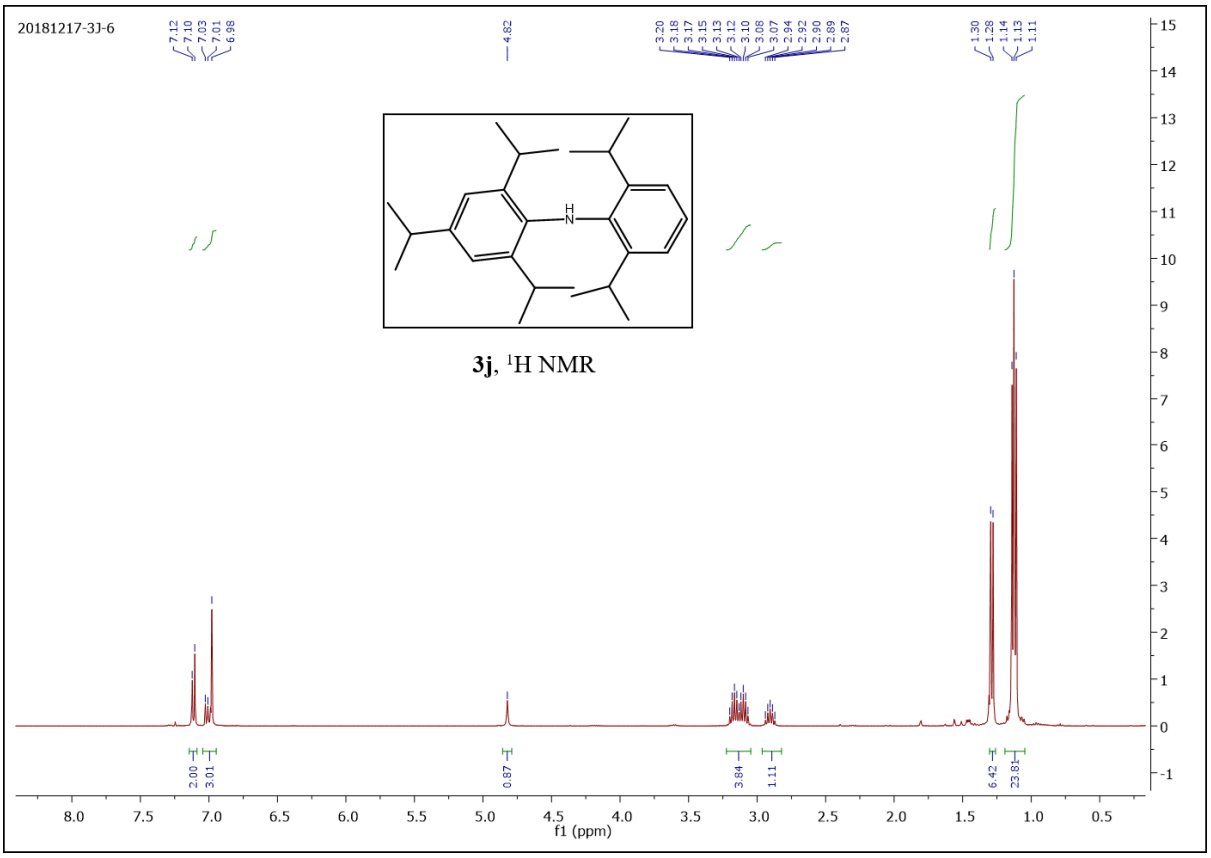
3h, ^{13}C NMR



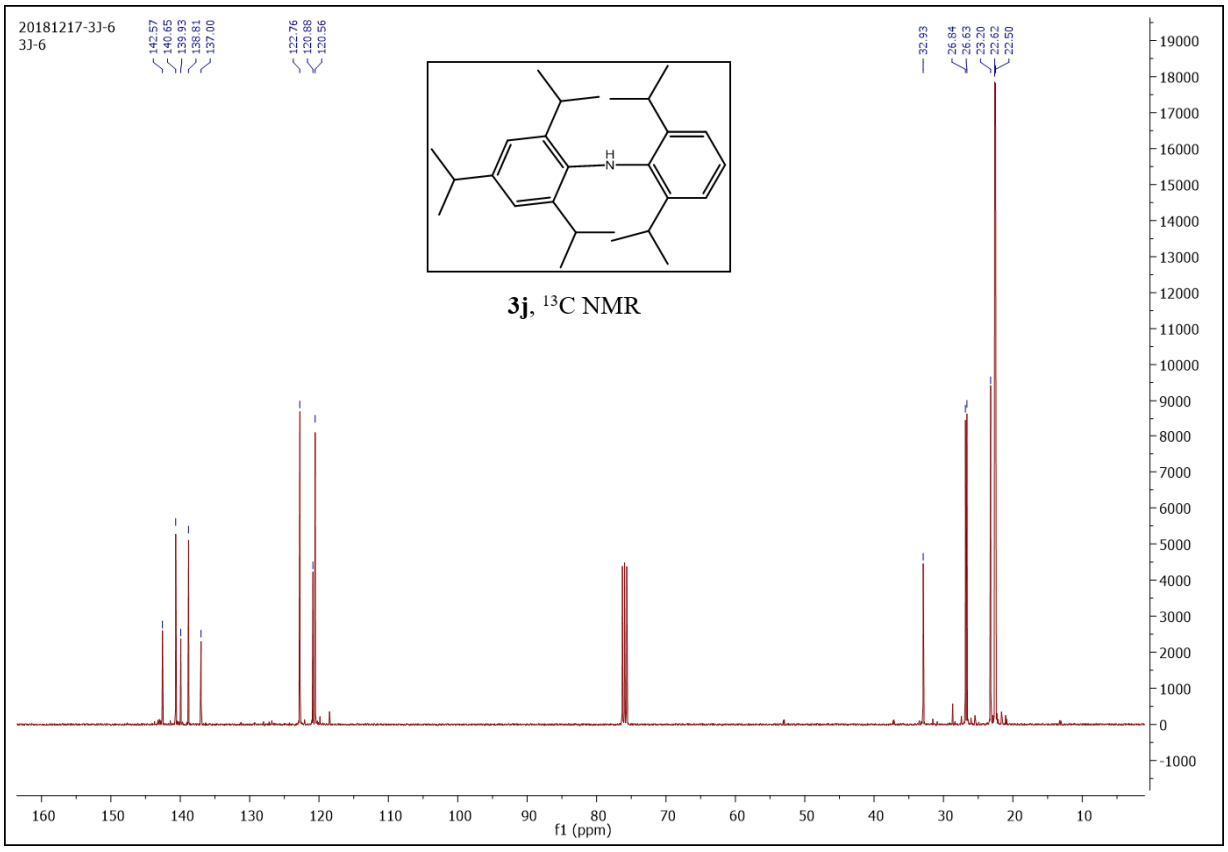
3i, ^{1}H NMR



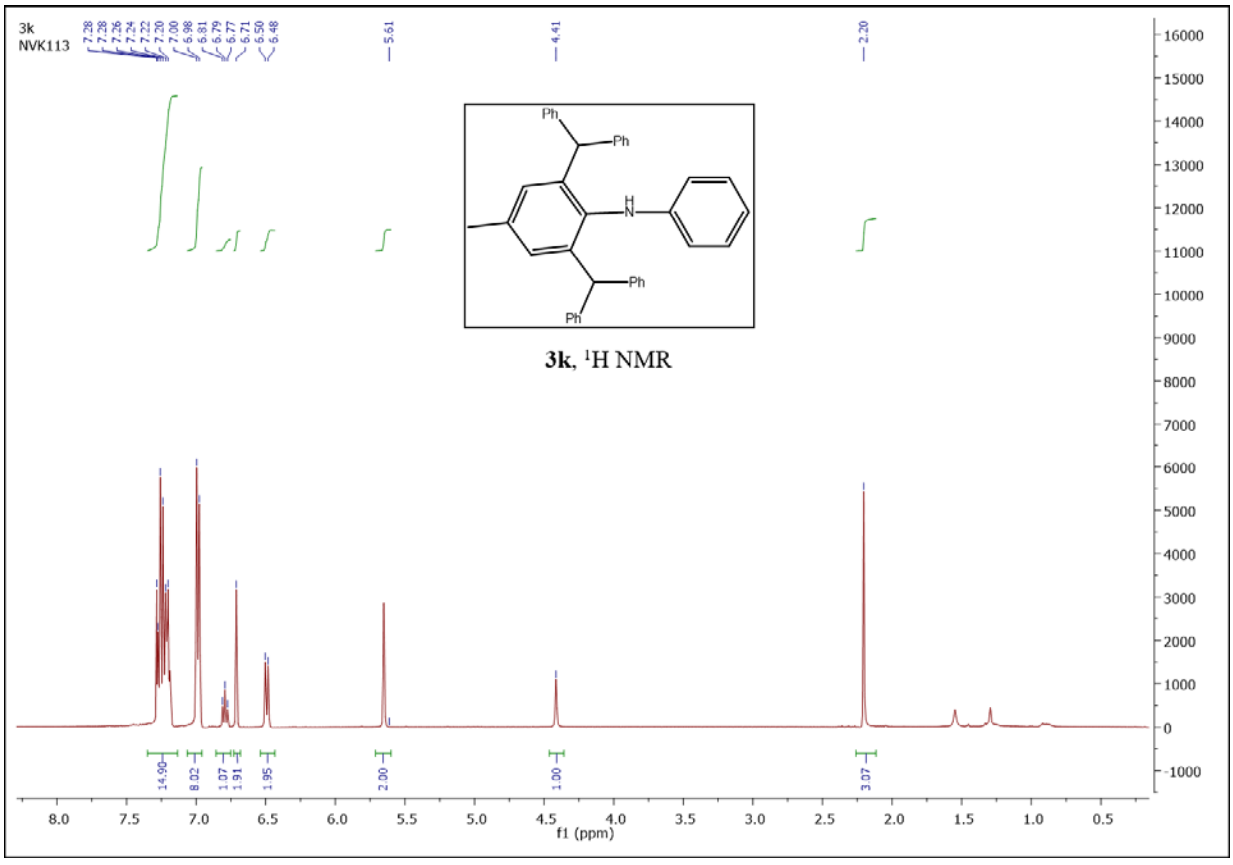
3i, ^{13}C NMR



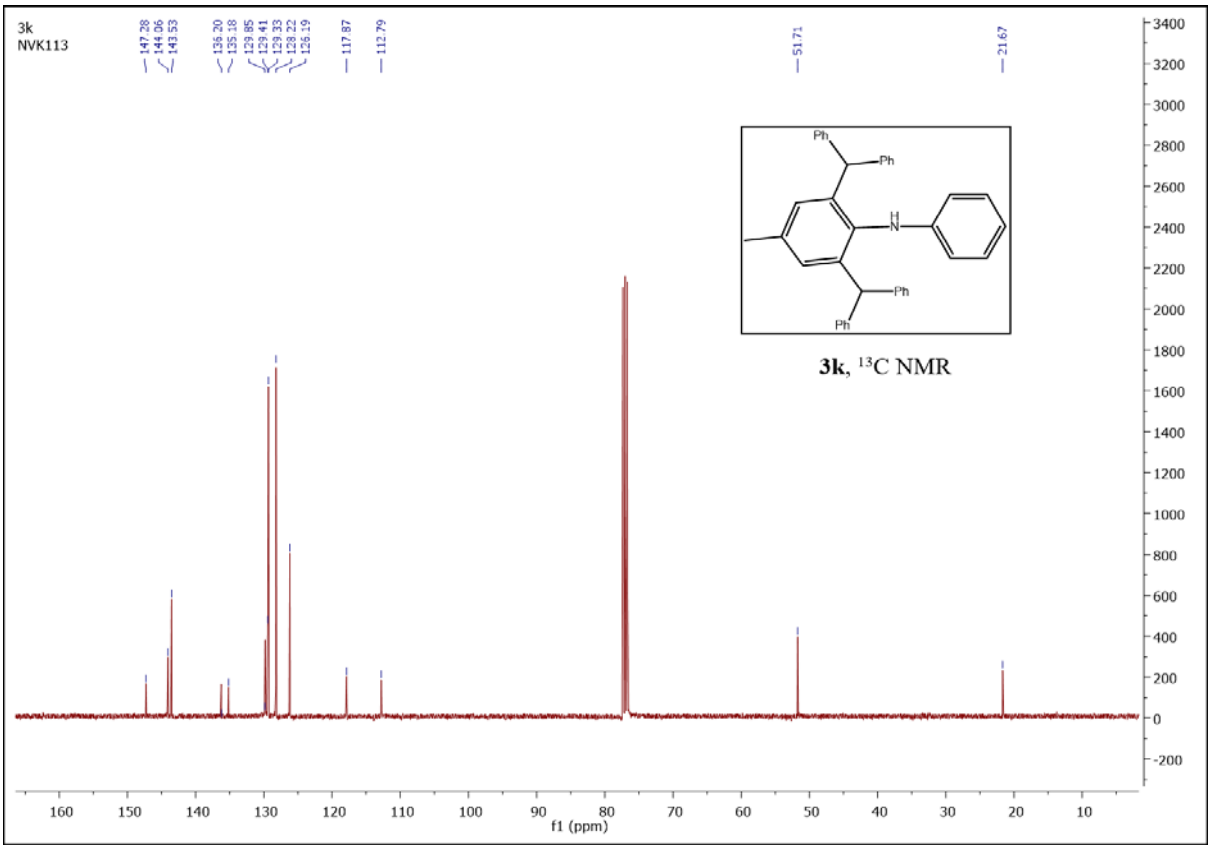
3j, ^{1}H NMR



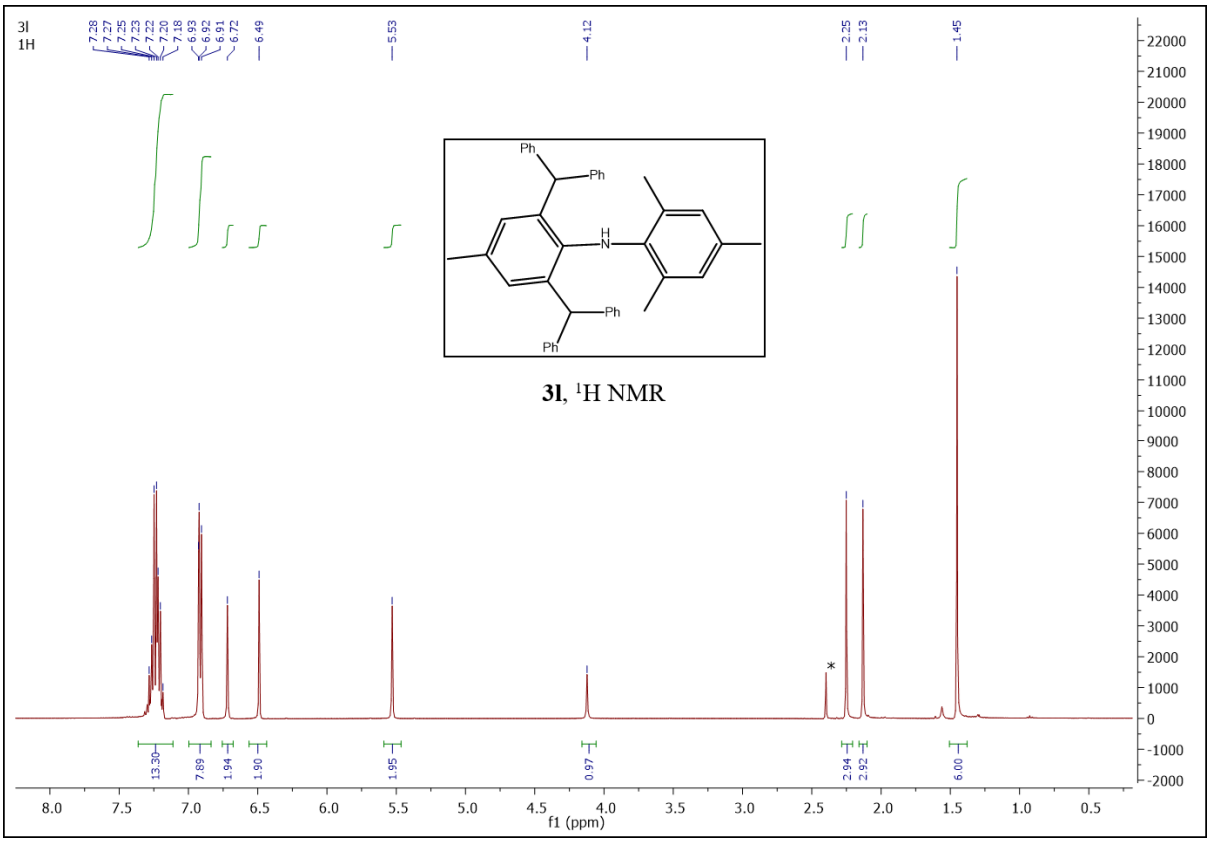
3j, ^{13}C NMR



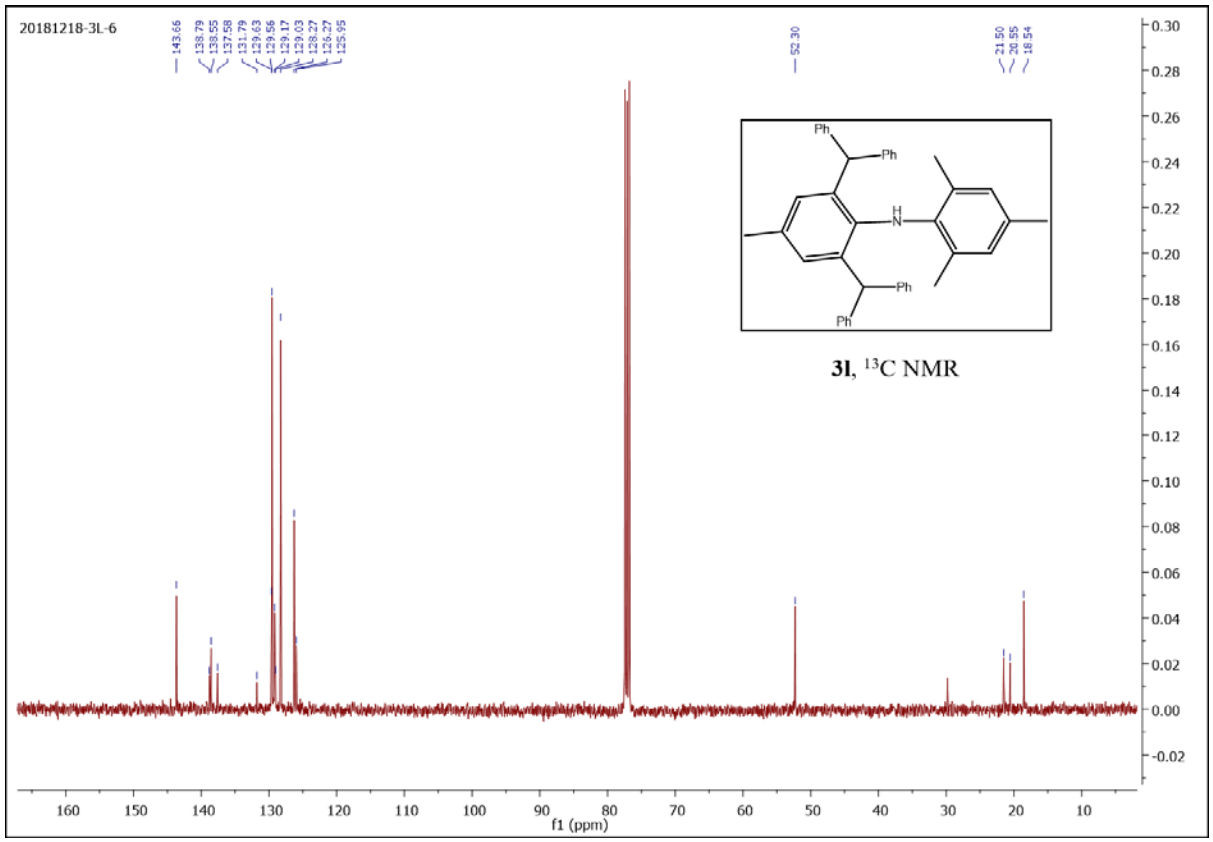
3k, ^{1}H NMR



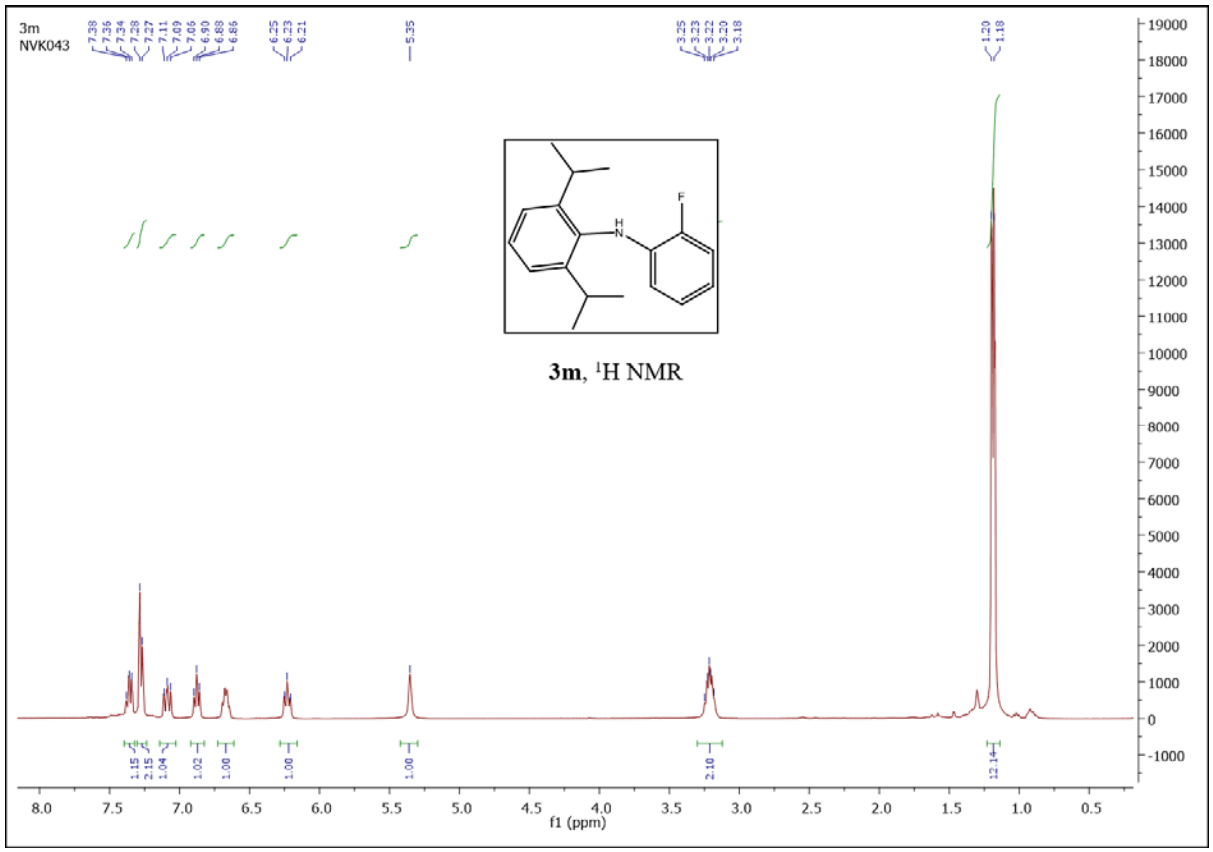
3k, ^{13}C NMR



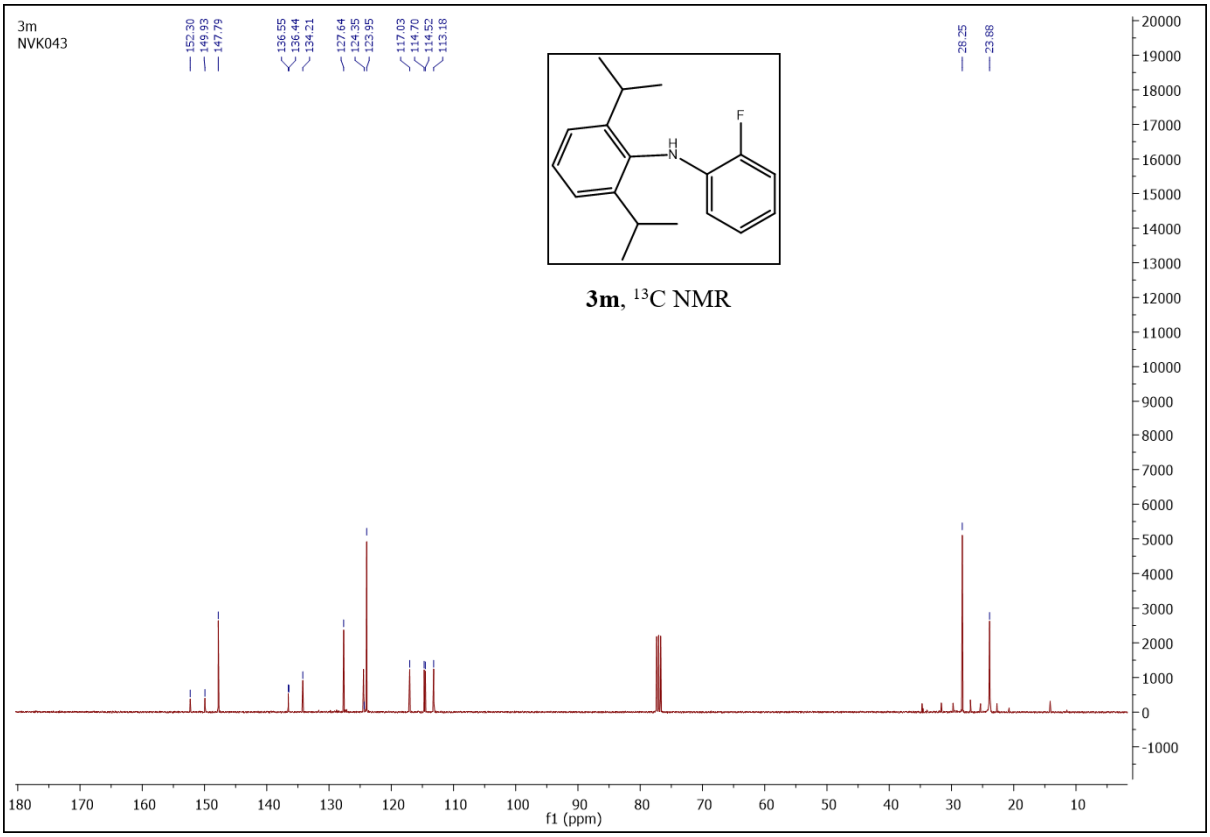
3l, ^{1}H NMR



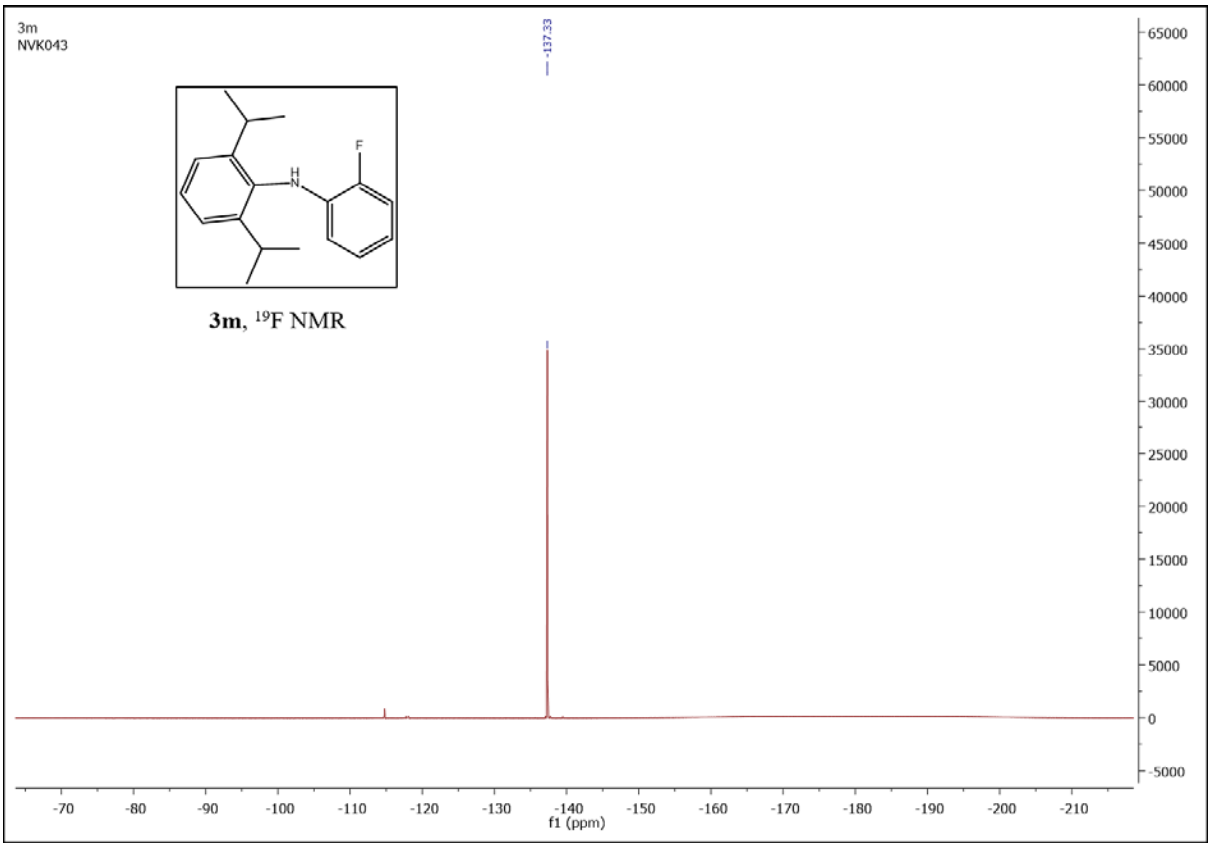
3l, ^{13}C NMR



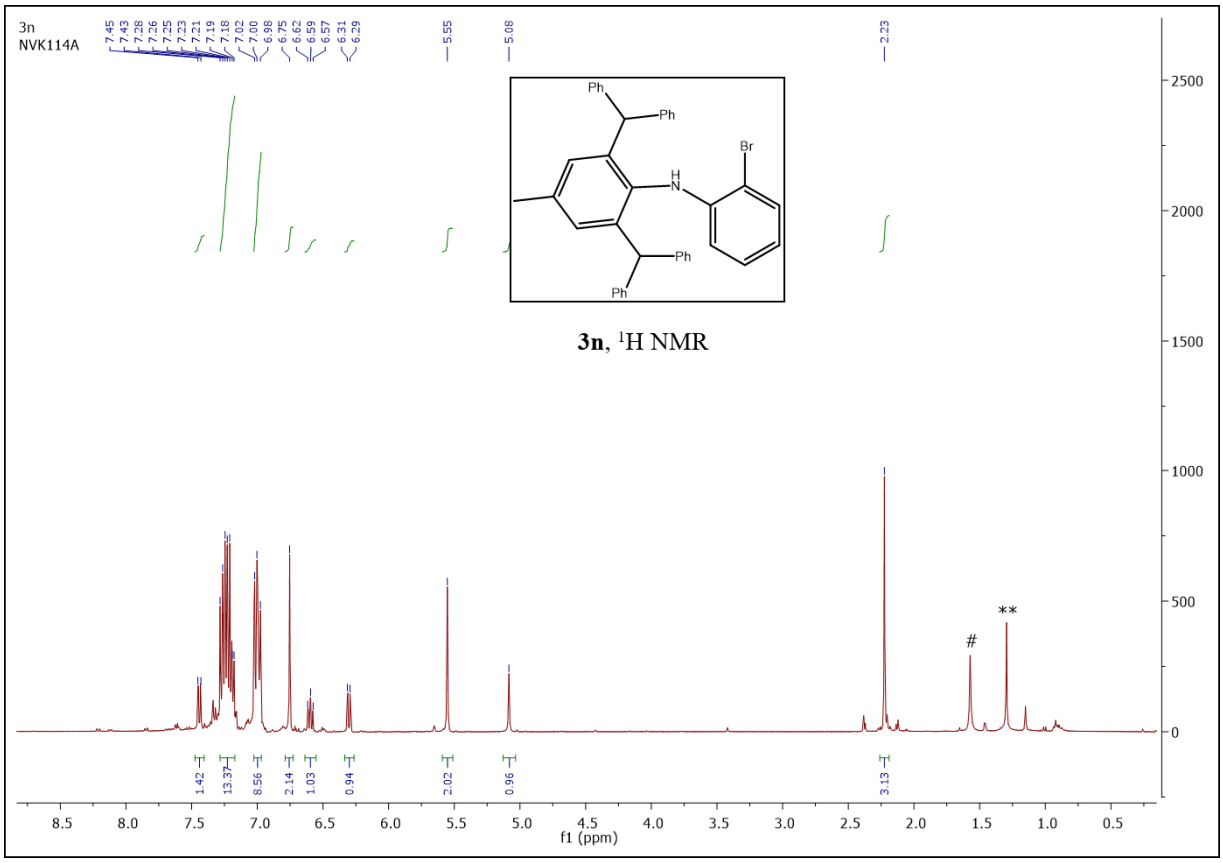
3m, ^{1}H NMR



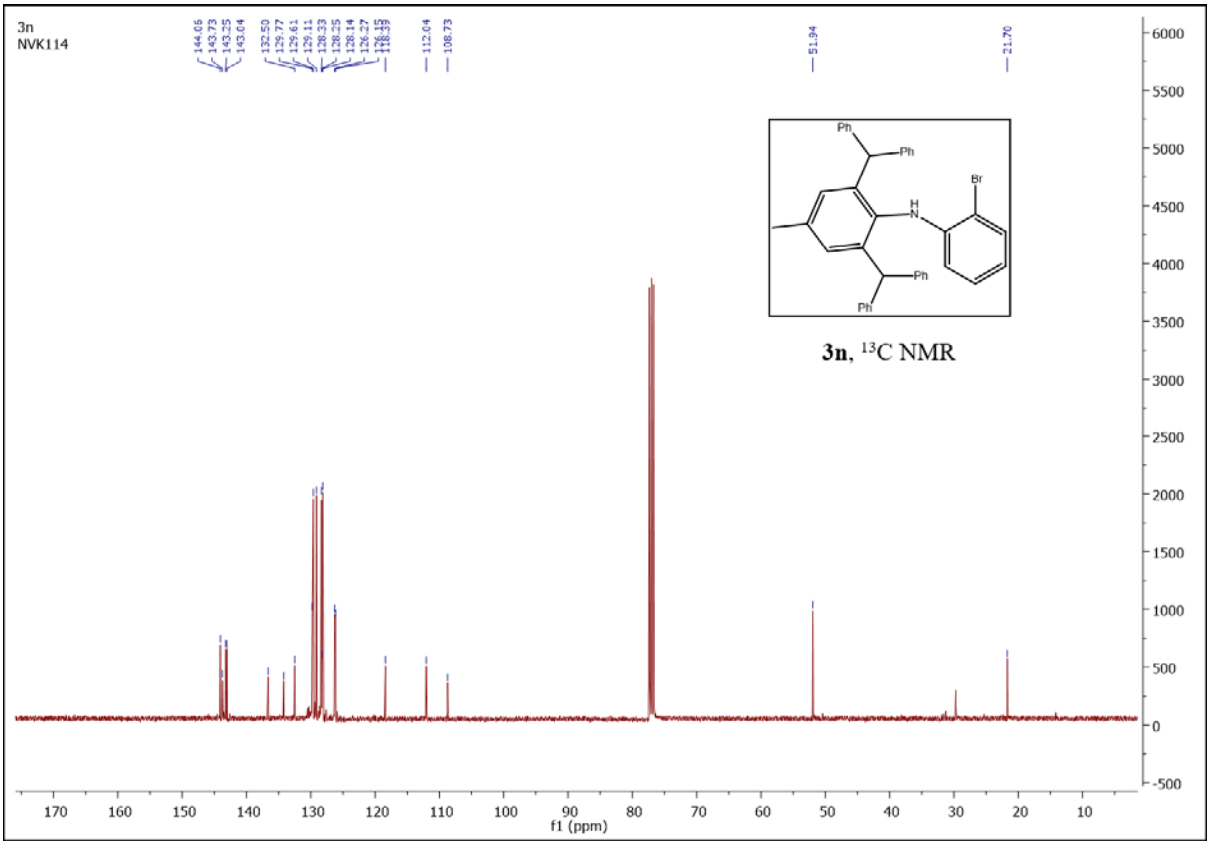
3m, ^{13}C NMR



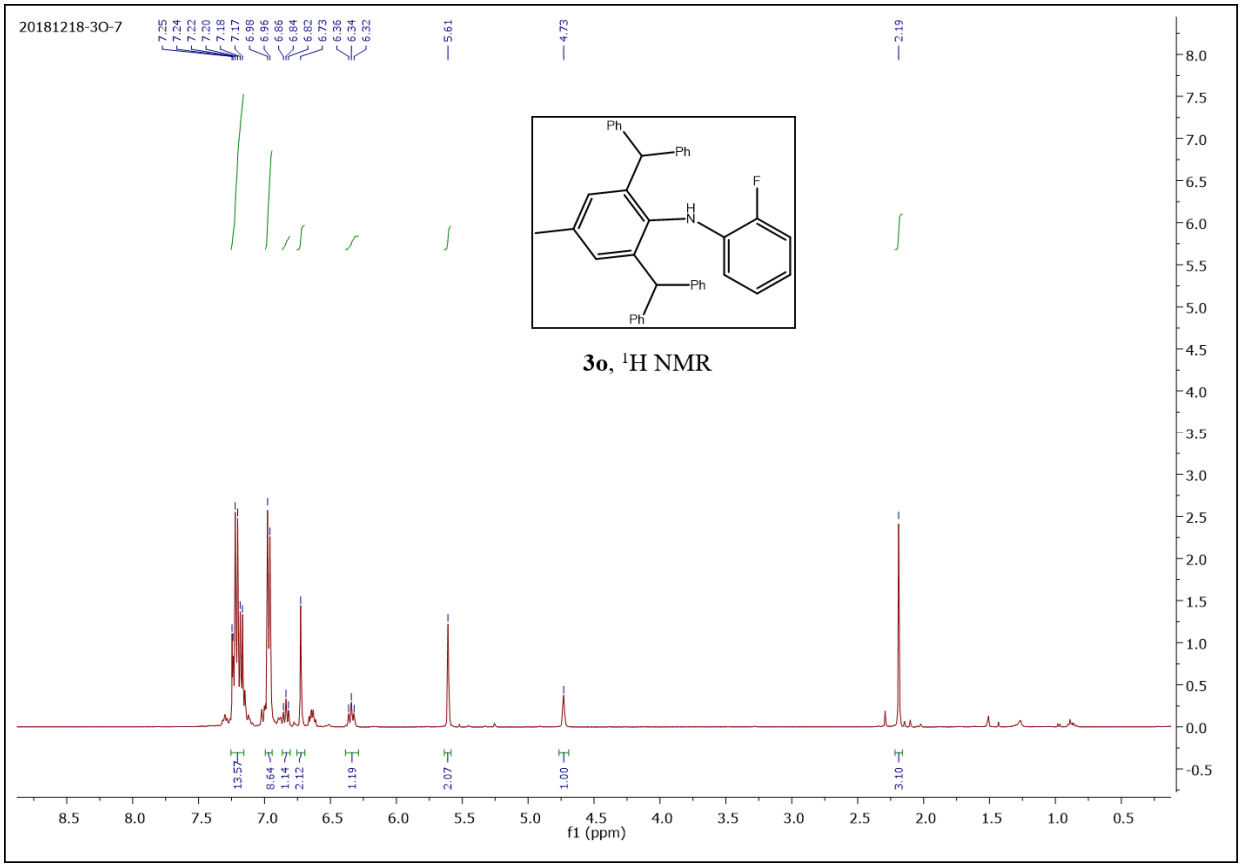
3m, ^{19}F NMR



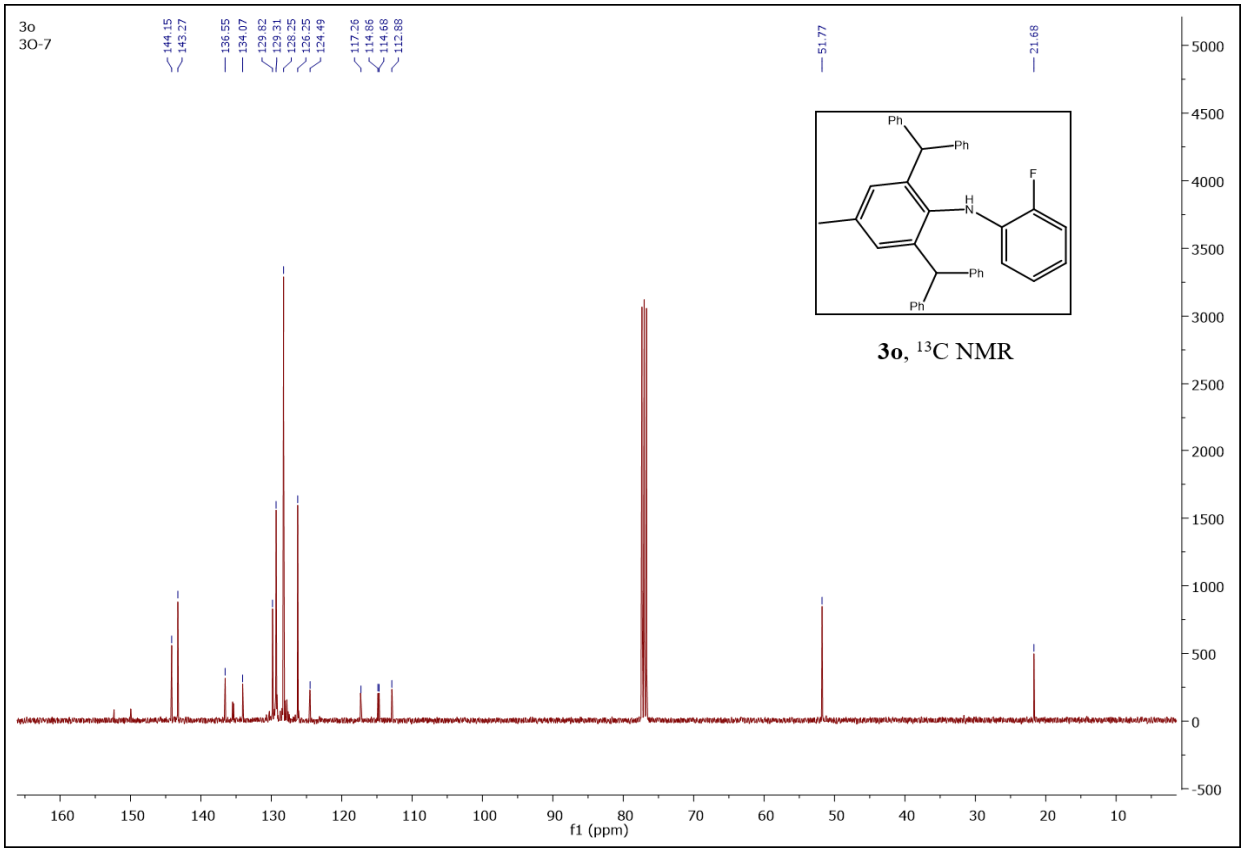
3n, ^{1}H NMR



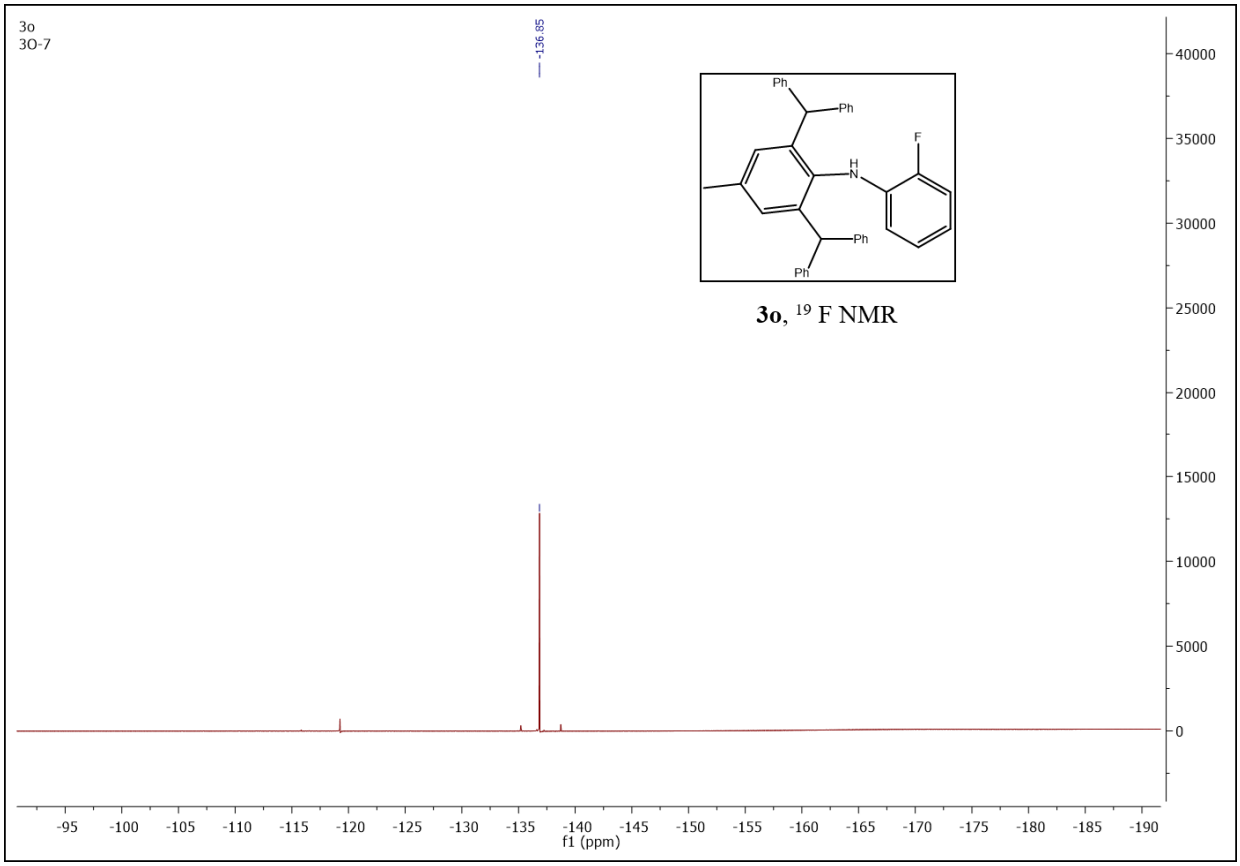
3n, ^{13}C NMR



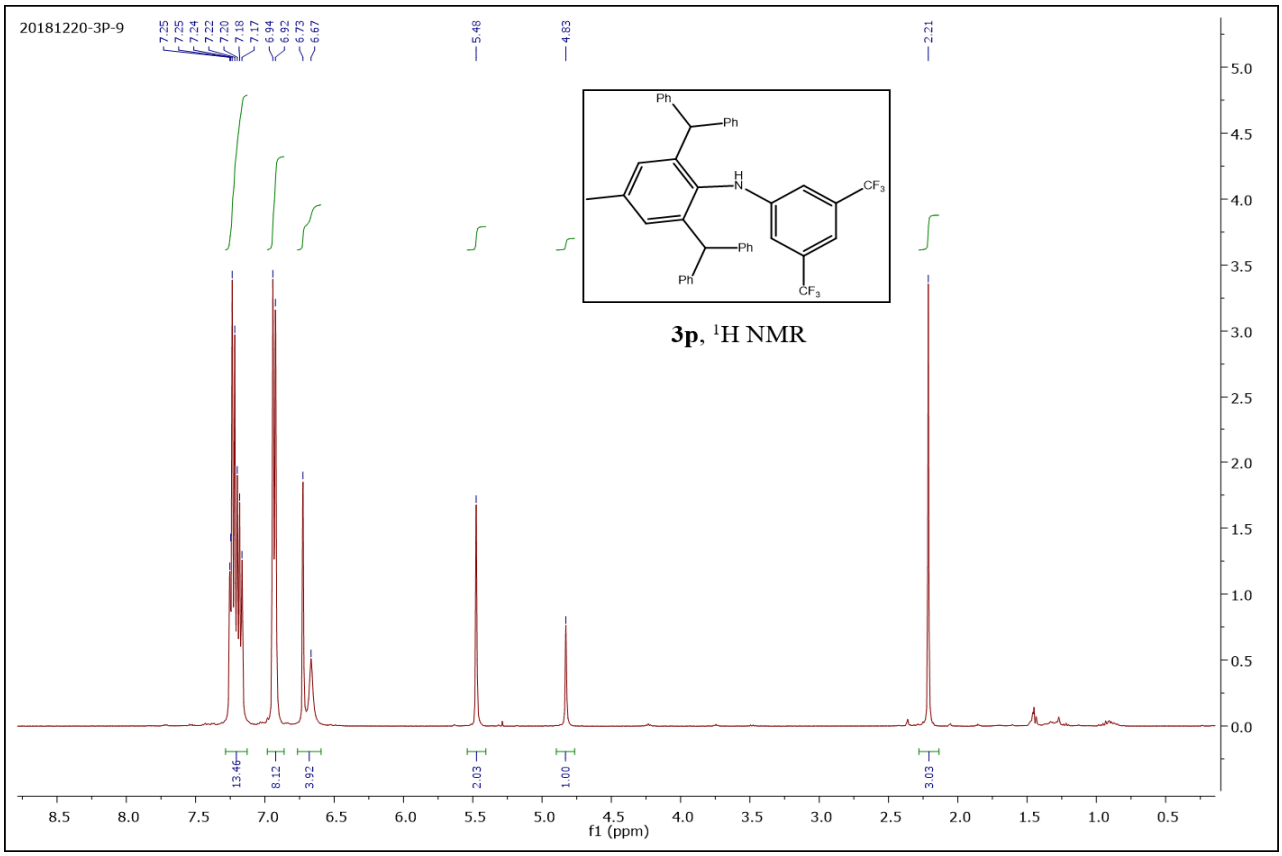
3o, ^{1}H NMR



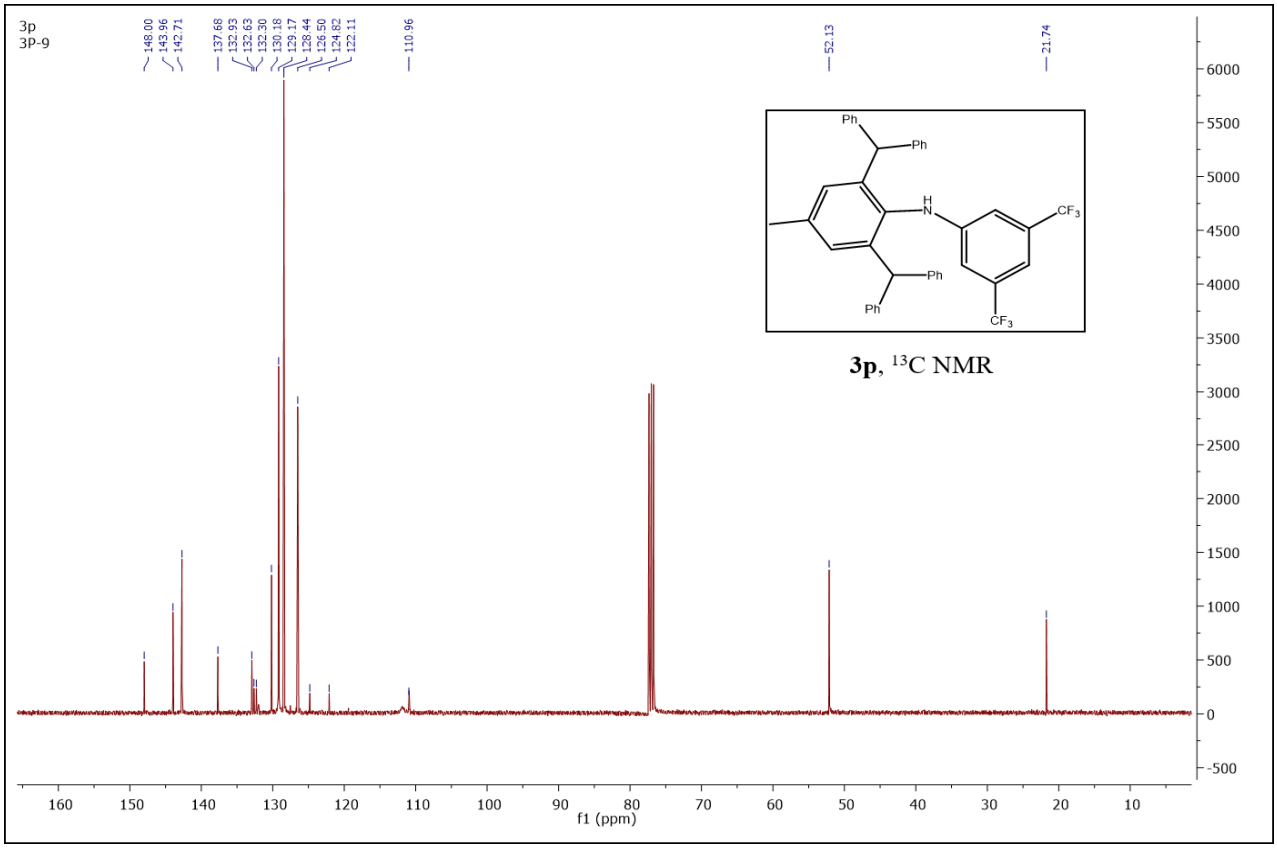
3o, ^{13}C NMR


3o
3O-7
-136.85
Ph
Ph
F
H
N
Ph
Ph
40000
35000
30000
25000
20000
15000
10000
5000
0
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
-185
-190
f1 (ppm)

3o, ^{19} F NMR



3p, ^{1}H NMR



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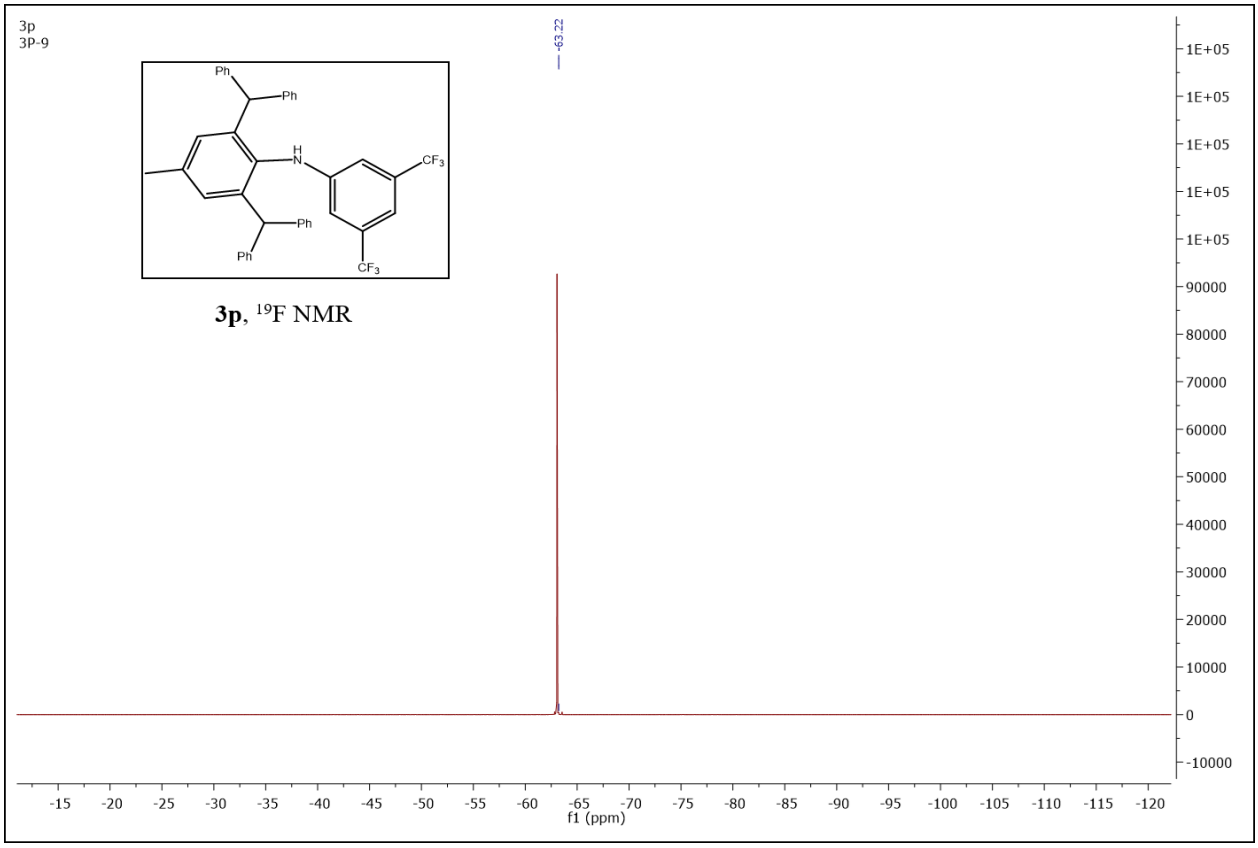
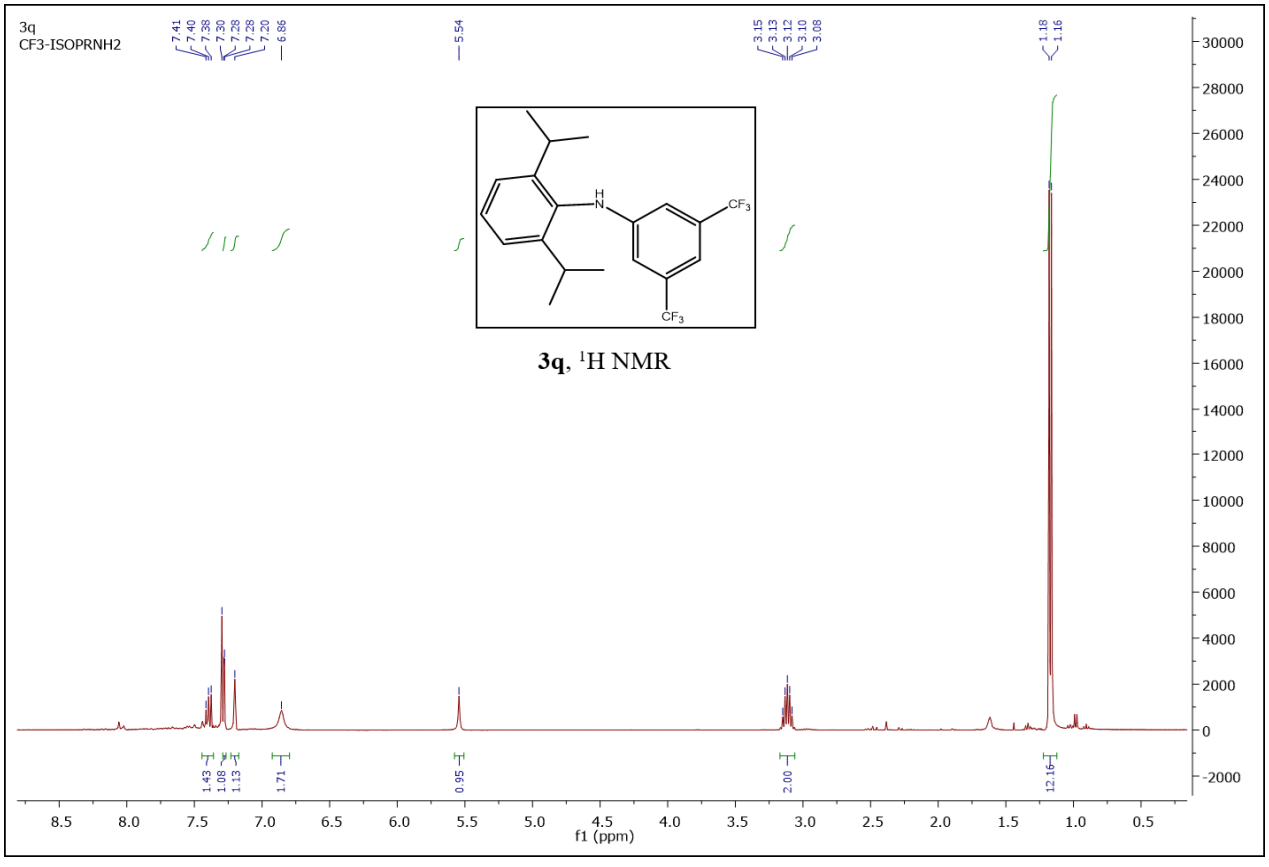
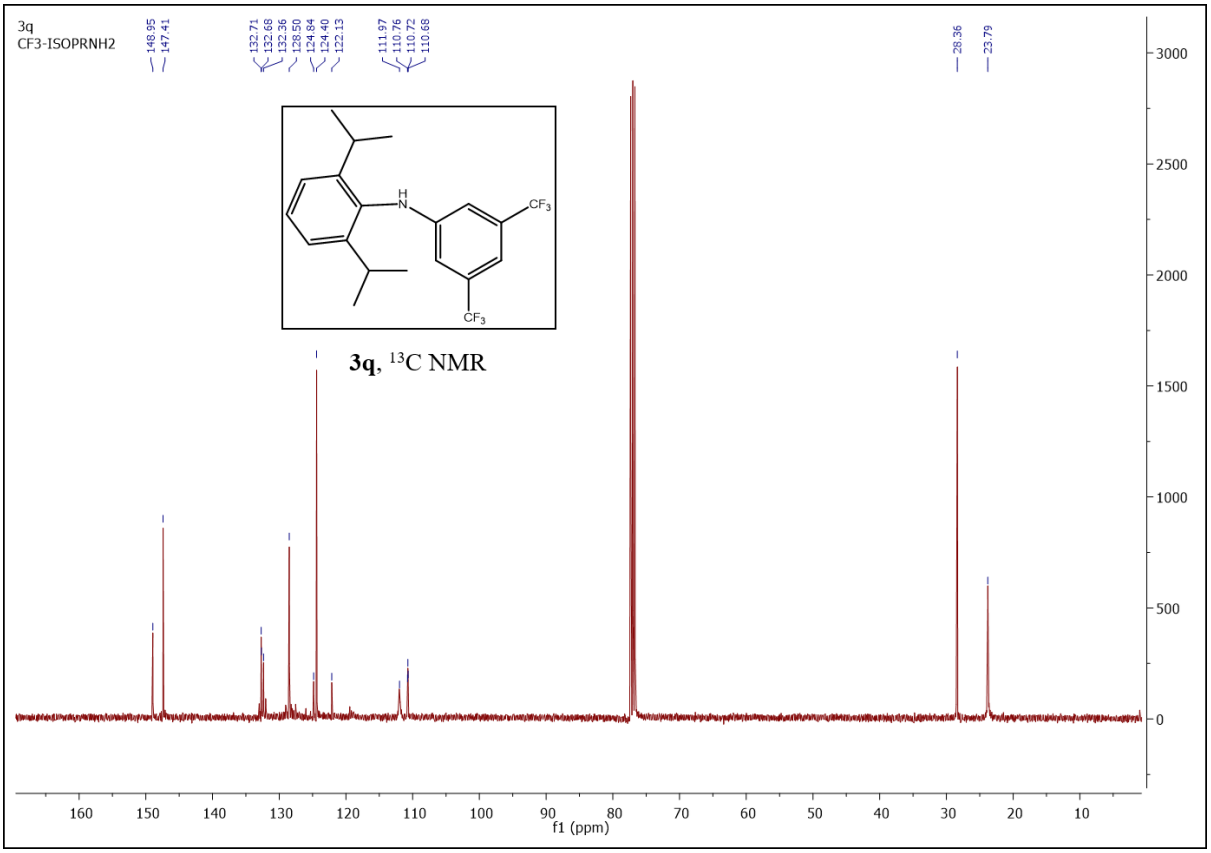


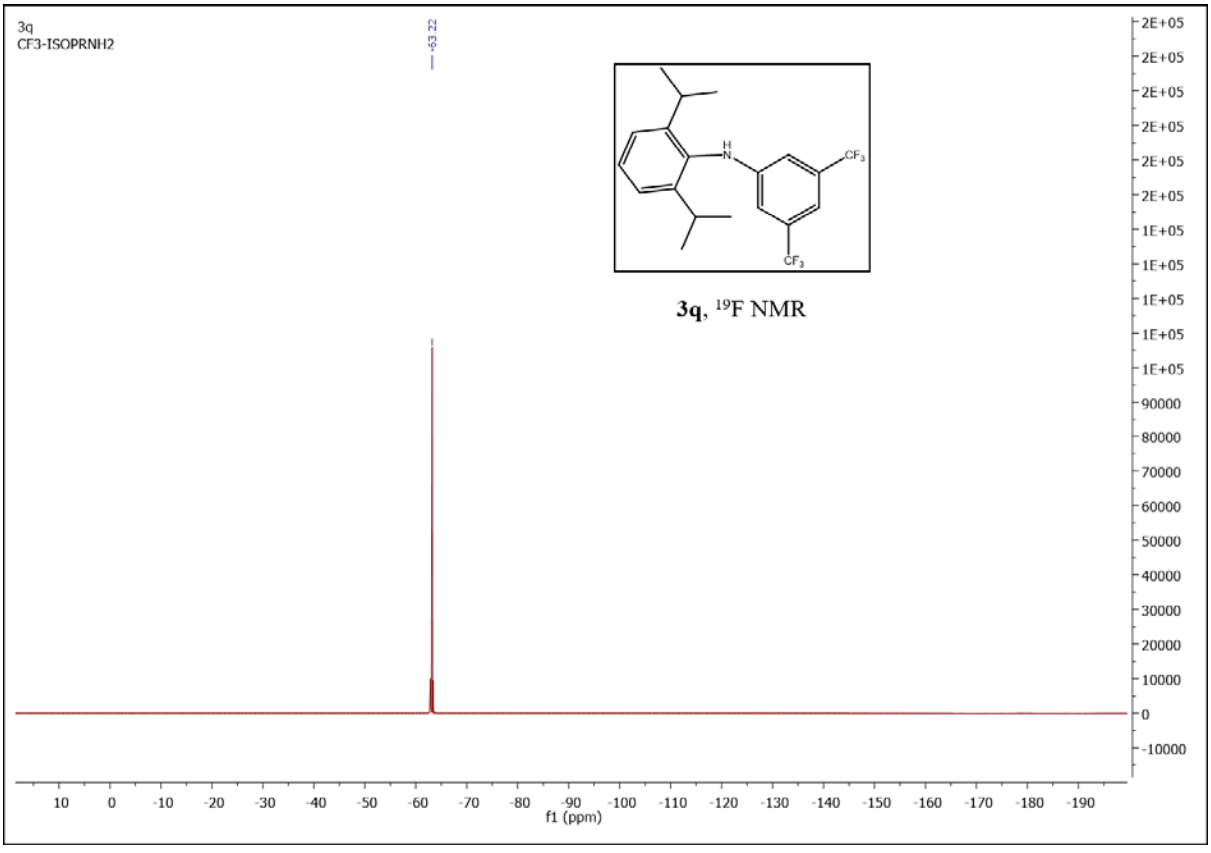
3p, ^{19}F NMR



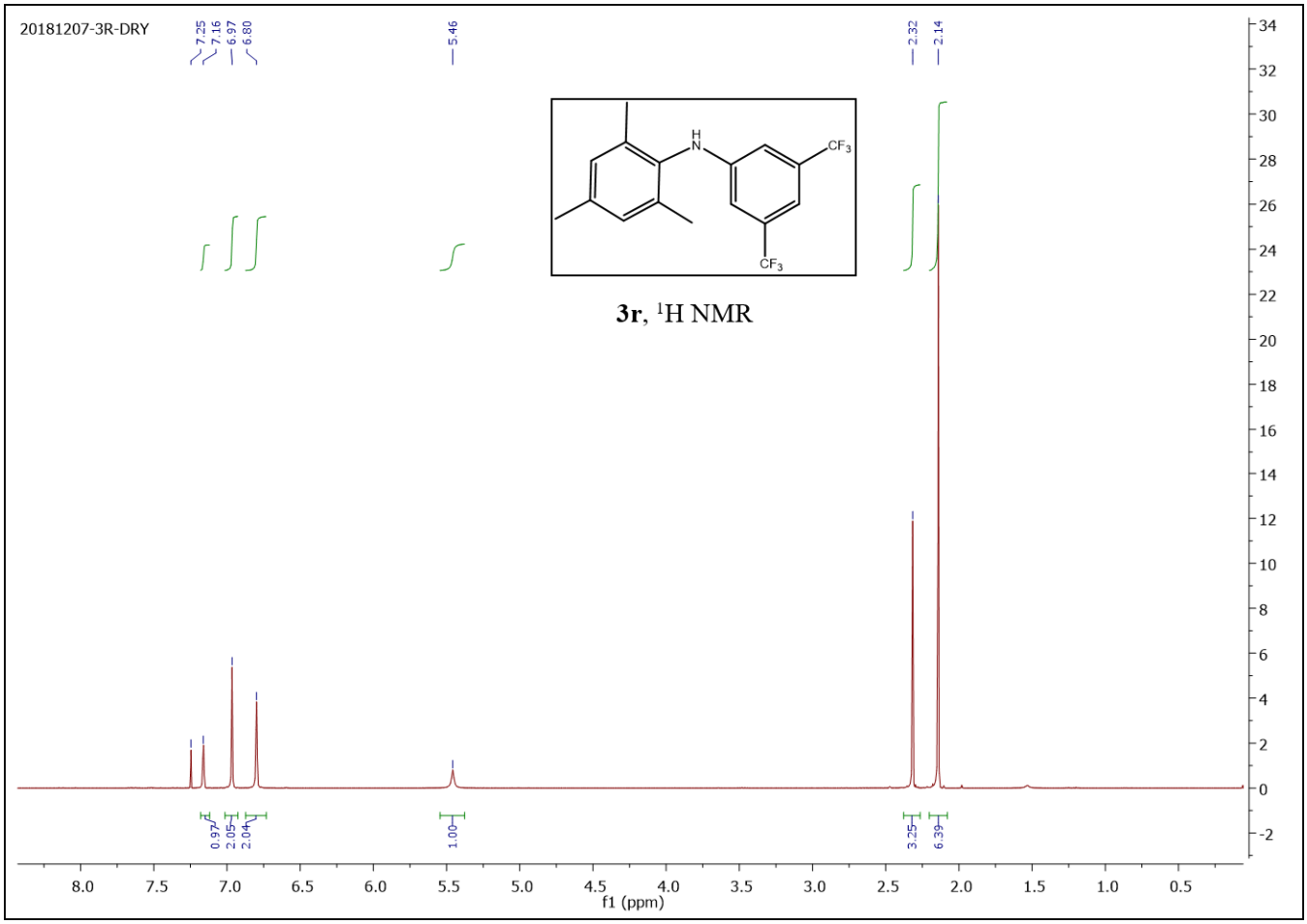
3q, ^{1}H NMR



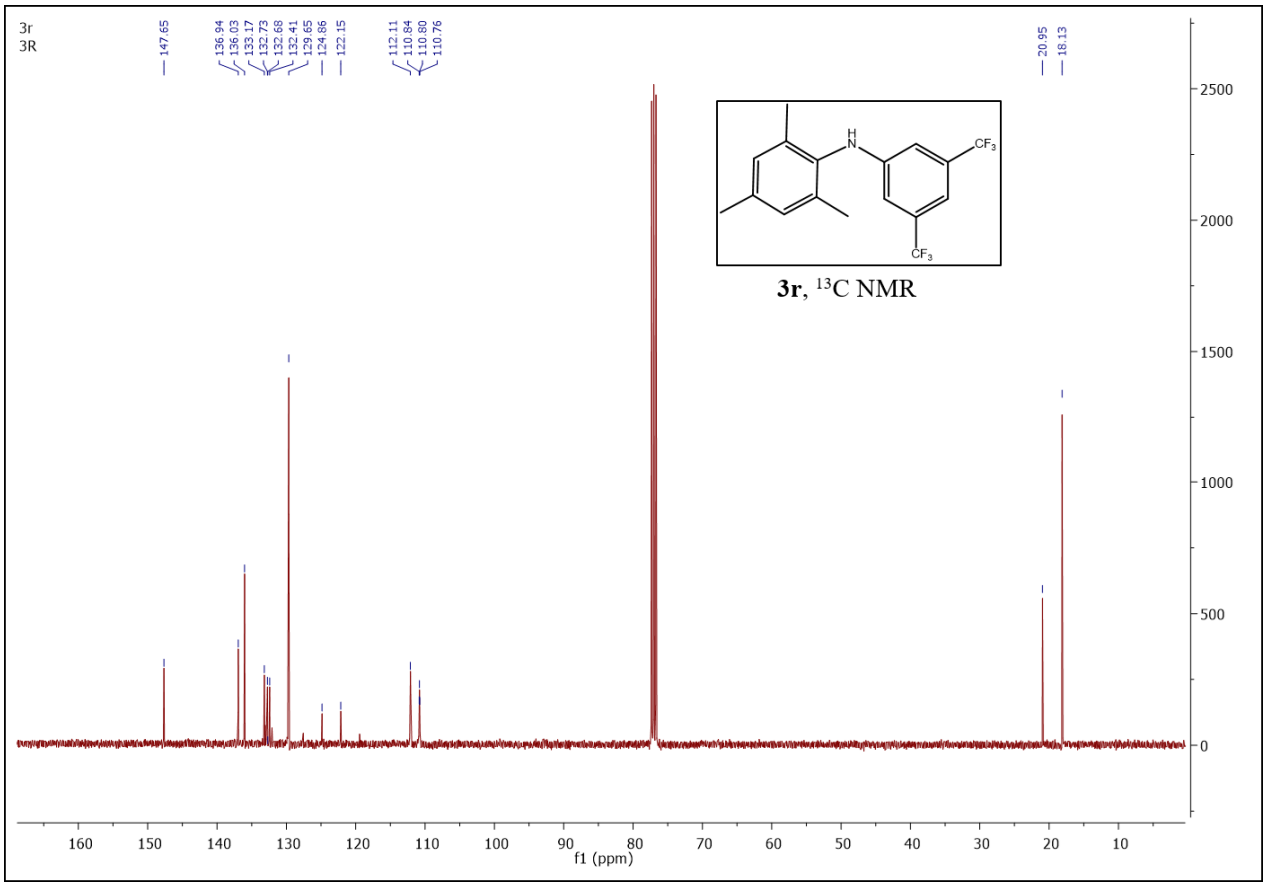
3q, ^{13}C NMR



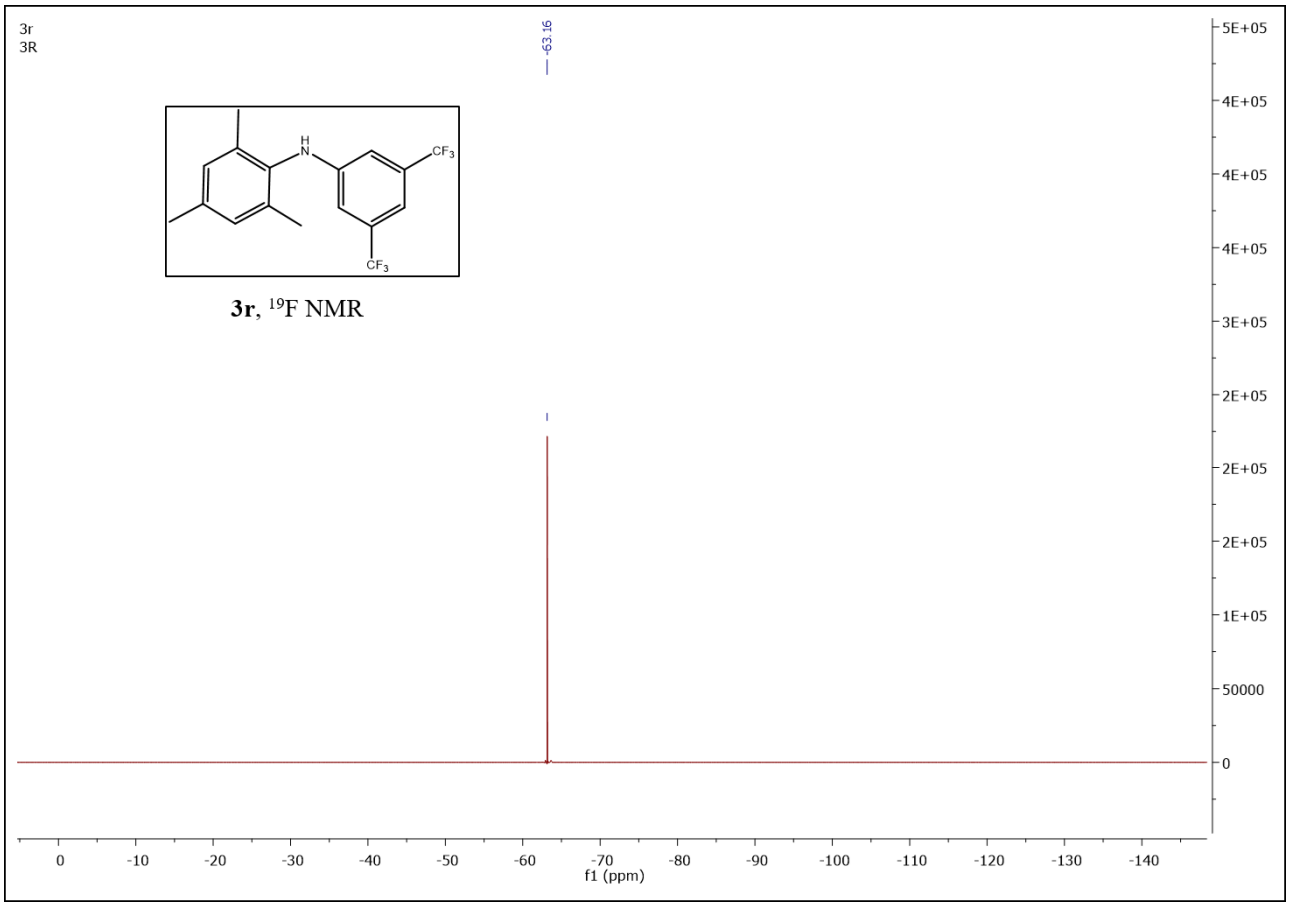
3q, ^{19}F NMR


20181207-3R-DRY
7.25
7.16
6.97
6.80
5.46
2.32
2.14
H
N
CF3
CF3
0.97
2.05
2.04
1.00
3.25
6.39
f1 (ppm)

3r, ^{1}H NMR


3r
3R
147.65
136.94
136.03
133.17
132.73
132.68
132.41
129.65
124.86
122.15
112.11
110.84
110.80
110.76
20.95
18.13
H
N
CF3
CF3
2500
2000
1500
1000
500
0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

3r, ^{13}C NMR


3r
3R
-63.16
5E+05
4E+05
4E+05
4E+05
3E+05
2E+05
2E+05
2E+05
1E+05
50000
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

3r, ^{19}F NMR

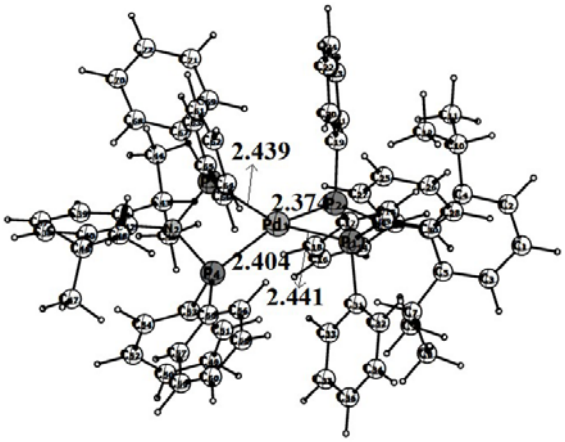
References

S1. S. Pal, N. Kathewad, R. Pant, and S. Khan, *Inorg. Chem*., 2015, **54**, 10172-10183

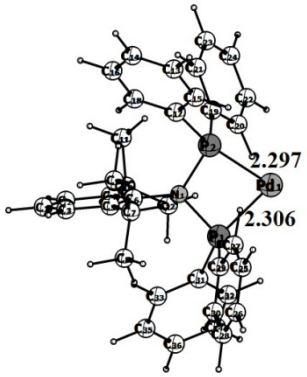
S4. Computational Section

Quantum mechanical calculations were carried out for Pd catalyzed Buchwald-Hartwig coupling reaction using Gaussian 09 programme package.[1] All geometries were optimized using the exchange functional of Becke in conjunction with the correlation functional of Perdew (BP86)[2] with def2-SVP basis set.[3] Single-point calculations were done by meta-hybrid GGA functional M06[4] with triple ζ-quality augmented by two set of polarization function (def2-TZVPP). Reaction energy (ΔE) and energy of activation ($\Delta E^{\ddagger}$) were calculated by adding electronic energy at the M06/def2-TZVPP level of theory with zero-point correction calculated at the BP86/def2-SVP level of theory. Gibbs free energy (ΔG) and Gibbs free energy of activation ($\Delta G^{\ddagger}$) were calculated by adding electronic energy calculated at the M06/def2-TZVPP level of theory with thermal correction to Gibbs free energy calculated at the BP86/def2-SVP level of theory.

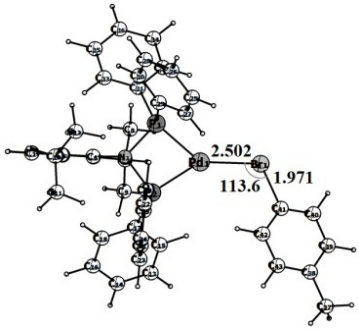
1. Gaussian 09, Revision A.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.;Robb, M. A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.;Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.;Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.;Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. J. A.; Peralta, J. E.;Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi,R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi,M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.;Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli,C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.;Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.;Cioslowski, J.; Fox, D. J., Gaussian Inc., Wallingford CT, 2009.
2. (a) Becke A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100; (b) Perdew, J. P., *Phys. Rev. B*, **1986**, *33*, 8822–8824; (c)) Perdew, J. P., *Phys. Rev. B*, **1986**, *34*, 7406–7406.
3. Weigend, F.; Ahlrichs, R. Phys. *Chem. Chem. Phys*., **2005**, *7*, 3297–3303.
4. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc,* **2008**, *120*, 215–241.



$Pd2_2$



Pd2



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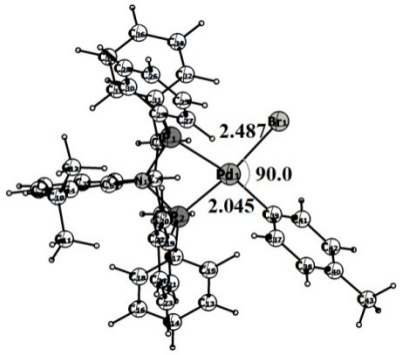

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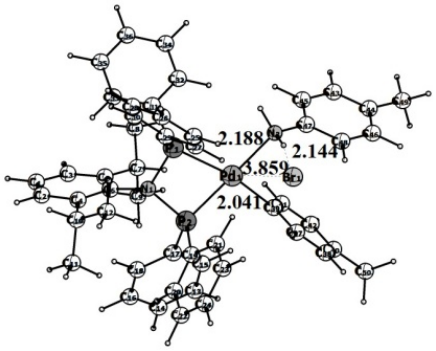

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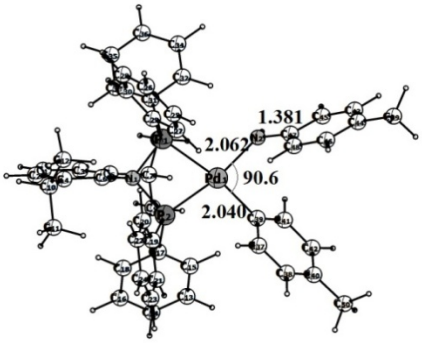

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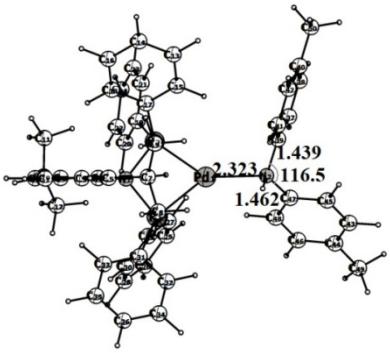

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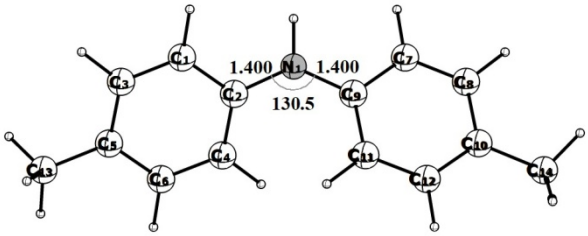

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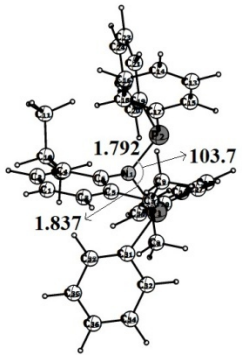

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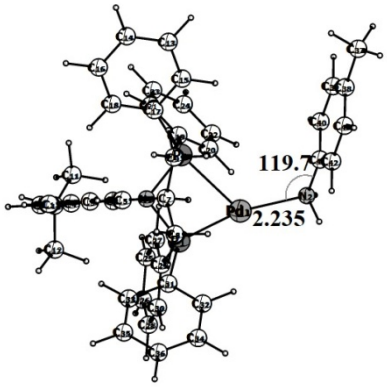

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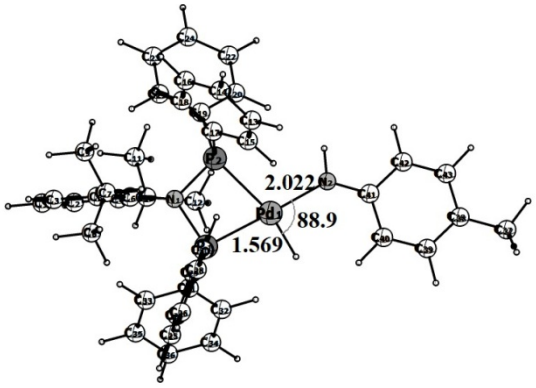

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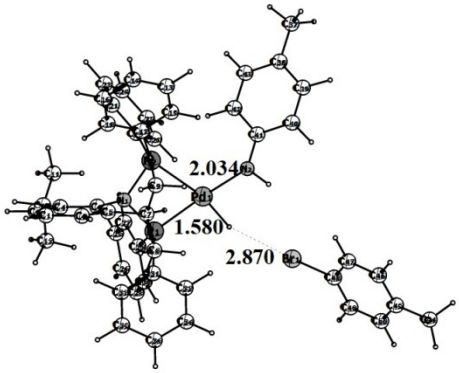

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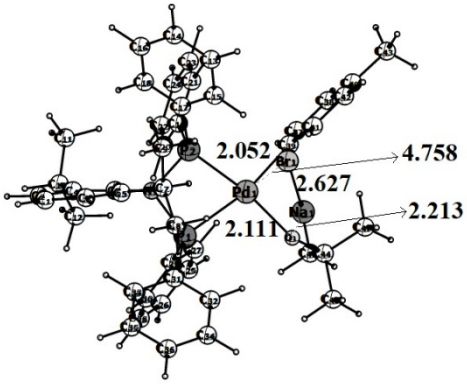

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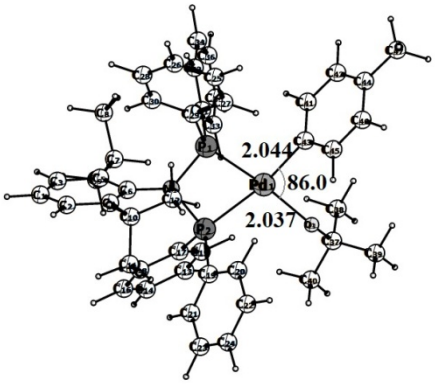

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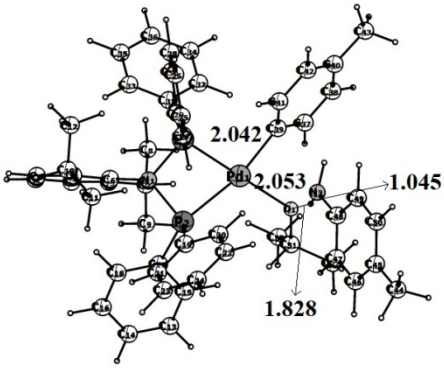

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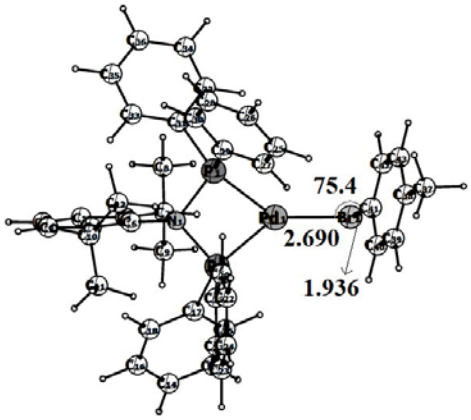

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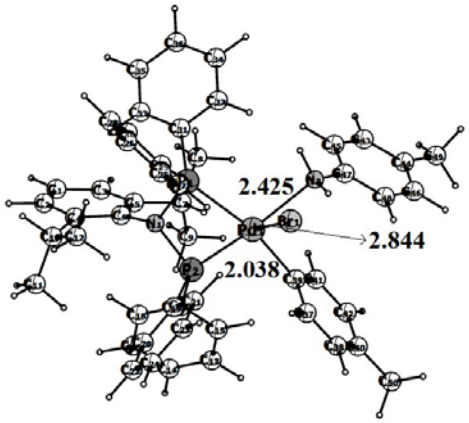
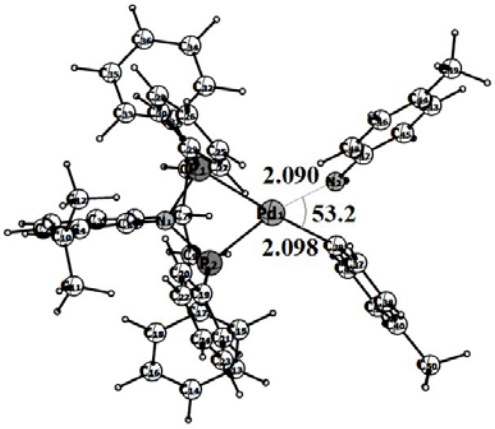


ts-2



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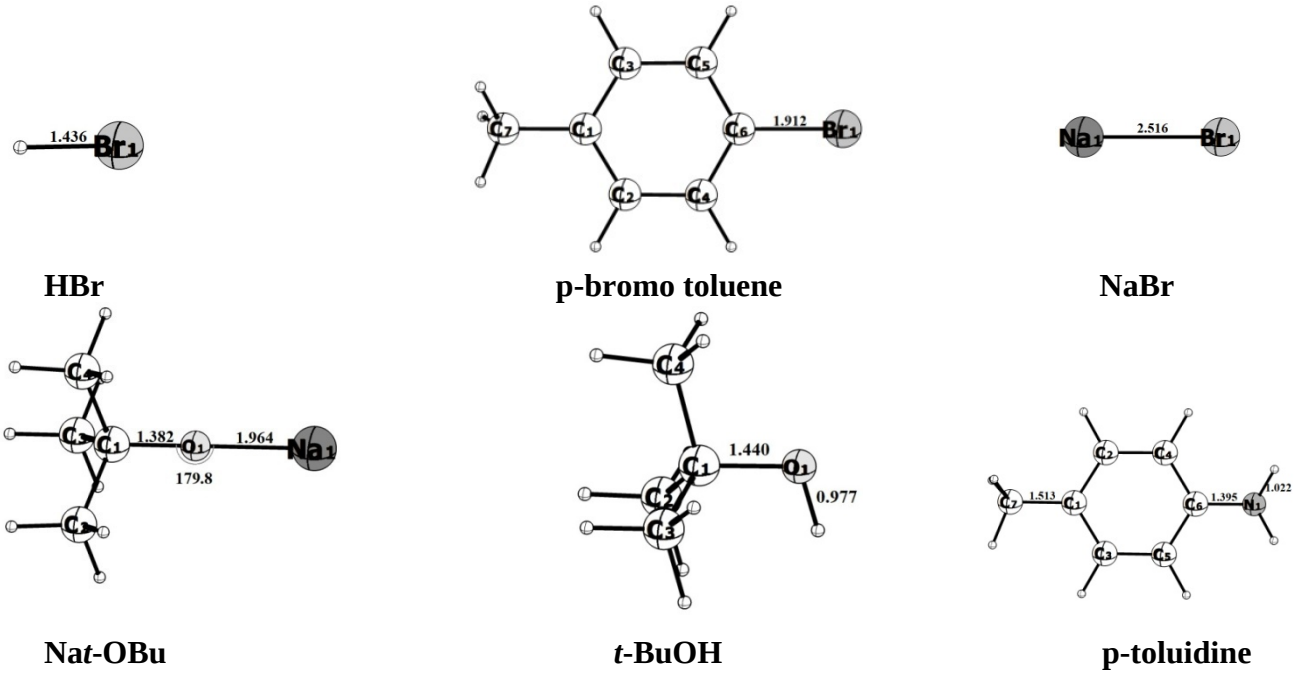


Figure S1. Optimized geometries of reactants, various intermediates and product at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory.

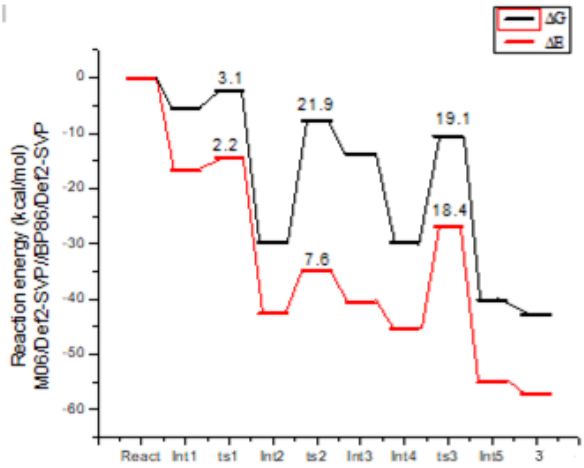
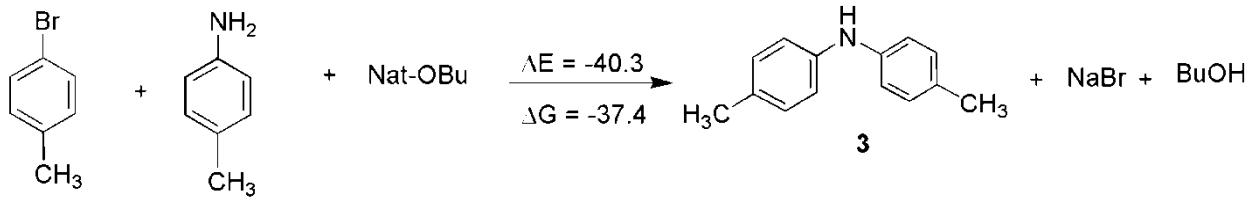
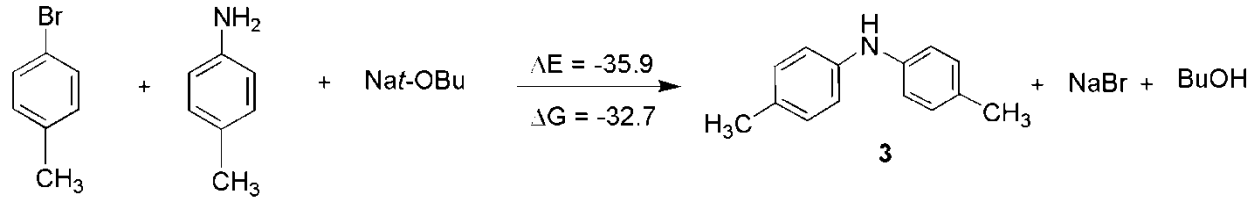


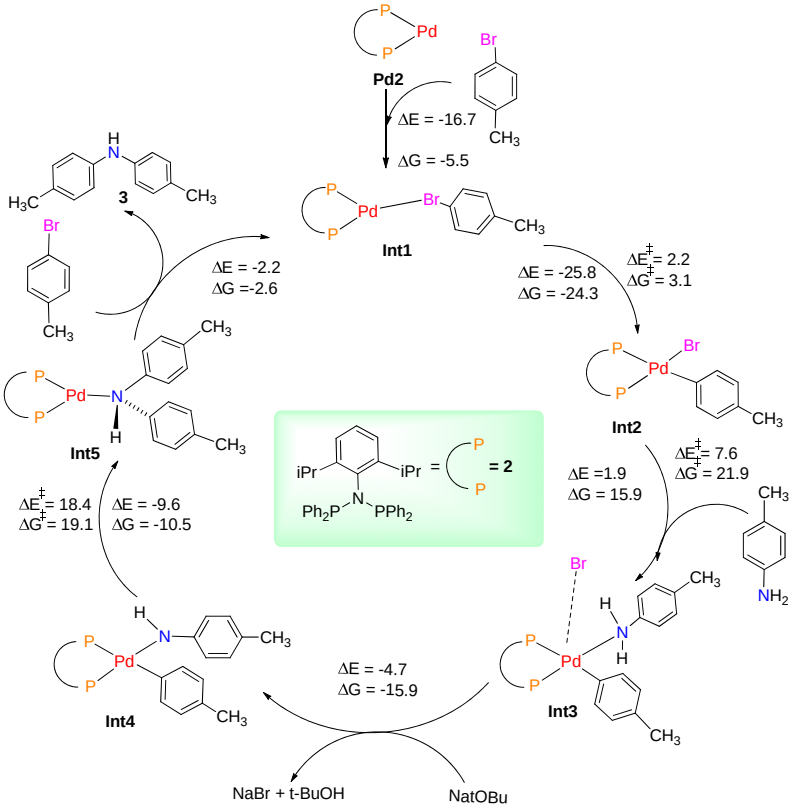
Figure S2. Reaction energy profile for the formation of **3** calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory with solvent as toluene using PCM. The energy of activation ($\Delta E^{\ddagger}$) and Gibb's free energy of activation ($\Delta G^{\ddagger}$) are given in kcal/mol.



Scheme S1. Total reaction energy and Gibbs free energy (ΔE, ΔG in kcal/mol) for the formation of **3** with solvent as toluene calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory.

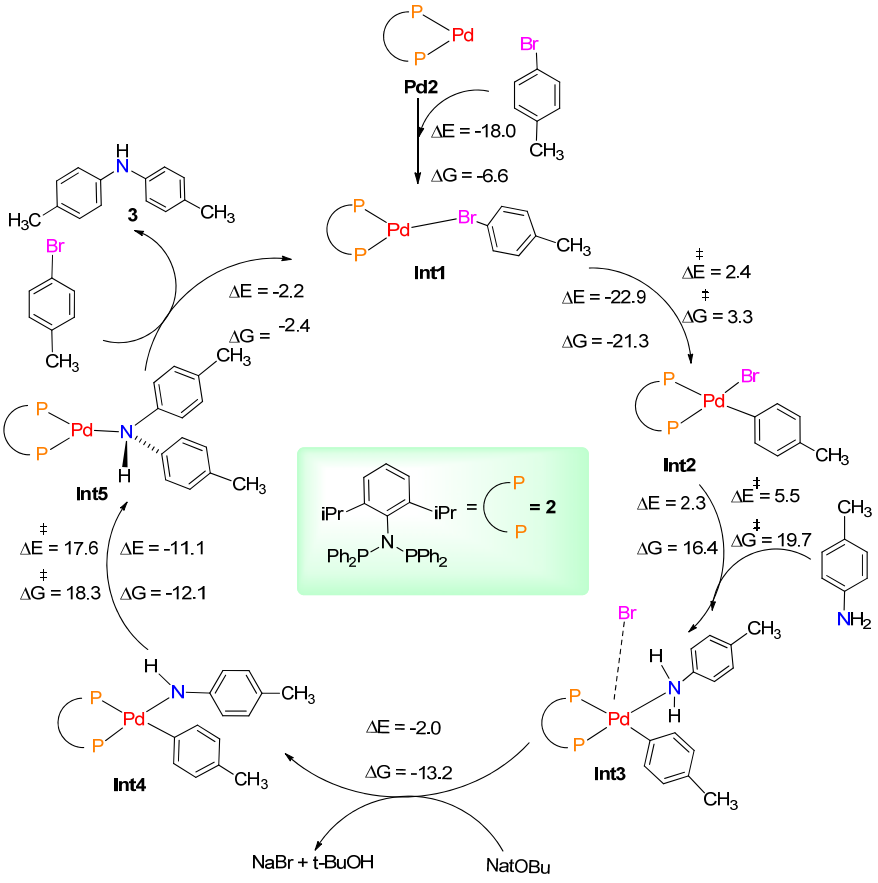


Scheme S2. Total reaction energy and Gibbs free energy (ΔE and ΔG in kcal/mol) for the formation of **3** in gaseous phases calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory.



Scheme S3. Catalytic cycle for the formation of **3** from p-bromo toluene and p-toluidine with solvent as toluene using PCM calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory. ΔE and ΔG (in

kcal/mol) represent the reaction energy and Gibb's free energy. $\Delta E^{\ddagger}$ and $\Delta G^{\ddagger}$ (in kcal/mol) represent activation energy and Gibb's free energy of activation respectively.



Scheme S4. Catalytic cycle for the formation of **3** from p-bromo toluene and p-amino toluene calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory. ΔE and ΔG (in kcal/mol) represent the reaction energies and Gibb's free energy. $\Delta E^{\ddagger}$ and $\Delta G^{\ddagger}$ (in kcal/mol) represent activation energy and Gibb's free energy of activation respectively.

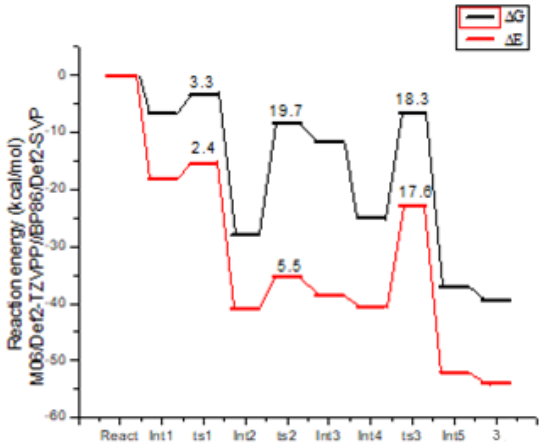
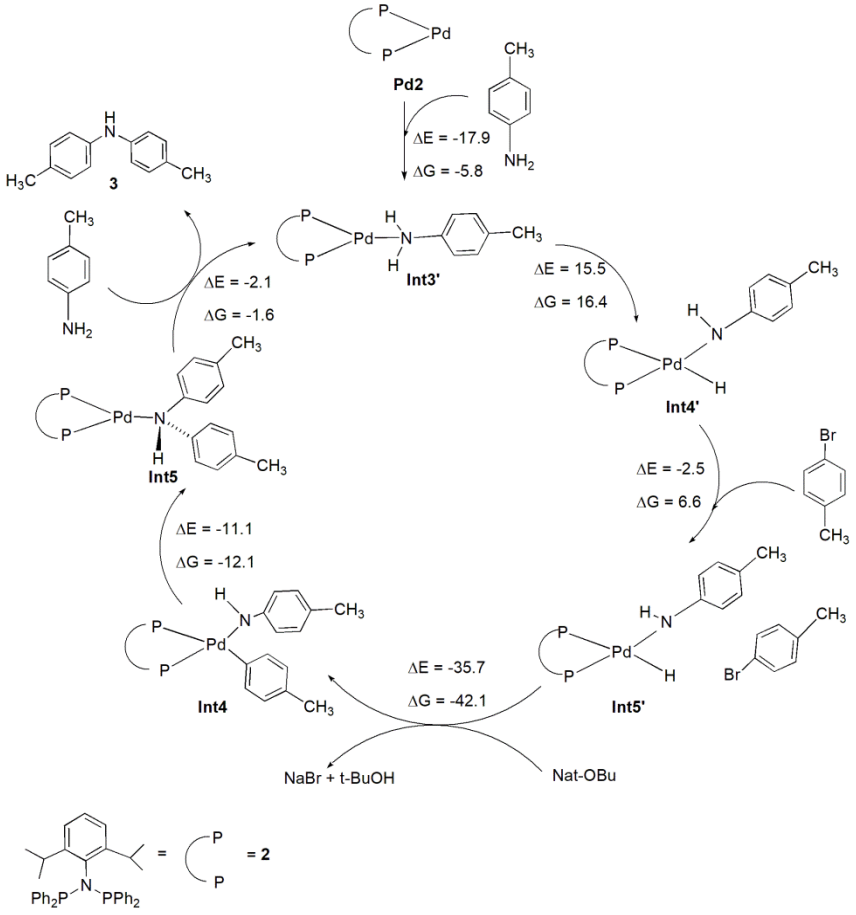
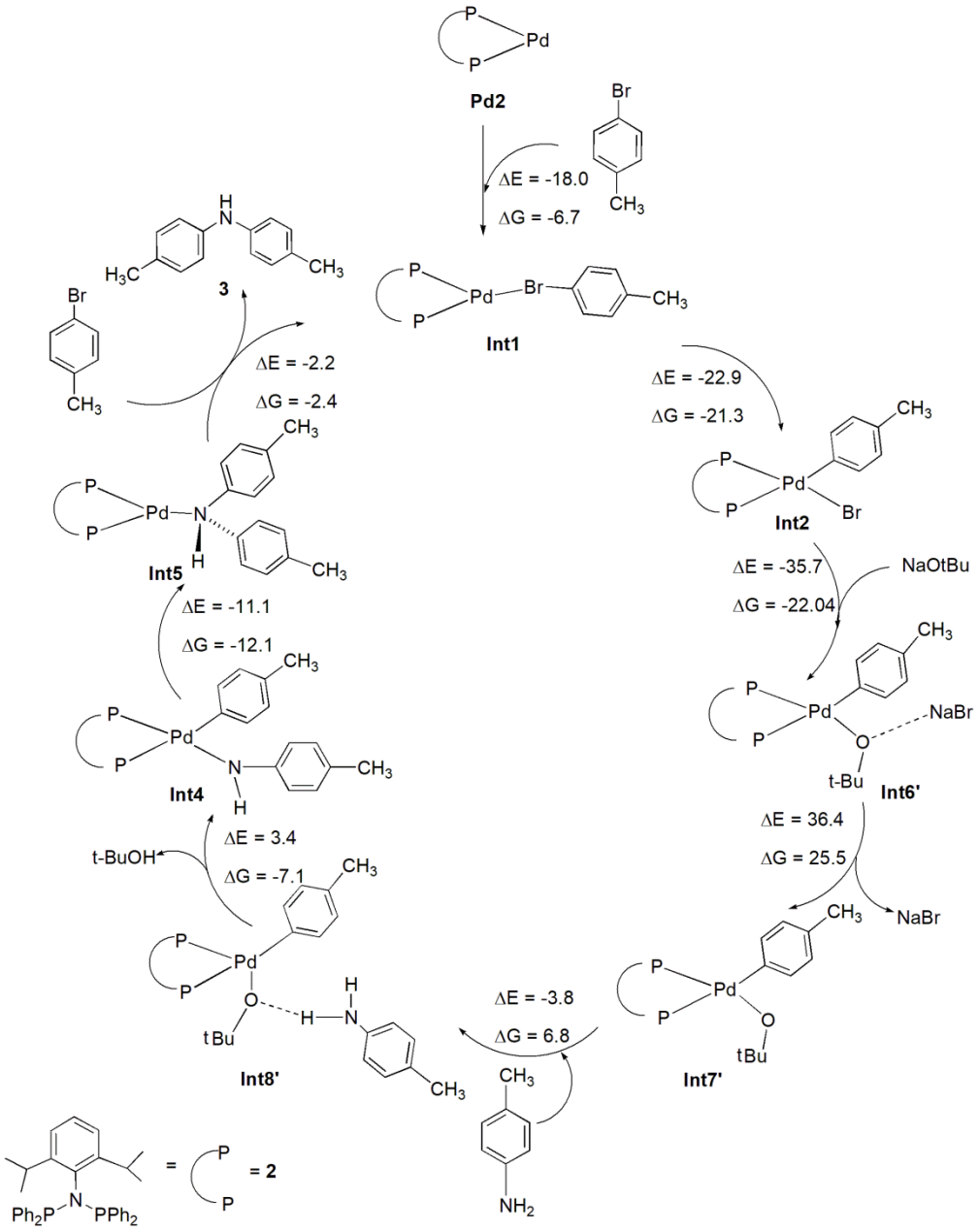


Figure S3. Reaction energy profile for the formation of **3** calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory. The energy of activation ($\Delta E^{\ddagger}$) and Gibb's free energy of activation ($\Delta G^{\ddagger}$) are given in kcal/mol.



Scheme S5. Catalytic cycle for the formation of **3** from p-bromo toluene and p-amino toluene calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory. ΔE and ΔG (in kcal/mol) represent the reaction energies and Gibb's free energy. $\Delta E^{\ddagger}$ and $\Delta G^{\ddagger}$ (in kcal/mol) represent activation energy and Gibb's free energy of activation respectively.



Scheme S6. Catalytic cycle for the formation of **3** from p-bromo toluene and p-amino toluene calculated at the M06/Def2-TZVPP//BP86/Def2-SVP level of theory. ΔE and ΔG (in kcal/mol) represent the reaction energies and Gibb's free energy, $\Delta E^{\ddagger}$ and $\Delta G^{\ddagger}$ (in kcal/mol) represent activation energy and Gibb's free energy of activation respectively.

2
Electronic energy (BP86) = -2129.730209 a.u.
Zero-point correction (BP86) = 0.612532 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.542493 a.u.
Electronic energy (M06) = -2130.933812 a.u.

6	0.707257000	-3.636285000	2.327257000
6	0.528134000	-2.387546000	2.929944000
6	0.636887000	-3.728864000	0.934598000
1	0.569807000	-2.307391000	4.029327000
1	0.773838000	-4.708772000	0.450577000
6	0.266020000	-1.212627000	2.186353000
6	0.402255000	-2.596486000	0.127979000
6	0.206008000	-1.313918000	0.752964000
1	0.893230000	-4.531924000	2.941228000
6	0.361707000	-2.832178000	-1.388603000
1	0.335601000	-1.843989000	-1.894050000
6	-0.912855000	-3.598995000	-1.811008000
6	1.611778000	-3.578225000	-1.903937000
1	1.643829000	-4.627735000	-1.540833000
1	1.597582000	-3.619921000	-3.013365000
1	2.550928000	-3.081832000	-1.592510000
1	-0.930958000	-4.616235000	-1.363660000
1	-0.945255000	-3.715373000	-2.914951000
1	-1.839007000	-3.078583000	-1.497528000
6	0.095780000	0.046397000	3.059510000
1	-0.206003000	-0.361137000	4.050806000
6	1.445551000	0.758845000	3.300178000
6	-1.009907000	1.033539000	2.660411000
1	-1.097297000	1.828094000	3.431743000
1	-0.797788000	1.514763000	1.690571000
1	-1.994706000	0.529178000	2.585457000
1	2.211988000	0.048918000	3.675859000
1	1.327433000	1.561858000	4.058505000
1	1.833460000	1.230340000	2.377058000
7	-0.076402000	-0.150182000	-0.066024000
15	-1.526690000	-0.155568000	-1.192711000
15	1.170532000	0.751377000	-0.983543000
6	4.542991000	-1.105427000	-2.428711000
6	5.151465000	-1.692272000	-1.306080000
6	3.327550000	-0.412470000	-2.285486000
1	6.100794000	-2.240965000	-1.414648000

1	2.845416000	0.040118000	-3.167731000
6	4.544274000	-1.576858000	-0.041656000
6	2.711692000	-0.280891000	-1.019007000
1	5.016958000	-2.035609000	0.841536000
6	3.338313000	-0.870490000	0.105164000
1	2.887230000	-0.772283000	1.103211000
1	5.011964000	-1.191051000	-3.421972000
6	1.734876000	2.195843000	0.052566000
6	0.785314000	3.191817000	0.391615000
6	3.099255000	2.454220000	0.328165000
1	-0.277061000	3.042649000	0.147162000
1	3.866244000	1.714468000	0.055002000
6	1.180684000	4.378114000	1.029070000
6	3.494502000	3.650528000	0.953898000
1	0.420271000	5.130322000	1.293613000
1	4.562377000	3.826083000	1.162465000
6	2.537731000	4.612865000	1.316315000
1	2.848053000	5.546985000	1.811279000
6	-2.159382000	3.772782000	-2.319516000
6	-2.967874000	4.316411000	-1.306182000
6	-1.734203000	2.435184000	-2.236673000
1	-3.306266000	5.363135000	-1.370222000
1	-1.099457000	2.005397000	-3.028411000
6	-3.353168000	3.516157000	-0.213922000
6	-2.101890000	1.625787000	-1.136359000
1	-3.996216000	3.935048000	0.577084000
6	-2.927465000	2.179575000	-0.130569000
1	-3.248589000	1.556755000	0.717809000
1	-1.860711000	4.390913000	-3.181316000
6	-2.966535000	-0.928065000	-0.287476000
6	-4.146860000	-0.922240000	-1.076531000
6	-3.008717000	-1.578559000	0.965149000
1	-4.133618000	-0.444402000	-2.071531000
1	-2.112236000	-1.632922000	1.595505000
6	-5.332958000	-1.511569000	-0.616364000
6	-4.198202000	-2.181735000	1.419540000
1	-6.236466000	-1.481723000	-1.246511000
1	-4.203984000	-2.684485000	2.400176000
6	-5.363906000	-2.147899000	0.638953000
1	-6.290807000	-2.621337000	0.999957000

Pd2

Electronic energy (BP86) = -2257.761114 a.u.
Zero-point correction (BP86) = 0.613670 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.541197 a.u.
Electronic energy (M06) = -2258.917819 a.u.

6	0.029533000	0.545537000	4.496910000
6	-0.352509000	-0.692878000	3.978705000
6	0.406804000	1.553504000	3.606979000
1	-0.638614000	-1.499366000	4.674359000
1	0.720225000	2.533675000	3.999893000
6	-0.388751000	-0.973505000	2.590546000
6	0.406972000	1.347512000	2.212812000
6	-0.004481000	0.072646000	1.674461000
1	0.042542000	0.718261000	5.584958000
6	0.912820000	2.517279000	1.366262000
1	0.799296000	2.231761000	0.303908000
6	2.410065000	2.779547000	1.644760000
6	0.120124000	3.823049000	1.583807000
1	0.235117000	4.206316000	2.620480000
1	0.500469000	4.612603000	0.901887000
1	-0.960409000	3.695224000	1.388696000
1	2.559380000	3.174842000	2.672601000
1	2.813502000	3.528883000	0.932306000
1	3.021776000	1.862536000	1.544365000
6	-0.928439000	-2.394619000	2.309858000
1	-0.638609000	-2.961784000	3.222704000
6	-2.475541000	-2.394249000	2.314901000
6	-0.343854000	-3.203067000	1.144143000
1	-0.881245000	-4.171392000	1.062566000
1	-0.432982000	-2.685445000	0.174007000
1	0.726100000	-3.427488000	1.312054000
1	-2.870418000	-1.918453000	3.236714000
1	-2.860423000	-3.435361000	2.276368000
1	-2.893399000	-1.852269000	1.446422000
7	-0.011407000	-0.120148000	0.233027000
15	1.390446000	-0.531117000	-0.854859000
15	-1.367111000	0.237814000	-0.926242000
6	-3.136908000	3.951421000	-0.623665000
6	-3.710537000	3.969321000	0.659370000
6	-2.401720000	2.830247000	-1.048986000
1	-4.291260000	4.844068000	0.993340000
1	-1.961368000	2.804597000	-2.060097000
6	-3.537872000	2.868352000	1.518961000
6	-2.231675000	1.714895000	-0.199753000
1	-3.979949000	2.880869000	2.528121000
6	-2.801567000	1.747863000	1.096057000
1	-2.678992000	0.891311000	1.775981000
1	-3.265189000	4.811893000	-1.299639000
6	-2.738054000	-1.031061000	-0.879029000
6	-2.457431000	-2.301627000	-1.444506000

6	-4.081738000	-0.734913000	-0.546017000
1	-1.426813000	-2.521592000	-1.774656000
1	-4.347114000	0.249985000	-0.136208000
6	-3.468371000	-3.256068000	-1.623086000
6	-5.098970000	-1.686834000	-0.744166000
1	-3.220476000	-4.238411000	-2.056374000
1	-6.137968000	-1.430297000	-0.481090000
6	-4.797878000	-2.953379000	-1.270414000
1	-5.596088000	-3.697838000	-1.419969000
6	3.179784000	2.991215000	-2.124648000
6	4.541588000	2.823099000	-1.805612000
6	2.242980000	2.013562000	-1.760348000
1	5.280057000	3.585059000	-2.101899000
1	1.185668000	2.130748000	-2.055936000
6	4.949332000	1.669885000	-1.116380000
6	2.635947000	0.853120000	-1.043338000
1	6.012637000	1.521346000	-0.867569000
6	4.007733000	0.696569000	-0.733188000
1	4.353323000	-0.198036000	-0.195074000
1	2.847231000	3.885661000	-2.675837000
6	2.401764000	-1.760849000	0.109022000
6	2.775157000	-2.933157000	-0.583816000
6	2.838624000	-1.585375000	1.443400000
1	2.433202000	-3.072160000	-1.623341000
1	2.570414000	-0.675980000	2.001358000
6	3.562412000	-3.916592000	0.040395000
6	3.616166000	-2.575007000	2.070009000
1	3.845897000	-4.825728000	-0.513791000
1	3.943934000	-2.431062000	3.112205000
6	3.978771000	-3.741649000	1.371638000
1	4.589206000	-4.514034000	1.866514000
46	-0.000664000	-0.329894000	-2.682636000

$Pd2_2$
Electronic energy (BP86) = -4387.541437 a.u.
Zero-point correction (BP86) = 1.229539 a.u.
Thermal correction to Gibbs free energy (BP86) = 1.113425 a.u.
Electronic energy (M06) = -4389.920177 a.u.

6	7.324843000	-0.267865000	-0.884889000
6	6.882150000	0.640160000	0.076852000
6	6.372167000	-1.019052000	-1.572665000
1	7.625589000	1.244409000	0.622783000
1	6.702374000	-1.735447000	-2.341114000
6	5.514181000	0.840382000	0.388204000
6	4.992670000	-0.896953000	-1.307107000

6	4.529495000	0.039472000	-0.307108000
1	8.399968000	-0.386503000	-1.094099000
6	4.097236000	-1.828450000	-2.132313000
1	3.047670000	-1.647862000	-1.831286000
6	4.447068000	-3.309628000	-1.862576000
6	4.199006000	-1.571891000	-3.652188000
1	5.219268000	-1.793214000	-4.032775000
1	3.497533000	-2.240565000	-4.194601000
1	3.956242000	-0.529219000	-3.923655000
1	5.464530000	-3.549459000	-2.238419000
1	3.735126000	-3.977136000	-2.389131000
1	4.415357000	-3.563208000	-0.785631000
6	5.341836000	2.016618000	1.379015000
1	6.315375000	2.041023000	1.916983000
6	5.288210000	3.355437000	0.604205000
6	4.284037000	1.932879000	2.485431000
1	4.223027000	2.907445000	3.013520000
1	3.281329000	1.697336000	2.097549000
1	4.546281000	1.160676000	3.232008000
1	6.142276000	3.441870000	-0.099542000
1	5.341382000	4.210031000	1.311544000
1	4.354130000	3.464119000	0.022762000
7	3.101018000	0.132475000	-0.035408000
15	2.056348000	-0.946085000	0.978620000
15	1.844968000	1.151883000	-0.838939000
6	3.976264000	2.094821000	-4.328841000
6	3.032750000	1.786983000	-5.326804000
6	3.671125000	1.876836000	-2.974080000
1	3.274046000	1.962229000	-6.387531000
1	4.416686000	2.132413000	-2.205994000
6	1.783675000	1.253651000	-4.965345000
6	2.412499000	1.347068000	-2.598981000
1	1.039296000	1.010451000	-5.740254000
6	1.476875000	1.035457000	-3.609489000
1	0.491521000	0.633533000	-3.320263000
1	4.959362000	2.507685000	-4.606536000
6	1.952243000	2.939161000	-0.282765000
6	1.623216000	3.225426000	1.064809000
6	2.141625000	4.031577000	-1.163370000
1	1.375722000	2.393685000	1.743075000
1	2.359166000	3.855082000	-2.226144000
6	1.569349000	4.546041000	1.535780000
6	2.054607000	5.357496000	-0.699308000
1	1.330190000	4.736909000	2.594241000
1	2.204765000	6.189252000	-1.406553000
6	1.789269000	5.621674000	0.654423000

1	1.739110000	6.659900000	1.019963000
6	2.683097000	-0.714595000	5.052343000
6	4.020560000	-1.106635000	5.233001000
6	2.132509000	-0.662748000	3.758514000
1	4.453647000	-1.147576000	6.245448000
1	1.084706000	-0.348891000	3.615439000
6	4.807537000	-1.443076000	4.115294000
6	2.910743000	-1.002669000	2.631239000
1	5.858784000	-1.744922000	4.250840000
6	4.258700000	-1.392074000	2.822469000
1	4.888002000	-1.650317000	1.956825000
1	2.061651000	-0.444868000	5.921184000
6	2.174656000	-2.766381000	0.520099000
6	2.737905000	-3.765418000	1.350606000
6	1.432526000	-3.193098000	-0.608206000
1	3.293049000	-3.485699000	2.256603000
1	0.927762000	-2.430104000	-1.221982000
6	2.583651000	-5.131375000	1.046510000
6	1.289214000	-4.551823000	-0.921077000
1	3.030433000	-5.887080000	1.712939000
1	0.700282000	-4.848430000	-1.803471000
6	1.866105000	-5.531186000	-0.092053000
1	1.742113000	-6.600812000	-0.325082000
46	-0.012299000	0.038135000	0.134439000
6	-6.821292000	1.091237000	-1.804533000
6	-6.827779000	0.244796000	-0.695255000
6	-5.596698000	1.578065000	-2.270376000
1	-7.791459000	-0.127210000	-0.308108000
1	-5.582473000	2.259147000	-3.135764000
6	-5.642454000	-0.162727000	-0.034538000
6	-4.377130000	1.236424000	-1.653328000
6	-4.384112000	0.333921000	-0.521997000
1	-7.765004000	1.380529000	-2.294146000
6	-3.124991000	1.901891000	-2.246060000
1	-2.248694000	1.613736000	-1.625435000
6	-3.247235000	3.445261000	-2.238121000
6	-2.837925000	1.471847000	-3.703703000
1	-3.676737000	1.757768000	-4.373991000
1	-1.930995000	1.995519000	-4.073410000
1	-2.673337000	0.386392000	-3.812393000
1	-3.953389000	3.789934000	-3.024071000
1	-2.262307000	3.906421000	-2.460322000
1	-3.603382000	3.843522000	-1.271928000
6	-5.930367000	-1.143636000	1.122158000
1	-6.870239000	-0.746434000	1.570339000
6	-6.284728000	-2.547283000	0.577238000

6	-4.927566000	-1.250541000	2.271764000
1	-5.362066000	-1.874765000	3.081203000
1	-3.978682000	-1.722050000	1.956874000
1	-4.688335000	-0.262340000	2.708086000
1	-7.070454000	-2.503895000	-0.204897000
1	-6.655335000	-3.197217000	1.398285000
1	-5.392633000	-3.040528000	0.144064000
7	-3.118411000	-0.046068000	0.076178000
15	-2.039988000	1.002750000	1.086077000
15	-1.928792000	-1.208423000	-0.609330000
6	-1.676728000	-2.265156000	-4.576645000
6	-3.000490000	-2.457335000	-5.008598000
6	-1.421997000	-1.850453000	-3.257946000
1	-3.206592000	-2.769657000	-6.044893000
1	-0.385176000	-1.666992000	-2.929697000
6	-4.061076000	-2.242681000	-4.110615000
6	-2.477903000	-1.639230000	-2.341357000
1	-5.102259000	-2.385542000	-4.441760000
6	-3.806291000	-1.846018000	-2.785612000
1	-4.655133000	-1.683990000	-2.106041000
1	-0.836907000	-2.425004000	-5.271698000
6	-2.195602000	-2.913239000	0.155698000
6	-1.353943000	-3.258770000	1.238129000
6	-3.068758000	-3.907850000	-0.343415000
1	-0.601845000	-2.525861000	1.574834000
1	-3.688210000	-3.705386000	-1.229095000
6	-1.422708000	-4.524033000	1.844375000
6	-3.137577000	-5.177852000	0.256346000
1	-0.749218000	-4.763950000	2.682230000
1	-3.829087000	-5.933617000	-0.150271000
6	-2.324582000	-5.486964000	1.360450000
1	-2.377461000	-6.483899000	1.826851000
6	-2.734154000	1.457850000	5.224510000
6	-2.360631000	0.205359000	5.736094000
6	-2.716089000	1.698332000	3.837499000
1	-2.382781000	0.016298000	6.821362000
1	-3.014505000	2.690463000	3.471561000
6	-1.948959000	-0.803403000	4.844705000
6	-2.313881000	0.690773000	2.927315000
1	-1.647248000	-1.791976000	5.226975000
6	-1.911149000	-0.554741000	3.464945000
1	-1.565223000	-1.345307000	2.786168000
1	-3.048236000	2.263668000	5.907855000
6	-2.808351000	2.697437000	1.016380000
6	-4.176367000	2.964575000	1.265644000
6	-1.927987000	3.783688000	0.828735000

1	-4.881744000	2.138027000	1.435555000
1	-0.863860000	3.588978000	0.627061000
6	-4.645661000	4.288154000	1.315286000
6	-2.394137000	5.109243000	0.902599000
1	-5.714673000	4.479681000	1.501429000
1	-1.686819000	5.941835000	0.761380000
6	-3.754761000	5.364326000	1.141004000
1	-4.125018000	6.401085000	1.189744000

Int1

Electronic energy (BP86) = -5102.560721 a.u.
Zero-point correction (BP86) = 0.728112 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.639535 a.u.
Electronic energy (M06) = -5103.851268 a.u.

6	4.636098000	2.574342000	-2.036983000
6	4.672271000	2.503364000	-0.641091000
6	3.566609000	1.983918000	-2.713799000
1	5.507827000	2.974483000	-0.096946000
1	3.525240000	2.043608000	-3.812983000
6	3.674971000	1.841805000	0.112611000
6	2.534458000	1.307926000	-2.029697000
6	2.587794000	1.213984000	-0.591284000
1	5.436176000	3.090349000	-2.591557000
6	1.412675000	0.732811000	-2.906920000
1	0.654639000	0.260307000	-2.242915000
6	1.918408000	-0.343779000	-3.895053000
6	0.707636000	1.840027000	-3.725272000
1	1.378544000	2.236861000	-4.517354000
1	-0.188581000	1.425538000	-4.232671000
1	0.384663000	2.692547000	-3.101339000
1	2.611171000	0.098185000	-4.643355000
1	1.061267000	-0.773764000	-4.454787000
1	2.447056000	-1.173242000	-3.392706000
6	3.880583000	1.933115000	1.634595000
1	4.934878000	2.272819000	1.742729000
6	3.021827000	3.049048000	2.267027000
6	3.789628000	0.613581000	2.411880000
1	4.056325000	0.779343000	3.477162000
1	2.775979000	0.178818000	2.378001000
1	4.495645000	-0.139729000	2.006618000
1	3.197725000	4.022198000	1.762262000
1	3.280865000	3.174217000	3.339814000
1	1.940594000	2.819556000	2.214926000
7	1.553153000	0.466347000	0.100975000
15	1.285713000	-1.334649000	-0.009326000

15	-0.136475000	1.023302000	0.407441000
6	-2.003107000	3.822371000	-1.960145000
6	-1.144828000	4.934963000	-1.950697000
6	-1.638743000	2.648210000	-1.277048000
1	-1.423578000	5.853749000	-2.491277000
1	-2.299355000	1.765091000	-1.295372000
6	0.074409000	4.871795000	-1.250326000
6	-0.422699000	2.579045000	-0.560971000
1	0.752191000	5.740398000	-1.242128000
6	0.432133000	3.706212000	-0.551778000
1	1.380134000	3.679887000	0.004110000
1	-2.957465000	3.862102000	-2.509040000
6	-0.248695000	1.689351000	2.141001000
6	0.186926000	0.896516000	3.230697000
6	-0.945790000	2.889788000	2.426525000
1	0.709037000	-0.052814000	3.044887000
1	-1.312989000	3.523694000	1.605926000
6	-0.039050000	1.301739000	4.554839000
6	-1.179859000	3.287494000	3.754314000
1	0.320977000	0.669760000	5.382585000
1	-1.721303000	4.227418000	3.949657000
6	-0.724206000	2.500450000	4.825583000
1	-0.904638000	2.816644000	5.865314000
6	0.794195000	-3.211868000	3.646960000
6	2.080031000	-3.647885000	4.013097000
6	0.611639000	-2.488560000	2.456428000
1	2.227107000	-4.224385000	4.940606000
1	-0.399918000	-2.169289000	2.140073000
6	3.175061000	-3.362641000	3.177673000
6	1.707700000	-2.174011000	1.617847000
1	4.182870000	-3.716621000	3.448753000
6	2.991008000	-2.636915000	1.988425000
1	3.855658000	-2.447864000	1.334888000
1	-0.074737000	-3.447787000	4.281993000
6	2.671460000	-2.057821000	-1.025180000
6	2.311363000	-3.236807000	-1.719143000
6	4.008239000	-1.602200000	-1.105594000
1	1.266759000	-3.589250000	-1.672904000
1	4.321702000	-0.687877000	-0.581644000
6	3.260779000	-3.948062000	-2.471132000
6	4.951744000	-2.306982000	-1.874913000
1	2.960801000	-4.864789000	-3.003628000
1	5.986424000	-1.933155000	-1.937400000
6	4.584037000	-3.480038000	-2.557095000
1	5.327779000	-4.027093000	-3.158302000
46	-1.029825000	-1.050906000	-0.167221000

1	-5.898100000	1.541918000	0.840145000
6	-8.440556000	0.843416000	0.017453000
1	-8.300907000	1.715003000	0.687372000
1	-9.228924000	0.197834000	0.458913000
1	-8.840084000	1.223853000	-0.947865000
6	-7.148629000	0.082569000	-0.184280000
6	-7.139399000	-1.153327000	-0.871217000
6	-5.947883000	-1.869087000	-1.078358000
6	-4.749273000	-1.331303000	-0.589175000
6	-4.714109000	-0.115454000	0.097199000
6	-5.918649000	0.583354000	0.295145000
1	-8.086159000	-1.569662000	-1.254794000
1	-5.957571000	-2.831358000	-1.613644000
1	-3.749220000	0.273258000	0.469981000
35	-3.068697000	-2.324287000	-0.862326000

Int2

Electronic energy (BP86) = -5102.603932 a.u.
Zero-point correction (BP86) = 0.729863 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.643778 a.u.
Electronic energy (M06) = -5103.894273 a.u.

6	4.158739000	3.422383000	-1.323749000
6	3.976798000	3.297026000	0.056701000
6	3.316673000	2.713314000	-2.182665000
1	4.623284000	3.869700000	0.742019000
1	3.442201000	2.821580000	-3.271302000
6	2.984521000	2.461028000	0.619493000
6	2.307017000	1.855041000	-1.697614000
6	2.149212000	1.701074000	-0.271337000
1	4.948210000	4.077187000	-1.725812000
6	1.436923000	1.178475000	-2.768702000
1	0.700640000	0.519525000	-2.258911000
6	2.249278000	0.311666000	-3.758896000
6	0.655241000	2.224585000	-3.599753000
1	1.345290000	2.802608000	-4.250715000
1	-0.072737000	1.713492000	-4.263350000
1	0.104025000	2.946987000	-2.973171000
1	2.918955000	0.942081000	-4.382145000
1	1.556899000	-0.211735000	-4.450556000
1	2.871469000	-0.449964000	-3.259135000
6	2.895016000	2.545105000	2.153401000
1	3.826848000	3.077919000	2.445818000
6	1.737215000	3.457366000	2.611593000
6	2.922042000	1.215491000	2.917454000
1	2.970390000	1.406569000	4.010346000

1	2.026385000	0.600812000	2.721535000
1	3.812716000	0.613816000	2.646159000
1	1.794655000	4.453579000	2.125245000
1	1.783416000	3.615362000	3.709856000
1	0.747894000	3.014613000	2.386990000
7	1.169278000	0.747645000	0.226441000
15	1.262453000	-1.057126000	0.106983000
15	-0.604549000	0.943175000	0.293169000
6	-2.702728000	3.348342000	-2.300518000
6	-2.124891000	4.617315000	-2.126952000
6	-2.198379000	2.238745000	-1.598982000
1	-2.518439000	5.484410000	-2.681148000
1	-2.651836000	1.243483000	-1.730430000
6	-1.041823000	4.780733000	-1.242839000
6	-1.117233000	2.399972000	-0.705047000
1	-0.583684000	5.773022000	-1.105955000
6	-0.542263000	3.680949000	-0.526040000
1	0.292879000	3.825776000	0.174294000
1	-3.552475000	3.213670000	-2.987912000
6	-1.144181000	1.452778000	1.996201000
6	-0.750154000	0.680133000	3.113409000
6	-2.076092000	2.498910000	2.189952000
1	-0.056958000	-0.163742000	2.985476000
1	-2.422952000	3.097081000	1.335450000
6	-1.241203000	0.971782000	4.395076000
6	-2.573882000	2.781786000	3.474508000
1	-0.912948000	0.363471000	5.252754000
1	-3.298920000	3.600809000	3.605346000
6	-2.153960000	2.026226000	4.581218000
1	-2.544067000	2.250913000	5.586630000
6	0.994113000	-3.217685000	3.605892000
6	2.319378000	-3.361362000	4.048638000
6	0.717267000	-2.482599000	2.439749000
1	2.539530000	-3.944074000	4.957437000
1	-0.318488000	-2.406851000	2.065940000
6	3.368816000	-2.780717000	3.312230000
6	1.762686000	-1.871387000	1.706695000
1	4.412142000	-2.909400000	3.641981000
6	3.095065000	-2.050173000	2.145313000
1	3.930781000	-1.635408000	1.562674000
1	0.168384000	-3.695288000	4.156569000
6	2.682784000	-1.541435000	-0.953185000
6	2.451965000	-2.674974000	-1.767905000
6	3.969979000	-0.954695000	-0.912758000
1	1.445828000	-3.131428000	-1.796552000
1	4.162426000	-0.064587000	-0.295138000

6	3.502247000	-3.213102000	-2.531924000
6	5.009480000	-1.496431000	-1.688010000
1	3.315466000	-4.095019000	-3.164767000
1	6.007112000	-1.029963000	-1.661400000
6	4.778841000	-2.625408000	-2.495458000
1	5.598423000	-3.046131000	-3.099762000
46	-1.088961000	-1.200832000	-0.314981000
6	-3.884843000	-0.665632000	0.679555000
6	-5.285257000	-0.537469000	0.596671000
6	-3.118172000	-0.990995000	-0.459796000
1	-5.857702000	-0.288121000	1.507281000
6	-5.968113000	-0.715871000	-0.624799000
6	-3.796527000	-1.177610000	-1.684973000
1	-3.236343000	-1.458110000	-2.591031000
6	-5.194768000	-1.032795000	-1.762705000
1	-5.697815000	-1.185895000	-2.733661000
1	-3.396463000	-0.506886000	1.655441000
6	-7.476302000	-0.611951000	-0.704039000
1	-7.960287000	-1.595118000	-0.508731000
1	-7.879139000	0.100801000	0.045046000
1	-7.813132000	-0.280369000	-1.707910000
35	-1.281039000	-3.564708000	-1.064275000

Int3

Electronic energy (BP86) = -5429.136183 a.u.
Zero-point correction (BP86) = 0.872027 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.775176 a.u.
Electronic energy (M06) = -5430.682173 a.u.

6	5.711119000	0.462372000	-2.295162000
6	5.724940000	0.368838000	-0.901402000
6	4.482338000	0.528146000	-2.959715000
1	6.692311000	0.347008000	-0.372186000
1	4.465978000	0.630815000	-4.056173000
6	4.539903000	0.317064000	-0.126562000
6	3.259531000	0.453137000	-2.263655000
6	3.285033000	0.308912000	-0.825305000
1	6.656073000	0.497049000	-2.860495000
6	1.984670000	0.572622000	-3.116613000
1	1.107111000	0.445255000	-2.446194000
6	1.887110000	-0.489891000	-4.235205000
6	1.882816000	1.962617000	-3.790646000
1	2.687577000	2.091539000	-4.545639000
1	0.913685000	2.054068000	-4.323979000
1	1.958939000	2.797753000	-3.073180000
1	2.679095000	-0.340832000	-4.999928000

1	0.912403000	-0.392719000	-4.757330000
1	1.971598000	-1.523947000	-3.860811000
6	4.812994000	0.403746000	1.391340000
1	5.796476000	-0.104307000	1.511634000
6	5.052275000	1.881325000	1.790688000
6	3.865512000	-0.269750000	2.389332000
1	4.290857000	-0.170801000	3.410114000
1	2.860574000	0.190135000	2.407806000
1	3.745725000	-1.348780000	2.186132000
1	5.780499000	2.381299000	1.119508000
1	5.443399000	1.938784000	2.828137000
1	4.105893000	2.457798000	1.769023000
7	2.028482000	0.100268000	-0.135829000
15	1.107594000	-1.439025000	-0.068012000
15	0.752337000	1.279489000	0.277673000
6	0.211058000	4.862179000	-1.668832000
6	1.499256000	5.420841000	-1.722896000
6	0.010899000	3.588638000	-1.107616000
1	1.652160000	6.419598000	-2.161955000
1	-1.002222000	3.158992000	-1.067033000
6	2.594493000	4.698978000	-1.215585000
6	1.107396000	2.859898000	-0.595027000
1	3.608727000	5.126442000	-1.258654000
6	2.404156000	3.425570000	-0.652697000
1	3.274409000	2.873574000	-0.271541000
1	-0.652951000	5.418426000	-2.064975000
6	0.835028000	1.804800000	2.054959000
6	1.531516000	2.951305000	2.507488000
6	0.076636000	1.054256000	2.982443000
1	2.073205000	3.593253000	1.797441000
1	-0.554704000	0.202776000	2.663988000
6	1.508866000	3.301911000	3.867165000
6	0.053258000	1.412253000	4.340381000
1	2.055774000	4.196562000	4.205478000
1	-0.563287000	0.811627000	5.027838000
6	0.778049000	2.528682000	4.788663000
1	0.756921000	2.814098000	5.852805000
6	0.886610000	-3.412057000	3.532948000
6	2.000016000	-4.265897000	3.551055000
6	0.671699000	-2.549655000	2.442718000
1	2.166957000	-4.944304000	4.403278000
1	-0.247412000	-1.931362000	2.454702000
6	2.893866000	-4.269901000	2.462178000
6	1.572891000	-2.533386000	1.354852000
1	3.760128000	-4.950842000	2.459389000
6	2.679241000	-3.418909000	1.367739000

1	3.375574000	-3.460084000	0.518371000
1	0.151273000	-3.409300000	4.353184000
6	1.622840000	-2.506974000	-1.484062000
6	0.581003000	-3.166239000	-2.174950000
6	2.964434000	-2.805302000	-1.825156000
1	-0.466161000	-2.924092000	-1.934163000
1	3.797206000	-2.288295000	-1.326246000
6	0.866277000	-4.117468000	-3.169489000
6	3.245883000	-3.752039000	-2.824653000
1	0.041189000	-4.623142000	-3.695305000
1	4.293871000	-3.970583000	-3.083898000
6	2.200859000	-4.414791000	-3.493356000
1	2.428260000	-5.159253000	-4.272687000
46	-0.969561000	-0.193979000	-0.038497000
6	-3.076268000	1.712455000	1.021289000
6	-4.126397000	2.642539000	0.908699000
6	-2.454386000	1.203094000	-0.136888000
1	-4.601872000	3.023602000	1.829134000
6	-4.589636000	3.089389000	-0.348949000
6	-2.912422000	1.632326000	-1.399746000
1	-2.457013000	1.244882000	-2.326726000
6	-3.968067000	2.562236000	-1.499862000
1	-4.313897000	2.881001000	-2.498511000
1	-2.776534000	1.350842000	2.018876000
6	-5.047263000	-1.935721000	-2.751704000
6	-6.216719000	-1.469778000	-2.114824000
6	-3.827404000	-2.026134000	-2.061661000
1	-2.925269000	-2.381504000	-2.587040000
6	-6.120298000	-1.109185000	-0.751473000
6	-3.751820000	-1.661504000	-0.704137000
1	-7.018517000	-0.751409000	-0.221098000
6	-4.911839000	-1.201111000	-0.047716000
1	-4.849734000	-0.935637000	1.019788000
1	-5.088667000	-2.231822000	-3.813224000
7	-2.509375000	-1.746869000	0.015255000
1	-2.042094000	-2.640475000	-0.189029000
6	-7.526510000	-1.343811000	-2.861276000
1	-7.484741000	-1.842618000	-3.850515000
1	-8.366976000	-1.791312000	-2.289832000
1	-7.790710000	-0.277782000	-3.037257000
6	-5.729274000	4.080884000	-0.449223000
1	-5.552658000	4.973082000	0.188657000
1	-5.877104000	4.431753000	-1.490689000
1	-6.688498000	3.631769000	-0.110209000
1	-2.661782000	-1.715404000	1.082087000
35	-2.674599000	-1.407428000	3.204049000

Int4

Electronic energy (BP86) = -2854.383877 a.u.
Zero-point correction (BP86) = 0.857968 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.762807 a.u.
Electronic energy (M06) = -2855.953747 a.u.

6	5.749658000	0.053422000	-1.664107000
6	5.638659000	0.004963000	-0.271288000
6	4.585840000	0.139503000	-2.430168000
1	6.552616000	-0.037626000	0.343461000
1	4.666861000	0.199946000	-3.526757000
6	4.389667000	0.010579000	0.391297000
6	3.303090000	0.147583000	-1.841808000
6	3.193143000	0.049734000	-0.406723000
1	6.739766000	0.036096000	-2.146465000
6	2.126338000	0.302856000	-2.817279000
1	1.179408000	0.302424000	-2.233469000
6	2.035238000	-0.834634000	-3.860848000
6	2.218921000	1.644423000	-3.583611000
1	3.053809000	1.621975000	-4.316754000
1	1.284817000	1.822744000	-4.155839000
1	2.383870000	2.508152000	-2.915403000
1	2.920750000	-0.832542000	-4.532167000
1	1.140947000	-0.683581000	-4.500960000
1	1.960386000	-1.836294000	-3.402730000
6	4.493959000	0.035579000	1.925462000
1	5.573778000	-0.145580000	2.123102000
6	4.199484000	1.434802000	2.505018000
6	3.746152000	-1.077623000	2.670356000
1	3.976819000	-1.033535000	3.755667000
1	2.651854000	-0.995795000	2.552773000
1	4.050912000	-2.079680000	2.305541000
1	4.839141000	2.206659000	2.028553000
1	4.408096000	1.452652000	3.595491000
1	3.140427000	1.726482000	2.370954000
7	1.871108000	-0.059075000	0.192977000
15	0.770782000	-1.487085000	0.043002000
15	0.639904000	1.231984000	0.372046000
6	0.550173000	4.583378000	-2.015368000
6	1.814979000	5.165240000	-1.825248000
6	0.229288000	3.366857000	-1.387135000
1	2.066909000	6.115836000	-2.322685000
1	-0.763236000	2.910362000	-1.531193000
6	2.760831000	4.534371000	-0.995116000
6	1.172882000	2.734716000	-0.547798000

1	3.753176000	4.987506000	-0.842752000
6	2.440896000	3.330169000	-0.347963000
1	3.177938000	2.859706000	0.318555000
1	-0.196367000	5.074156000	-2.659256000
6	0.639700000	1.872889000	2.115734000
6	0.660208000	0.977731000	3.209942000
6	0.434256000	3.250189000	2.370064000
1	0.799988000	-0.097959000	3.035597000
1	0.393958000	3.968800000	1.538186000
6	0.510427000	1.446938000	4.523983000
6	0.275908000	3.715624000	3.687621000
1	0.539473000	0.732193000	5.361778000
1	0.118801000	4.791692000	3.865987000
6	0.317968000	2.819082000	4.768443000
1	0.195539000	3.187246000	5.799654000
6	-0.663296000	-3.007089000	3.596884000
6	0.227269000	-4.040201000	3.933942000
6	-0.441477000	-2.236643000	2.442439000
1	0.050752000	-4.651660000	4.833059000
1	-1.161752000	-1.451127000	2.155610000
6	1.332143000	-4.309654000	3.104317000
6	0.680887000	-2.481341000	1.615130000
1	2.021183000	-5.132661000	3.352575000
6	1.553774000	-3.542813000	1.949624000
1	2.403797000	-3.786554000	1.294424000
1	-1.548671000	-2.809612000	4.221808000
6	1.489283000	-2.751012000	-1.081639000
6	0.511723000	-3.471059000	-1.810780000
6	2.852414000	-3.109621000	-1.194134000
1	-0.551335000	-3.188141000	-1.711771000
1	3.624531000	-2.558709000	-0.637402000
6	0.898087000	-4.531896000	-2.647166000
6	3.228247000	-4.167464000	-2.040520000
1	0.132407000	-5.086581000	-3.212357000
1	4.292243000	-4.437451000	-2.131901000
6	2.255722000	-4.878296000	-2.766917000
1	2.558053000	-5.706284000	-3.427927000
46	-1.146214000	-0.060185000	-0.313692000
6	-2.903478000	2.210330000	0.612630000
6	-3.894885000	3.204274000	0.507051000
6	-2.553951000	1.405040000	-0.495707000
1	-4.147703000	3.809529000	1.395355000
6	-4.569269000	3.443605000	-0.709398000
6	-3.228017000	1.644538000	-1.714687000
1	-3.000672000	1.034460000	-2.603865000
6	-4.209246000	2.648909000	-1.818621000

1	-4.717168000	2.807675000	-2.786045000
1	-2.401706000	2.069664000	1.584901000
6	-6.029701000	-2.503859000	-1.335160000
6	-6.507824000	-2.295425000	-0.021115000
6	-4.715355000	-2.190300000	-1.702390000
1	-4.382351000	-2.365143000	-2.740875000
6	-5.589810000	-1.758819000	0.909951000
6	-3.779073000	-1.664031000	-0.759739000
1	-5.924847000	-1.570353000	1.945150000
6	-4.268396000	-1.452897000	0.561962000
1	-3.584312000	-1.023184000	1.311506000
1	-6.710994000	-2.917305000	-2.099782000
7	-2.457199000	-1.446181000	-1.095528000
1	-2.331944000	-1.496521000	-2.116530000
6	-7.943226000	-2.594860000	0.354014000
1	-8.071498000	-2.660529000	1.454664000
1	-8.642834000	-1.806325000	-0.007791000
1	-8.293530000	-3.555253000	-0.082323000
6	-5.663606000	4.484392000	-0.809376000
1	-6.654181000	4.054811000	-0.539118000
1	-5.483711000	5.337690000	-0.123085000
1	-5.755625000	4.886248000	-1.839520000

Int5

Electronic energy (BP86) = -2854.389252 a.u.
Zero-point correction (BP86) = 0.859150 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.762468 a.u.
Electronic energy (M06) = -2855.970244 a.u.

6	5.215842000	1.297058000	-2.328520000
6	5.410572000	0.872330000	-1.010463000
6	3.916950000	1.323736000	-2.840885000
1	6.431376000	0.852775000	-0.593375000
1	3.752352000	1.662414000	-3.876129000
6	4.343689000	0.457874000	-0.179944000
6	2.804243000	0.927068000	-2.069371000
6	3.007975000	0.473398000	-0.716619000
1	6.072122000	1.606361000	-2.949197000
6	1.436952000	1.029034000	-2.759751000
1	0.649791000	0.750036000	-2.022597000
6	1.310066000	0.068355000	-3.964252000
6	1.150693000	2.469277000	-3.244189000
1	1.801880000	2.740712000	-4.102866000
1	0.099779000	2.553884000	-3.592955000
1	1.308454000	3.222029000	-2.450043000
1	2.038869000	0.328628000	-4.761963000

1	0.294588000	0.147633000	-4.408129000
1	1.477574000	-0.987494000	-3.683979000
6	4.772651000	0.069314000	1.245087000
1	5.881017000	-0.008987000	1.181391000
6	4.499681000	1.199344000	2.259754000
6	4.290898000	-1.303625000	1.737668000
1	4.712162000	-1.519365000	2.742323000
1	3.190862000	-1.359547000	1.807971000
1	4.624678000	-2.113938000	1.057102000
1	4.977884000	2.147004000	1.933965000
1	4.917429000	0.936227000	3.254966000
1	3.417784000	1.384820000	2.396430000
7	1.864889000	0.020321000	0.056102000
15	0.868105000	-1.473424000	-0.312049000
15	0.583455000	1.080195000	0.761985000
6	-0.164516000	4.888223000	-0.613627000
6	1.076322000	5.545127000	-0.552467000
6	-0.260178000	3.530670000	-0.256847000
1	1.155963000	6.606132000	-0.839802000
1	-1.229071000	3.005962000	-0.316053000
6	2.218739000	4.844313000	-0.121921000
6	0.879533000	2.822697000	0.185714000
1	3.193506000	5.355556000	-0.070139000
6	2.121697000	3.494536000	0.256315000
1	3.016525000	2.966912000	0.615509000
1	-1.064124000	5.428752000	-0.948632000
6	0.918484000	1.304831000	2.577846000
6	1.318803000	0.224776000	3.400943000
6	0.573366000	2.528775000	3.207772000
1	1.603669000	-0.732038000	2.944291000
1	0.254812000	3.390278000	2.601261000
6	1.380242000	0.362350000	4.797270000
6	0.632387000	2.661659000	4.604490000
1	1.704925000	-0.493916000	5.410339000
1	0.364196000	3.625350000	5.067467000
6	1.035190000	1.580287000	5.409114000
1	1.082741000	1.688013000	6.504579000
6	0.049583000	-3.538207000	3.186952000
6	0.956386000	-4.613959000	3.198877000
6	0.089211000	-2.598251000	2.144412000
1	0.923731000	-5.359282000	4.009971000
1	-0.633404000	-1.760671000	2.118017000
6	1.898523000	-4.737120000	2.162244000
6	1.041998000	-2.699655000	1.100706000
1	2.607802000	-5.580735000	2.158755000
6	1.942488000	-3.791093000	1.123059000

1	2.680687000	-3.912792000	0.316077000
1	-0.699043000	-3.433775000	3.988811000
6	1.795246000	-2.452285000	-1.611694000
6	0.947756000	-3.273074000	-2.394369000
6	3.187412000	-2.492243000	-1.858540000
1	-0.141648000	-3.236835000	-2.218003000
1	3.876895000	-1.872121000	-1.269495000
6	1.470890000	-4.116313000	-3.388124000
6	3.707499000	-3.321084000	-2.869705000
1	0.792154000	-4.750682000	-3.980945000
1	4.793985000	-3.330998000	-3.054712000
6	2.855555000	-4.135868000	-3.635706000
1	3.269606000	-4.782752000	-4.425793000
46	-1.123193000	-0.246753000	-0.052586000
6	-4.470986000	1.544259000	0.420330000
6	-4.982327000	2.840268000	0.552655000
6	-3.825631000	1.154653000	-0.774711000
1	-5.480035000	3.121672000	1.495899000
6	-4.869739000	3.797334000	-0.485073000
6	-3.715356000	2.090115000	-1.822895000
1	-3.221868000	1.799826000	-2.765572000
6	-4.223401000	3.392268000	-1.670711000
1	-4.124363000	4.105498000	-2.505960000
1	-4.558765000	0.823314000	1.247376000
6	-6.274724000	-2.466696000	-0.770593000
6	-5.810386000	-3.506179000	0.070119000
6	-5.464046000	-1.365616000	-1.082583000
1	-5.844837000	-0.564562000	-1.736567000
6	-4.505626000	-3.396824000	0.594931000
6	-4.157424000	-1.279881000	-0.557804000
1	-4.118232000	-4.186775000	1.259614000
6	-3.686356000	-2.295347000	0.288523000
1	-2.660213000	-2.208937000	0.689331000
1	-7.292025000	-2.522566000	-1.192967000
7	-3.278150000	-0.168601000	-0.915556000
1	-2.958835000	-0.297262000	-1.886651000
6	-6.686892000	-4.700479000	0.376720000
1	-6.255345000	-5.330132000	1.180019000
1	-7.704268000	-4.389050000	0.694353000
1	-6.813955000	-5.344926000	-0.520815000
6	-5.431176000	5.192438000	-0.320574000
1	-5.265889000	5.808784000	-1.226728000
1	-6.525214000	5.170046000	-0.124671000
1	-4.964905000	5.723139000	0.537607000

3

Electronic energy (BP86) = -596.607833 a.u.
Zero-point correction (BP86) = 0.245244 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.202530 a.u.
Electronic energy (M06) = -597.0291125 a.u.

6	-2.382560000	1.405757000	0.412606000
6	-1.271035000	0.627922000	-0.004480000
6	-3.681401000	0.885896000	0.376622000
1	-4.519276000	1.523571000	0.705376000
6	-1.521981000	-0.688192000	-0.463943000
6	-3.939601000	-0.433988000	-0.058529000
1	-0.696487000	-1.306852000	-0.842910000
6	-2.830218000	-1.197167000	-0.478677000
1	-2.992067000	-2.224290000	-0.846879000
1	-2.214887000	2.435746000	0.770383000
6	2.377729000	1.407225000	-0.416618000
6	3.678455000	0.887901000	-0.387714000
6	1.271546000	0.631400000	0.013597000
1	4.513668000	1.523610000	-0.726455000
6	3.941355000	-0.427623000	0.052798000
6	1.528038000	-0.682053000	0.481438000
1	0.705674000	-1.297495000	0.872509000
6	2.835443000	-1.189484000	0.489559000
1	3.000562000	-2.213291000	0.865918000
1	2.207009000	2.435143000	-0.778708000
7	-0.000630000	1.215803000	0.008866000
1	-0.002063000	2.237097000	0.005180000
6	-5.341796000	-1.000993000	-0.056763000
1	-6.075361000	-0.283992000	-0.482303000
1	-5.403004000	-1.937802000	-0.646727000
1	-5.686121000	-1.238336000	0.974484000
6	5.339180000	-1.004972000	0.037238000
1	6.110901000	-0.208594000	0.053232000
1	5.518090000	-1.669467000	0.908112000
1	5.518846000	-1.615448000	-0.876071000

ts-1
Electronic energy (BP86) = -5102.549318 a.u.
Zero-point correction (BP86) = 0.727756 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.640605 a.u.
Electronic energy (M06) = -5103.8472743 a.u.

6	-5.614125000	0.647722000	-0.120014000
6	-5.062549000	0.652378000	1.164808000
6	-4.766685000	0.469524000	-1.215960000
1	-5.724069000	0.788922000	2.036684000
1	-5.193227000	0.458480000	-2.231520000

6	-3.676567000	0.494339000	1.398303000
6	-3.374502000	0.302960000	-1.060482000
6	-2.806030000	0.324760000	0.264818000
1	-6.698322000	0.781527000	-0.263554000
6	-2.572958000	0.098840000	-2.354346000
1	-1.504379000	-0.060040000	-2.084875000
6	-2.647360000	1.321559000	-3.298142000
6	-3.055757000	-1.145222000	-3.136538000
1	-4.066311000	-0.978327000	-3.567695000
1	-2.369017000	-1.350806000	-3.984446000
1	-3.104355000	-2.051994000	-2.506969000
1	-1.997971000	1.154959000	-4.183556000
1	-2.323414000	2.258265000	-2.810444000
1	-3.682387000	1.473228000	-3.673274000
6	-3.294874000	0.485367000	2.889289000
1	-4.187550000	0.916191000	3.395726000
6	-3.159608000	-0.948711000	3.444366000
6	-2.116322000	1.379480000	3.295863000
1	-1.998287000	1.374282000	4.400146000
1	-1.165288000	1.043165000	2.848521000
1	-2.284139000	2.430738000	2.985390000
1	-4.074446000	-1.544420000	3.241917000
1	-3.011208000	-0.923120000	4.544857000
1	-2.293668000	-1.481142000	3.007791000
7	-1.368305000	0.191892000	0.416700000
15	-0.130714000	1.412118000	-0.160058000
15	-0.446590000	-1.351335000	0.260053000
6	-1.826971000	-4.563564000	-1.907437000
6	-3.111308000	-4.823429000	-1.399276000
6	-1.081873000	-3.479364000	-1.410389000
1	-3.702267000	-5.666087000	-1.792816000
1	-0.080710000	-3.254451000	-1.815874000
6	-3.641666000	-4.002723000	-0.386328000
6	-1.600761000	-2.656196000	-0.385794000
1	-4.648375000	-4.201972000	0.014705000
6	-2.889753000	-2.932076000	0.126663000
1	-3.309675000	-2.313902000	0.932366000
1	-1.405475000	-5.200252000	-2.701710000
6	-0.115877000	-2.030279000	1.960848000
6	0.506634000	-1.216700000	2.939480000
6	-0.291876000	-3.406604000	2.252948000
1	0.678787000	-0.150277000	2.736570000
1	-0.760822000	-4.072546000	1.513611000
6	0.910608000	-1.750528000	4.172551000
6	0.124285000	-3.940068000	3.484788000
1	1.380882000	-1.090309000	4.919149000

1	-0.028344000	-5.012532000	3.688367000
6	0.722461000	-3.116373000	4.454012000
1	1.042040000	-3.535833000	5.421292000
6	2.803161000	2.231386000	2.648566000
6	2.346073000	3.367759000	3.339677000
6	2.013881000	1.658391000	1.637285000
1	2.965717000	3.825551000	4.127654000
1	2.382073000	0.784778000	1.065973000
6	1.100063000	3.927760000	3.005522000
6	0.745829000	2.194821000	1.308329000
1	0.740842000	4.827978000	3.530122000
6	0.308971000	3.350013000	1.997804000
1	-0.652640000	3.816479000	1.736861000
1	3.785446000	1.793334000	2.886545000
6	-1.071428000	2.935613000	-0.705211000
6	-0.381375000	3.688771000	-1.684826000
6	-2.307923000	3.426150000	-0.223680000
1	0.574874000	3.303928000	-2.079283000
1	-2.875657000	2.868677000	0.534409000
6	-0.901847000	4.901186000	-2.165802000
6	-2.836699000	4.631296000	-0.721172000
1	-0.345699000	5.472381000	-2.926474000
1	-3.805985000	4.993620000	-0.341974000
6	-2.137910000	5.373361000	-1.689321000
1	-2.558073000	6.316355000	-2.074310000
46	1.191999000	-0.342208000	-1.012615000
1	5.997787000	1.963704000	-0.331887000
6	6.790589000	0.268201000	1.690939000
1	6.734480000	1.321398000	2.034773000
1	7.835899000	0.094776000	1.351542000
1	6.617265000	-0.390714000	2.565363000
6	5.805120000	-0.008990000	0.577554000
6	5.167355000	-1.263494000	0.463482000
6	4.280562000	-1.547468000	-0.591168000
6	4.027835000	-0.545260000	-1.542744000
6	4.638437000	0.716870000	-1.462640000
6	5.520988000	0.972120000	-0.399698000
1	5.363842000	-2.045242000	1.215314000
1	3.793083000	-2.529502000	-0.669717000
1	4.424486000	1.489065000	-2.215817000
35	2.860871000	-0.939234000	-3.035930000

ts-2

Electronic energy (BP86) = -5429.130958 a.u.
Zero-point correction (BP86) = 0.871352 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.774811 a.u.

Electronic energy (M06) = -5430.6723744 a.u.

1	6	4.148669000	1.825877000	3.631659000
2	6	4.762917000	1.080971000	2.621954000
3	6	2.752848000	1.917152000	3.656149000
4	1	5.861474000	0.981760000	2.618532000
5	1	2.262230000	2.478647000	4.466896000
6	6	4.030025000	0.425901000	1.601060000
7	6	1.956054000	1.324851000	2.656983000
8	6	2.604557000	0.600033000	1.587042000
9	1	4.756056000	2.321958000	4.405514000
10	6	0.433467000	1.480825000	2.815211000
11	1	-0.059826000	0.986096000	1.949394000
12	6	-0.039581000	2.952567000	2.847428000
13	6	-0.070979000	0.801870000	4.112244000
14	1	0.296410000	1.344726000	5.009556000
15	1	-1.180181000	0.827414000	4.144647000
16	1	0.249717000	-0.251160000	4.201418000
17	1	0.367150000	3.485552000	3.733289000
18	1	-1.146230000	2.983893000	2.927671000
19	1	0.252127000	3.521497000	1.947873000
20	6	4.918294000	-0.481666000	0.719727000
21	1	5.881047000	0.074416000	0.652543000
22	6	5.240853000	-1.789922000	1.485802000
23	6	4.512334000	-0.805319000	-0.721430000
24	1	5.318451000	-1.405470000	-1.193644000
25	1	3.581163000	-1.397682000	-0.781790000
26	1	4.379673000	0.105589000	-1.330639000
27	1	5.589263000	-1.594943000	2.520723000
28	1	6.035435000	-2.356455000	0.956171000
29	1	4.351976000	-2.450641000	1.539624000
30	7	1.790717000	0.125310000	0.488215000
31	15	1.127358000	1.150060000	-0.833476000
32	15	0.643902000	-1.246144000	0.472920000
33	6	-0.825852000	-3.102832000	3.844279000
34	6	0.289468000	-3.236165000	4.687942000
35	6	-0.704932000	-2.456683000	2.601568000
36	1	0.192066000	-3.742019000	5.661808000
37	1	-1.586812000	-2.352702000	1.952342000
38	6	1.532418000	-2.719228000	4.282051000
39	6	0.540382000	-1.933461000	2.186950000
40	1	2.413743000	-2.815452000	4.935889000
41	6	1.662044000	-2.074703000	3.039757000
42	1	2.642162000	-1.674276000	2.749198000
43	1	-1.805747000	-3.501751000	4.150337000
44	6	1.382261000	-2.705812000	-0.423863000

45	6	2.155821000	-3.709231000	0.206404000
46	6	1.083956000	-2.838821000	-1.799429000
47	1	2.352939000	-3.663362000	1.287398000
48	1	0.420264000	-2.106420000	-2.294872000
49	6	2.658941000	-4.791297000	-0.534086000
50	6	1.587436000	-3.924937000	-2.535708000
51	1	3.261495000	-5.562428000	-0.027894000
52	1	1.337055000	-4.010471000	-3.604982000
53	6	2.383625000	-4.898200000	-1.909333000
54	1	2.774550000	-5.751649000	-2.486370000
55	6	2.802381000	0.325157000	-4.517441000
56	6	3.900388000	1.194403000	-4.615590000
57	6	1.993569000	0.326497000	-3.366948000
58	1	4.530218000	1.194582000	-5.519832000
59	1	1.090868000	-0.306787000	-3.336784000
60	6	4.178523000	2.085062000	-3.562045000
61	6	2.283597000	1.195527000	-2.291357000
62	1	5.024894000	2.786482000	-3.637883000
63	6	3.373658000	2.092171000	-2.412276000
64	1	3.599333000	2.810627000	-1.611352000
65	1	2.551917000	-0.352336000	-5.349018000
66	6	1.242220000	2.931360000	-0.330669000
67	6	0.198300000	3.763805000	-0.792888000
68	6	2.337668000	3.530941000	0.337230000
69	1	-0.652309000	3.315821000	-1.326810000
70	1	3.171017000	2.918378000	0.708082000
71	6	0.232923000	5.153726000	-0.590185000
72	6	2.366828000	4.920753000	0.547217000
73	1	-0.592763000	5.780666000	-0.961935000
74	1	3.222678000	5.368113000	1.077068000
75	6	1.317814000	5.735696000	0.087158000
76	1	1.347425000	6.824114000	0.253927000
77	46	-0.937238000	-0.190360000	-0.788538000
78	6	-2.612929000	-2.722476000	-0.980030000
79	6	-3.665625000	-3.580598000	-0.613290000
80	6	-2.419934000	-1.500960000	-0.301590000
81	1	-3.797333000	-4.528495000	-1.163442000
82	6	-4.558542000	-3.254659000	0.432638000
83	6	-3.300026000	-1.166126000	0.747144000
84	1	-3.172792000	-0.226032000	1.307614000
85	6	-4.356148000	-2.031368000	1.103343000
86	1	-5.034412000	-1.740778000	1.924143000
87	1	-1.956532000	-2.998084000	-1.818754000
88	6	-4.777824000	3.395733000	0.968355000
89	6	-6.034717000	2.754427000	0.904107000
90	6	-3.683818000	2.945612000	0.214251000

91	1	-2.712947000	3.460343000	0.297225000
92	6	-6.147501000	1.634685000	0.051058000
93	6	-3.814801000	1.831729000	-0.644906000
94	1	-7.111584000	1.104328000	-0.022498000
95	6	-5.063319000	1.175370000	-0.711162000
96	1	-5.179015000	0.296719000	-1.364296000
97	1	-4.648817000	4.270257000	1.627970000
98	7	-2.705270000	1.355882000	-1.393691000
99	1	-2.139652000	2.118156000	-1.783648000
100	6	-7.220582000	3.265604000	1.692093000
101	1	-7.899502000	2.441052000	1.992242000
102	1	-6.902786000	3.798136000	2.611786000
103	1	-7.826905000	3.982240000	1.093949000
104	6	-5.702035000	-4.177447000	0.796461000
105	1	-5.368196000	-5.233870000	0.873500000
106	1	-6.164384000	-3.894653000	1.763875000
107	1	-6.504350000	-4.151559000	0.026141000
108	1	-2.937006000	0.734650000	-2.193201000
109	35	-1.456553000	-0.600446000	-3.554443000

ts-3

Electronic energy (BP86) = -2854.359380 a.u.
Zero-point correction (BP86) = 0.857289 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.763236 a.u.
Electronic energy (M06) = -2855.9230638 a.u.

6	5.665809000	-0.048602000	-1.750519000
6	5.587972000	-0.260276000	-0.370425000
6	4.485964000	0.162510000	-2.466453000
1	6.514634000	-0.415393000	0.206601000
1	4.539095000	0.340847000	-3.552008000
6	4.357864000	-0.283583000	0.325696000
6	3.221123000	0.151364000	-1.840429000
6	3.143593000	-0.089942000	-0.421948000
1	6.641855000	-0.042985000	-2.261330000
6	2.020134000	0.418430000	-2.759586000
1	1.091775000	0.412865000	-2.143793000
6	1.856580000	-0.655753000	-3.859385000
6	2.129563000	1.802065000	-3.443469000
1	2.937231000	1.805158000	-4.206574000
1	1.182356000	2.043435000	-3.969584000
1	2.340855000	2.616134000	-2.726485000
1	2.721747000	-0.648623000	-4.556351000
1	0.948275000	-0.442124000	-4.461326000
1	1.760178000	-1.676955000	-3.449285000
6	4.497912000	-0.478216000	1.844308000
1	5.571879000	-0.732203000	1.985188000

6	4.284591000	0.836491000	2.622775000
6	3.719030000	-1.662985000	2.435481000
1	3.955306000	-1.777904000	3.514518000
1	2.626334000	-1.541547000	2.337156000
1	3.992905000	-2.613669000	1.933058000
1	4.987902000	1.620763000	2.272516000
1	4.470174000	0.680564000	3.706733000
1	3.254220000	1.225477000	2.519367000
7	1.834672000	-0.172612000	0.210532000
15	0.634230000	-1.509038000	-0.084570000
15	0.702782000	1.193767000	0.466142000
6	0.977752000	4.851923000	-1.382936000
6	2.309292000	5.251644000	-1.179822000
6	0.536806000	3.599860000	-0.916944000
1	2.656869000	6.228590000	-1.552388000
1	-0.504251000	3.280835000	-1.090593000
6	3.199096000	4.401988000	-0.495489000
6	1.424870000	2.747754000	-0.223077000
1	4.243563000	4.711812000	-0.331884000
6	2.759342000	3.161157000	-0.006362000
1	3.458268000	2.515635000	0.543081000
1	0.273586000	5.512145000	-1.913530000
6	0.658366000	1.639830000	2.269965000
6	0.890229000	0.703024000	3.300957000
6	0.203008000	2.934732000	2.622494000
1	1.248376000	-0.304661000	3.054011000
1	0.005708000	3.684373000	1.840701000
6	0.688107000	1.052121000	4.647312000
6	-0.003606000	3.277527000	3.968282000
1	0.886197000	0.307115000	5.434486000
1	-0.355776000	4.290578000	4.220434000
6	0.239359000	2.339351000	4.987511000
1	0.079768000	2.611936000	6.042837000
6	-0.896187000	-2.823429000	3.520336000
6	-0.240836000	-4.042494000	3.767831000
6	-0.578004000	-2.075080000	2.375176000
1	-0.496178000	-4.637642000	4.659186000
1	-1.113406000	-1.133260000	2.165314000
6	0.730235000	-4.507639000	2.862623000
6	0.414479000	-2.519472000	1.468500000
1	1.237999000	-5.468732000	3.043299000
6	1.054905000	-3.755517000	1.721431000
1	1.808548000	-4.139388000	1.017514000
1	-1.670447000	-2.457772000	4.213271000
6	1.400589000	-2.788590000	-1.180153000
6	0.457907000	-3.483337000	-1.976778000

6	2.762461000	-3.164422000	-1.245013000
1	-0.604555000	-3.189862000	-1.941025000
1	3.516428000	-2.642269000	-0.639441000
6	0.866326000	-4.532875000	-2.816366000
6	3.167428000	-4.204596000	-2.100345000
1	0.119939000	-5.064315000	-3.427811000
1	4.232752000	-4.481310000	-2.148895000
6	2.224210000	-4.891376000	-2.885348000
1	2.548398000	-5.705995000	-3.552453000
46	-1.173597000	0.164247000	-0.448806000
6	-3.582675000	1.765663000	0.399500000
6	-4.251455000	2.995549000	0.491929000
6	-2.804011000	1.450511000	-0.750236000
1	-4.829274000	3.212078000	1.407492000
6	-4.209250000	3.959179000	-0.542246000
6	-2.764832000	2.412241000	-1.802740000
1	-2.187797000	2.201493000	-2.719777000
6	-3.451605000	3.631027000	-1.690167000
1	-3.393925000	4.352032000	-2.524673000
1	-3.660811000	1.046558000	1.229345000
6	-6.173033000	-2.173278000	-1.433020000
6	-6.207248000	-2.728407000	-0.131324000
6	-5.116039000	-1.362650000	-1.859917000
1	-5.128179000	-0.935697000	-2.877102000
6	-5.120391000	-2.436113000	0.719496000
6	-4.013312000	-1.084177000	-1.003673000
1	-5.107768000	-2.855037000	1.740100000
6	-4.043944000	-1.639549000	0.300654000
1	-3.192090000	-1.454099000	0.973581000
1	-7.004603000	-2.375489000	-2.129809000
7	-2.958566000	-0.287075000	-1.437272000
1	-3.037396000	-0.046162000	-2.428712000
6	-7.364072000	-3.593259000	0.318972000
1	-7.213780000	-3.966814000	1.352184000
1	-8.326386000	-3.035466000	0.303635000
1	-7.498978000	-4.478804000	-0.340044000
6	-4.975422000	5.259545000	-0.440679000
1	-4.550946000	6.038714000	-1.107392000
1	-6.044727000	5.135943000	-0.727641000
1	-4.968202000	5.661424000	0.594680000

$PhCH_3Br$

Electronic energy (BP86) = -2844.768065 a.u.
Zero-point correction (BP86) = 0.114151 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.080082 a.u.
Electronic energy (M06) = -2844.906432 a.u.

6	-2.479485000	0.002852000	-0.008155000
6	-1.749163000	1.210584000	-0.008580000
6	-1.749444000	-1.207102000	-0.008586000
1	-2.289535000	2.171759000	-0.014065000
1	-2.289999000	-2.168309000	-0.013910000
6	-0.343542000	1.222480000	-0.004273000
6	-0.345549000	-1.219384000	-0.004342000
1	0.207615000	2.174641000	-0.006320000
1	0.206535000	-2.171075000	-0.006543000
6	0.350663000	0.001833000	-0.000939000
35	2.263114000	-0.001053000	0.002837000
6	-3.991685000	-0.002479000	0.012701000
1	-4.408630000	0.980230000	-0.285433000
1	-4.406967000	-0.772307000	-0.670253000
1	-4.378759000	-0.230788000	1.030282000

$PhCH_3NH_2$
Electronic energy (BP86) = -326.543539 a.u.
Zero-point correction (BP86) = 0.139885 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.106691 a.u.
Electronic energy (M06) = -326.7886757 a.u.

6	-1.414494000	0.004438000	-0.003169000
6	-0.677308000	-1.201550000	-0.001260000
6	-0.674667000	1.205617000	-0.001378000
1	-1.215382000	-2.164860000	-0.006225000
1	-1.211270000	2.169540000	-0.006424000
6	0.723353000	-1.212202000	0.003964000
6	0.728492000	1.213129000	0.003626000
1	1.264027000	-2.173688000	0.008175000
1	1.270431000	2.173776000	0.007282000
6	1.459693000	0.000320000	0.007860000
7	2.853196000	-0.004193000	0.071305000
1	3.312959000	-0.853570000	-0.262709000
1	3.318058000	0.844848000	-0.256456000
6	-2.927936000	-0.001372000	-0.004650000
1	-3.337613000	-0.566857000	-0.869742000
1	-3.339201000	-0.477936000	0.912233000
1	-3.337183000	1.027828000	-0.055228000

Na(t-OBu)
Electronic energy (BP86) = -395.027443 a.u.
Zero-point correction (BP86) = 0.119437 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.086313 a.u.
Electronic energy (M06) = -395.3250242 a.u.

6	-0.621356000	0.000014000	-0.000178000
6	-1.154579000	-0.005064000	1.460251000
6	-1.160958000	-1.260356000	-0.733366000
1	-2.272383000	-1.311269000	-0.758110000
1	-0.788676000	-1.271091000	-1.780378000
1	-0.781672000	-2.175504000	-0.229861000
1	-0.775229000	0.889887000	1.998803000
1	-0.777927000	-0.905124000	1.992226000
1	-2.265817000	-0.003656000	1.521777000
6	-1.157686000	1.267157000	-0.723639000
1	-0.777278000	2.177386000	-0.212094000
1	-0.783340000	1.285394000	-1.769763000
1	-2.269042000	1.320506000	-0.749827000
8	0.760735000	-0.001541000	-0.003406000
11	2.724814000	-0.000427000	-0.000357000

_t_-BuOH

Electronic energy (BP86) = -233.362865 a.u.
Zero-point correction (BP86) = 0.119437 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.086313 a.u.
Electronic energy (M06) = -233.60479 a.u.

6	0.006221000	-0.000215000	0.017129000
6	-0.709584000	-1.258640000	-0.513349000
6	-0.673336000	1.278940000	-0.511550000
1	-0.178376000	2.177705000	-0.090233000
1	-0.632735000	1.341723000	-1.619446000
1	-1.745021000	1.306842000	-0.215498000
1	-0.670303000	-1.321528000	-1.621258000
1	-1.781881000	-1.255536000	-0.218088000
1	-0.241420000	-2.171869000	-0.092560000
6	1.495146000	-0.020656000	-0.357209000
1	1.632252000	-0.020822000	-1.457446000
1	2.007418000	0.868210000	0.064068000
1	1.982373000	-0.924943000	0.060980000
8	-0.015992000	-0.001028000	1.456839000
1	-0.955058000	0.011870000	1.724635000

NaBr

Electronic energy (BP86) = -2736.426014 a.u.
Zero-point correction (BP86) = 0.000670 a.u.
Thermal correction to Gibbs free energy (BP86) = -0.022960 a.u.
Electronic energy (M06) = -2736.454177 a.u.

11	0.000000000	0.000000000	-1.914553000

35 0.000000000 0.000000000 0.601717000

HBr
Electronic energy (BP86) = -2574.713252 a.u.
Zero-point correction (BP86) = 0.005811 a.u.
Thermal correction to Gibbs free energy (BP86) = -0.013430 a.u.
Electronic energy (M06) = -2574.667502 a.u.

1 0.000000000 0.000000000 -1.396155000
35 0.000000000 0.000000000 0.039890000

Int3'
Electronic energy (BP86) = -2584.334815 a.u.
Zero-point correction (BP86) = 0.755823 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.669385 a.u.
Electronic energy (M06) = -2585.7288447 a.u.

6 2.945467000 2.461582000 -3.522334000
6 3.404961000 2.709045000 -2.224973000
6 1.868260000 1.589976000 -3.701560000
1 4.251891000 3.399281000 -2.073626000
1 1.499451000 1.389700000 -4.720165000
6 2.815320000 2.117659000 -1.083274000
6 1.240025000 0.953680000 -2.611161000
6 1.708389000 1.219337000 -1.275140000
1 3.423464000 2.949283000 -4.387004000
6 0.081317000 0.005931000 -2.950665000
1 -0.255807000 -0.487508000 -2.011675000
6 0.514263000 -1.104920000 -3.934765000
6 -1.130554000 0.756586000 -3.549981000
1 -0.870562000 1.212828000 -4.529568000
1 -1.968132000 0.048718000 -3.725183000
1 -1.499221000 1.563054000 -2.889302000
1 0.727644000 -0.689624000 -4.943185000
1 -0.303999000 -1.846116000 -4.053933000
1 1.417195000 -1.644510000 -3.593278000
6 3.490800000 2.513083000 0.242799000
1 4.056963000 3.436681000 -0.013520000
6 2.558355000 2.905253000 1.397386000
6 4.557926000 1.485889000 0.679599000
1 5.119947000 1.865624000 1.559122000
1 4.107394000 0.517781000 0.970224000
1 5.290345000 1.299535000 -0.133874000
1 1.877328000 3.729733000 1.103562000
1 3.157112000 3.261111000 2.262459000
1 1.938060000 2.057549000 1.735008000

7	1.043925000	0.576623000	-0.157437000
15	1.285642000	-1.138524000	0.301585000
15	-0.718838000	0.861312000	0.271851000
6	-3.215196000	3.747402000	-1.210594000
6	-2.409574000	4.797234000	-1.688448000
6	-2.621052000	2.602795000	-0.656213000
1	-2.869833000	5.690275000	-2.140815000
1	-3.257788000	1.768639000	-0.313377000
6	-1.011908000	4.693105000	-1.589326000
6	-1.213074000	2.488649000	-0.538118000
1	-0.370032000	5.508476000	-1.960870000
6	-0.415797000	3.555576000	-1.012741000
1	0.679260000	3.506731000	-0.947768000
1	-4.312864000	3.812441000	-1.284357000
6	-0.791209000	1.491843000	2.049566000
6	-1.072234000	0.530597000	3.049885000
6	-0.725697000	2.851739000	2.433127000
1	-1.131794000	-0.534899000	2.741803000
1	-0.539517000	3.627598000	1.675703000
6	-1.258513000	0.905806000	4.390929000
6	-0.911736000	3.230693000	3.774010000
1	-1.471950000	0.137131000	5.151490000
1	-0.854600000	4.295953000	4.051121000
6	-1.176215000	2.261111000	4.757950000
1	-1.325574000	2.562944000	5.807300000
6	3.072329000	-0.577154000	4.016848000
6	4.126054000	-1.509492000	4.026145000
6	2.257639000	-0.437883000	2.882965000
1	4.763775000	-1.620607000	4.917646000
1	1.428742000	0.283023000	2.903023000
6	4.353951000	-2.299963000	2.886867000
6	2.487035000	-1.214877000	1.722055000
1	5.172811000	-3.037633000	2.880108000
6	3.545792000	-2.155790000	1.745599000
1	3.744727000	-2.785742000	0.866041000
1	2.876998000	0.047472000	4.903394000
6	2.283151000	-1.972302000	-1.025437000
6	1.830044000	-3.245068000	-1.438356000
6	3.485852000	-1.465670000	-1.570133000
1	0.886730000	-3.628170000	-1.011252000
1	3.870873000	-0.486118000	-1.254197000
6	2.563276000	-4.002448000	-2.368693000
6	4.205809000	-2.214334000	-2.517042000
1	2.200225000	-4.997068000	-2.673715000
1	5.135951000	-1.803230000	-2.940982000
6	3.750300000	-3.484698000	-2.915145000

1	4.322749000	-4.070807000	-3.652060000
46	-0.816612000	-1.776812000	0.651210000
1	-5.949032000	-2.526925000	-2.354180000
6	-7.639065000	-0.680115000	-1.190332000
1	-7.430044000	0.264405000	-1.740477000
1	-8.370405000	-0.435477000	-0.392972000
1	-8.131525000	-1.369777000	-1.905808000
6	-6.371296000	-1.277954000	-0.621489000
6	-5.891868000	-0.905371000	0.653822000
6	-4.699785000	-1.430815000	1.174858000
6	-3.951807000	-2.364570000	0.429554000
6	-4.413467000	-2.746353000	-0.845829000
6	-5.604882000	-2.208967000	-1.356052000
1	-6.465436000	-0.184073000	1.259375000
1	-4.344682000	-1.111816000	2.168139000
1	-3.835373000	-3.470069000	-1.443577000
7	-2.727296000	-2.896976000	0.951778000
1	-2.765144000	-3.010398000	1.973878000
1	-2.508976000	-3.816351000	0.546770000

Int4'

Electronic energy (BP86) = -2584.328453 a.u.
Zero-point correction (BP86) = 0.751778 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.666697 a.u.
Electronic energy (M06) = -2585.6999567 a.u.

46	1.667009000	-0.370588000	-0.055740000
6	-5.435478000	-0.084098000	-1.306798000
6	-4.434841000	-0.056080000	-2.279903000
6	-5.075832000	0.025581000	0.040247000
1	-4.724829000	-0.143772000	-3.339561000
1	-5.859247000	0.025220000	0.814779000
6	-3.057156000	0.067168000	-1.970328000
6	-3.725218000	0.120126000	0.429317000
6	-2.697125000	0.112326000	-0.576723000
1	-6.492916000	-0.187221000	-1.598802000
6	-3.445080000	0.240649000	1.929061000
1	-2.349409000	0.346540000	2.059468000
6	-3.902553000	-1.012058000	2.706813000
6	-4.122181000	1.495442000	2.525802000
1	-5.227949000	1.389793000	2.544862000
1	-3.785103000	1.656595000	3.571010000
1	-3.888378000	2.413188000	1.949816000
1	-5.002882000	-1.149279000	2.637064000
1	-3.646615000	-0.915154000	3.782489000
1	-3.419962000	-1.933952000	2.328257000

6	-2.177518000	0.124558000	-3.250682000
1	-2.524164000	-0.759345000	-3.835289000
6	-2.535389000	1.375790000	-4.096600000
6	-0.648699000	0.011042000	-3.188173000
1	-0.260106000	-0.046733000	-4.226637000
1	-0.171556000	0.893720000	-2.722994000
1	-0.297252000	-0.893533000	-2.665732000
1	-3.625555000	1.487509000	-4.263119000
1	-2.046725000	1.309126000	-5.091062000
1	-2.172571000	2.300504000	-3.604389000
7	-1.311006000	0.056729000	-0.166234000
15	-0.330309000	-1.416770000	0.070515000
15	-0.066413000	1.319098000	0.035852000
6	1.054380000	2.483361000	3.825592000
6	0.070311000	3.397181000	4.240058000
6	0.953372000	1.862081000	2.568170000
1	0.147003000	3.885897000	5.224535000
1	1.739066000	1.163207000	2.226121000
6	-1.004043000	3.703257000	3.383595000
6	-0.135173000	2.146688000	1.707181000
1	-1.768182000	4.434100000	3.694727000
6	-1.100234000	3.092441000	2.122687000
1	-1.925716000	3.373662000	1.452993000
1	1.914001000	2.256733000	4.476591000
6	-0.507378000	2.751308000	-1.048157000
6	0.571523000	3.363358000	-1.727458000
6	-1.797700000	3.321924000	-1.150900000
1	1.575501000	2.910758000	-1.672666000
1	-2.660003000	2.847153000	-0.659230000
6	0.368820000	4.533230000	-2.478963000
6	-1.995251000	4.490686000	-1.906928000
1	1.218669000	4.999112000	-3.001928000
1	-3.005401000	4.923489000	-1.984106000
6	-0.913884000	5.101531000	-2.566215000
1	-1.073451000	6.018420000	-3.155493000
6	-1.408472000	-4.162160000	3.037836000
6	-1.107827000	-3.458348000	4.214967000
6	-1.235736000	-3.552578000	1.781568000
1	-1.240341000	-3.938695000	5.197414000
1	-1.466571000	-4.125234000	0.871842000
6	-0.621905000	-2.140164000	4.130944000
6	-0.757045000	-2.225554000	1.687533000
1	-0.368807000	-1.583084000	5.046930000
6	-0.437241000	-1.534028000	2.879754000
1	-0.024123000	-0.515343000	2.828795000
1	-1.777592000	-5.198879000	3.090867000

6	-0.849628000	-2.699954000	-1.151221000
6	0.176024000	-3.358048000	-1.867517000
6	-2.196702000	-3.081352000	-1.357498000
1	1.223304000	-3.050659000	-1.709590000
1	-3.008571000	-2.594814000	-0.796351000
6	-0.139552000	-4.379811000	-2.778929000
6	-2.506041000	-4.093537000	-2.282599000
1	0.668149000	-4.887487000	-3.329632000
1	-3.557741000	-4.378947000	-2.444109000
6	-1.480509000	-4.743752000	-2.993087000
1	-1.728493000	-5.538516000	-3.714719000
1	2.465848000	-1.719803000	0.003838000
1	7.894224000	1.682235000	-0.454582000
6	9.020365000	-0.853089000	-0.477136000
1	9.681045000	0.036223000	-0.408933000
1	9.254543000	-1.361870000	-1.440097000
1	9.322436000	-1.554256000	0.332347000
6	7.560634000	-0.466894000	-0.376834000
6	6.542415000	-1.445999000	-0.285950000
6	5.187562000	-1.108965000	-0.210125000
6	4.752157000	0.249122000	-0.214060000
6	5.784185000	1.233458000	-0.309849000
6	7.138519000	0.879808000	-0.385445000
1	6.822254000	-2.514562000	-0.275637000
1	4.420689000	-1.898240000	-0.141757000
1	5.501144000	2.301247000	-0.318076000
7	3.427660000	0.622027000	-0.119573000
1	3.330881000	1.641909000	-0.149368000

Int5'

Electronic energy (BP86) = -5429.096076 a.u.
Zero-point correction (BP86) = 0.866764 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.762202 a.u.
Electronic energy (M06) = -5430.609848 a.u.

6	-4.271322000	-2.740006000	3.520361000
6	-4.882842000	-2.645969000	2.267001000
6	-2.969210000	-2.260303000	3.670285000
1	-5.904547000	-3.037900000	2.132017000
1	-2.473177000	-2.345083000	4.649801000
6	-4.240762000	-2.064243000	1.149577000
6	-2.263610000	-1.665377000	2.602406000
6	-2.912063000	-1.538382000	1.319634000
1	-4.805827000	-3.191509000	4.371291000
6	-0.826984000	-1.227086000	2.923208000
1	-0.379621000	-0.776705000	2.010041000

6	0.045153000	-2.435734000	3.340741000
6	-0.749918000	-0.178817000	4.057567000
1	-1.067993000	-0.618526000	5.026977000
1	0.299176000	0.162122000	4.180402000
1	-1.375332000	0.710264000	3.868212000
1	-0.253657000	-2.807604000	4.344149000
1	1.110320000	-2.131350000	3.406421000
1	-0.028594000	-3.283037000	2.636186000
6	-5.065394000	-2.136169000	-0.146274000
1	-6.076234000	-2.448758000	0.197268000
6	-5.279177000	-0.808415000	-0.885478000
6	-4.581690000	-3.271735000	-1.072890000
1	-5.264855000	-3.379834000	-1.941874000
1	-3.568852000	-3.082854000	-1.476392000
1	-4.566667000	-4.241897000	-0.533481000
1	-5.740853000	-0.050301000	-0.220070000
1	-5.963881000	-0.956100000	-1.747245000
1	-4.336233000	-0.382249000	-1.268593000
7	-2.218389000	-0.844892000	0.242747000
15	-0.839526000	-1.444856000	-0.729365000
15	-1.843791000	0.932009000	0.177679000
6	-1.898510000	3.515211000	3.339305000
6	-3.087790000	3.224868000	4.029704000
6	-1.537206000	2.764739000	2.206871000
1	-3.365333000	3.808166000	4.922292000
1	-0.600604000	2.990758000	1.670872000
6	-3.923971000	2.186047000	3.581047000
6	-2.378349000	1.723707000	1.748154000
1	-4.855607000	1.953272000	4.120908000
6	-3.579021000	1.439670000	2.441070000
1	-4.243122000	0.629407000	2.105652000
1	-1.238194000	4.326295000	3.683954000
6	-2.949610000	1.790632000	-1.050565000
6	-2.425515000	1.942035000	-2.358034000
6	-4.178516000	2.415823000	-0.735810000
1	-1.434787000	1.514817000	-2.594108000
1	-4.583283000	2.356918000	0.285606000
6	-3.134688000	2.657298000	-3.337531000
6	-4.883639000	3.133678000	-1.715371000
1	-2.707024000	2.769226000	-4.346340000
1	-5.839597000	3.615098000	-1.454111000
6	-4.368840000	3.249935000	-3.019741000
1	-4.920699000	3.822304000	-3.782400000
6	-2.713920000	-1.758731000	-4.440653000
6	-2.068991000	-2.861672000	-5.027687000
6	-2.389486000	-1.362527000	-3.133823000

1	-2.320205000	-3.170022000	-6.054948000
1	-2.900099000	-0.494477000	-2.695960000
6	-1.098079000	-3.564447000	-4.294967000
6	-1.426467000	-2.070698000	-2.381362000
1	-0.581026000	-4.426969000	-4.744900000
6	-0.777779000	-3.175463000	-2.982619000
1	-0.011616000	-3.737474000	-2.428421000
1	-3.475447000	-1.196339000	-5.003993000
6	-0.159048000	-2.992957000	-0.003292000
6	1.235111000	-3.074148000	0.202076000
6	-0.969669000	-4.124382000	0.249452000
1	1.863599000	-2.189440000	0.009631000
1	-2.055490000	-4.079693000	0.080028000
6	1.814582000	-4.277119000	0.643007000
6	-0.387181000	-5.316335000	0.710500000
1	2.904764000	-4.332044000	0.789272000
1	-1.025039000	-6.190927000	0.914465000
6	1.005301000	-5.396812000	0.901182000
1	1.459013000	-6.337071000	1.253225000
46	0.386807000	0.456498000	-0.642863000
1	-0.896139000	5.852661000	-0.977495000
6	1.034283000	7.788963000	-0.524896000
1	1.680229000	8.241180000	-1.310751000
1	1.323043000	8.270775000	0.435998000
1	-0.010513000	8.091102000	-0.744358000
6	1.173213000	6.283211000	-0.470648000
6	2.415236000	5.666750000	-0.179523000
6	2.561300000	4.278367000	-0.135310000
6	1.456935000	3.393262000	-0.371353000
6	0.215123000	4.022202000	-0.686922000
6	0.087662000	5.419580000	-0.725047000
1	3.299434000	6.299049000	0.016122000
1	3.547386000	3.839987000	0.096431000
1	-0.652512000	3.393722000	-0.933689000
7	1.612578000	2.033649000	-0.259489000
1	2.601977000	1.774738000	-0.194572000
1	1.665775000	-0.189281000	-1.309456000
1	9.241010000	-2.031006000	-1.099253000
6	10.451262000	-0.817854000	1.066467000
1	10.983448000	-1.656285000	0.574234000
1	10.555145000	-0.943031000	2.164302000
1	10.987884000	0.118359000	0.796544000
6	8.999211000	-0.754608000	0.647943000
6	8.063770000	0.003476000	1.387732000
6	6.717967000	0.094488000	0.997958000
6	6.289875000	-0.585814000	-0.155490000

6	7.193591000	-1.350100000	-0.911555000
6	8.536261000	-1.428100000	-0.502709000
1	8.392915000	0.538471000	2.294241000
1	6.003607000	0.689297000	1.586582000
1	6.851624000	-1.880679000	-1.812745000
35	4.455717000	-0.470477000	-0.70017100

Int6'

Electronic energy (BP86) = -5497.679921 a.u.
Zero-point correction (BP86) = 0.851923 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.754510 a.u.
Electronic energy (M06) = -5499.2439813 a.u.

6	4.769222000	-0.656647000	-3.212374000
6	4.918765000	0.505455000	-2.448926000
6	3.567280000	-1.359623000	-3.137341000
1	5.849720000	1.089931000	-2.530429000
1	3.424303000	-2.255457000	-3.760868000
6	3.912640000	0.972842000	-1.572907000
6	2.514675000	-0.957923000	-2.285157000
6	2.700523000	0.204672000	-1.452392000
1	5.579494000	-0.997160000	-3.876825000
6	1.231046000	-1.790501000	-2.398736000
1	0.470874000	-1.382001000	-1.697997000
6	1.401652000	-3.290537000	-2.070056000
6	0.658339000	-1.693607000	-3.834216000
1	1.278678000	-2.286108000	-4.540834000
1	-0.368040000	-2.116095000	-3.843418000
1	0.625889000	-0.654004000	-4.210316000
1	2.101061000	-3.779500000	-2.781427000
1	0.413418000	-3.786062000	-2.176185000
1	1.777327000	-3.473239000	-1.047831000
6	4.245357000	2.318019000	-0.906381000
1	5.293999000	2.519072000	-1.217807000
6	3.419237000	3.477483000	-1.499895000
6	4.275542000	2.314856000	0.628306000
1	4.595784000	3.307062000	1.010985000
1	3.291426000	2.079287000	1.068781000
1	4.993704000	1.560664000	1.010175000
1	3.536187000	3.517728000	-2.602838000
1	3.762240000	4.450123000	-1.087762000
1	2.341089000	3.388623000	-1.269337000
7	1.688085000	0.521902000	-0.446034000
15	1.398882000	-0.434093000	1.055738000
15	0.050859000	1.207955000	-0.672389000
6	-1.961639000	0.574663000	-4.212755000

6	-1.272692000	1.393024000	-5.121891000
6	-1.526581000	0.476333000	-2.879442000
1	-1.613327000	1.466077000	-6.167067000
1	-2.053801000	-0.199050000	-2.190700000
6	-0.135079000	2.110650000	-4.702439000
6	-0.405506000	1.215861000	-2.448392000
1	0.417081000	2.741730000	-5.416810000
6	0.296299000	2.031197000	-3.369609000
1	1.172092000	2.612336000	-3.044359000
1	-2.833170000	-0.016971000	-4.532828000
6	0.002212000	3.017094000	-0.265197000
6	0.771682000	3.577753000	0.777790000
6	-0.978808000	3.820039000	-0.895262000
1	1.536455000	2.973717000	1.283848000
1	-1.606520000	3.402471000	-1.695992000
6	0.587227000	4.915201000	1.163888000
6	-1.164589000	5.156093000	-0.500947000
1	1.208375000	5.337352000	1.969653000
1	-1.931481000	5.766096000	-1.004184000
6	-0.381408000	5.710053000	0.525299000
1	-0.526588000	6.758857000	0.829378000
6	1.886351000	1.858647000	4.453852000
6	3.162231000	1.517447000	4.934405000
6	1.402076000	1.276363000	3.270154000
1	3.540352000	1.965908000	5.866884000
1	0.386560000	1.515611000	2.914010000
6	3.945868000	0.584104000	4.231616000
6	2.193479000	0.358061000	2.539507000
1	4.939031000	0.298378000	4.613494000
6	3.465193000	0.003733000	3.046777000
1	4.082471000	-0.740310000	2.521675000
1	1.254418000	2.568366000	5.010849000
6	2.273831000	-2.044747000	1.010714000
6	1.539342000	-3.100041000	1.603438000
6	3.594004000	-2.272339000	0.558132000
1	0.507598000	-2.906931000	1.952117000
1	4.174260000	-1.464624000	0.087949000
6	2.124136000	-4.371200000	1.739353000
6	4.164145000	-3.550146000	0.690917000
1	1.548858000	-5.190304000	2.198930000
1	5.188264000	-3.727915000	0.326248000
6	3.433737000	-4.597936000	1.280854000
1	3.887774000	-5.596784000	1.379901000
46	-0.978235000	-0.102933000	0.871722000
6	-3.247537000	1.801732000	1.222950000
6	-4.559369000	2.305170000	1.139276000

6	-2.873887000	0.614426000	0.549866000
1	-4.816232000	3.230657000	1.684134000
6	-5.548279000	1.654299000	0.368903000
6	-3.853741000	-0.024593000	-0.241162000
1	-3.624804000	-0.926542000	-0.841531000
6	-5.164549000	0.488329000	-0.324996000
1	-5.901006000	-0.038158000	-0.956198000
1	-2.510617000	2.356654000	1.828169000
6	-6.964015000	2.185406000	0.302476000
1	-7.525169000	1.961242000	1.236800000
1	-6.983841000	3.288265000	0.173624000
1	-7.530084000	1.733645000	-0.537108000
35	-2.710766000	-3.228022000	-2.270189000
6	-2.295340000	-1.669623000	3.327387000
6	-1.890654000	-2.955351000	4.088401000
6	-1.853919000	-0.436837000	4.142378000
1	-2.137006000	0.492045000	3.604699000
1	-2.330714000	-0.412730000	5.145565000
1	-0.753386000	-0.444230000	4.281717000
1	-2.391063000	-3.021467000	5.077849000
1	-0.793260000	-2.981547000	4.251656000
1	-2.173991000	-3.858757000	3.505713000
8	-1.628439000	-1.716147000	2.067870000
11	-2.365767000	-2.830054000	0.303864000
6	-3.832191000	-1.645899000	3.143511000
1	-4.177284000	-2.543781000	2.582904000
1	-4.148376000	-0.746642000	2.578923000
1	-4.363008000	-1.650025000	4.119885000

Int7'

Electronic energy (BP86) = -2761.199864 a.u.
Zero-point correction (BP86) = 0.849474 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.758204 a.u.
Electronic energy (M06) = -2762.7616141 a.u.

6	-4.985182000	-2.522280000	-1.243298000
6	-4.234204000	-1.917338000	-2.251130000
6	-4.482924000	-2.517962000	0.060463000
1	-4.608547000	-1.948786000	-3.287880000
1	-5.049281000	-3.017444000	0.861984000
6	-2.995869000	-1.268869000	-2.014733000
6	-3.257008000	-1.900995000	0.376029000
6	-2.504520000	-1.234643000	-0.660452000
1	-5.943844000	-3.012161000	-1.476963000
6	-2.767880000	-2.072391000	1.815571000
1	-1.876465000	-1.431880000	1.944958000

6	-2.355640000	-3.542773000	2.058398000
6	-3.792612000	-1.652410000	2.888466000
1	-4.698436000	-2.295420000	2.872891000
1	-3.341316000	-1.754968000	3.897546000
1	-4.116144000	-0.602280000	2.766343000
1	-3.245001000	-4.208697000	2.033944000
1	-1.872883000	-3.655966000	3.051355000
1	-1.641273000	-3.910914000	1.296826000
6	-2.410096000	-0.679700000	-3.321204000
1	-2.715690000	-1.430527000	-4.084780000
6	-3.148984000	0.620340000	-3.720461000
6	-0.890990000	-0.551289000	-3.489319000
1	-0.673716000	-0.113494000	-4.486186000
1	-0.417416000	0.099697000	-2.734270000
1	-0.395563000	-1.538498000	-3.448394000
1	-4.249690000	0.480047000	-3.707988000
1	-2.856930000	0.923487000	-4.747891000
1	-2.908184000	1.458835000	-3.041394000
7	-1.275025000	-0.540930000	-0.310438000
15	0.377651000	-1.167027000	-0.019388000
15	-1.040601000	1.192142000	0.115122000
6	-2.835152000	2.437838000	3.619348000
6	-4.211750000	2.342667000	3.354423000
6	-1.900702000	2.050217000	2.642433000
1	-4.944339000	2.656945000	4.114713000
1	-0.822292000	2.147819000	2.846165000
6	-4.651996000	1.837146000	2.117584000
6	-2.331370000	1.559319000	1.388952000
1	-5.730058000	1.745423000	1.909993000
6	-3.721101000	1.439066000	1.142232000
1	-4.081720000	1.030130000	0.186072000
1	-2.482479000	2.825395000	4.588220000
6	-1.432404000	2.410815000	-1.224657000
6	-0.391444000	2.662964000	-2.153979000
6	-2.578907000	3.240491000	-1.255158000
1	0.548212000	2.092798000	-2.083943000
1	-3.380978000	3.111465000	-0.516031000
6	-0.525935000	3.667210000	-3.125035000
6	-2.702637000	4.255196000	-2.219024000
1	0.294954000	3.844617000	-3.837405000
1	-3.602715000	4.890431000	-2.224981000
6	-1.683806000	4.463062000	-3.164959000
1	-1.782828000	5.260572000	-3.918716000
6	2.217851000	-3.321899000	-3.009281000
6	1.319563000	-4.371742000	-3.267872000
6	1.919275000	-2.357069000	-2.031048000

1	1.554610000	-5.122764000	-4.039046000
1	2.620450000	-1.531253000	-1.830233000
6	0.119968000	-4.464208000	-2.538371000
6	0.714324000	-2.443856000	-1.299110000
1	-0.587294000	-5.285303000	-2.736203000
6	-0.182198000	-3.509238000	-1.553061000
1	-1.125395000	-3.591300000	-0.991986000
1	3.160140000	-3.246343000	-3.574426000
6	0.587156000	-2.116303000	1.566043000
6	1.060771000	-3.446735000	1.599003000
6	0.486373000	-1.400975000	2.784455000
1	1.178297000	-4.014556000	0.664495000
1	0.175652000	-0.344032000	2.770422000
6	1.404284000	-4.052220000	2.822040000
6	0.810287000	-2.012918000	4.004161000
1	1.780116000	-5.087755000	2.827519000
1	0.721788000	-1.441500000	4.941640000
6	1.273053000	-3.342671000	4.026480000
1	1.544541000	-3.818024000	4.982438000
46	1.376316000	0.853539000	0.163762000
6	2.312060000	3.646377000	1.047456000
6	2.762339000	2.929699000	2.342187000
6	3.422450000	4.629014000	0.597536000
1	3.123622000	5.126309000	-0.348367000
1	3.616027000	5.414169000	1.360089000
1	4.363900000	4.073767000	0.409870000
1	2.929045000	3.642135000	3.179517000
1	3.700191000	2.365613000	2.162614000
1	1.986473000	2.196151000	2.656170000
6	1.008979000	4.441923000	1.314119000
1	1.122071000	5.182600000	2.136049000
1	0.698241000	4.982883000	0.396572000
1	0.183936000	3.751788000	1.588911000
8	2.128750000	2.737612000	-0.014958000
6	3.878742000	-0.772417000	0.800023000
6	5.227437000	-1.155969000	0.645752000
6	3.310007000	0.218827000	-0.027028000
1	5.648512000	-1.927844000	1.313610000
6	6.044737000	-0.580790000	-0.348236000
6	4.129395000	0.811699000	-1.014114000
1	3.723523000	1.621107000	-1.640664000
6	5.466376000	0.407094000	-1.177842000
1	6.081867000	0.881876000	-1.962466000
1	3.278397000	-1.262635000	1.583423000
6	7.495828000	-0.980907000	-0.510207000
1	7.729769000	-1.909630000	0.049031000

1	7.758764000	-1.150189000	-1.576124000
1	8.180606000	-0.188206000	-0.134854000

Int8'

Electronic energy (BP86) = -3048.503616 a.u.
Zero-point correction (BP86) = 0.964677 a.u.
Thermal correction to Gibbs free energy (BP86) = 0.861643 a.u.
Electronic energy (M06) = -3050.2712408 a.u.

6	-6.147182000	-1.350104000	0.458404000
6	-5.432339000	-1.437756000	1.656190000
6	-5.473297000	-0.967534000	-0.703434000
1	-5.958188000	-1.733965000	2.579022000
1	-6.031345000	-0.889903000	-1.649773000
6	-4.047009000	-1.162559000	1.737905000
6	-4.092481000	-0.679595000	-0.702728000
6	-3.356839000	-0.786257000	0.533571000
1	-7.224479000	-1.579091000	0.432967000
6	-3.499440000	-0.259963000	-2.056157000
1	-2.415786000	-0.051404000	-1.917590000
6	-4.163983000	1.026826000	-2.600882000
6	-3.645807000	-1.358521000	-3.135401000
1	-4.713979000	-1.516474000	-3.395943000
1	-3.125780000	-1.045334000	-4.064786000
1	-3.228087000	-2.330821000	-2.821602000
1	-5.216764000	0.832973000	-2.897798000
1	-3.626722000	1.375059000	-3.507453000
1	-4.168744000	1.850726000	-1.866324000
6	-3.483649000	-1.256817000	3.167822000
1	-4.240209000	-1.867618000	3.708928000
6	-2.152534000	-1.995685000	3.346227000
6	-3.483482000	0.117682000	3.872350000
1	-3.224782000	-0.000740000	4.945851000
1	-2.740748000	0.809059000	3.430257000
1	-4.482729000	0.597925000	3.816607000
1	-2.195901000	-3.014215000	2.911736000
1	-1.925571000	-2.106862000	4.427450000
1	-1.307236000	-1.462530000	2.877528000
7	-1.927820000	-0.518660000	0.521378000
15	-1.169808000	1.089634000	0.480621000
15	-0.628873000	-1.510558000	-0.275924000
6	-1.379805000	-4.618217000	-2.868574000
6	-2.481188000	-5.293030000	-2.314970000
6	-0.879909000	-3.458153000	-2.252972000
1	-2.878961000	-6.197571000	-2.801952000
1	-0.020464000	-2.930918000	-2.695861000

6	-3.071975000	-4.808123000	-1.135007000
6	-1.470076000	-2.960571000	-1.068891000
1	-3.934100000	-5.331519000	-0.691979000
6	-2.568748000	-3.654688000	-0.508550000
1	-3.048401000	-3.296402000	0.412825000
1	-0.906942000	-4.989913000	-3.791297000
6	0.434546000	-2.435005000	0.949417000
6	1.721326000	-1.896586000	1.195880000
6	0.103762000	-3.688893000	1.516059000
1	2.033819000	-0.949216000	0.719472000
1	-0.865163000	-4.159720000	1.294613000
6	2.637780000	-2.576735000	2.018669000
6	1.017055000	-4.361438000	2.342753000
1	3.638595000	-2.145934000	2.176814000
1	0.741858000	-5.336100000	2.776832000
6	2.283912000	-3.805008000	2.600842000
1	3.003353000	-4.342004000	3.239654000
6	0.673920000	1.202999000	4.187803000
6	0.264623000	2.432974000	4.734109000
6	0.209299000	0.801825000	2.925728000
1	0.634253000	2.750827000	5.721998000
1	0.565639000	-0.146104000	2.496875000
6	-0.605448000	3.260514000	4.005173000
6	-0.691550000	1.612859000	2.197198000
1	-0.918723000	4.233344000	4.416372000
6	-1.080346000	2.857682000	2.744319000
1	-1.754221000	3.523629000	2.186739000
1	1.370115000	0.552954000	4.740728000
6	-2.430131000	2.357802000	0.042366000
6	-2.079972000	3.324873000	-0.925782000
6	-3.675142000	2.459456000	0.708594000
1	-1.106712000	3.253808000	-1.436280000
1	-3.961185000	1.724205000	1.474406000
6	-2.961399000	4.379835000	-1.221920000
6	-4.557091000	3.506863000	0.395348000
1	-2.673312000	5.132028000	-1.972901000
1	-5.527985000	3.572104000	0.911443000
6	-4.201261000	4.470219000	-0.566917000
1	-4.893546000	5.293906000	-0.803841000
46	0.524970000	0.554190000	-0.930494000
6	1.495205000	3.050790000	-2.280743000
6	2.076944000	4.328092000	-2.379049000
6	1.297092000	2.442069000	-1.021111000
1	2.214667000	4.780406000	-3.376817000
6	2.501931000	5.036238000	-1.232656000
6	1.711788000	3.145649000	0.128835000

1	1.579192000	2.711902000	1.132775000
6	2.311068000	4.417886000	0.020017000
1	2.630556000	4.941366000	0.937955000
1	1.206995000	2.519213000	-3.200121000
6	3.164824000	6.391765000	-1.351004000
1	4.234522000	6.295553000	-1.642297000
1	2.677402000	7.021097000	-2.124820000
1	3.135644000	6.946730000	-0.391228000
1	8.150077000	0.208076000	1.901966000
6	8.898972000	-2.356177000	1.182073000
1	9.660654000	-2.253920000	0.375546000
1	8.724680000	-3.444173000	1.320385000
1	9.362471000	-1.968907000	2.113302000
6	7.618825000	-1.620949000	0.848312000
6	6.608898000	-2.214902000	0.058046000
6	5.435147000	-1.531455000	-0.287417000
6	5.208978000	-0.194132000	0.145112000
6	6.223015000	0.404367000	0.942950000
6	7.389229000	-0.296117000	1.281053000
1	6.743711000	-3.250225000	-0.300597000
1	4.666212000	-2.034778000	-0.895077000
1	6.082810000	1.438399000	1.300870000
7	4.031912000	0.466095000	-0.149135000
1	3.449525000	0.179622000	-0.967756000
1	4.019673000	1.477200000	0.001356000
6	1.933261000	-0.936750000	-3.144611000
1	1.686739000	-1.925676000	-2.655687000
6	3.276599000	-1.115454000	-3.875511000
6	0.804430000	-0.620798000	-4.143678000
1	-0.159537000	-0.484625000	-3.607341000
1	1.027734000	0.322972000	-4.686137000
1	0.673594000	-1.429042000	-4.896371000
1	3.553839000	-0.174479000	-4.395971000
1	3.222873000	-1.932082000	-4.627010000
1	4.087049000	-1.356492000	-3.158314000
8	2.082366000	0.066874000	-2.175840000