Electronic Supplementary Information

Copper(I)-catalyzed heteroannulation of [60]fullerene with ketoxime acetates: preparation of novel 1-fulleropyrrolines

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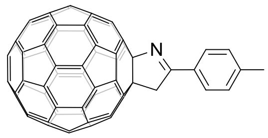
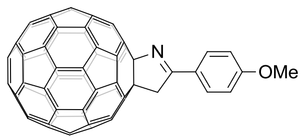
General procedure for the synthesis of 2a–k from the CuBr-catalyzed reaction of C_{60} with 1a–k. A mixture of C_{60} (0.05 mmol), oxime acetates **1** (0.075 mmol), CuBr (0.01 mmol), and $NaHSO_3$ (0.5 mmol) was dissolved in CB (8 mL). Then the solution was vigorously stirred at 150 °C and stopped at the designated time. The resulting solution was directly separated on a silica gel column with CS_2/CH_2Cl_2 as the eluent to give recovered C_{60} and then the desired product **2**.

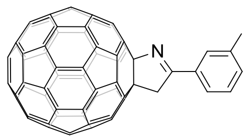


Preparation of **2a**: By following the general procedure, the reaction of C_{60} (35.9 mg, 0.05 mmol) with **1a** (14.3 mg, 0.075 mmol), CuBr (1.4 mg, 0.01 mmol), and $NaHSO_3$ (52.3 mg, 0.5 mmol) at 150 °C afforded **2a** (12.8 mg, 30%) and recovered C_{60} (14.7 mg, 41%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.16 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 5.13 (s, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$ all 2C unless indicated) δ 172.58 (1C, C=N), 155.54, 150.18, 147.59 (1C), 147.43 (1C), 146.40, 146.28, 146.16, 146.03, 145.97, 145.70 (4C), 145.26, 145.22, 145.20, 144.98, 144.46, 144.36, 142.96, 142.60, 142.59, 142.53, 142.27, 142.16 (1C, aryl *C*), 142.09, 141.89 (4C), 141.72, 140.21, 139.73, 136.14, 135.16, 130.65 (1C, aryl *C*), 129.65 (aryl *C*), 128.59 (aryl *C*), 100.81 (1C, sp^3-*C* of C_{60}), 65.20 (1C, sp^3-*C* of C_{60}), 50.87 (1C), 21.84 (1C); FT-IR ν/cm^{-1} (KBr) 3027, 2913, 2853, 1795, 1611, 1567, 1506, 1420, 1334, 1177, 1108, 1043, 810, 770, 555, 522; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.06), 311 (4.58), 429 (3.47); MALDI-TOF MS m/z calcd for $C_{69}H_9N$ $[M]^+$ 851.0730, found 851.0742.

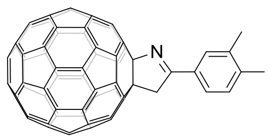


Preparation of **2b**. By following the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with **1b** (15.6 mg, 0.075 mmol), CuBr (1.6 mg, 0.01 mmol), and $NaHSO_3$ (52.3 mg, 0.5 mmol) at 150 °C afforded **2b** (11.5 mg, 27%) and recovered C_{60} (16.9 mg, 47%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.21 (d, J = 8.8 Hz, 2H), 7.08 (d, J = 8.8 Hz, 2H), 5.11 (s, 2H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 171.92 (1C, C=N), 162.48 (1C, aryl *C*), 155.63, 150.34, 147.59 (1C), 147.42 (1C), 146.38, 146.26, 146.15, 146.02, 145.96, 145.71, 145.68, 145.25, 145.21, 145.19, 144.98, 144.46, 144.36, 142.95, 142.59, 142.58, 142.52, 142.26, 142.08, 141.92, 141.89, 141.71, 140.20, 139.70, 136.10, 135.19, 130.26 (aryl *C*), 125.99 (1C, aryl *C*), 114.25 (aryl *C*), 100.73 (1C, sp^3-*C* of C_{60}), 65.30 (1C, sp^3-*C* of C_{60}), 55.18 (1C), 50.80 (1C); FT-IR ν/cm^{-1} (KBr) 2990, 2953, 2917, 2830, 1795, 1603, 1567, 1506, 1458, 1421, 1336, 1310, 1248, 1172, 1109, 1027, 900, 830, 796, 773, 727, 603, 556, 523; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.08), 310 (4.74), 429 (3.53); MALDI-TOF MS m/z calcd for $C_{69}H_9NO$ $[M]^+$ 867.0679, found

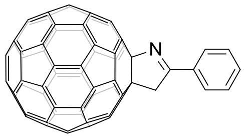
867.0635.



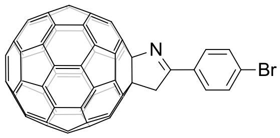
Preparation of **2c**. By following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1c** (14.5 mg, 0.075 mmol), CuBr (1.6 mg, 0.01 mmol), and $NaHSO_3$ (51.9 mg, 0.5 mmol) at 150 ^oC afforded **2c** (10.4 mg, 24%) and recovered C_{60} (16.1 mg, 45%): amorphous brown solid; ^1H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.16 (s, 1H), 8.04 (d, J = 7.6 Hz, 1H), 7.49 (dd, J = 7.6 Hz, 7.6 Hz, 1H), 7.43 (d, J = 7.6 Hz, 1H), 5.14 (s, 2H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 172.98 (1C, C=N), 155.44, 150.02, 147.58 (1C), 147.41 (1C), 146.36, 146.27, 146.14, 146.02, 145.96, 145.69 (4C), 145.25, 145.21, 145.19, 144.95, 144.44, 144.35, 142.94, 142.59, 142.58, 142.51, 142.25, 142.08, 141.88 (4C), 141.71, 140.22, 139.72, 138.51 (1C, aryl *C*), 136.15, 135.12, 133.19 (1C, aryl *C*), 132.65 (1C, aryl *C*), 129.09 (1C, aryl *C*), 128.85 (1C, aryl *C*), 125.79 (1C, aryl *C*), 100.79 (1C, sp^3-*C* of C_{60}), 65.13 (1C, sp^3-*C* of C_{60}), 50.90 (1C), 21.64 (1C); FT-IR ν/cm^{-1} (KBr) 3028, 2913, 2853, 1795, 1618, 1507, 1425, 1337, 1180, 1109, 1041, 1001, 782, 692, 566, 525; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.12), 310 (4.64), 429 (3.55); MALDI-TOF MS *m*/*z* calcd for $C_{69}H_9N$ $[M]^+$ 851.0730, found 851.0741.



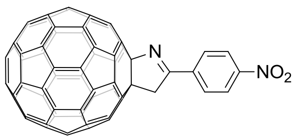
Preparation of **2d**. By following the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with **1d** (15.4 mg, 0.075 mmol), CuBr (1.5 mg, 0.01 mmol), and $NaHSO_3$ (52.3 mg, 0.50 mmol) at 150 ^oC afforded **2d** (11.1 mg, 26%) and recovered C_{60} (15.3 mg, 44%): amorphous brown solid; ^1H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.09 (s, 1H), 7.95 (dd, J = 7.7 Hz, 1.6 Hz, 1H), 7.34 (d, J = 7.7 Hz, 1H), 5.12 (s, 2H), 2.45 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 172.75 (1C, C=N), 155.55, 150.17, 147.55(1C), 147.38 (1C), 146.36, 146.24, 146.11, 145.99, 145.93, 145.67, 145.66, 145.22, 145.17, 145.16, 144.95, 144.42, 144.33, 142.91, 142.55 (4C), 142.50, 142.23, 142.05, 141.87, 141.86, 141.68, 140.86 (1C, aryl *C*), 140.18, 139.68, 137.05 (1C, aryl *C*), 136.10, 135.13, 130.96 (1C, aryl *C*), 130.18 (1C, aryl *C*), 129.62 (1C, aryl *C*), 126.27 (1C, aryl *C*), 100.74 (1C, sp^3-*C* of C_{60}), 65.14 (1C, sp^3-*C* of C_{60}), 50.84 (1C), 20.15 (1C), 19.98 (1C); FT-IR ν/cm^{-1} (KBr) 3021, 2932, 2912, 2852, 1794, 1614, 1567, 1503, 1422, 1329, 1248, 1182, 1111, 1040, 1002, 902, 875, 814, 769, 730, 596, 570, 557, 524; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (5.06), 309 (4.56), 429 (3.48); ESI FT-ICR MS *m*/*z* calcd for $C_{70}H_{12}N$ $[M+H]^+$ 866.0964, found 866.0957.



Preparation of **2e**. By following the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with **1e** (13.3 mg, 0.075 mmol), CuBr (1.4 mg, 0.01 mmol), and $NaHSO_3$ (52.5 mg, 0.5 mmol) at 150 ^oC afforded **2e** (10.7 mg, 26%) and recovered C_{60} (14.7 mg, 41%): amorphous brown solid; ^1H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.31-8.27 (m, 2H), 7.64-7.58 (m, 3H), 5.16 (s, 2H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 172.76 (1C, C=N), 155.42, 150.03, 147.61 (1C), 147.45 (1C), 146.40, 146.30, 146.18, 146.05, 145.99, 145.73, 145.72, 145.29, 145.25, 145.22, 144.97, 144.47, 144.38, 142.97, 142.63, 142.61, 142.53, 142.29, 142.11, 141.91, 141.89, 141.74, 140.25, 139.76, 136.17, 135.15, 133.32 (1C, aryl *C*), 131.82 (1C, aryl *C*), 128.93 (aryl *C*), 128.54 (aryl *C*), 99.84 (1C, sp^3-*C* of C_{60}), 65.19 (1C, sp^3-*C* of C_{60}), 50.88 (1C); FT-IR ν/cm^{-1} (KBr) 3056, 2912, 1798, 1617, 1574, 1502, 1425, 1339, 1177, 1109, 1038, 758, 688, 562, 523; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.03), 310 (4.52), 429 (3.43); MALDI-TOF MS *m*/*z* calcd for $C_{68}H_7N$ $[M]^+$ 837.0573, found 837.0621.

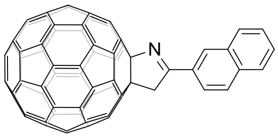


Preparation of **2f**. By following the general procedure, the reaction of C_{60} (35.9 mg, 0.05 mmol) with **1f** (19.3 mg, 0.075 mmol), CuBr (1.5 mg, 0.01 mmol), and $NaHSO_3$ (52.0 mg, 0.5 mmol) at 150 ^oC afforded **2f** (11.9 mg, 26%) and recovered C_{60} (15.8 mg, 44%): amorphous brown solid; ^1H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 5.13 (s, 2H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 172.03 (1C, C=N), 155.16, 149.70, 147.65 (1C), 147.48 (1C), 146.34, 146.31, 146.21, 146.09, 146.03, 145.77, 145.70, 145.32, 145.28, 145.25, 144.90, 144.46, 144.38, 143.00, 142.66 (4C), 142.51, 142.29, 142.12, 141.92, 141.86, 141.76, 140.28, 139.79, 136.22, 135.13, 132.26 (aryl *C*), 132.15 (1C, aryl *C*), 129.97 (aryl *C*), 127.08 (1C, aryl *C*), 100.85 (1C, sp^3-*C* of C_{60}), 65.19 (1C, sp^3-*C* of C_{60}), 50.73 (1C); FT-IR ν/cm^{-1} (KBr) 2961, 2910, 1796, 1617, 1586, 1506, 1486, 1421, 1395, 1331, 1178, 1107, 1067, 1043, 1007, 816, 768, 558, 523; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (5.00), 312 (4.63), 428 (3.46); MALDI-TOF MS *m*/*z* calcd for $C_{68}H_6N^{79}Br$ $[M]^+$ 914.9678, found 914.9717.

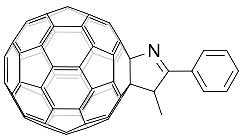


Preparation of **2g**. By following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1g** (16.9 mg, 0.075 mmol), CuBr (1.6 mg, 0.01 mmol), and $NaHSO_3$

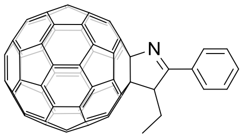
(52.2 mg, 0.5 mmol) at 150 °C afforded **2g** (7.8 mg, 18%) and recovered C_{60} (20.2 mg, 56%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.51 (d, J = 8.9 Hz, 2H), 8.48 (d, J = 8.9 Hz, 2H), 5.19 (s, 2H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 171.31 (1C, C=N), 154.62, 149.72 (1C, aryl *C*), 149.09, 147.64 (1C), 147.47 (1C), 146.36, 146.21, 146.19, 146.09, 146.03, 145.80, 145.62, 145.33, 145.32, 145.25, 144.76, 144.41, 144.34, 143.00, 142.67 (4C), 142.45, 142.28, 142.10, 141.91, 141.75 (4C), 140.32, 139.84, 138.65 (1C, aryl *C*), 136.24, 135.02, 129.34 (aryl *C*), 124.03 (aryl *C*), 100.99 (1C, sp^3-*C* of C_{60}), 65.07 (1C, sp^3-*C* of C_{60}), 50.80 (1C); FT-IR ν/cm^{-1} (KBr) 3071, 2911, 2849, 1794, 1593, 1517, 1421, 1335, 1179, 1106, 1046, 902, 851, 730, 688, 562, 524; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.03), 311 (4.53), 429 (3.45); ESI FT-ICR MS m/z calcd for $C_{68}H_7N_2O_2$ $[M+H]^+$ 883.0502, found 883.0516.



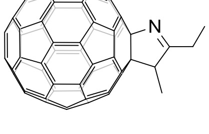
Preparation of **2h**. By following the general procedure, the reaction of C_{60} (36.1 mg, 0.05 mmol) with **1h** (17.2 mg, 0.075 mmol), CuBr (1.5 mg, 0.01 mmol), and $NaHSO_3$ (52.5 mg, 0.50 mmol) at 150 °C afforded **2h** (10.9 mg, 25%) and recovered C_{60} (18.6 mg, 52%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.60-8.58 (m, 1H), 8.56 (dd, J = 8.5 Hz, 1.7 Hz, 1H), 8.06-8.01 (m, 2H), 7.97-7.93 (m, 1H), 7.65-7.56 (m, 2H), 5.29 (s, 2H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 2C unless indicated) δ 172.90 (1C, C=N), 155.50, 150.10, 147.65 (1C), 147.48 (1C), 146.44, 146.34, 146.21, 146.09, 146.02, 145.77, 145.75, 145.32, 145.28, 145.25, 145.01, 144.50, 144.41, 143.00, 142.65 (4C), 142.57, 142.31, 142.14, 141.94 (4C), 141.78, 140.29, 139.80, 136.26, 135.21, 135.12 (1C, aryl *C*), 133.05 (1C, aryl *C*), 130.90 (1C, aryl *C*), 129.52 (1C, aryl *C*), 129.04 (1C, aryl *C*), 128.86 (1C, aryl *C*), 128.07 (1C, aryl *C*), 127.97 (1C, aryl *C*), 126.91 (1C, aryl *C*), 125.03 (1C, aryl *C*), 100.97 (1C, sp^3-*C* of C_{60}), 65.28 (1C, sp^3-*C* of C_{60}), 50.93 (1C); FT-IR ν/cm^{-1} (KBr) 3054, 2916, 2850, 1794, 1613, 1572, 1464, 1425, 1354, 1263, 1185, 1109, 1040, 857, 817, 770, 744, 598, 558, 525 ; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.19), 310 (4.80), 428 (3.60); MALDI-TOF MS m/z calcd for $C_{72}H_9N$ $[M]^+$ 887.0730, found 887.0696.



Preparation of **2i**. By following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1i** (14.4 mg, 0.075 mmol), CuBr (1.4 mg, 0.01 mmol), and $NaHSO_3$ (52.2 mg, 0.50 mmol) at 150 °C afforded **2i** (13.5 mg, 31%) and recovered C_{60} (12.7 mg, 35%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.25-8.19 (m, 2H), 7.63-7.58 (m, 3H), 5.49 (q, J = 7.6 Hz, 1H), 2.09 (d, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 1C unless indicated) δ 177.71 (C=N), 156.18, 152.45, 150.78, 150.44, 147.59, 147.44, 146.57, 146.29 (2C), 146.25 (2C), 146.08, 146.05, 146.00, 145.96, 145.93, 145.78, 145.71, 145.67, 145.62, 145.57, 145.27 (2C), 145.23 (2C), 145.17, 145.06, 144.86, 144.52, 144.41, 144.40, 144.29, 143.00, 142.92, 142.66, 142.61 (2C), 142.56, 142.55, 142.28, 142.25, 142.21, 142.10 (2C), 141.91, 141.87, 141.86, 141.76, 141.74, 141.53, 140.23 (2C), 139.75, 139.56, 136.56 (2C), 135.84, 134.62, 133.03 (aryl *C*), 131.29 (aryl *C*), 128.93 (2C, aryl *C*), 128.85 (2C, aryl *C*), 99.28 (sp^3-*C* of C_{60}), 70.36 (sp^3-*C* of C_{60}), 55.84, 20.72; FT-IR ν/cm^{-1} (KBr) 3056, 2969, 2925, 1806, 1617, 1572, 1506, 1448, 1427, 1379, 1328, 1183, 1109, 1021, 913, 770, 691, 648, 597, 568, 559, 526; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (5.10), 311 (4.61), 429 (3.52); MALDI-TOF MS *m*/*z* calcd for $C_{69}H_9N$ $[M]^+$ 851.0730, found 851.0717.

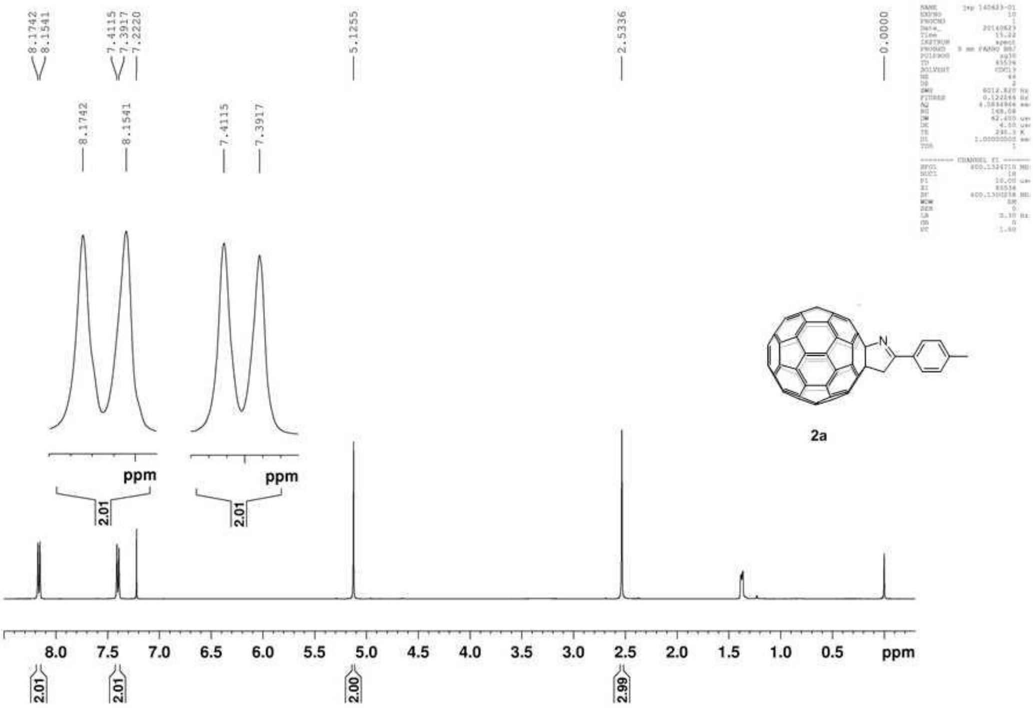


Preparation of **2j**. By following the general procedure, the reaction of C_{60} (35.7 mg, 0.05 mmol) with **1j** (15.7 mg, 0.075 mmol), CuBr (1.4 mg, 0.01 mmol), and $NaHSO_3$ (52.5 mg, 0.50 mmol) at 150 °C afforded **2j** (15.4 mg, 35%) and recovered C_{60} (15.7 mg, 44%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.24-8.18 (m, 2H), 7.64-7.59 (m, 3H), 5.41 (dd, *J* = 6.3 Hz, 4.1 Hz, 1H), 2.66-2.56 (m, 2H), 1.40 (dd, *J* = 7.4 Hz, 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 1C unless indicated) δ 176.78 (C=N), 156.70, 151.87, 150.80, 150.69, 147.54, 147.42, 146.69, 146.28, 146.27, 146.24, 146.13, 146.09, 146.06, 146.02, 145.98, 145.95, 145.92, 145.76, 145.62, 145.57, 145.56, 145.28 (2C), 145.25, 145.22, 145.13, 145.01, 144.57, 144.49, 144.42, 144.39, 144.26, 143.00, 142.93, 142.69, 142.64 (2C), 142.54, 142.53, 142.28, 142.19, 142.11 (3C), 141.90, 141.85 (2C), 141.69, 141.67, 141.51, 140.29, 140.23, 139.71, 139.14, 137.22, 136.68, 135.44, 134.51, 133.66 (aryl *C*), 131.19 (aryl *C*), 128.91 (2C, aryl *C*), 128.48 (2C, aryl *C*), 99.65 (sp^3-*C* of C_{60}), 70.47 (sp^3-*C* of C_{60}), 62.15, 26.71, 12.46; FT-IR ν/cm^{-1} (KBr) 3052, 3025, 2965, 2926, 2871, 1780, 1617, 1571, 1509, 1426, 1380, 1350, 1329, 1183, 1103, 1026, 799, 766, 690, 647, 597, 568, 559, 525; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (5.11), 312 (4.66), 429 (3.53); MALDI-TOF MS *m*/*z* calcd for $C_{70}H_{11}N$ $[M]^+$ 865.0886, found 865.0911.

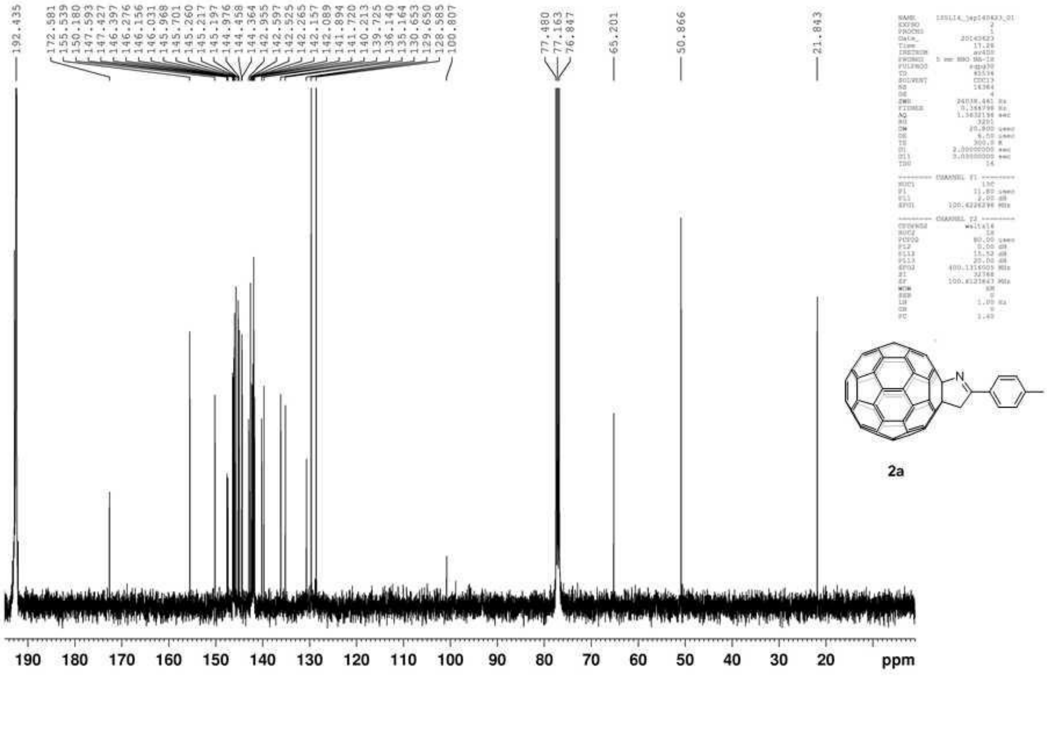


Preparation of **2k**. By following the general procedure, the reaction of C_{60} (36.2 mg, 0.05 mmol) with **1k** (11.0 μL, 0.075 mmol), CuBr (1.5 mg, 0.01 mmol), and $NaHSO_3$ (51.9 mg, 0.50 mmol) at 150 °C afforded **2k** (6.8 mg, 17%) and recovered C_{60} (12.6 mg, 35%): amorphous brown solid; ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 4.82 (q, *J* = 7.6 Hz, 1H), 2.99 (dq, *J* = 16.7 Hz, 7.4 Hz, 1H), 2.86 (dq, *J* = 16.7 Hz, 7.4 Hz, 1H), 2.01 (d, *J* = 7.6 Hz, 3H), 1.63 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$, all 1C unless indicated) δ 182.17 (C=N), 156.64, 152.24, 151.24, 150.52, 147.53, 147.38, 146.51, 146.26, 146.22, 146.21 (2C), 146.03 (2C), 145.95, 145.92, 145.88 (2C), 145.71, 145.61, 145.59, 145.57, 145.26, 145.23, 145.20 (2C), 145.03, 145.02, 144.75, 144.47, 144.41, 144.32, 144.27, 142.96, 142.90, 142.55 (4C), 142.53, 142.32, 142.22, 142.18, 142.05, 142.03, 141.84, 141.79 (3C), 141.64, 141.58, 140.15, 140.11, 139.75, 139.56, 136.46, 135.97, 135.83, 134.34, 99.23 (sp^3-*C* of C_{60}), 70.26 (sp^3-*C* of C_{60}), 58.35, 25.52, 18.33, 11.09; FT-IR ν/cm^{-1} (KBr) 2962, 2926, 2867, 1796, 1509, 1453, 1426, 1375, 1184, 1115, 1006, 766, 611, 574, 556, 526; UV–vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (5.00), 312 (4.51), 429 (3.45); MALDI-TOF MS *m*/*z* calcd for $C_{65}H_9N$ $[M]^+$ 803.0730, found 803.0759.

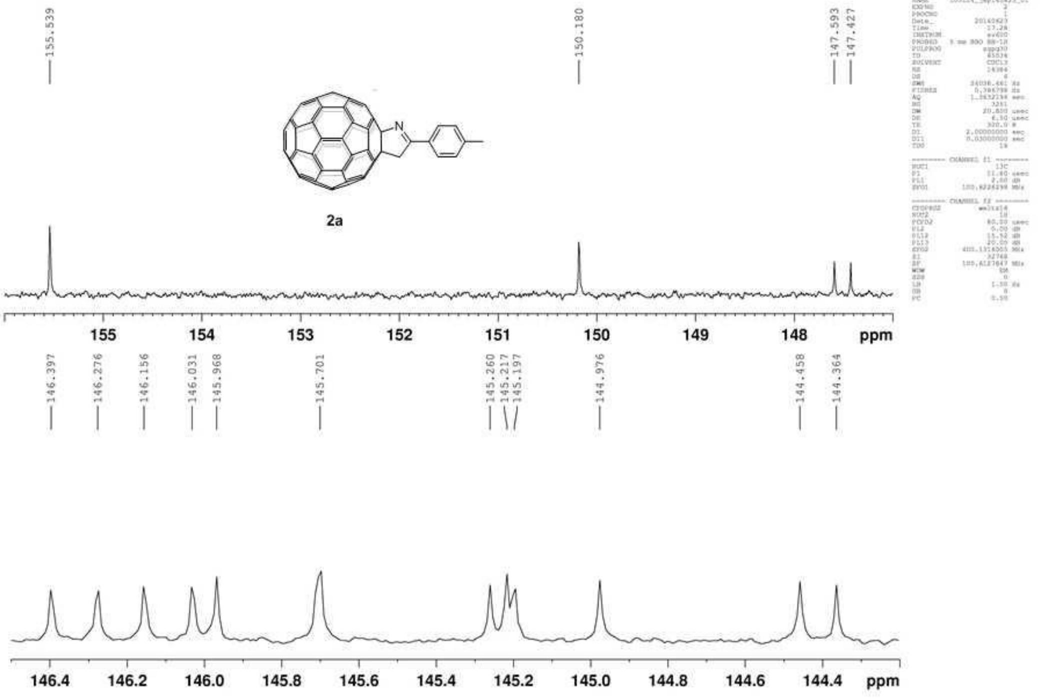
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2a



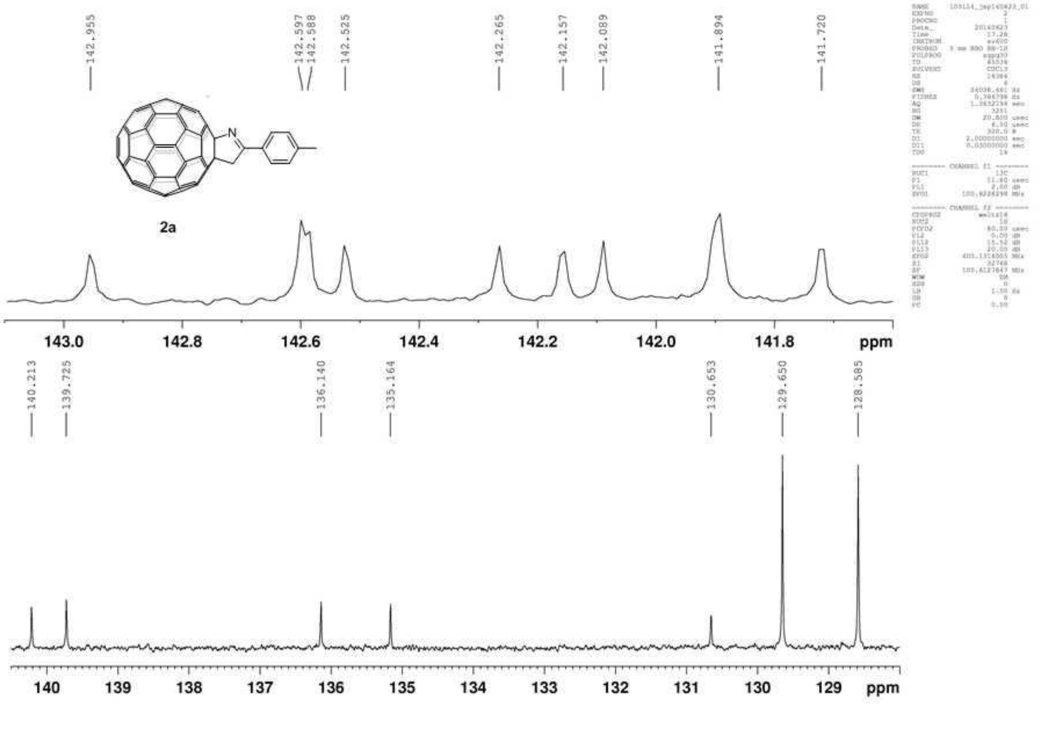
¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2a



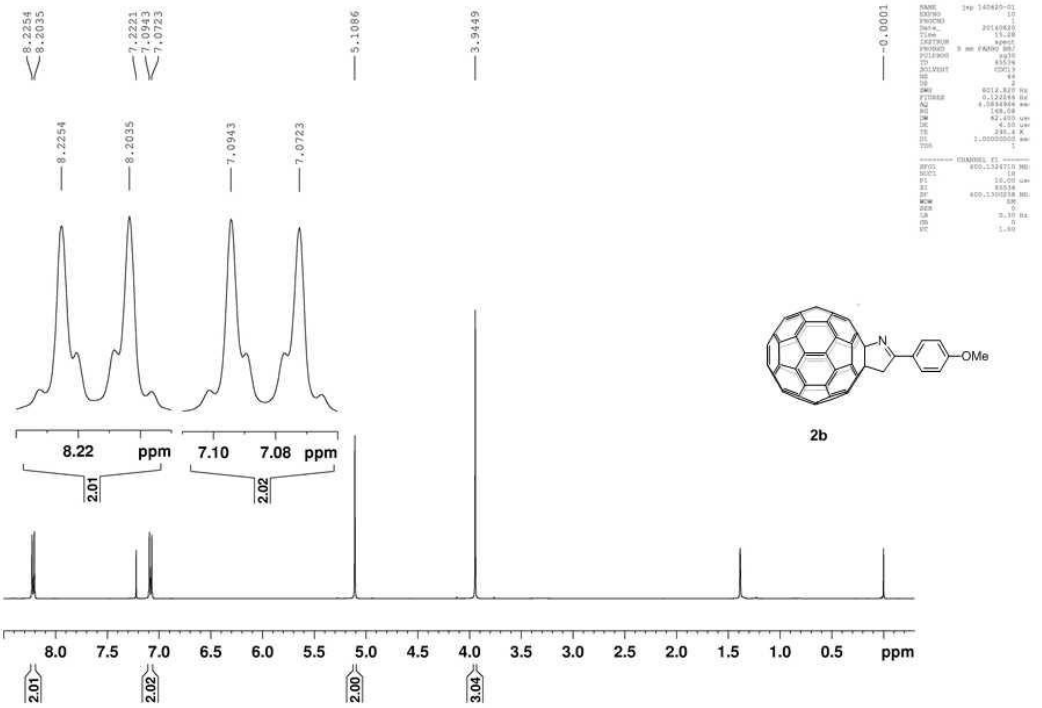
Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2a



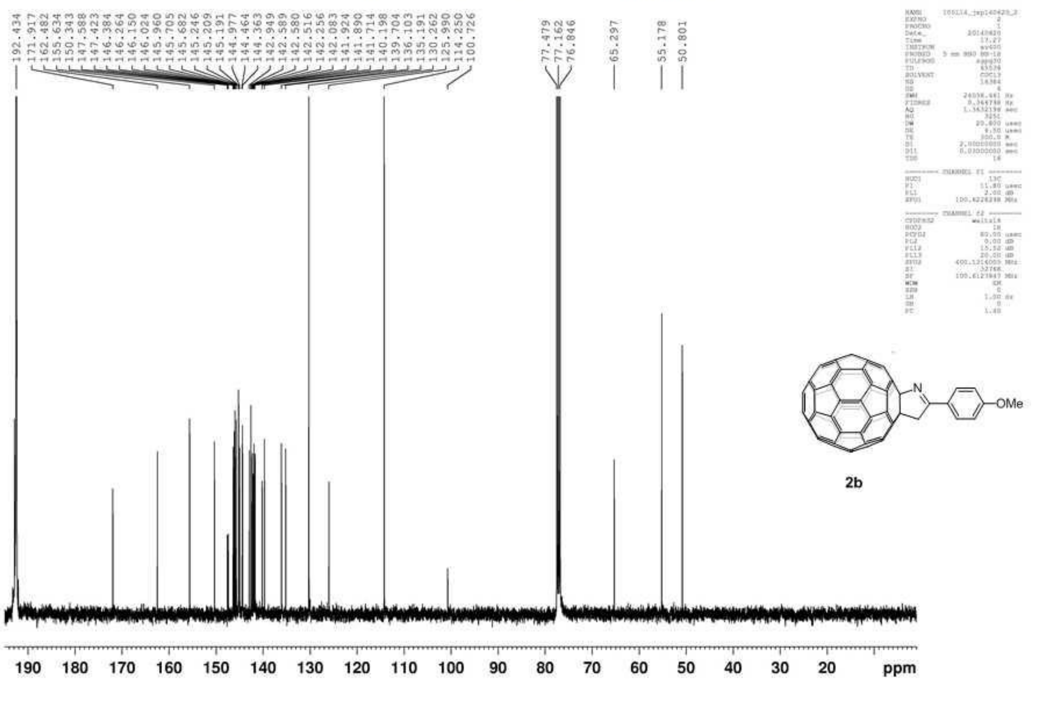
Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2a



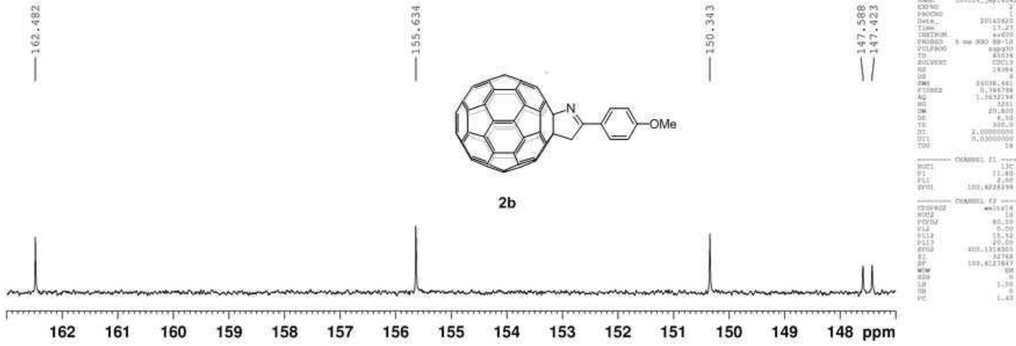
^1H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2b

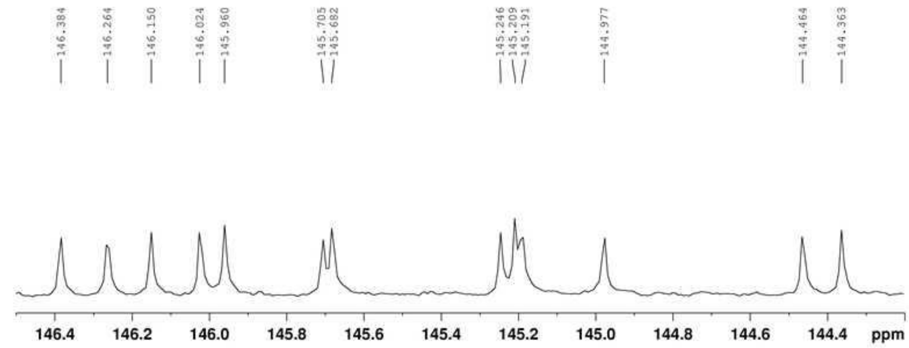


^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2b

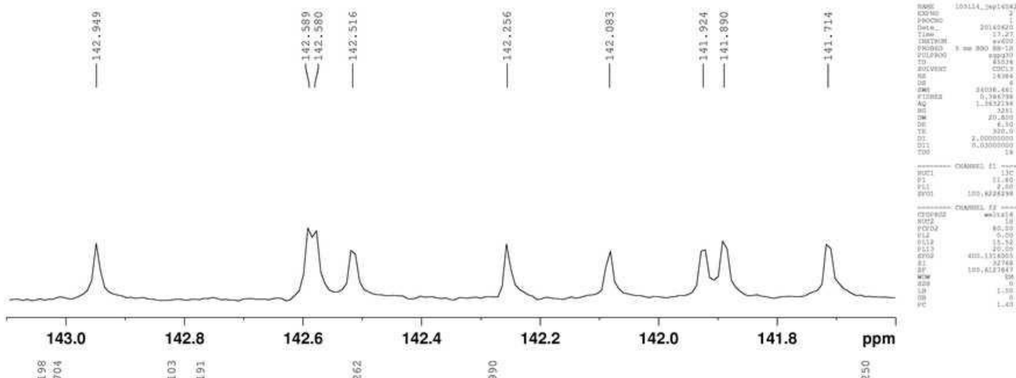


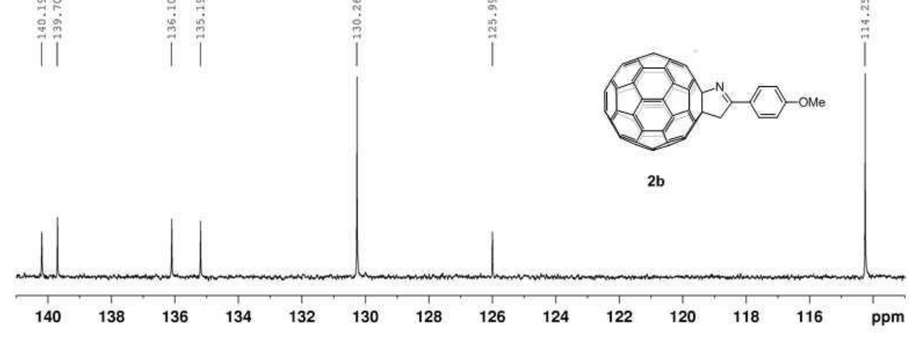
Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2b



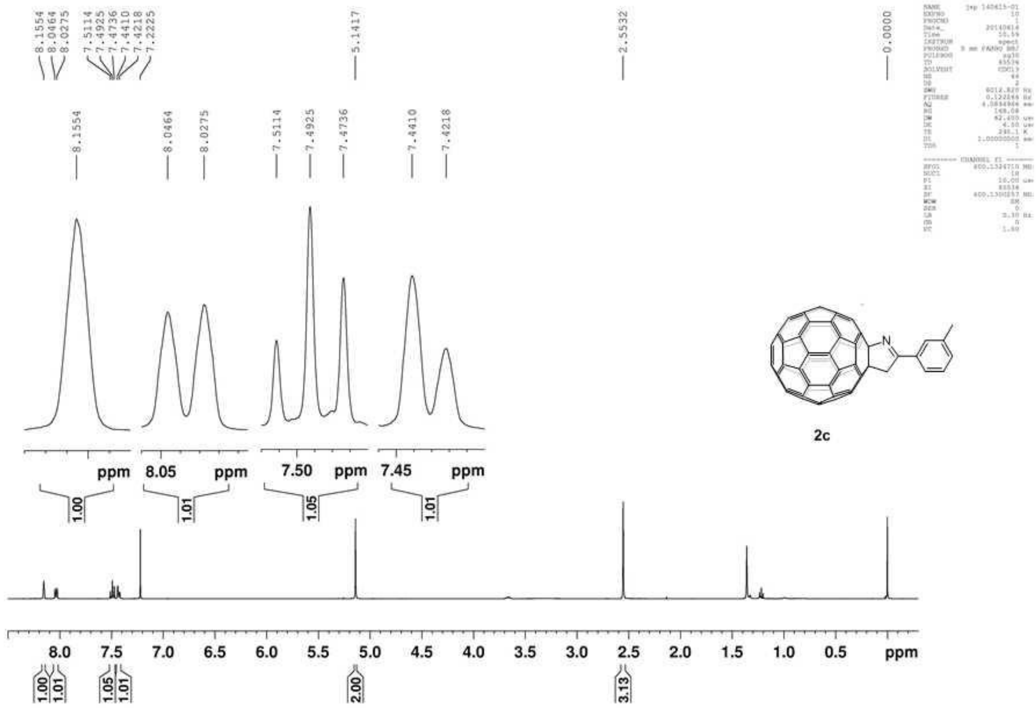


Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2b

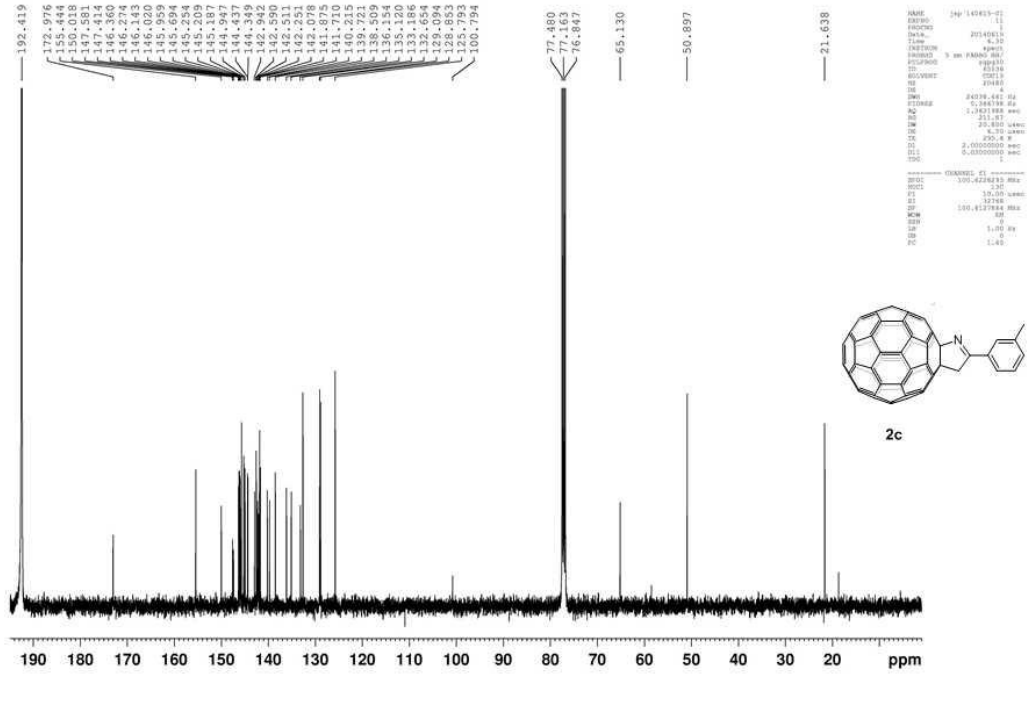




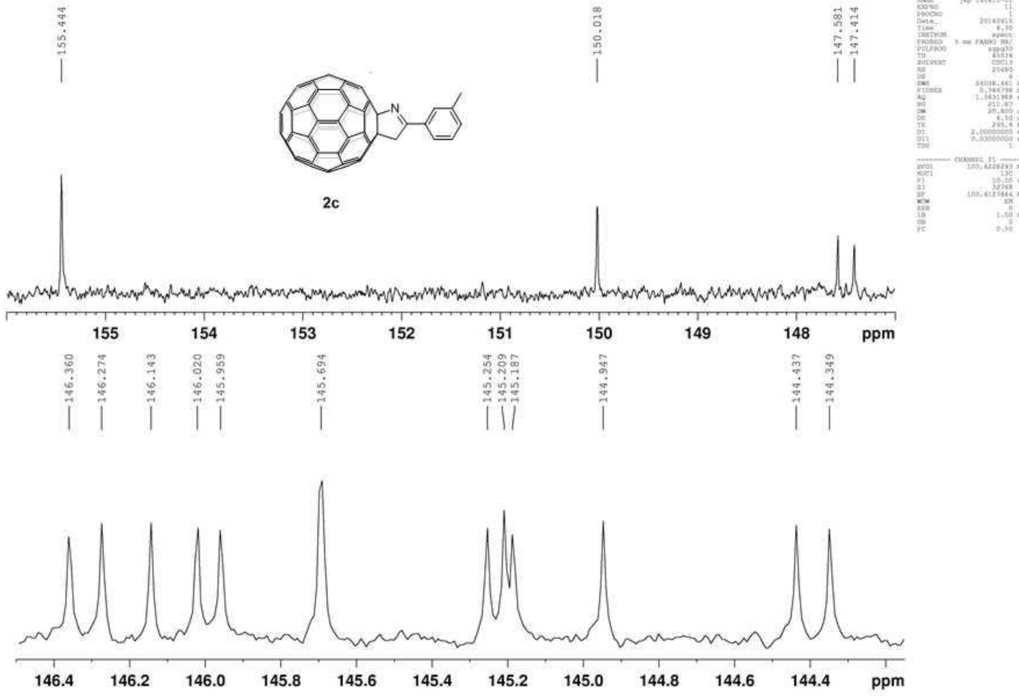
^{1}H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2c



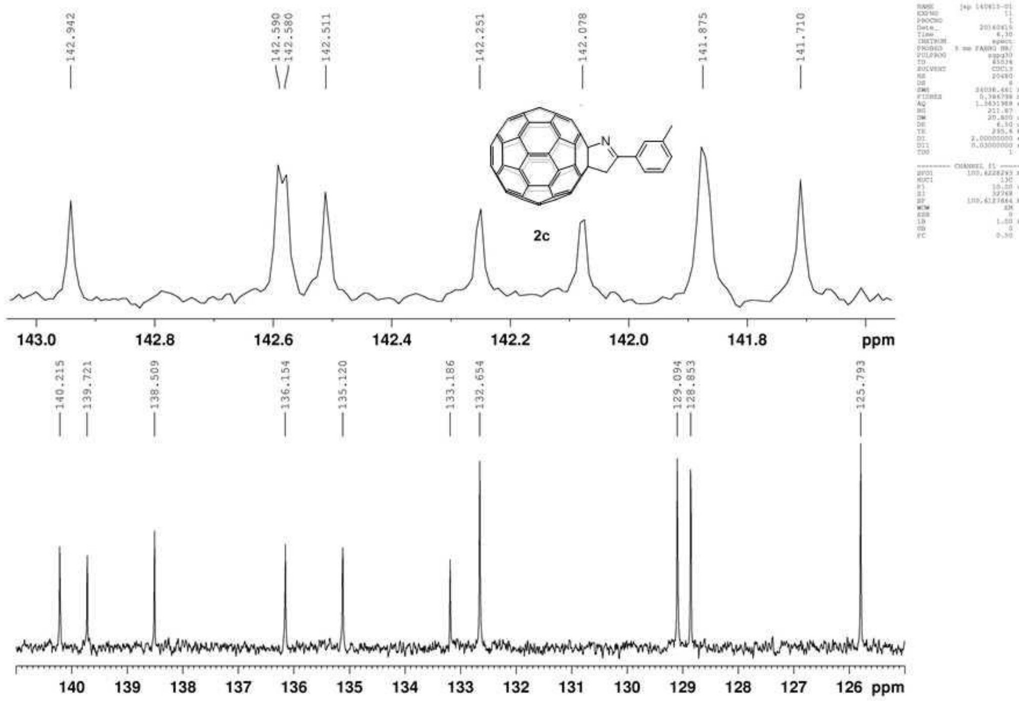
^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2c



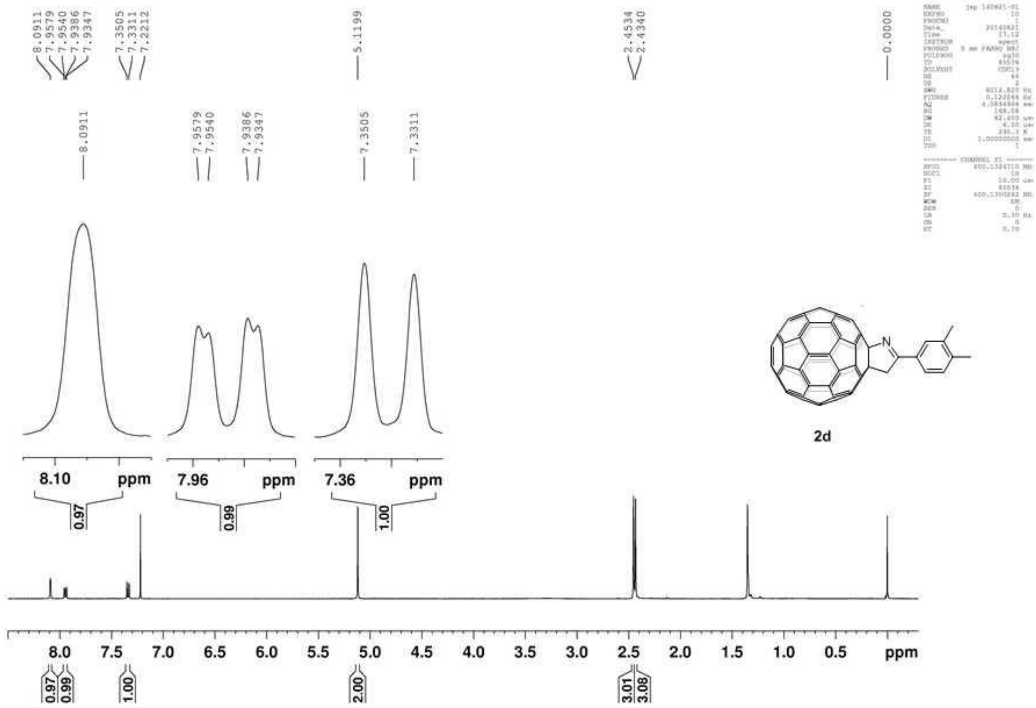
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2c



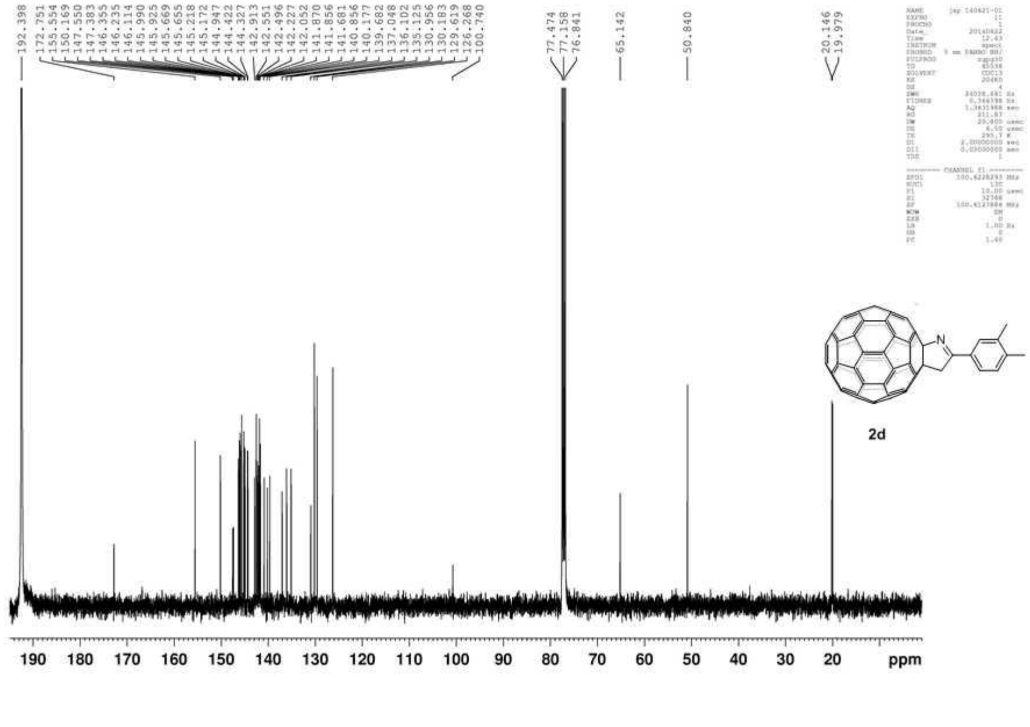
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2c



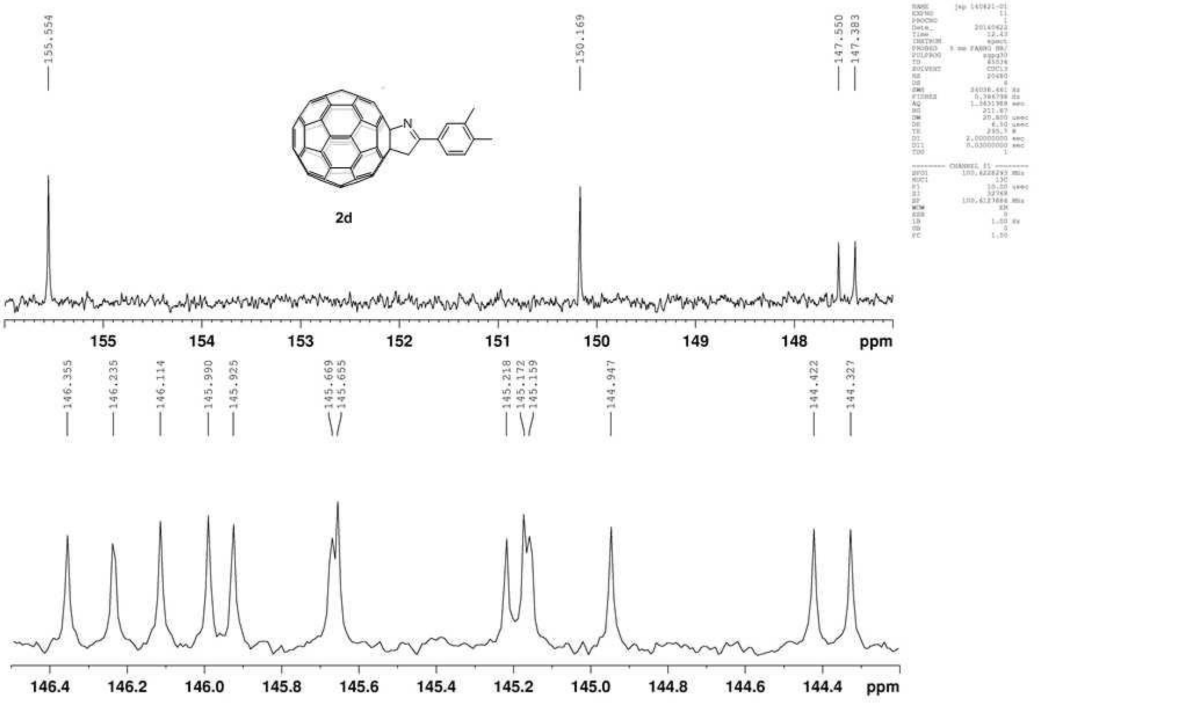
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2d



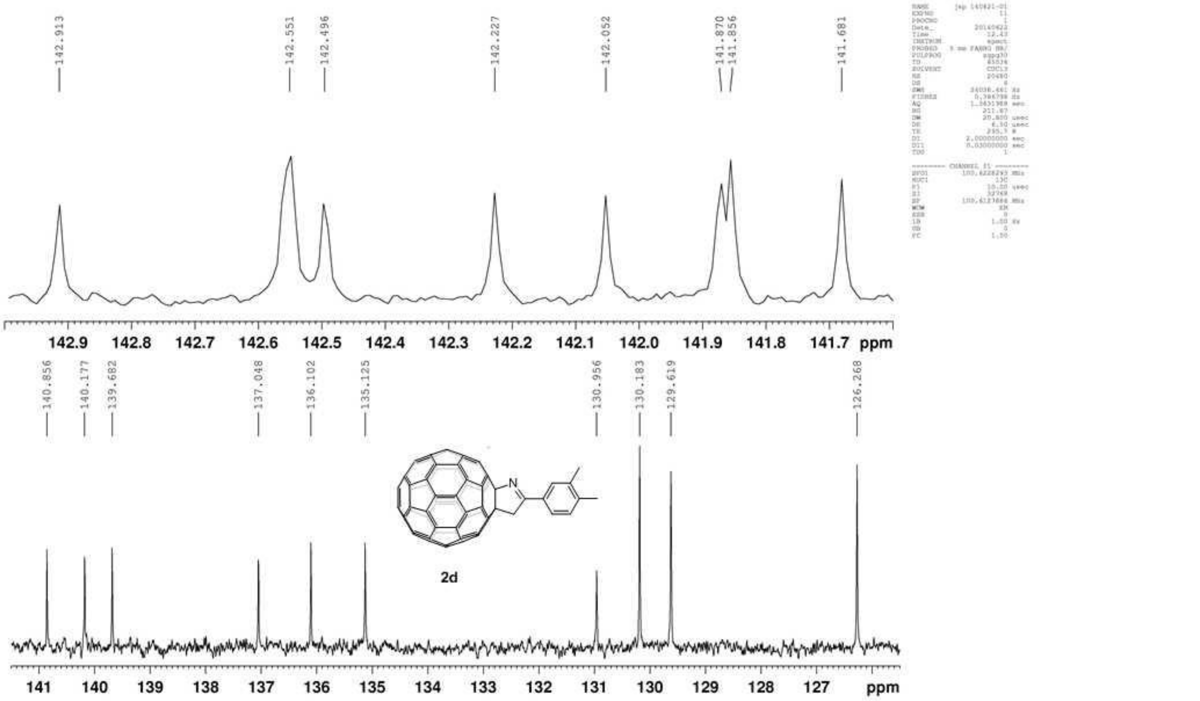
¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2d



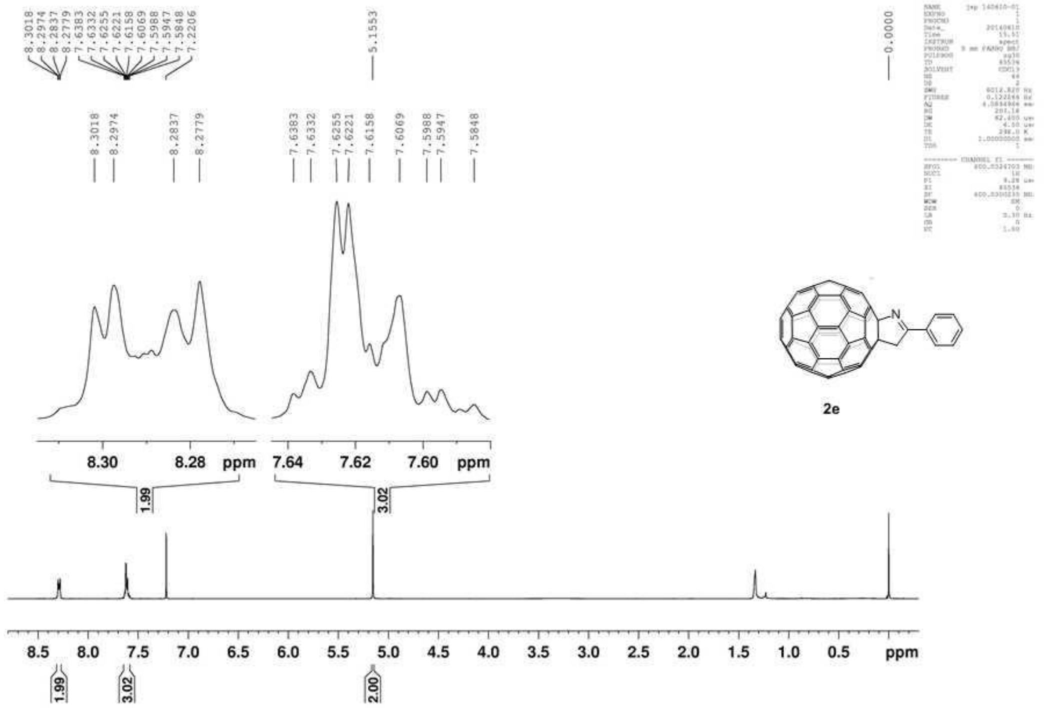
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2d



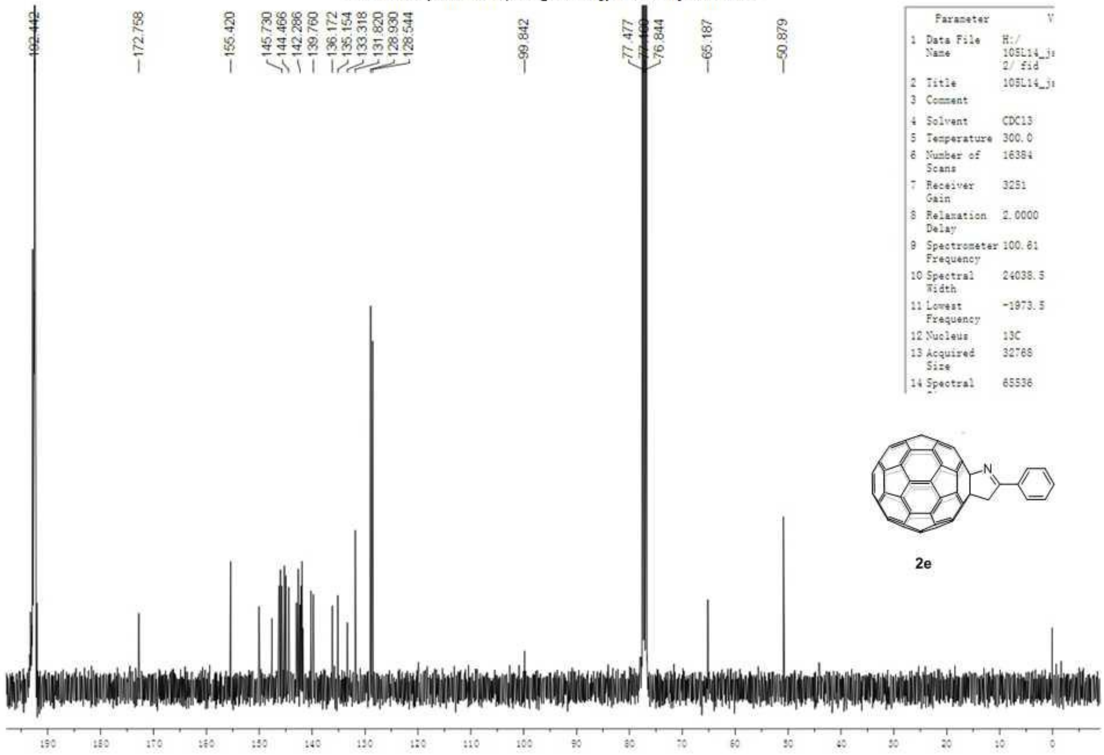
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2d



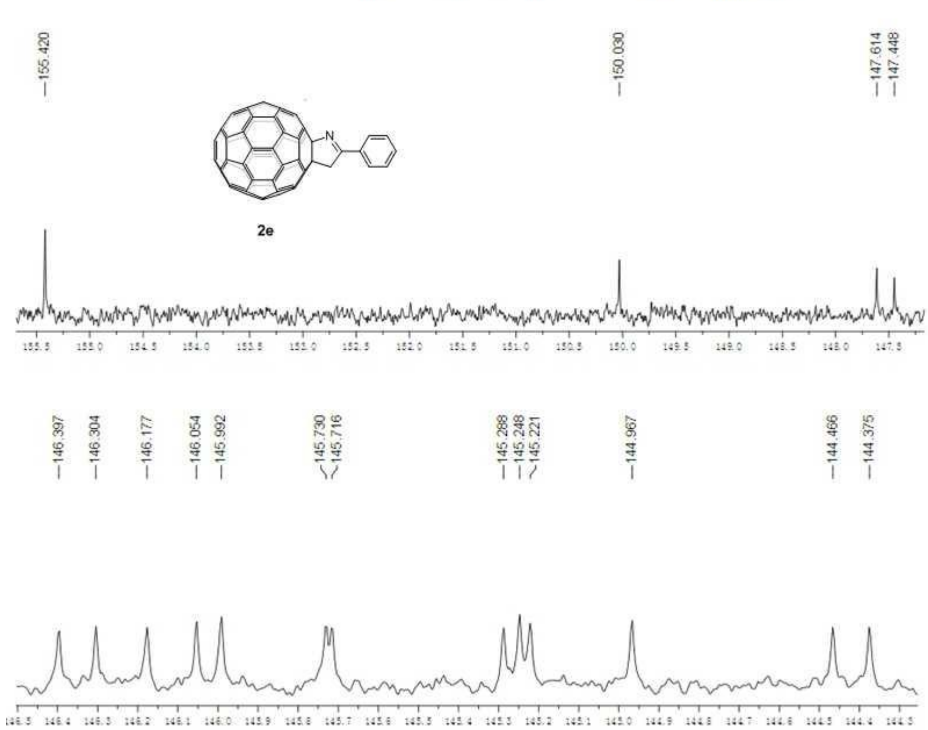
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2e



¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2e



Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2e



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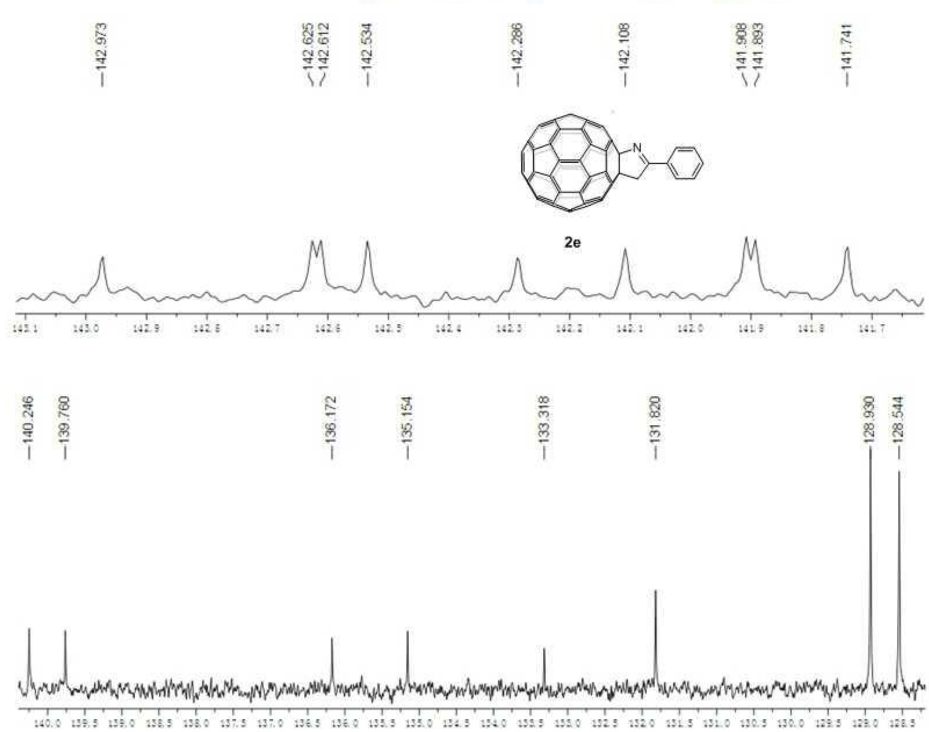
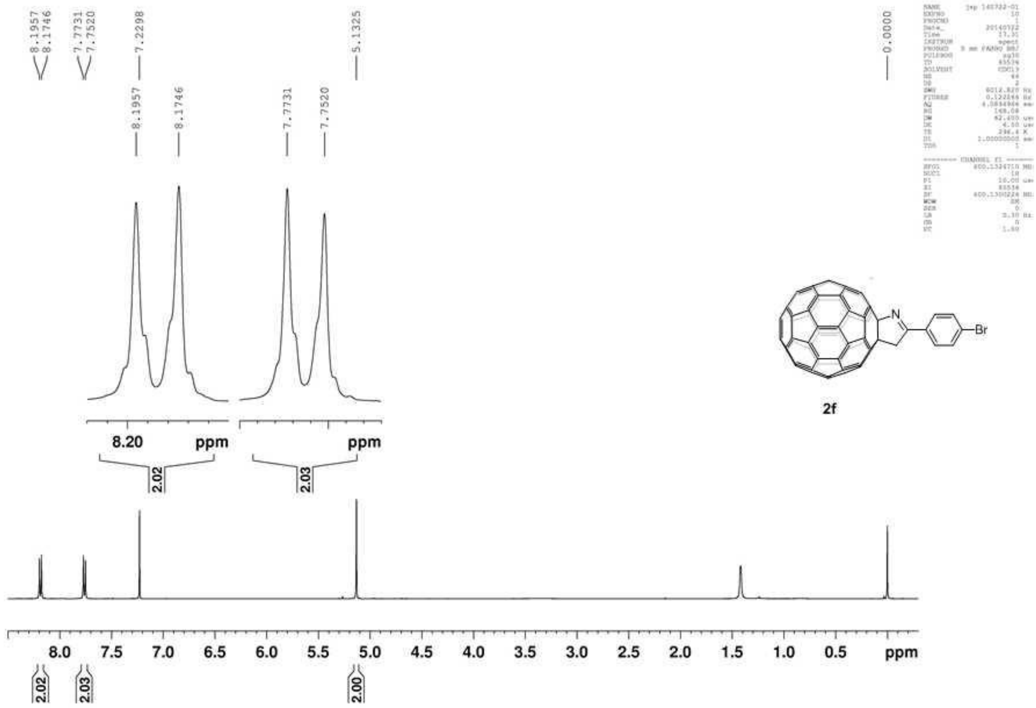
10 Spectral Width	24038.5
11 Lowest Frequency	-1973.5
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral	65536

Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2e

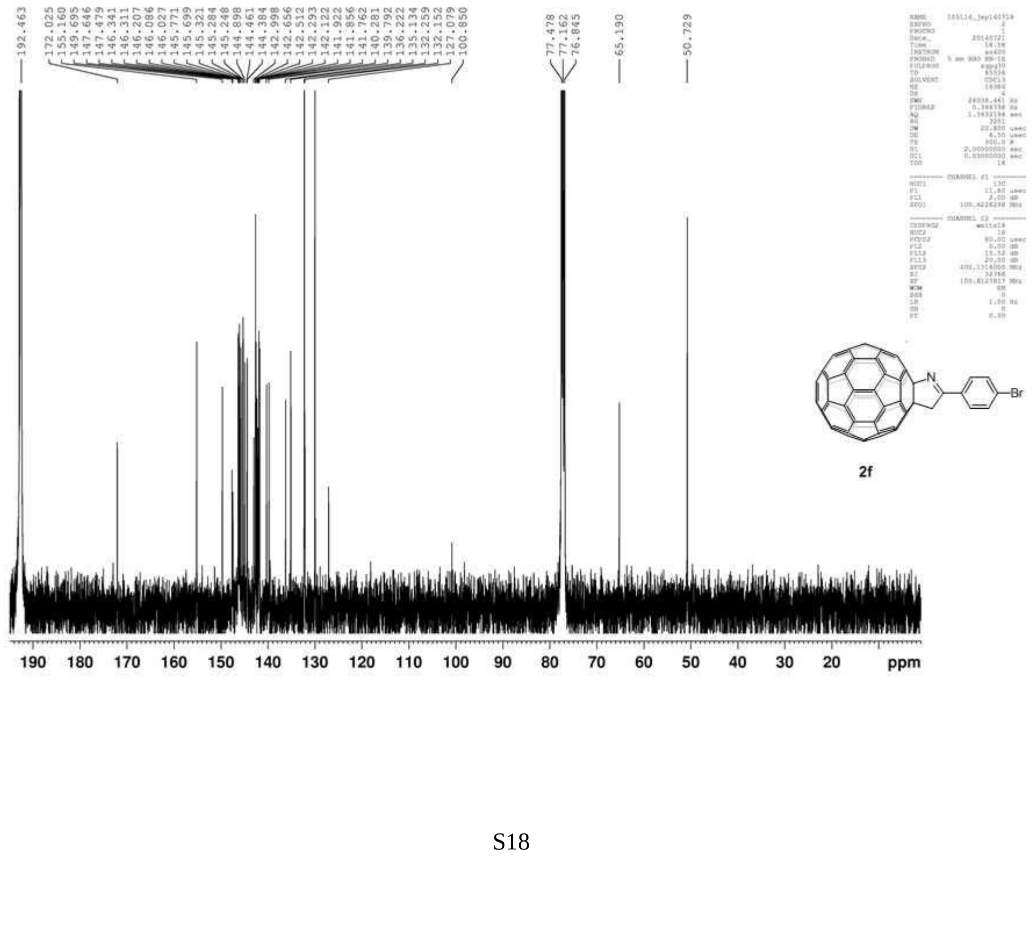


Parameter	V
1 Data File Name	H:/ 105L14_js 2/ fid
2 Title	105L14_js
3 Comment	
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16384
7 Receiver Gain	3251
8 Relaxation Delay	2.0000
9 Spectrometer Frequency	100.61
10 Spectral Width	24038.5
11 Lowest Frequency	-1973.5
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral	65536

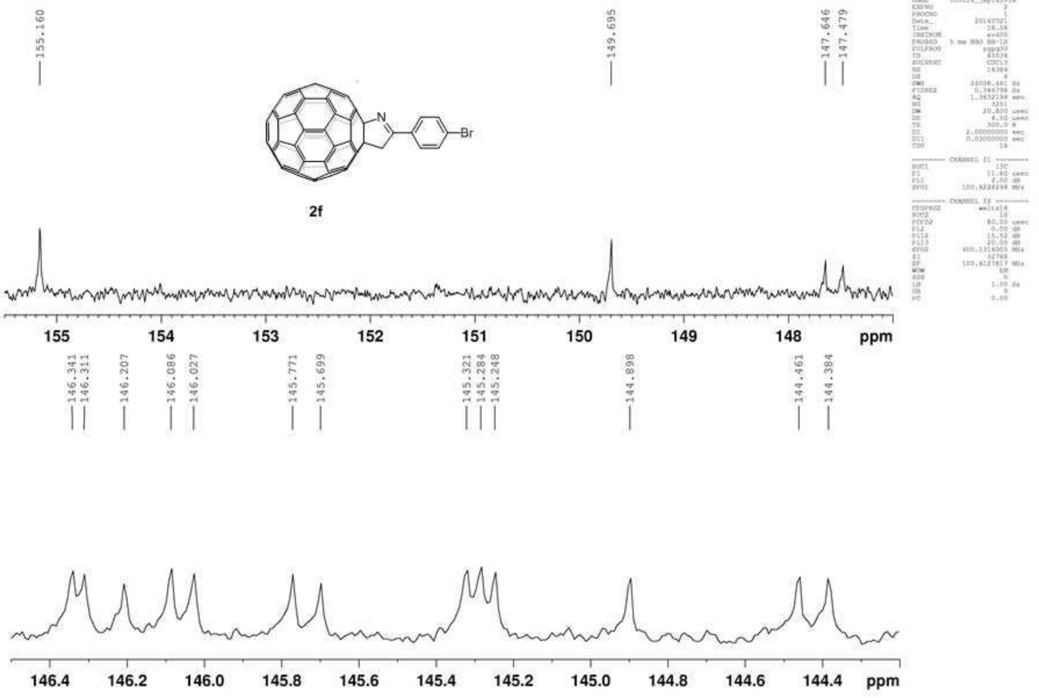
^{1}H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2f



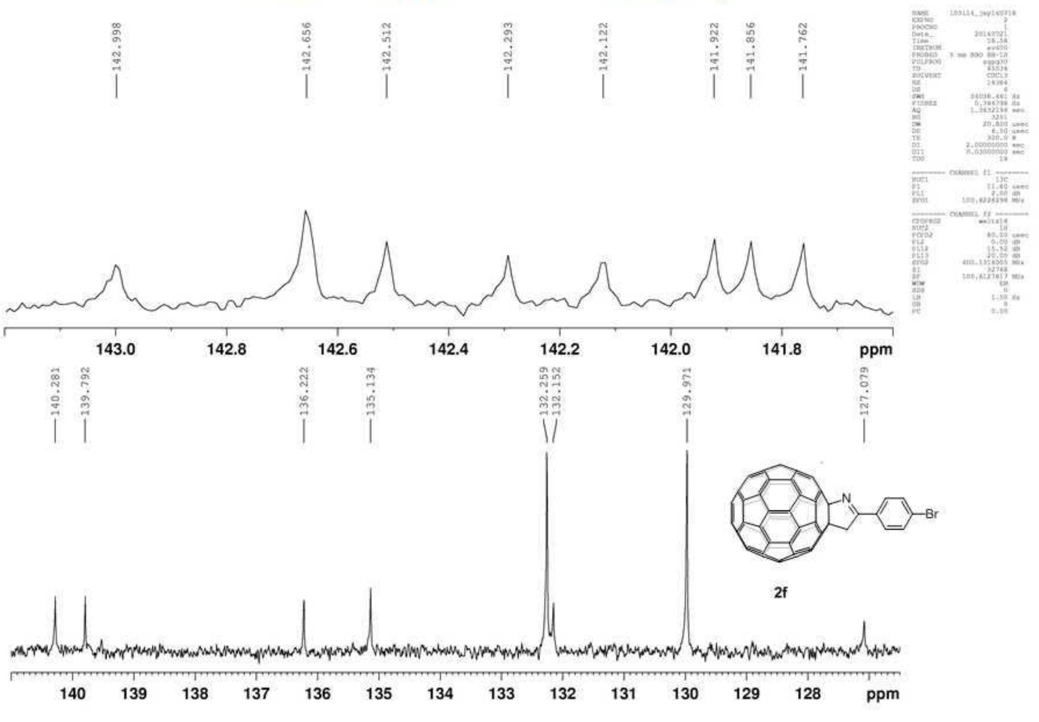
^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2f



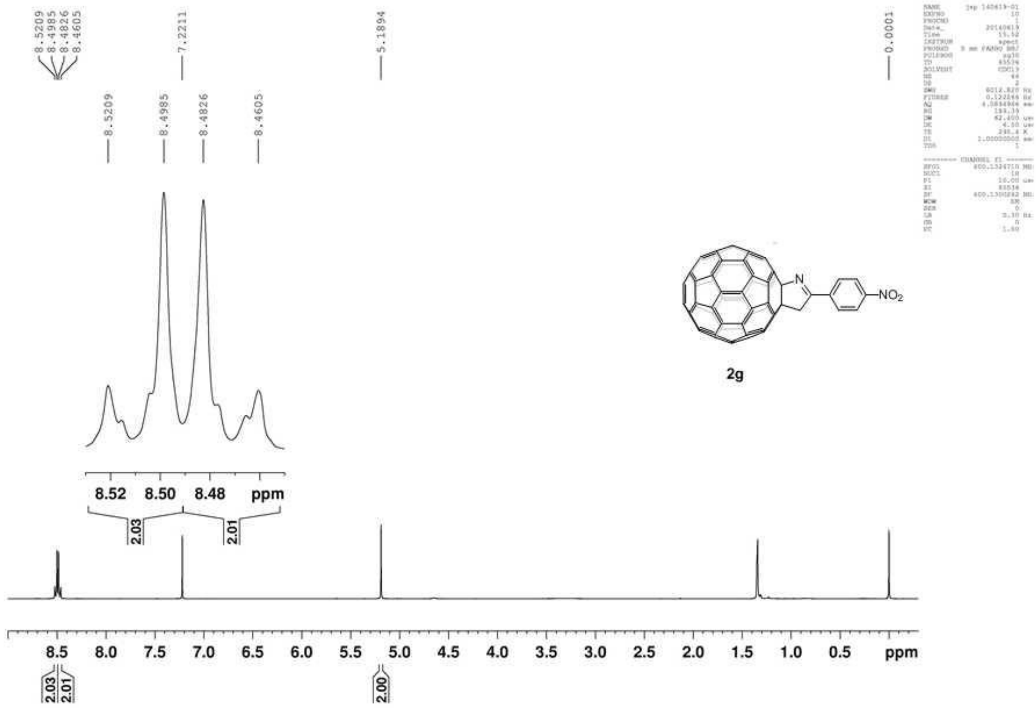
Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2f



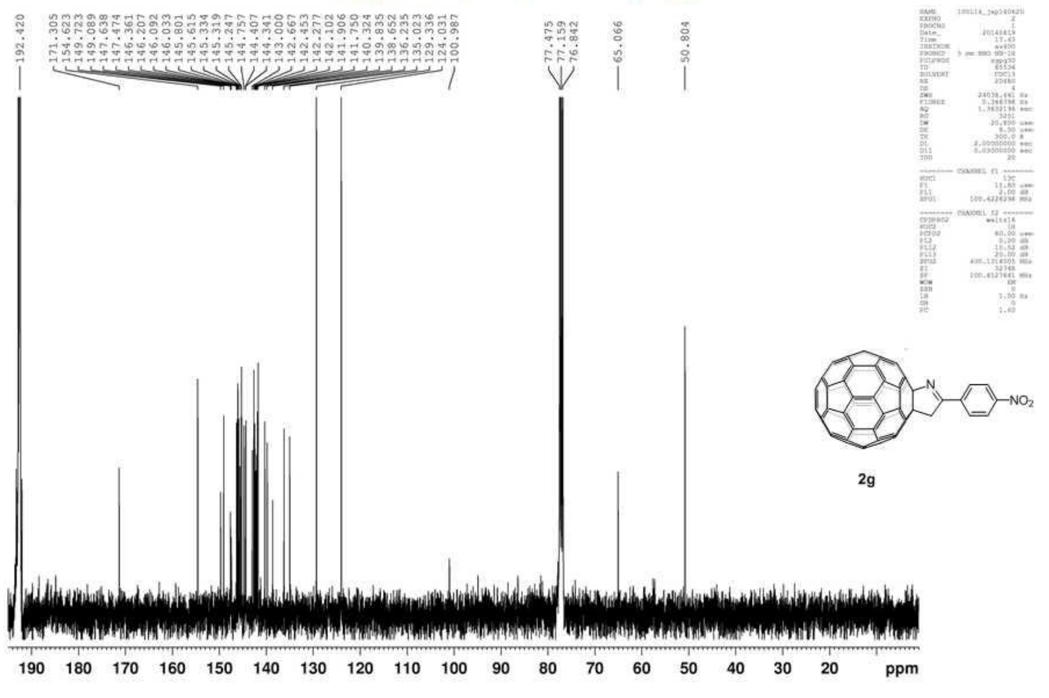
Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2f



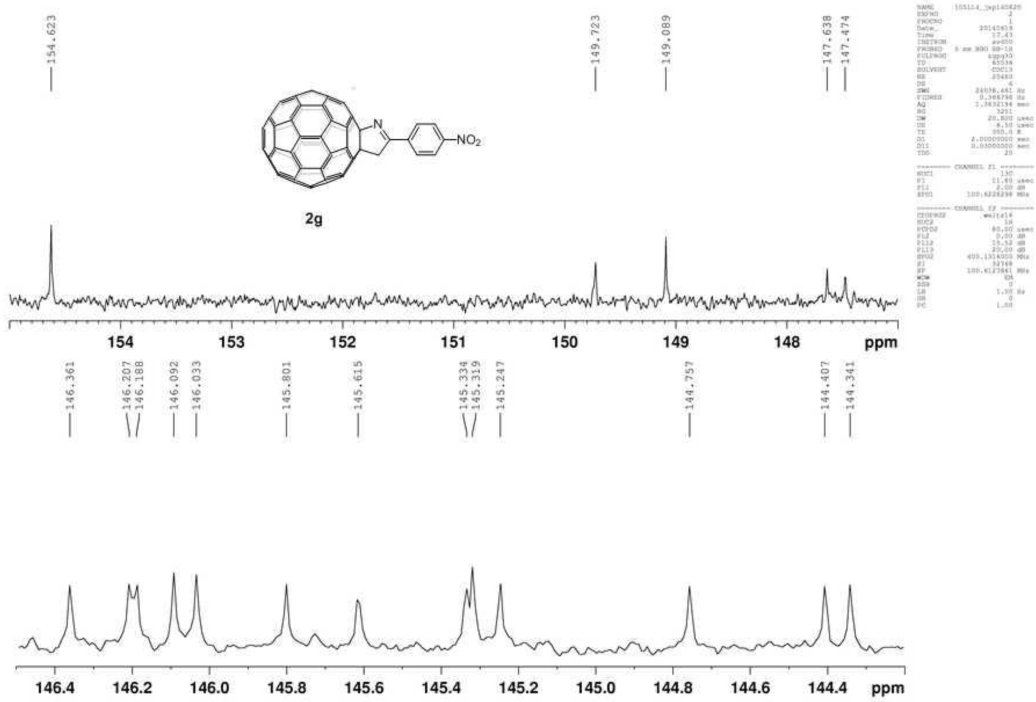
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2g



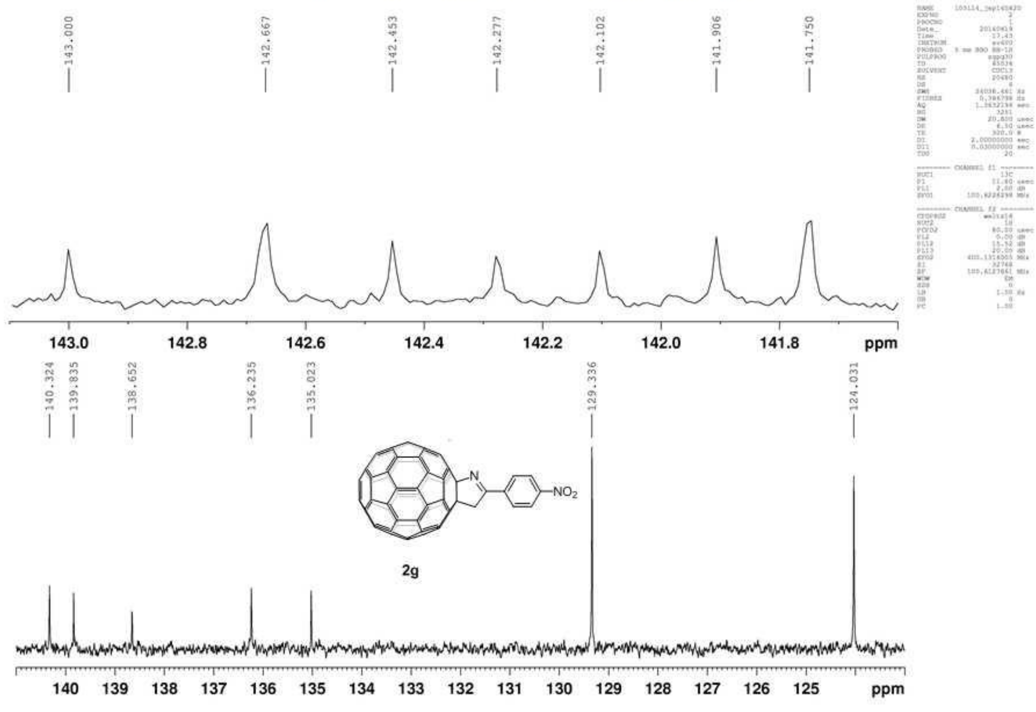
¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2g



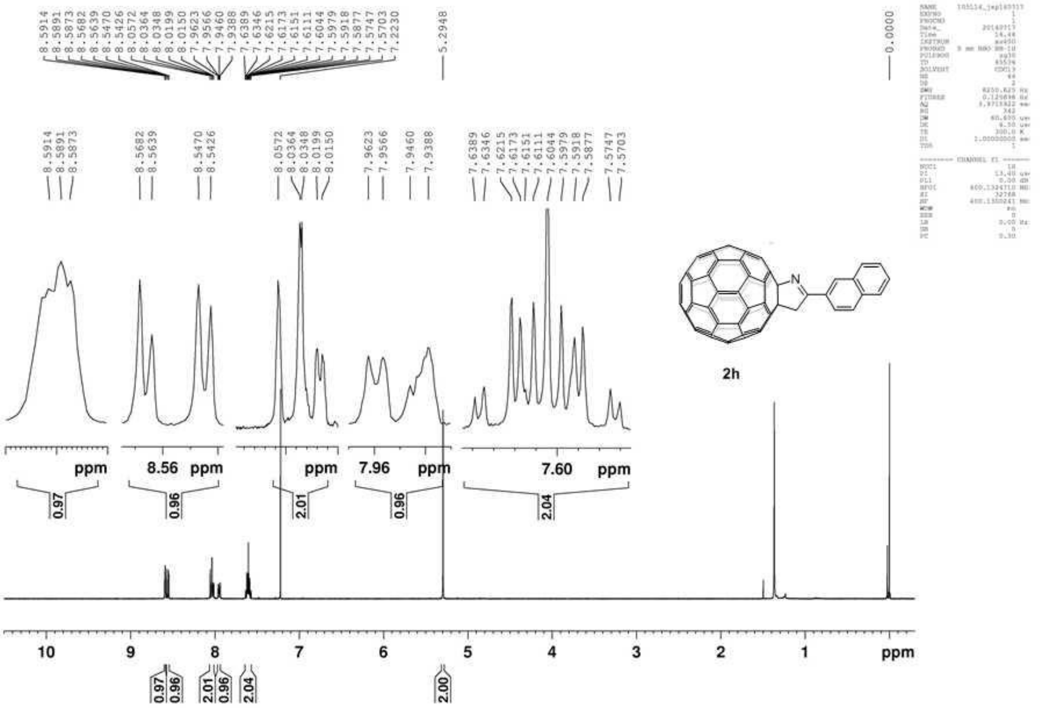
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2g



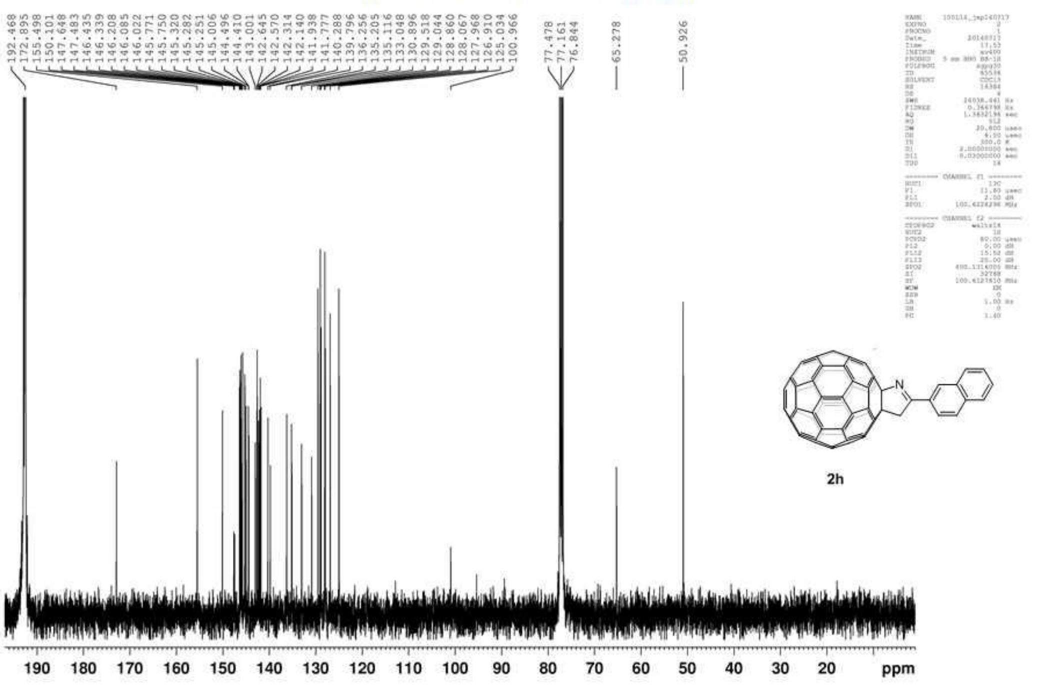
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2g



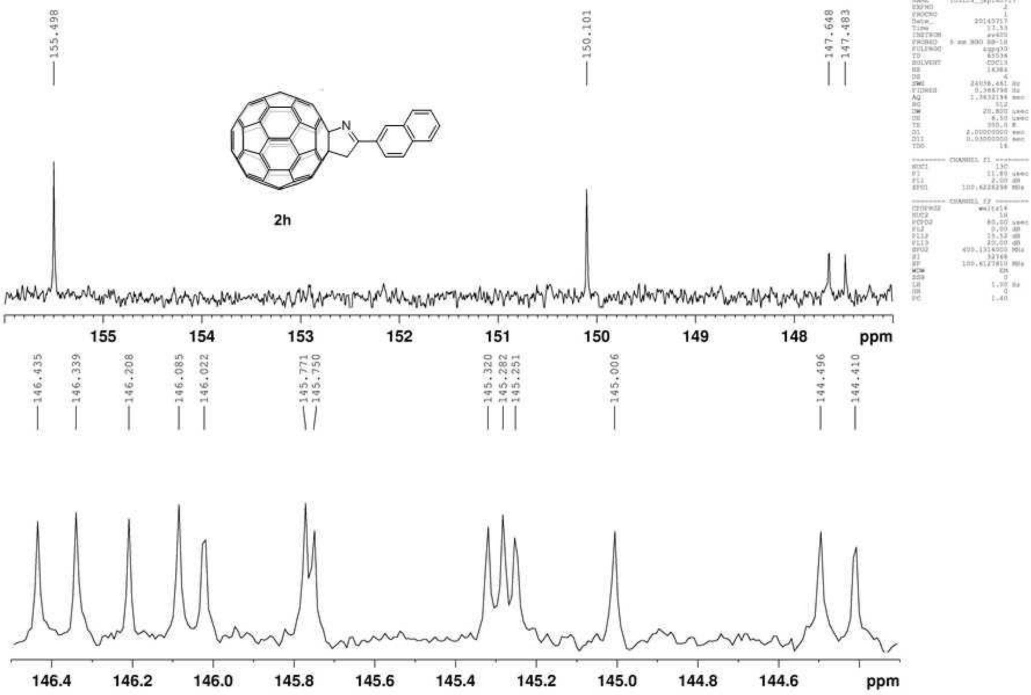
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2h



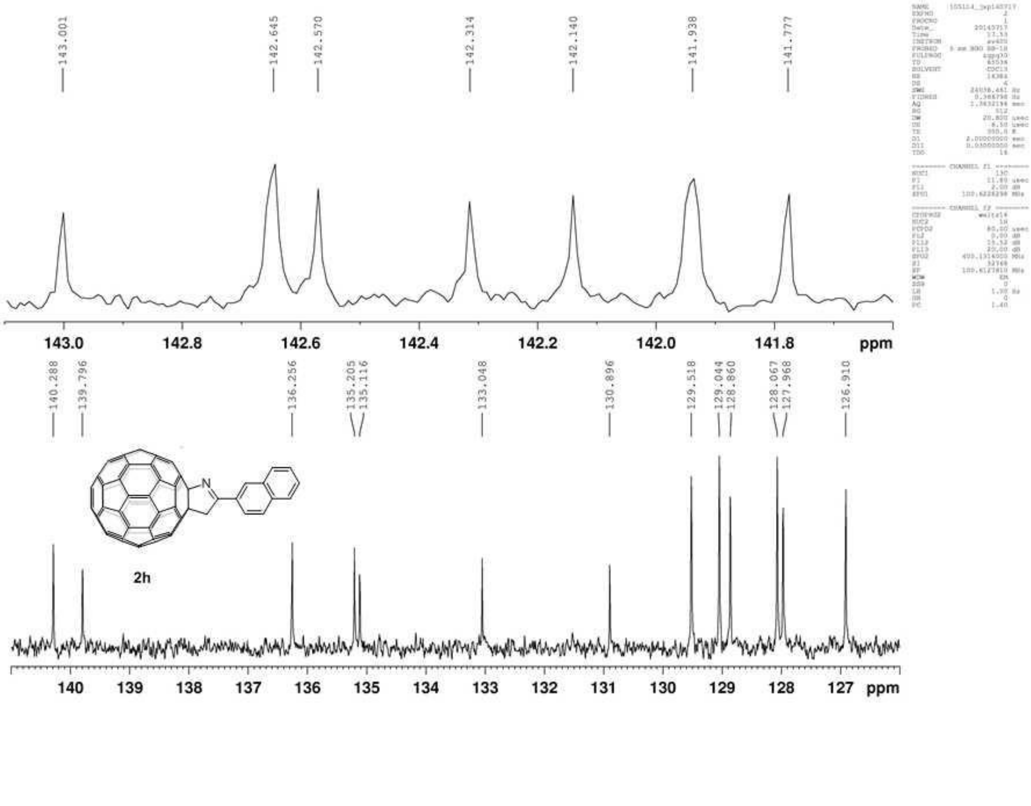
¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2h



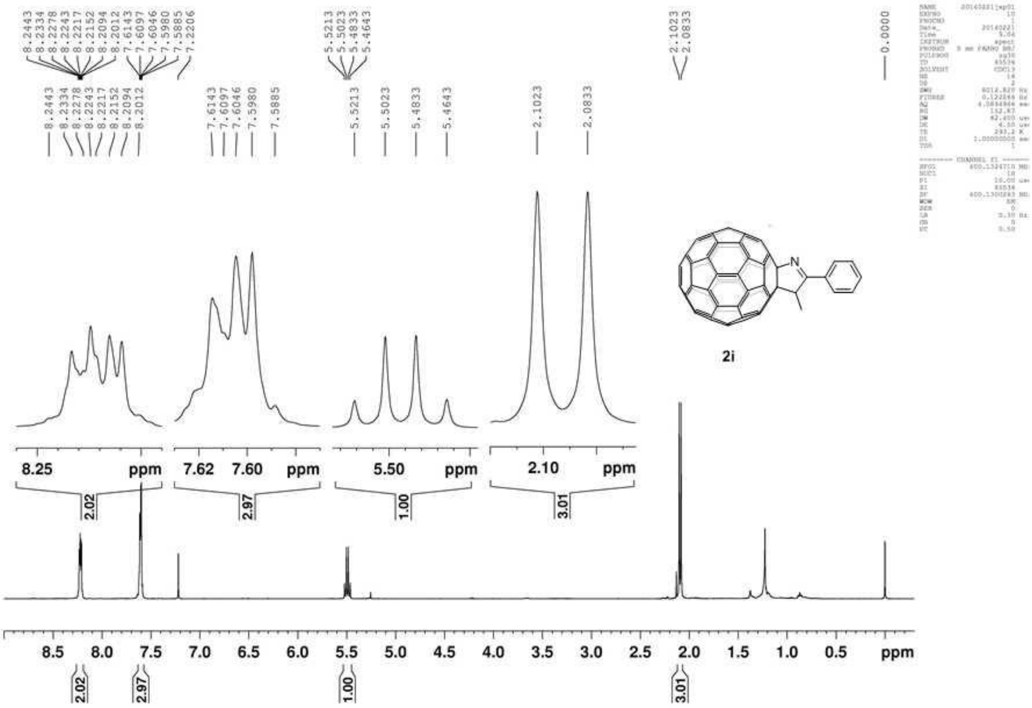
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2h



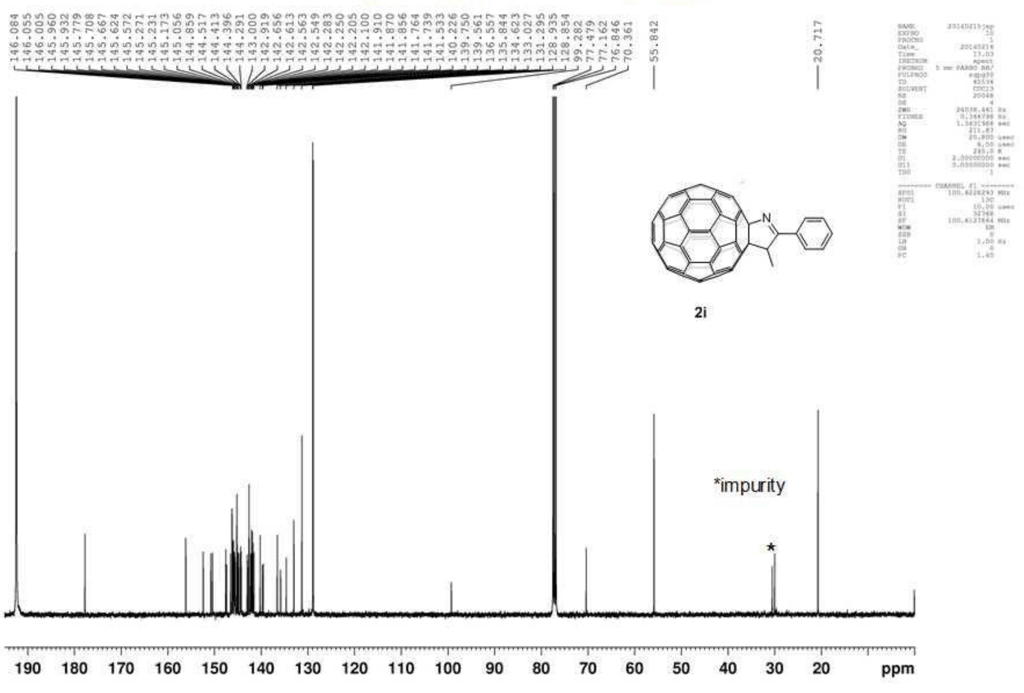
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2h



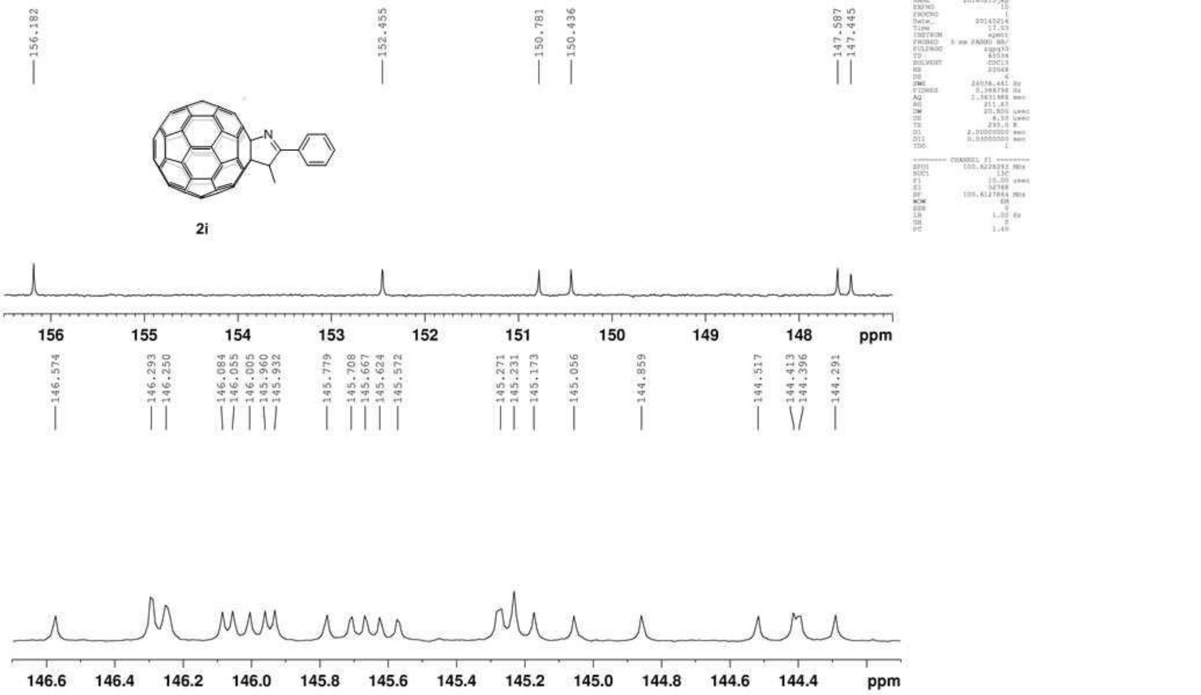
^{1}H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2i



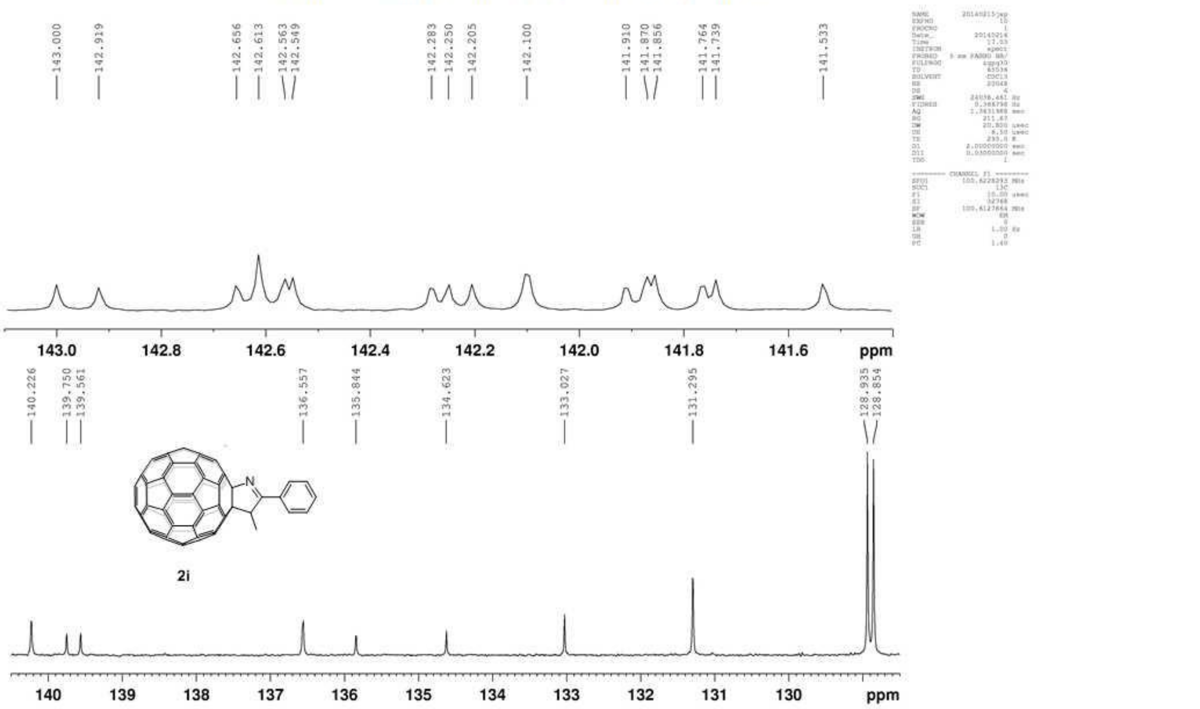
^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2i



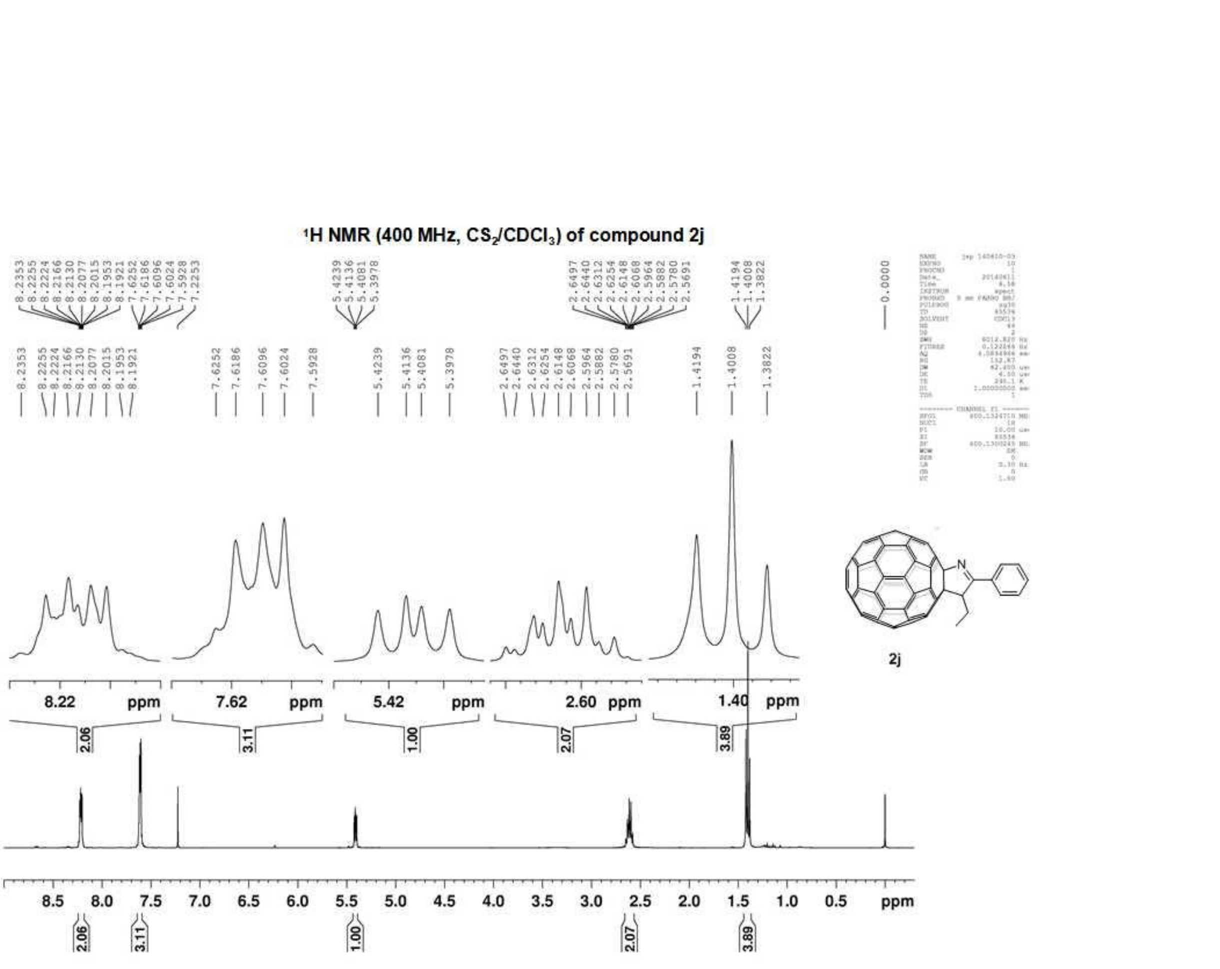
Expanded ^{13}C NMR (100 MHz, CS_2/$CDCl_3$) of compound 2i



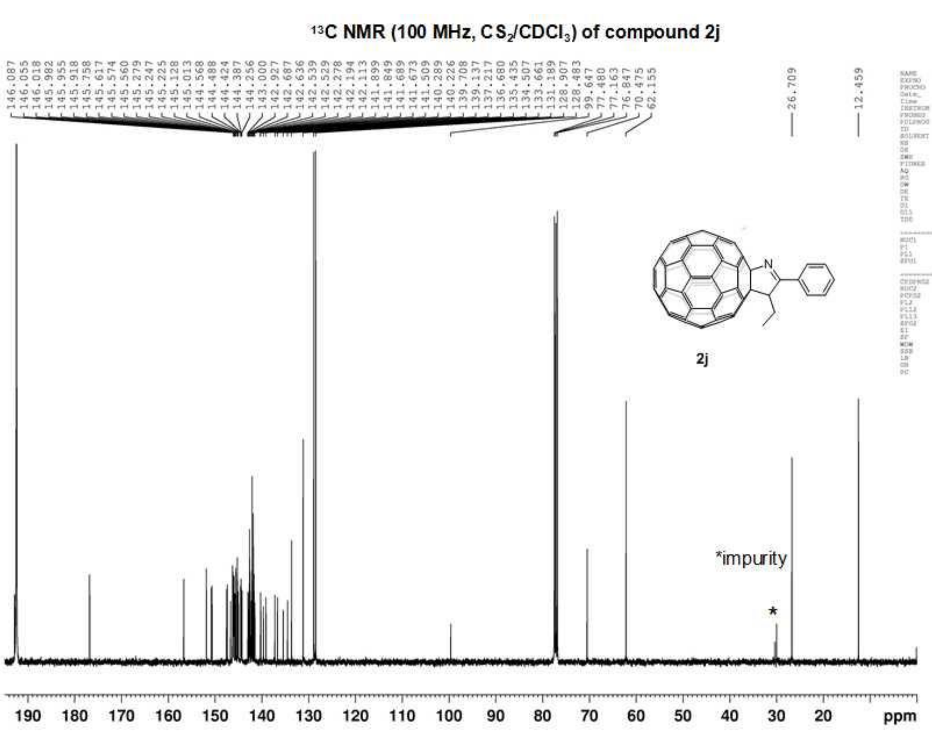
Expanded ^{13}C NMR (100 MHz, CS_2/$CDCl_3$) of compound 2i



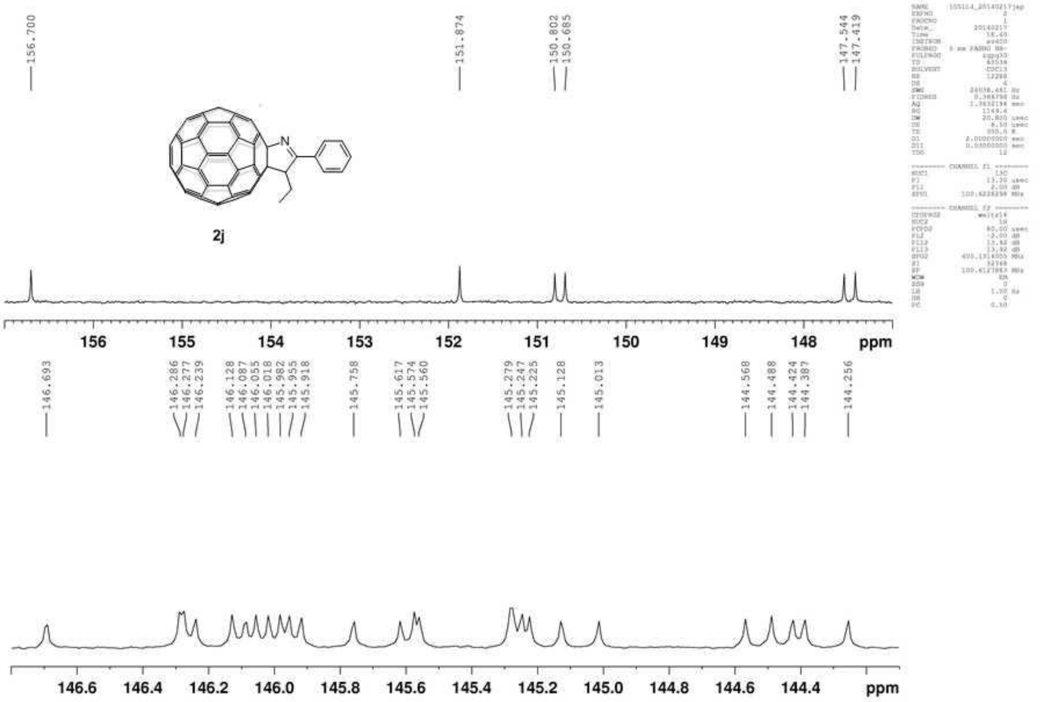
[1]H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2j



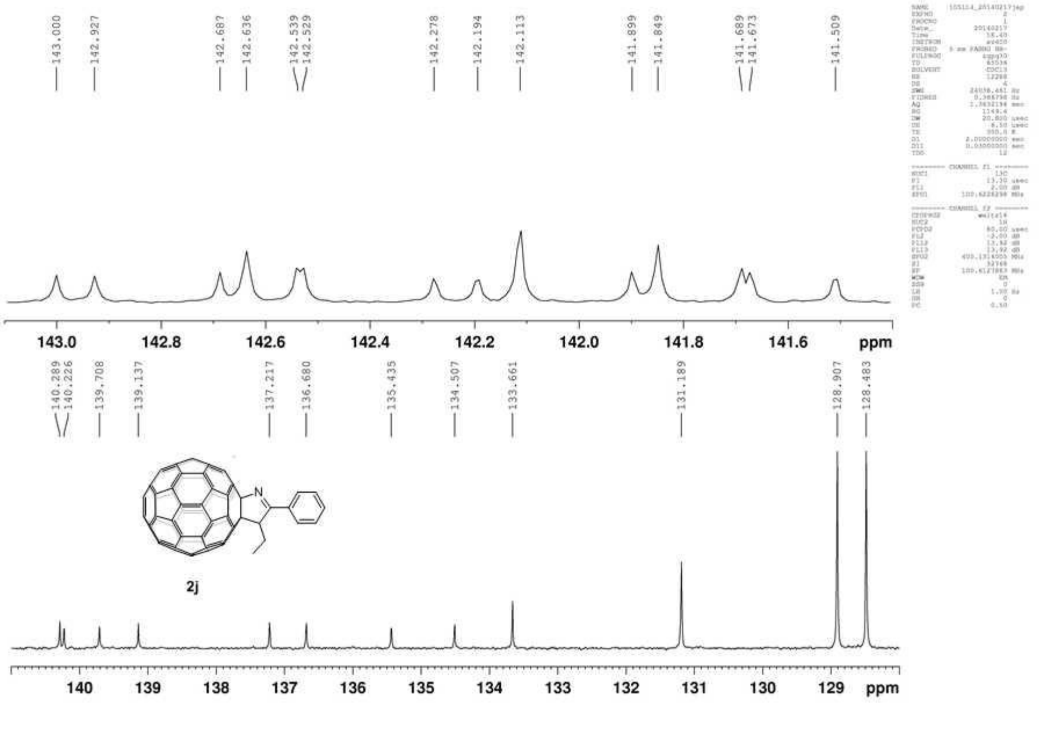
[13]C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2j



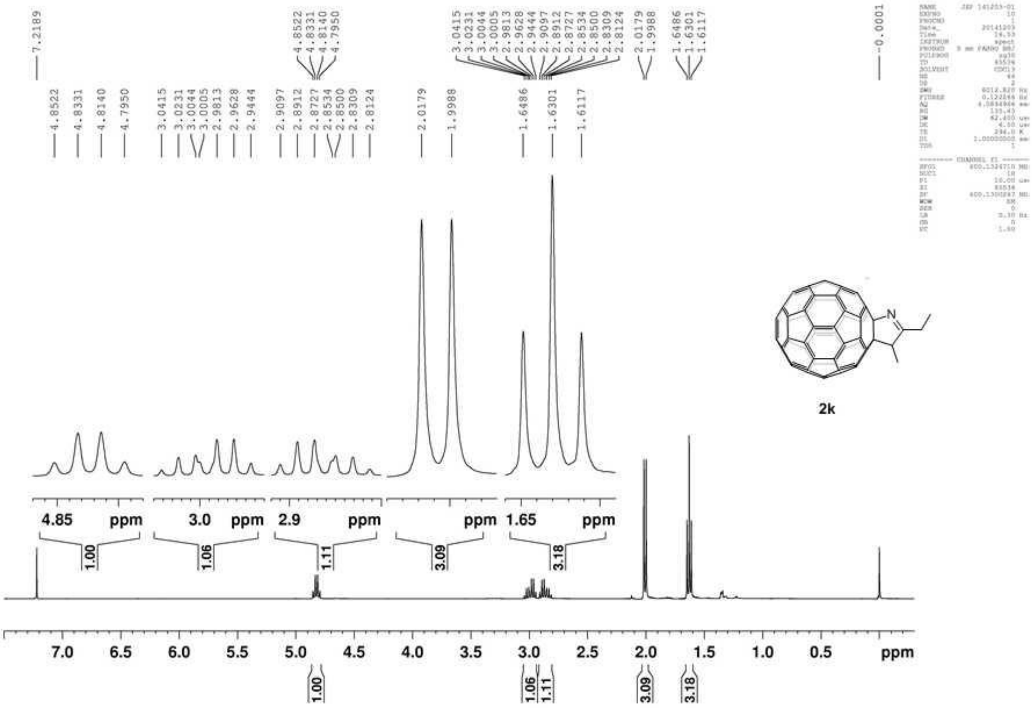
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2j



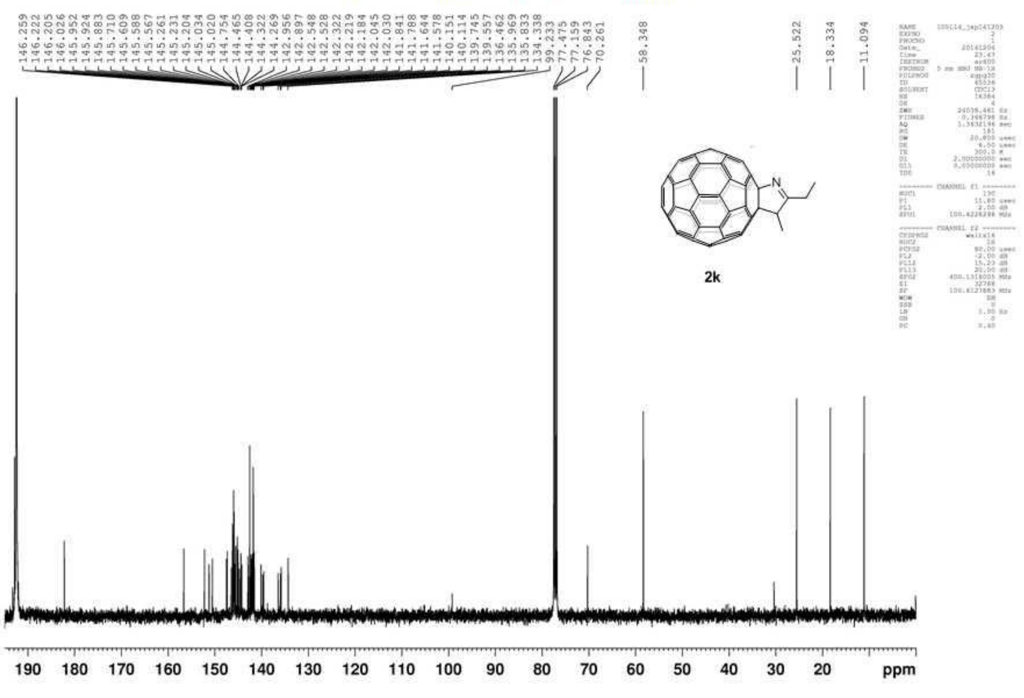
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2j



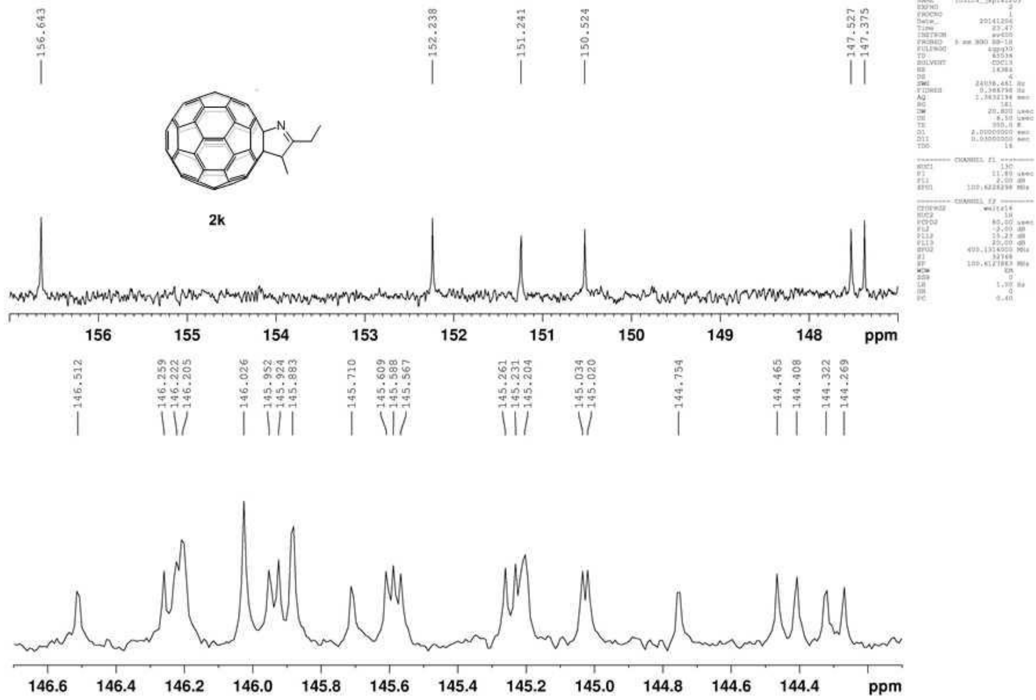
¹H NMR (400 MHz, $CS_2/CDCl_3$) of compound 2k



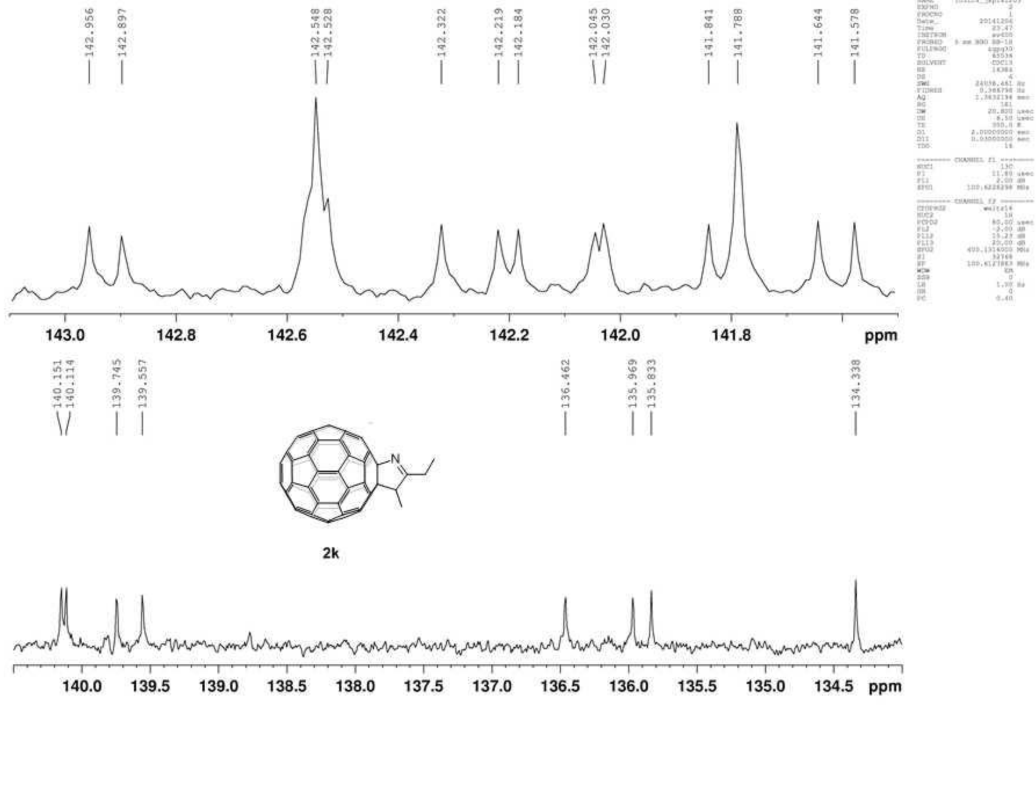
¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2k

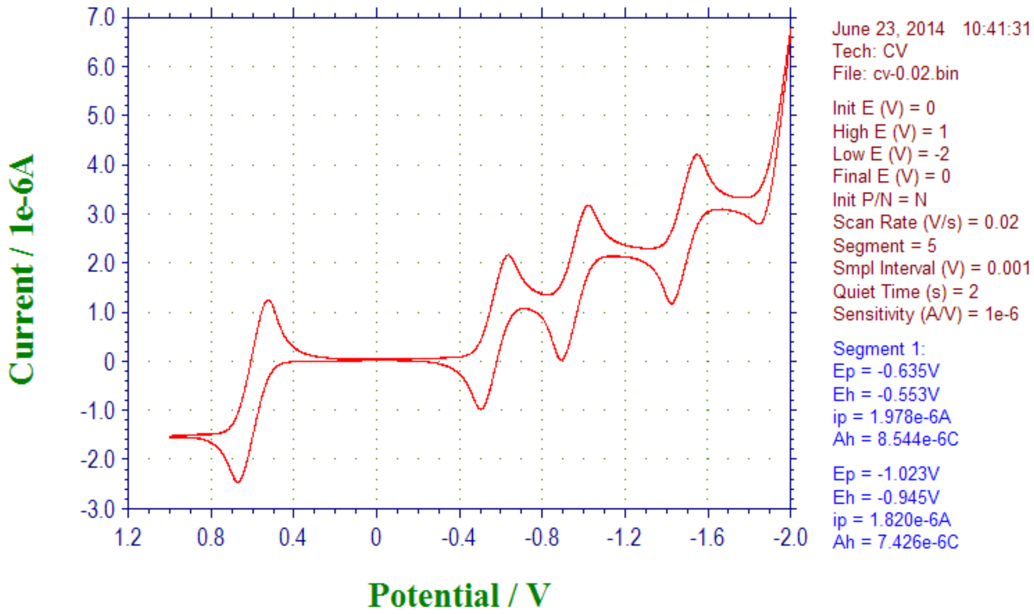


Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2k

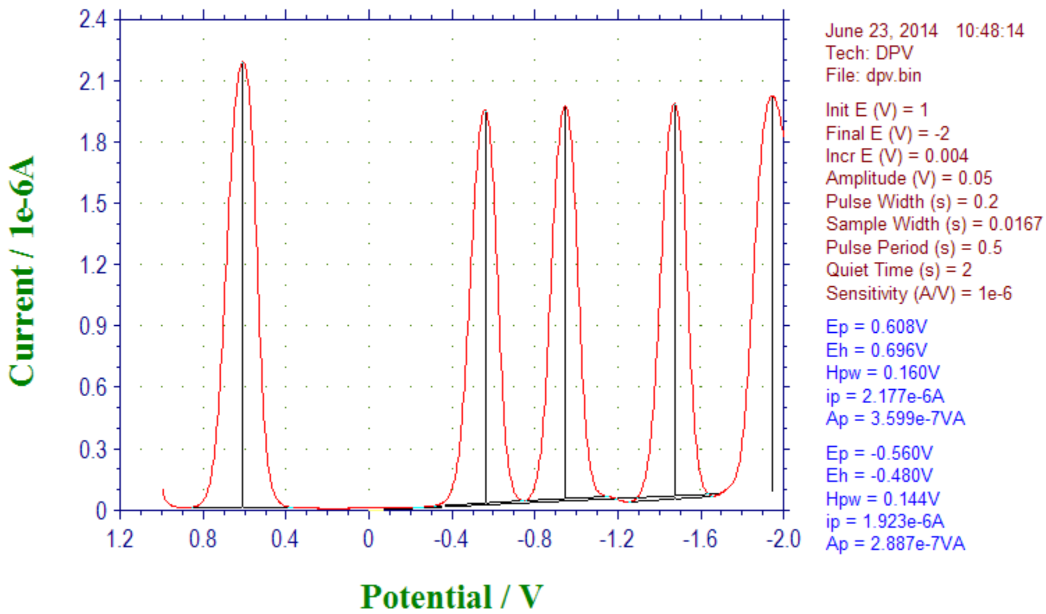


Expanded ¹³C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2k

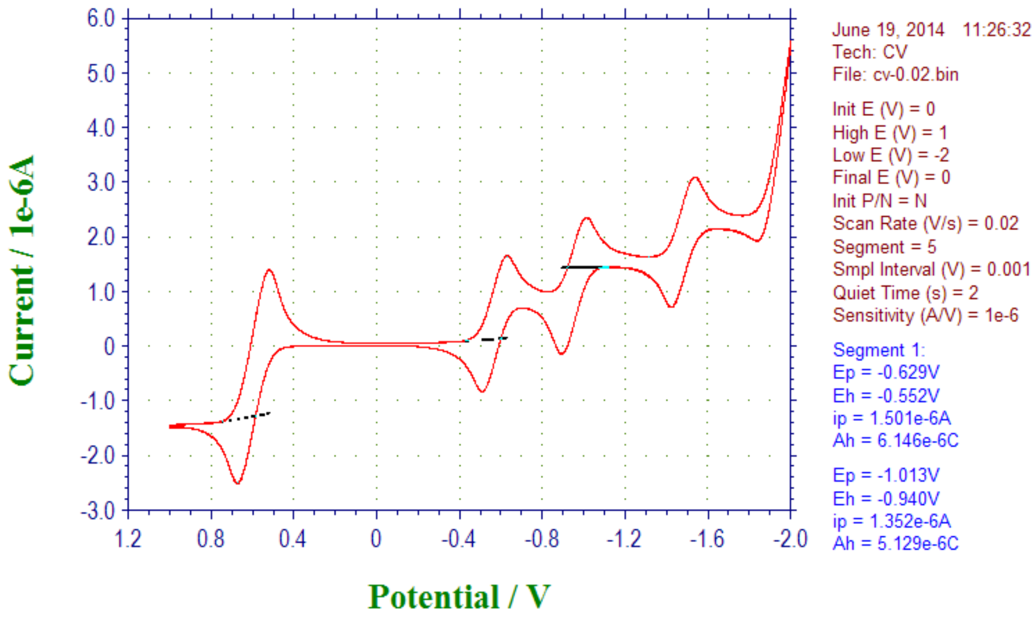




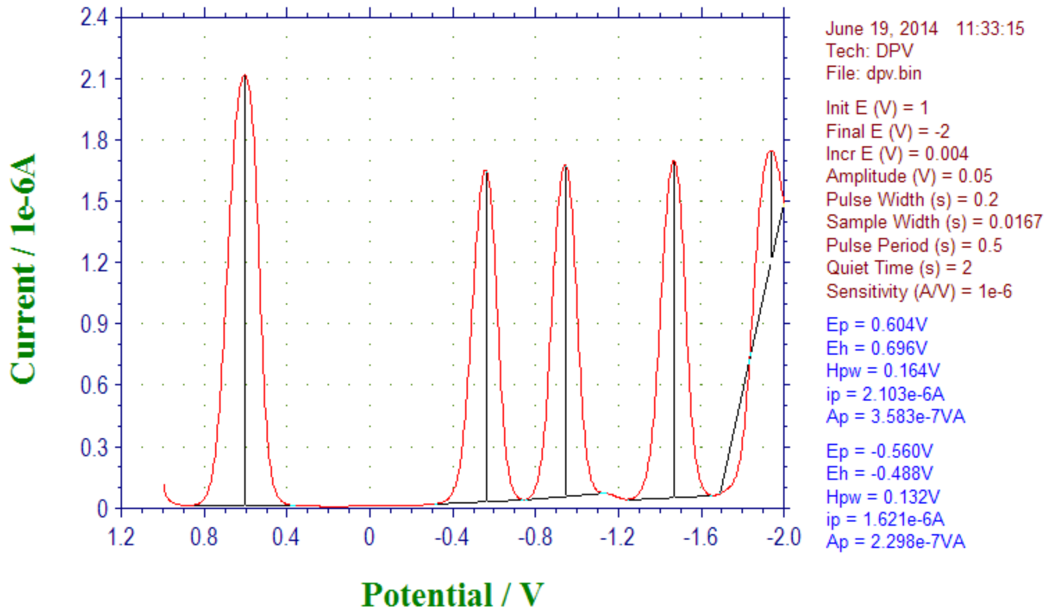
Cyclic voltammogram of compound **2a** (scanning rate: 20 mV s^{-1})



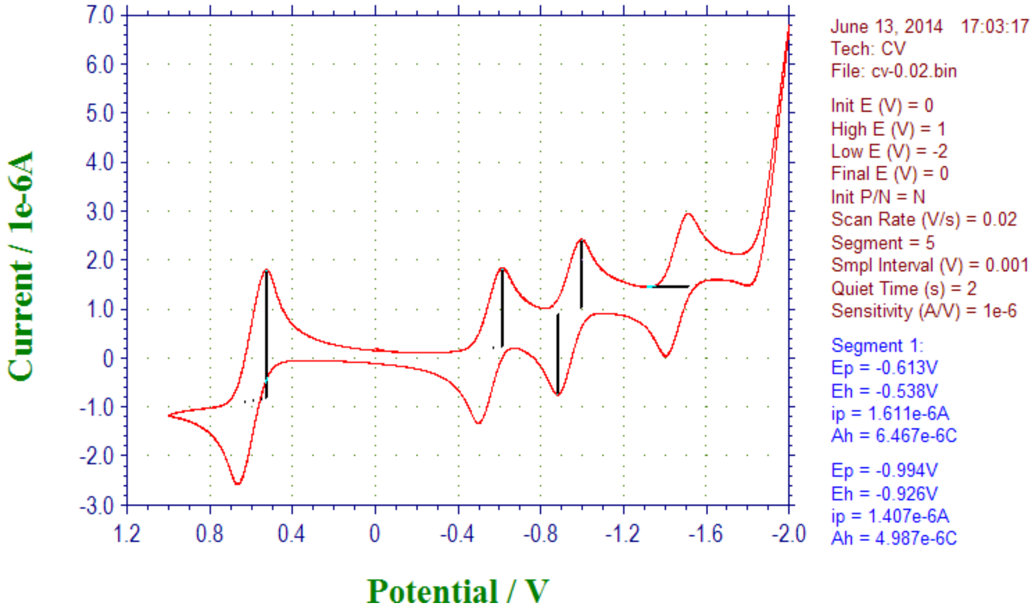
Differential pulse voltammogram of compound **2a**



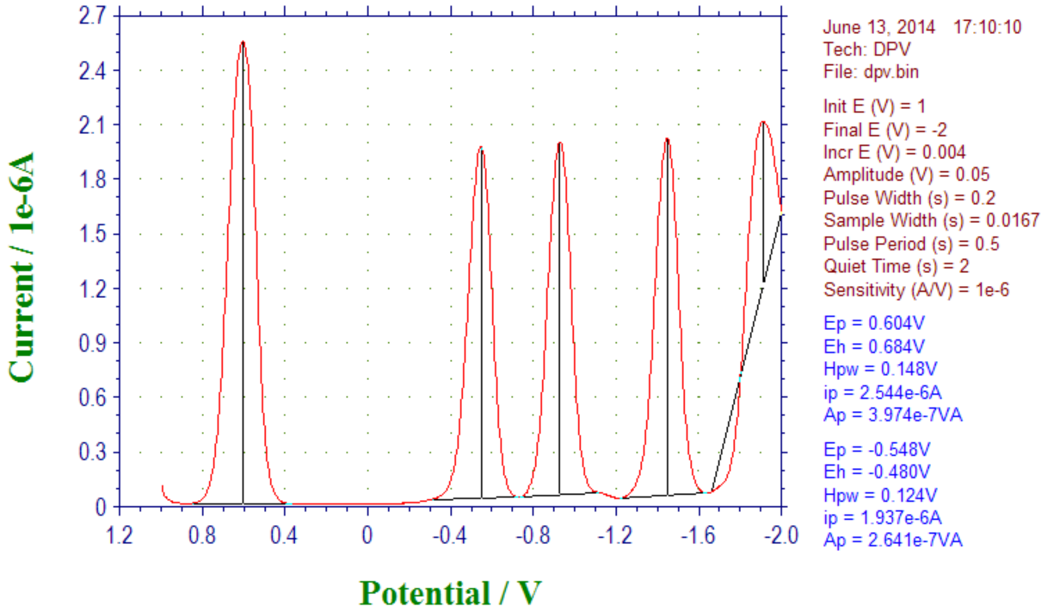
Cyclic voltammogram of compound **2b** (scanning rate: 20 mV s^{-1})



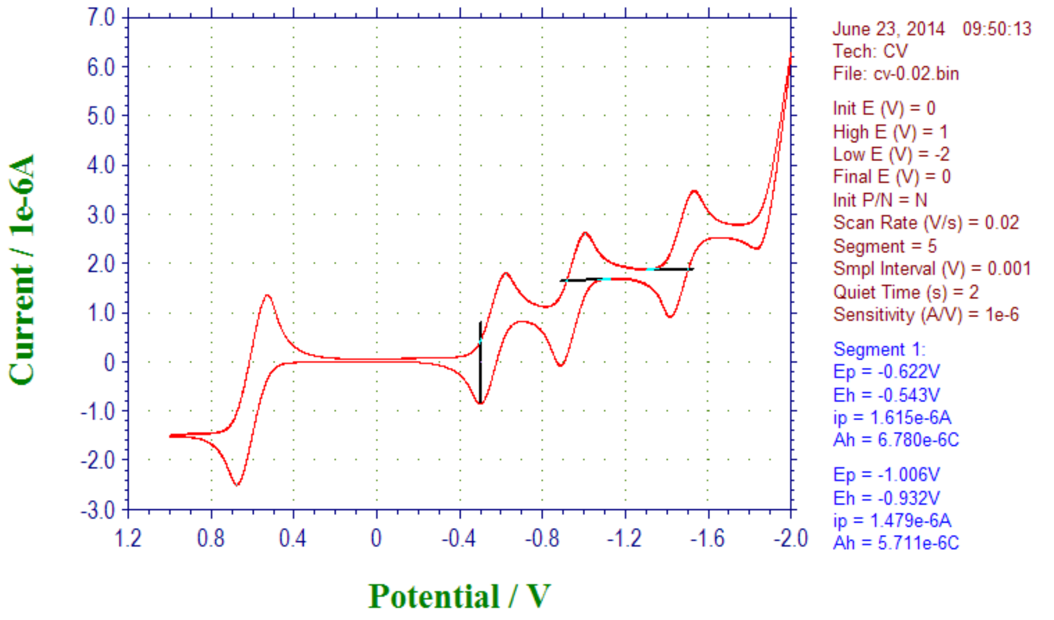
Differential pulse voltammogram of compound **2b**



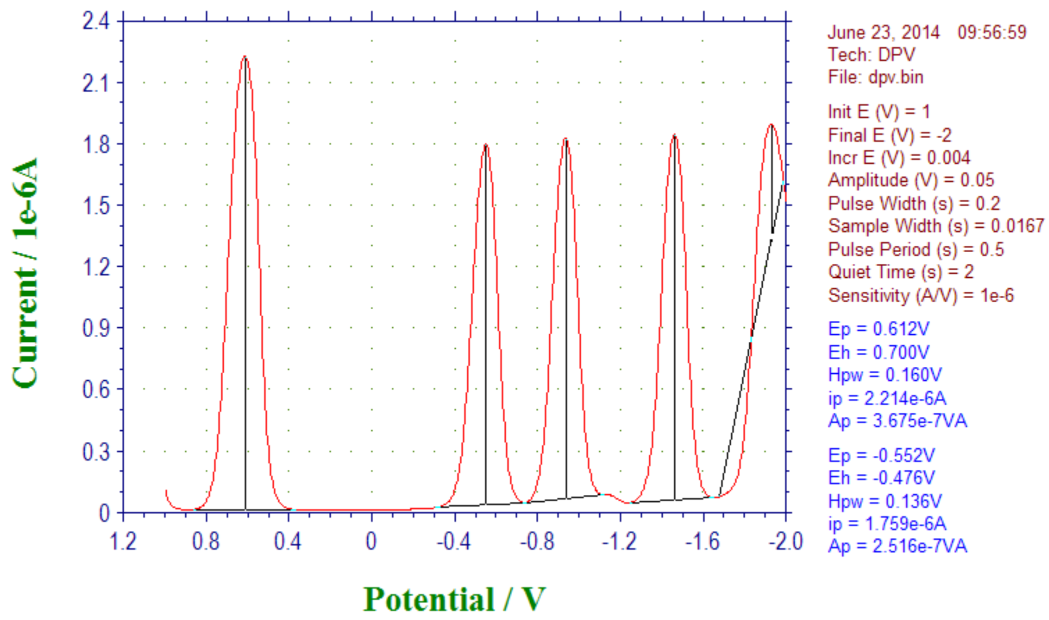
Cyclic voltammogram of compound **2c** (scanning rate: 20 mV s^{-1})



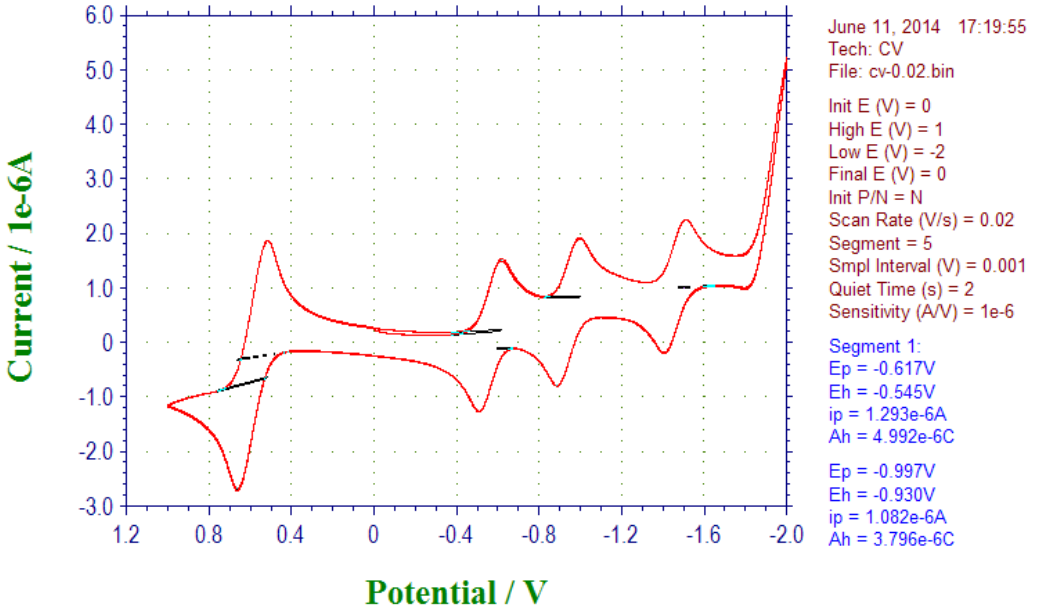
Differential pulse voltammogram of compound **2c**



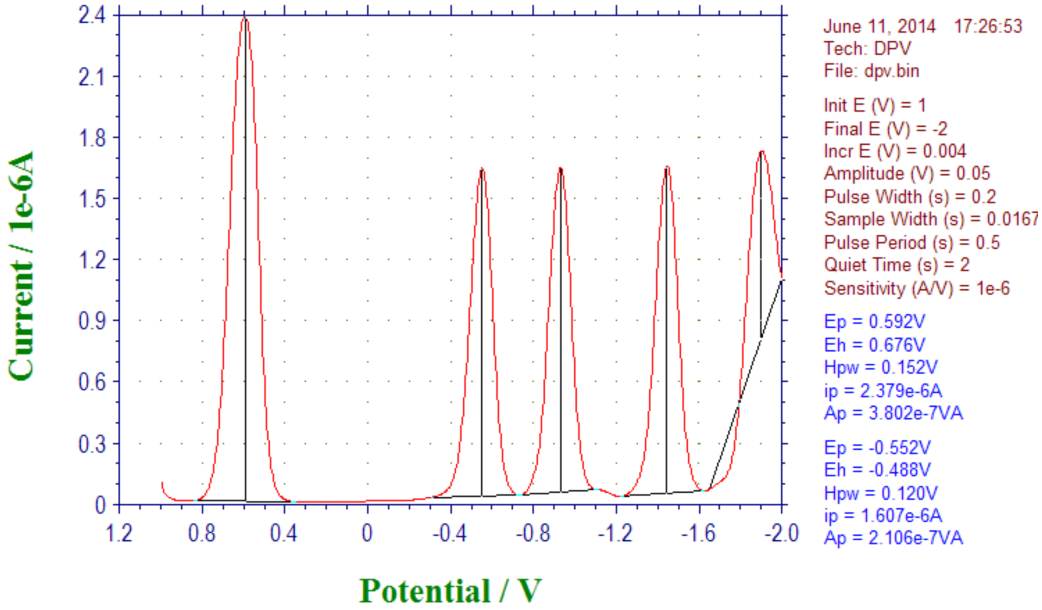
Cyclic voltammogram of compound **2d** (scanning rate: 20 mV s^{-1})



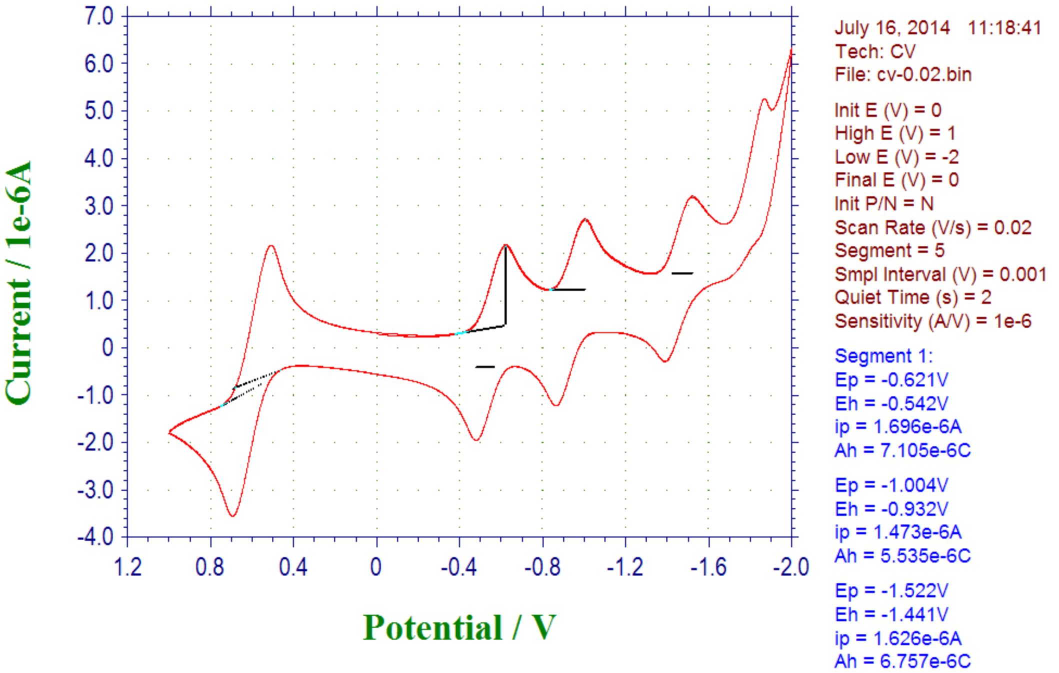
Differential pulse voltammogram of compound **2d**



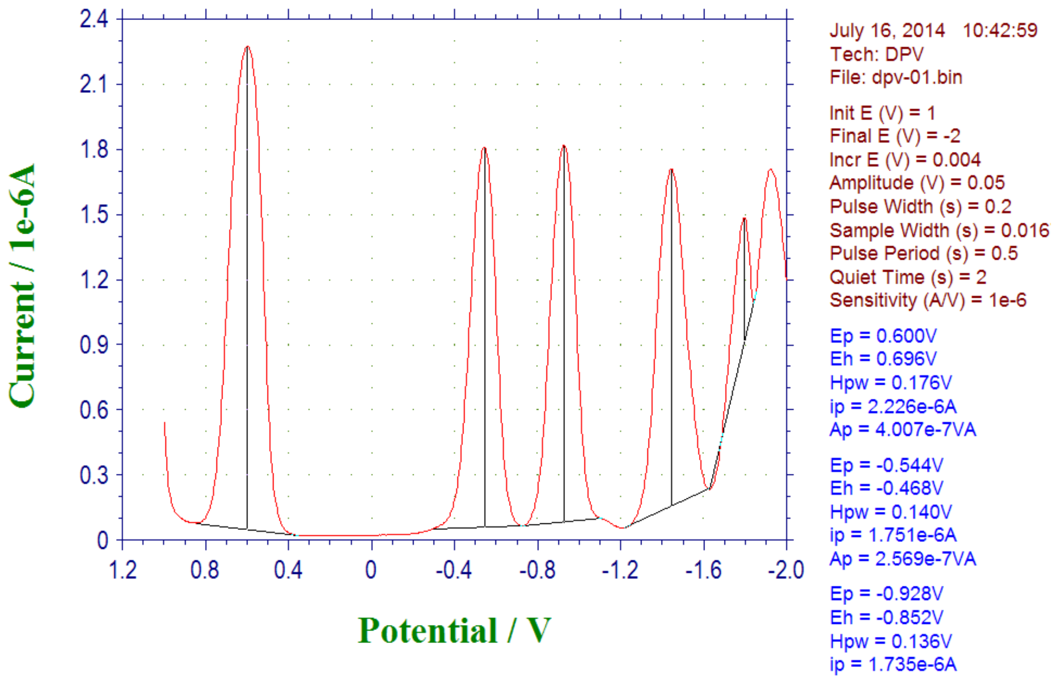
Cyclic voltammogram of compound **2e** (scanning rate: 20 mV s^{-1})



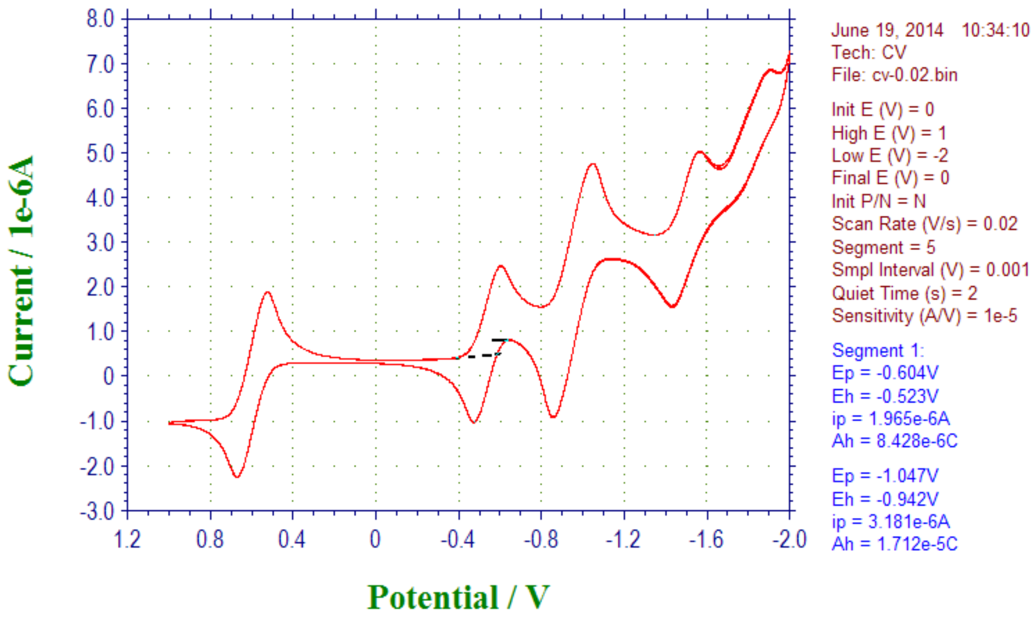
Differential pulse voltammogram of compound **2e**



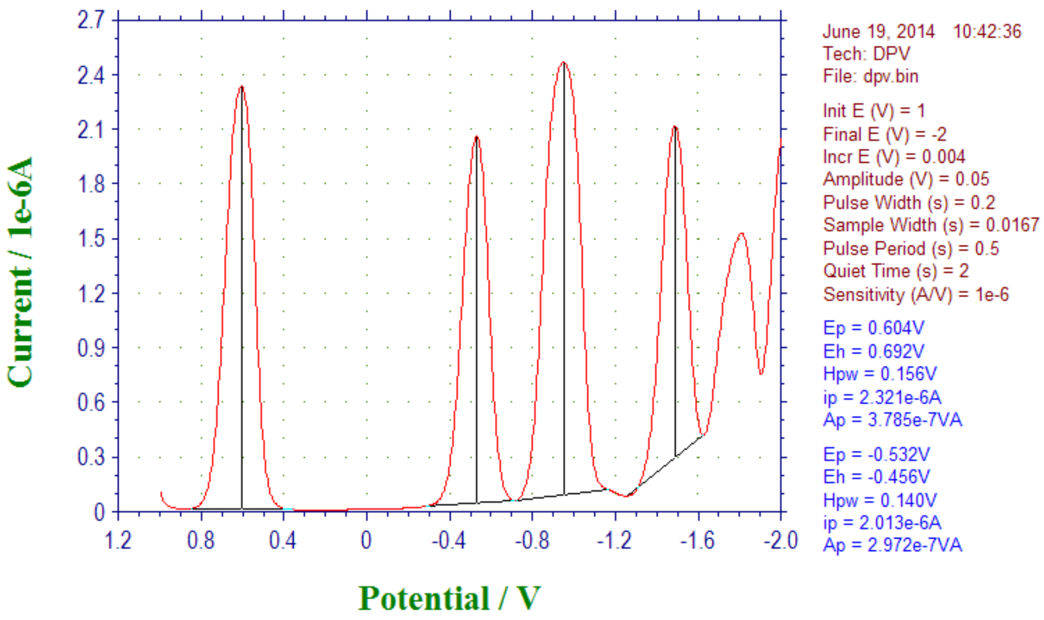
Cyclic voltammogram of compound **2f** (scanning rate: 20 mV s^{-1})



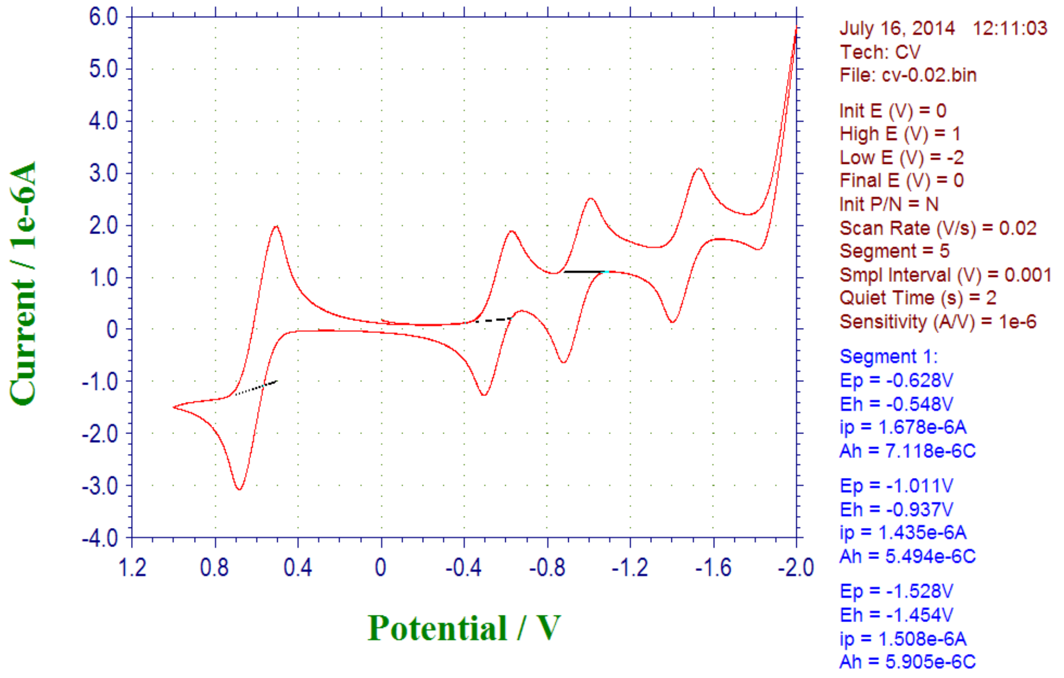
Differential pulse voltammogram of compound **2f**



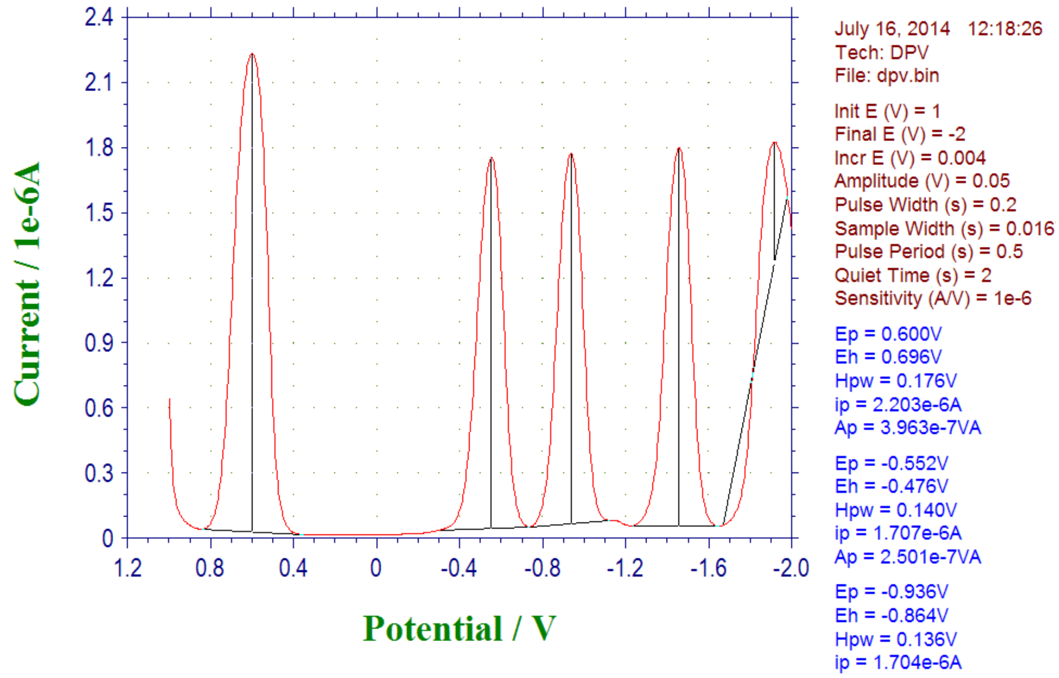
Cyclic voltammogram of compound **2g** (scanning rate: 20 mV s^{-1})



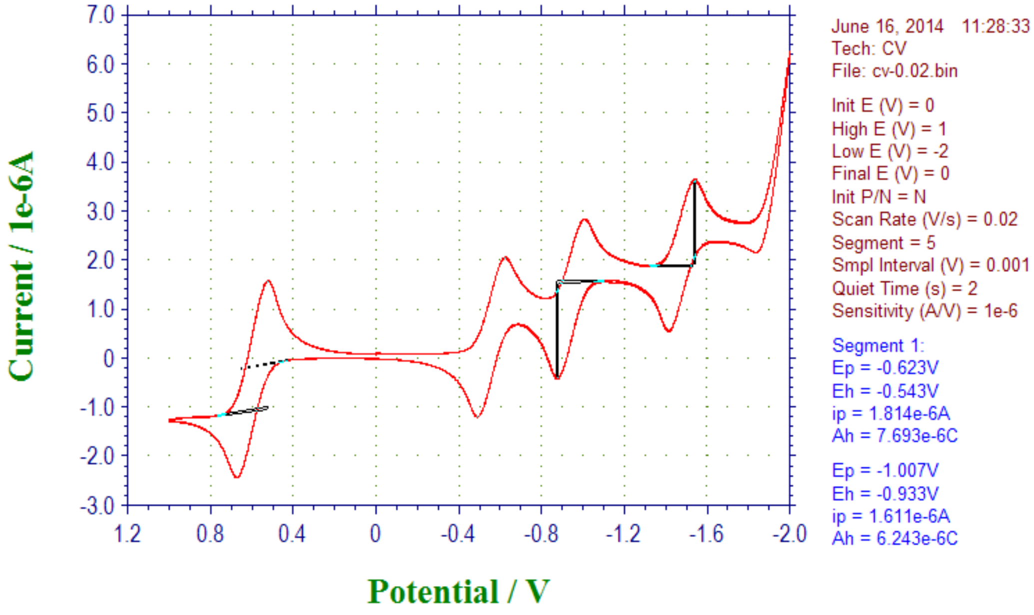
Differential pulse voltammogram of compound **2g**



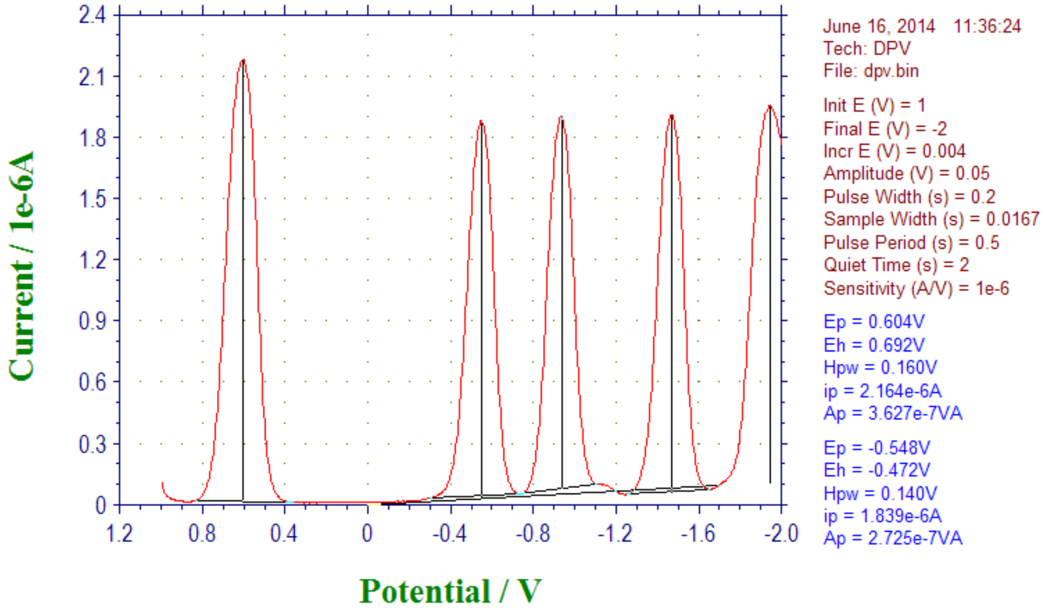
Cyclic voltammogram of compound **2h** (scanning rate: 20 mV s^{-1}**)**



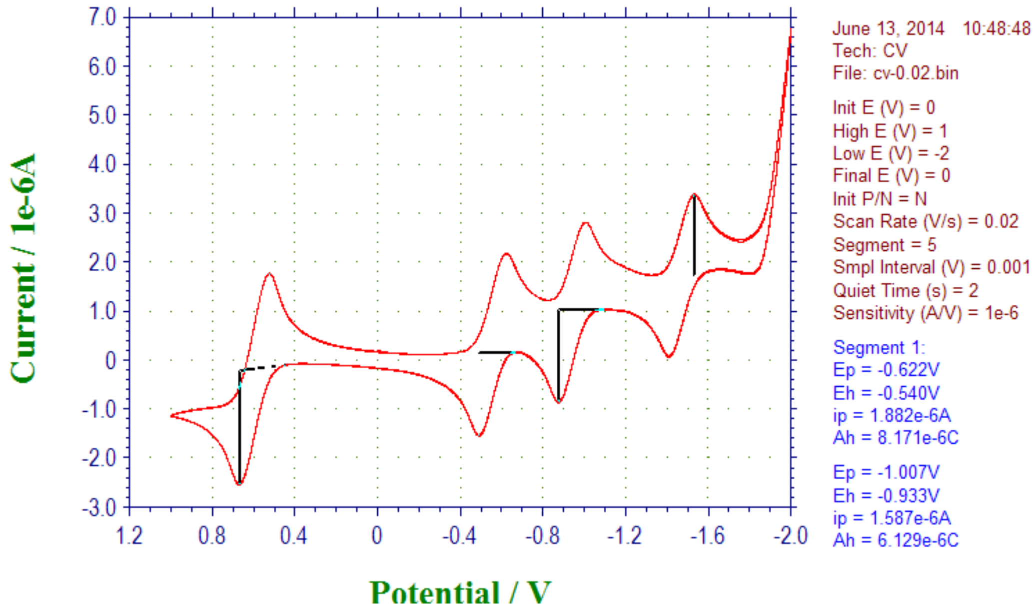
Differential pulse voltammogram of compound **2h**



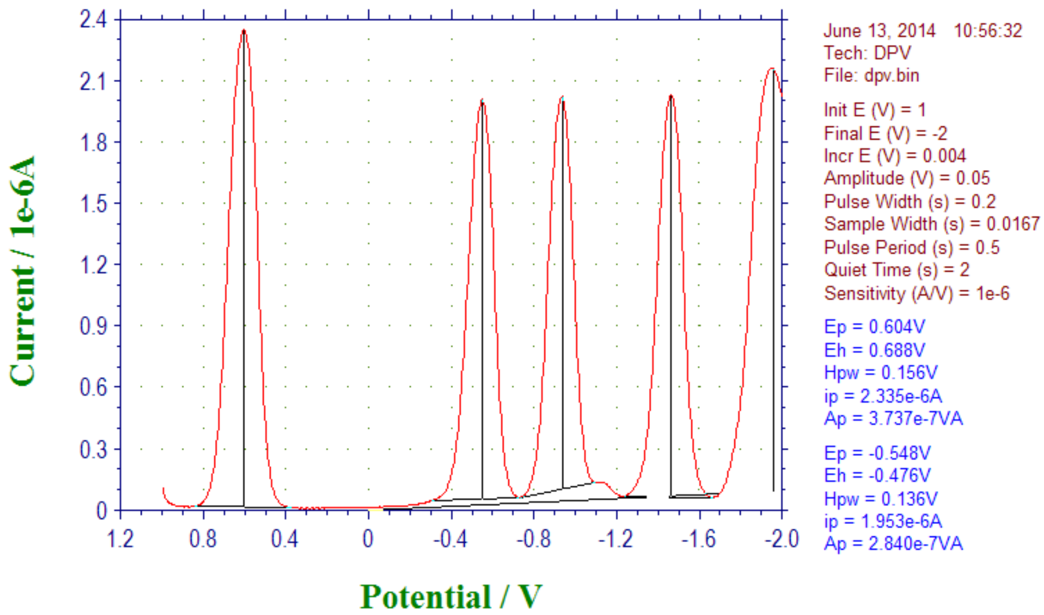
Cyclic voltammogram of compound **2i** (scanning rate: 20 mV s^{-1})



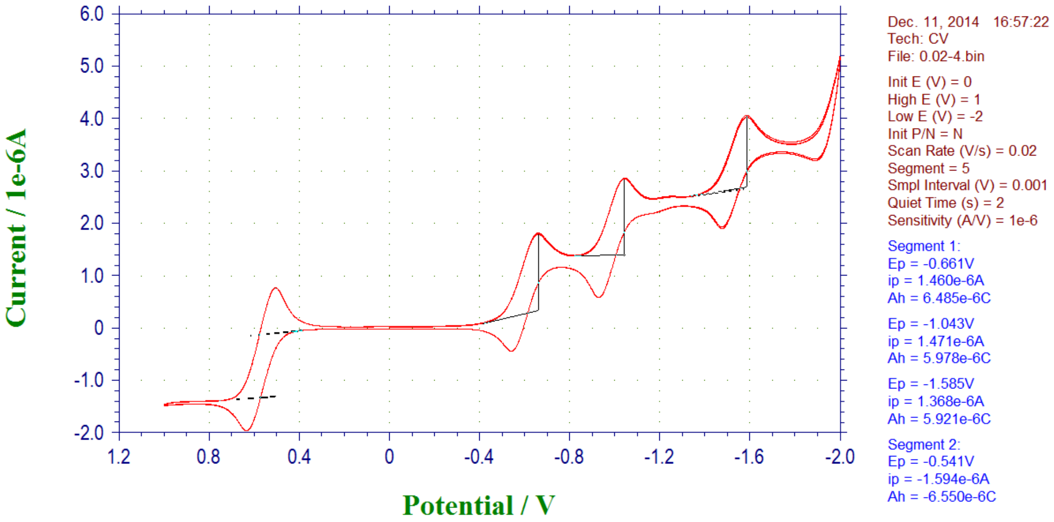
Differential pulse voltammogram of compound **2i**



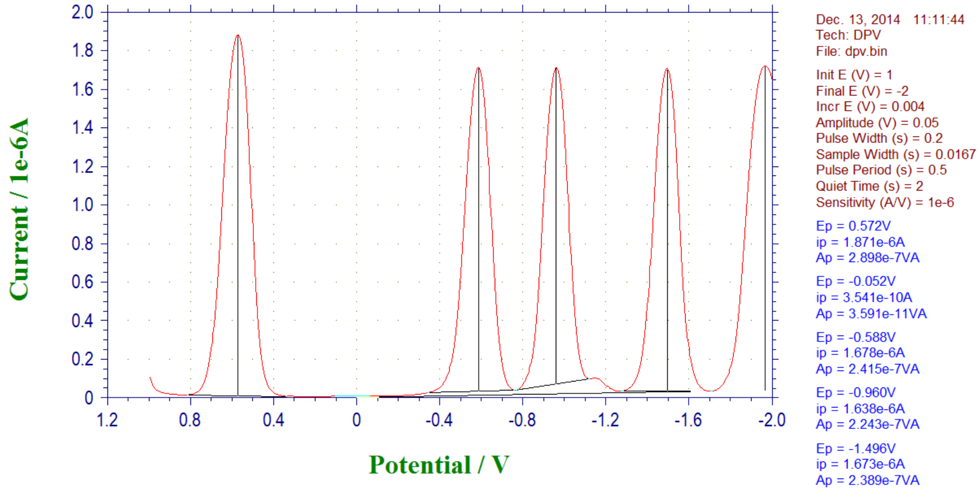
Cyclic voltammogram of compound **2j** (scanning rate: 20 mV s^{-1})



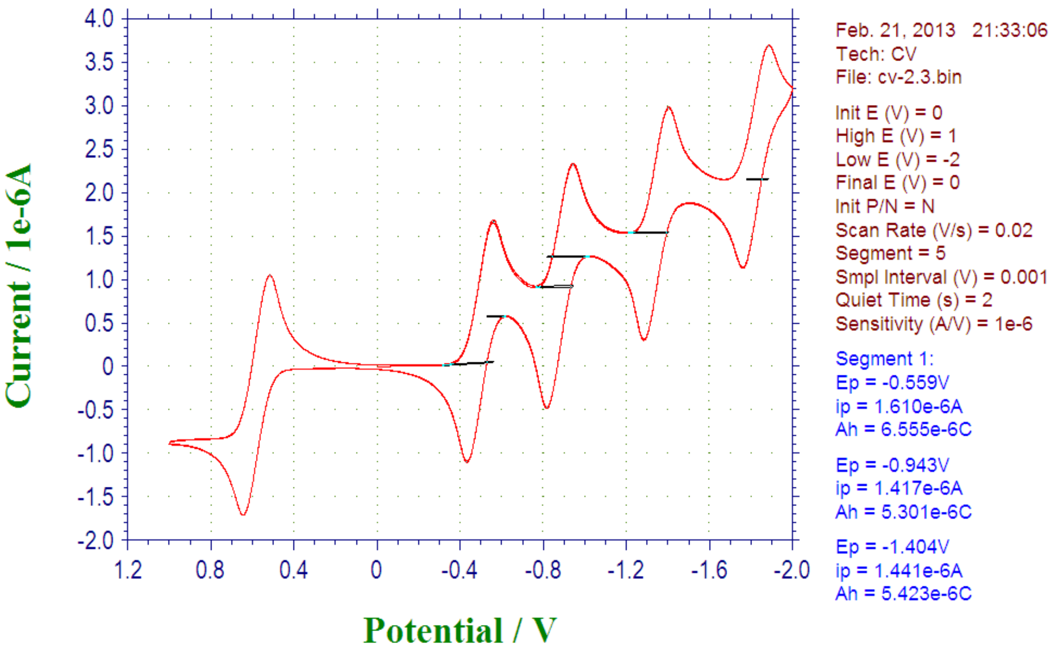
Differential pulse voltammogram of compound **2j**



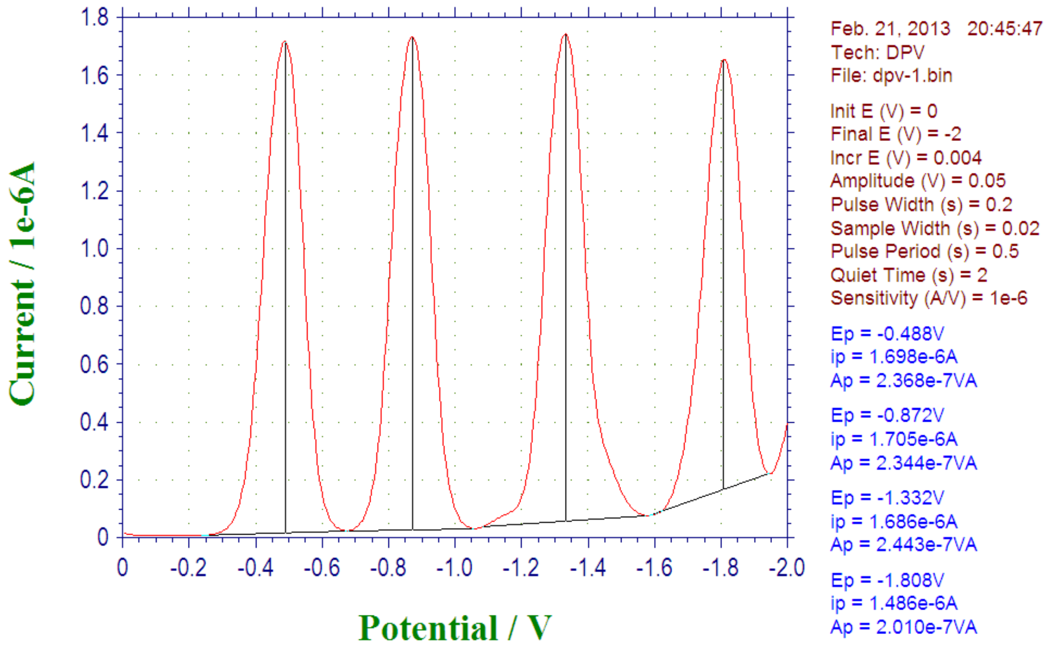
Cyclic voltammogram of compound **2k** (scanning rate: 20 mV s^{-1})



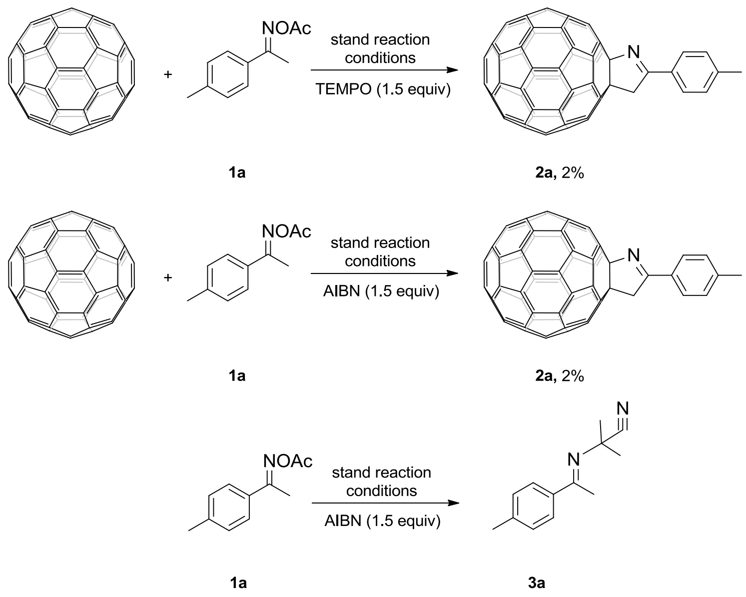
Differential pulse voltammogram of compound **2k**



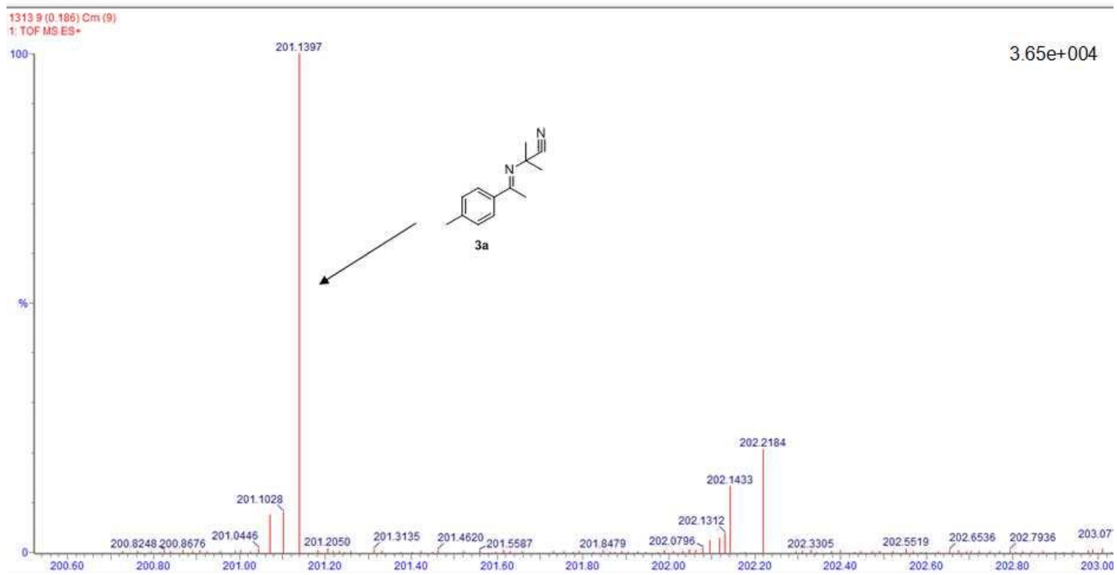
Cyclic voltammogram of C_{60} (scanning rate: 20 mV s^{-1})



Differential pulse voltammogram of C_{60}

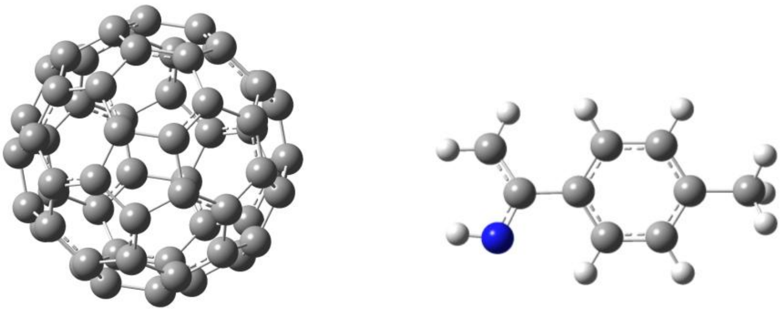


ESI-TOF-MS for the reaction mixture of **1a**, AIBN, CuBr and $NaHSO_3$

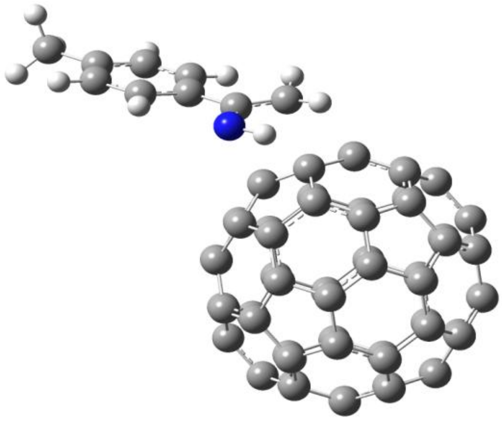


species	formula	calculated	found	error
3a	$C_{13}H_{17}N_2$ [M+H]	201.1392	201.1397	2.5 ppm

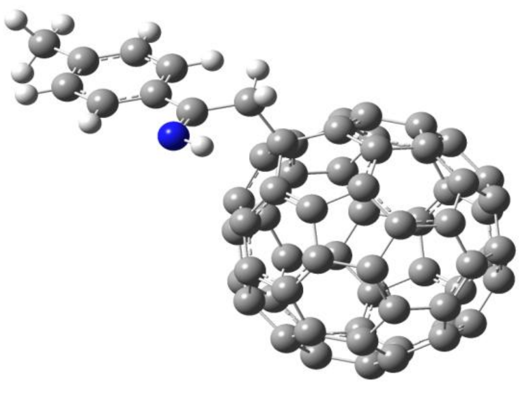
Figure S1. Mechanism study



C_{60} and **D-1a**
0.0 kcal/mol

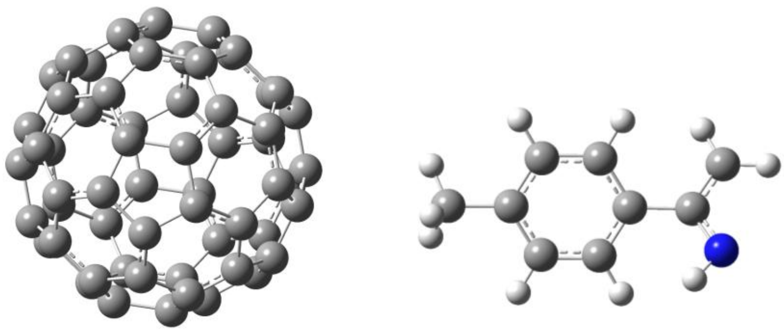


TS1 (from **D-1a** to **E-1a**)
6.1 kcal/mol

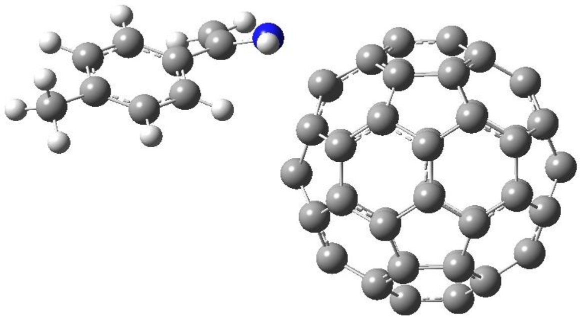


E-1a
-14.3 kcal/mol

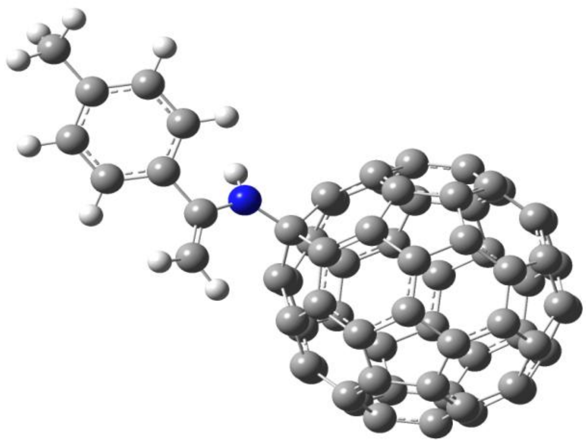
Figure S2. Relative energies (kcal/mol) for optimized C_{60}, **D-1a**, **TS1** and **E-1a** at the B3LYP/6-31G (d)



C_{60} and **G-1a**
0.2 kcal/mol



TS2 (from **G-1a** to **H-1a**)
9.7 kcal/mol



H-1a
-3.2 kcal/mol

Figure S3. Relative energies (kcal/mol) for optimized C_{60}, **G-1a**, **TS2** and **H-1a** at the B3LYP/6-31G (d)

The xyz coordinates for the lowest energy structure of C_{60}

C	-0.88158800	0.67024300	3.37263400
C	0.55213000	0.45528500	3.47640500
C	1.43848900	1.38641100	2.93371100
C	0.92821800	2.57143200	2.26453600
C	-0.44833400	2.77766500	2.16457300
C	-1.37149700	1.80779900	2.72970300
C	-1.51403800	-0.61925900	3.15040700
C	-0.47118800	-1.63097900	3.11735000
C	0.80577400	-0.96700100	3.31905100
C	1.93576300	-1.40165200	2.62486300
C	2.61537300	0.93387700	2.21117000
C	1.78982600	2.85126400	1.12796000
C	1.24004100	3.32576700	-0.06374300
C	-0.19356800	3.54023700	-0.16788000
C	-1.02069400	3.27204800	0.92358800
C	-2.29782900	2.60821800	0.72182800
C	-2.51415200	1.70278100	1.83791100
C	-3.12152600	0.46464700	1.62476900
C	-2.61168600	-0.72008300	2.29455900
C	-0.56722600	-2.70330500	2.22951400
C	-1.71032800	-2.80839000	1.33796400
C	-2.71149900	-1.83678300	1.36954900
C	-3.28399100	-1.34219100	0.12854500
C	-3.53763300	0.08019300	0.28636600
C	-3.32937900	0.94924700	-0.78543800
C	-2.69717000	2.23902400	-0.56341500
C	-1.83572600	2.51849400	-1.70023500
C	-0.60939800	3.15573300	-1.50632600
C	2.83216900	1.83889800	1.09480600
C	1.51403900	0.61925700	-3.15040700
C	2.61168500	0.72008100	-2.29455900
C	3.12152500	-0.46464600	-1.62476900
C	2.51415200	-1.70278100	-1.83791200
C	1.37149800	-1.80780000	-2.72970400
C	-0.55213000	-0.45528500	-3.47640500
C	-0.80577400	0.96700200	-3.31905100
C	0.47118600	1.63098000	-3.11735000
C	0.56722500	2.70330600	-2.22951400
C	1.71032800	2.80839000	-1.33796300
C	2.71149800	1.83678300	-1.36954800
C	3.53763200	-0.08019300	-0.28636600
C	3.32937800	-0.94924700	0.78543700
C	2.69716900	-2.23902400	0.56341600

C	2.29782900	-2.60821900	-0.72182800
C	1.02069500	-3.27204900	-0.92358900
C	0.44833400	-2.77766600	-2.16457300
C	-0.92821700	-2.57143100	-2.26453500
C	-1.43848800	-1.38641000	-2.93371000
C	-1.93576400	1.40165300	-2.62486300
C	-2.85875400	0.43189600	-2.05952200
C	-2.61537300	-0.93387700	-2.21116900
C	-2.83216900	-1.83889700	-1.09480500
C	-1.78982400	-2.85126300	-1.12795900
C	-1.24004100	-3.32576700	0.06374200
C	0.19356800	-3.54023700	0.16788100
C	0.60939800	-3.15573300	1.50632500
C	1.83572600	-2.51849400	1.70023400
C	3.28399000	1.34219200	-0.12854600
C	2.85875400	-0.43189600	2.05952200
C	0.88158900	-0.67024200	-3.37263400

Energy = -2286.17423945 a.u.

The xyz coordinates for the lowest energy structure of **D-1a**

C	-0.73230900	-0.00619500	0.01268100
C	-0.01717300	1.18992600	0.15849600
C	1.37730400	1.19484800	0.15515200
C	2.10538800	0.00952700	0.00385700
C	1.38596600	-1.18738600	-0.12954600
C	-0.00467300	-1.19880400	-0.12267600
H	-0.54378600	2.12859300	0.30558800
H	1.90743700	2.13645100	0.27985700
H	1.92631000	-2.12537900	-0.23963600
H	-0.55029200	-2.13130800	-0.21869500
C	-2.22770000	-0.04985000	0.01679300
N	-2.79277800	-1.21452800	0.29171100
H	-3.81379800	-1.11318000	0.25132600
C	-2.97610000	1.10633100	-0.29674600
H	-4.06116100	1.07716900	-0.25568900
H	-2.51686300	2.03364900	-0.61929700
C	3.61535000	0.01621300	-0.03202300
H	4.03318600	-0.83778800	0.51288900
H	3.98874900	-0.04580500	-1.06304500
H	4.02335100	0.93163300	0.40879600

Energy = -403.67471738 a.u.

The xyz coordinates for the lowest energy structure of **TS1**

C	1.56858200	0.97558800	1.97564700

C	0.55837100	0.74646200	2.99535300
C	0.09831200	-0.54684900	3.24569400
C	0.62874200	-1.66683900	2.48681200
C	1.59509900	-1.44630300	1.50114700
C	2.07439600	-0.09974500	1.24027200
C	1.25641900	2.22379400	1.30720200
C	0.05213300	2.76937700	1.91026100
C	-0.37955300	1.85578500	2.95478800
C	-1.74052900	1.62813400	3.16426900
C	-1.31869500	-0.78433700	3.46511700
C	-0.45718700	-2.59451900	2.23724600
C	-0.53067900	-3.26558800	1.01530300
C	0.48010000	-3.03756100	-0.00130200
C	1.52514600	-2.15077900	0.23995800
C	2.04063800	-1.27094500	-0.82690100
C	2.30255400	0.03027900	-0.18259800
C	1.99663900	1.22627400	-0.82458000
C	1.46427400	2.34474900	-0.06786500
C	-0.89451000	3.41694900	1.11496400
C	-0.67577900	3.54638700	-0.31661300
C	0.47950900	3.02012400	-0.89536700
C	0.40343900	2.31979400	-2.16708700
C	1.34025400	1.21379300	-2.12631200
C	1.00682400	-0.00639300	-2.71990700
C	1.32185800	-1.25239400	-2.05668800
C	0.23527400	-2.17513500	-2.30078800
C	-0.17915000	-3.05978300	-1.30205600
C	-1.66224700	-2.05074000	2.84048300
C	-3.74607800	-2.10409300	-1.27365100
C	-3.95614200	-2.22930300	0.10106600
C	-4.48745500	-1.11007600	0.85988800
C	-4.78800000	0.09051200	0.21522600
C	-4.57078200	0.22102900	-1.21613000
C	-3.05170500	-0.62548300	-2.96571600
C	-2.11318700	-1.73427400	-2.92246200
C	-2.54370400	-2.64845100	-1.87831400
C	-1.59317500	-3.29544100	-1.08361400
C	-1.81167300	-3.42384000	0.34810600
C	-2.96883600	-2.90287500	0.92782100
C	-3.83029600	-1.09336200	2.15683900
C	-3.50103400	0.12327300	2.75729500
C	-3.81368400	1.37297500	2.08484600
C	-4.44369200	1.35658800	0.83910800
C	-4.01324400	2.27016700	-0.20547700

C	-4.09169900	1.56858700	-1.47631000
C	-3.12194900	1.78759500	-2.45516300
C	-2.59152900	0.66825800	-3.21545100
C	-0.75331100	-1.50454900	-3.13155300
C	-0.27518200	-0.15975100	-3.39111100
C	-1.17426800	0.90597300	-3.43243100
C	-0.82958400	2.17206700	-2.80815300
C	-2.03203400	2.71645700	-2.20382400
C	-1.95783500	3.39093500	-0.98353900
C	-2.96792300	3.16292100	0.03532700
C	-2.31080700	3.17954700	1.33229900
C	-2.72559200	2.30259700	2.33609100
C	-2.89245000	-2.20141500	2.19907700
C	-2.21974600	0.28068800	3.42454900
C	-4.06121800	-0.85375700	-1.94533500
C	5.83605900	-0.86316200	-0.12121400
C	5.79767000	0.19054000	-1.04495400
C	6.67679400	1.26865000	-0.94017400
C	7.62722100	1.33188100	0.08341200
C	7.65964400	0.27864300	1.01132900
C	6.78400500	-0.79529300	0.91479600
H	5.06986100	0.19534700	-1.84969300
H	6.61970400	2.07451800	-1.66832900
H	8.38494000	0.30432000	1.82198300
H	6.81519500	-1.60329200	1.63730200
C	4.92223600	-2.04414500	-0.19645900
N	4.92827000	-2.87743300	0.80866200
H	4.25851400	-3.63528500	0.63877900
C	4.06625900	-2.22340800	-1.34636400
H	4.23640200	-1.66785400	-2.26103200
H	3.60237900	-3.19589600	-1.47791900
C	8.59949900	2.48297500	0.18237600
H	8.68485900	2.84804500	1.21242300
H	9.60631100	2.18102200	-0.13547800
H	8.29314600	3.32256100	-0.44970300

Energy = -2689.84021959 a.u.

The xyz coordinates for the lowest energy structure of **E-1a**

C	1.62970500	1.33888100	1.68057900
C	0.68526300	1.20987400	2.77775800
C	0.29607800	-0.05422200	3.22069600
C	0.83412800	-1.24635700	2.58795900
C	1.72950100	-1.12571600	1.51686800
C	2.13681200	0.19165200	1.05448800

C	1.23352300	2.47043200	0.87711200
C	0.03884900	3.04845100	1.46683100
C	-0.29989900	2.26926100	2.64651600
C	-1.63795600	2.02025000	2.95857700
C	-1.09432400	-0.31273900	3.55156300
C	-0.21448500	-2.23659800	2.52872400
C	-0.31772900	-3.05870800	1.40293700
C	0.63273100	-2.93482700	0.31791700
C	1.65504100	-2.00481000	0.38509300
C	2.25594000	-1.32064800	-0.86402200
C	2.31729200	0.14192600	-0.36865200
C	1.90987500	1.21708600	-1.13889500
C	1.36163000	2.40124000	-0.51312400
C	-0.97516900	3.54393200	0.64498900
C	-0.83510200	3.48316700	-0.80200300
C	0.30902900	2.92148200	-1.36728100
C	0.20200400	2.05717800	-2.53236600
C	1.18658200	1.00991000	-2.40477200
C	0.86929200	-0.29630600	-2.80161500
C	1.27666300	-1.42693600	-2.02508700
C	0.22377400	-2.39566600	-2.06503400
C	-0.09769900	-3.16639400	-0.93961500
C	-1.41092900	-1.66445100	3.12069000
C	-3.69696600	-2.34860200	-0.83419000
C	-3.83040000	-2.29453900	0.55658500
C	-4.36993500	-1.10554300	1.18899300
C	-4.75832800	-0.01370300	0.41033300
C	-4.62162500	-0.06889200	-1.03615300
C	-3.16456600	-1.08485100	-2.74609500
C	-2.17631200	-2.14150600	-2.60934700
C	-2.50846700	-2.92250200	-1.42979500
C	-1.48099200	-3.41537000	-0.61192100
C	-1.62081000	-3.35284600	0.83470400
C	-2.77097800	-2.81069100	1.40691600
C	-3.64944700	-0.89006500	2.43506200
C	-3.34613200	0.40906900	2.85075000
C	-3.74704300	1.54334200	2.03776200
C	-4.43753800	1.33551200	0.84057500
C	-4.10291400	2.11584600	-0.33705500
C	-4.21592000	1.24872700	-1.49849100
C	-3.31125200	1.37121100	-2.55269500
C	-2.77541700	0.18029100	-3.18956900
C	-0.84264000	-1.88790000	-2.92173000
C	-0.44008300	-0.57773100	-3.38108300

C	-1.38290700	0.43864400	-3.51402800
C	-1.05989500	1.78808800	-3.08294200
C	-2.24819000	2.36333600	-2.48806600
C	-2.14148700	3.19711800	-1.37052800
C	-3.08558600	3.06983900	-0.27649200
C	-2.36471800	3.28594300	0.96936700
C	-2.69099500	2.53808100	2.10354900
C	-2.66330300	-1.94445600	2.57099700
C	-2.04307800	0.70275600	3.42072900
C	-4.10552600	-1.21194700	-1.64611000
C	5.71473600	-0.82197900	-0.12558800
C	5.74889000	0.24921500	-1.02910000
C	6.71966200	1.24703400	-0.92342800
C	7.68960800	1.21114300	0.08147700
C	7.65454600	0.13680000	0.98715500
C	6.69143000	-0.85617600	0.88910500
H	5.01342900	0.33146000	-1.82187700
H	6.71844300	2.06700500	-1.63761700
H	8.39707200	0.08358000	1.78071300
H	6.67157100	-1.68125700	1.59239400
C	4.70589700	-1.91865600	-0.19055600
N	4.75309400	-2.83835900	0.70320500
H	4.01233100	-3.53061100	0.55329300
C	3.64847400	-1.92099100	-1.29155600
H	3.98490900	-1.39197900	-2.18660500
H	3.46944400	-2.95972000	-1.59044000
C	8.74395100	2.28510100	0.19928600
H	8.69838500	2.78189600	1.17646600
H	9.75284700	1.86493800	0.10144400
H	8.62494900	3.05223500	-0.57215200

Energy = -2689.87617243 a.u.

The xyz coordinates for the lowest energy structure of **G-1a**

C	-2.09481800	0.01619900	-0.01370400
C	-1.38170500	-1.16326300	-0.26652300
C	0.01091000	-1.18012500	-0.25348000
C	0.74356700	-0.01202400	0.00362200
C	0.03228400	1.17159400	0.24665500
C	-1.36111600	1.18206200	0.24108300
H	-1.92477600	-2.08028600	-0.48423600
H	0.53701000	-2.10546600	-0.47571800
H	0.57340600	2.08899700	0.46233400
H	-1.88837500	2.11226000	0.44119400
C	2.24160000	-0.04517200	0.02757700

N	2.93605200	-1.05498400	0.52605300
H	2.29330600	-1.75834300	0.90900600
C	-3.60517200	0.02447300	0.00652300
H	-4.01956000	-0.71805000	-0.68377700
H	-3.99014700	-0.21278100	1.00747100
H	-4.00512500	1.00552900	-0.27059100
C	2.97001700	1.03466700	-0.51265800
H	4.05292400	1.00547700	-0.46964400
H	2.48556800	1.87708000	-0.99297100

Energy = -403.67440382 a.u.

The xyz coordinates for the lowest energy structure of **TS2**

C	-0.11891200	1.91733600	2.75819000
C	1.06112500	1.16507900	2.39050200
C	1.71477000	1.43964700	1.18756800
C	1.22661700	2.50299800	0.32400500
C	0.09576000	3.23649300	0.68618600
C	-0.59352800	2.93935000	1.92843900
C	-1.05840300	1.00324000	3.38934700
C	-0.45814000	-0.31932800	3.40543100
C	0.84981900	-0.22771900	2.78270900
C	1.32026200	-1.26380400	1.98770400
C	2.21632400	0.36795600	0.35360000
C	1.40901500	2.07569800	-1.04918000
C	0.45302800	2.39563900	-2.01404400
C	-0.72773300	3.15650600	-1.63885400
C	-0.90265800	3.56805900	-0.31715000
C	-2.21140700	3.47127600	0.30715400
C	-2.01890700	3.08087600	1.69480600
C	-2.92020500	2.20494800	2.30395300
C	-2.42859300	1.14504500	3.16857600
C	-1.25228100	-1.44984100	3.20369100
C	-2.67884800	-1.30321300	2.97128500
C	-3.25468000	-0.03189900	2.95251100
C	-4.25351600	0.29903800	1.95218300
C	-4.04542900	1.68110200	1.55017600
C	-4.22957500	2.05475700	0.21796100
C	-3.29314600	2.96767400	-0.41594700
C	-3.11100400	2.53901600	-1.79301600
C	-1.85419000	2.63140900	-2.39178000
C	2.01101400	0.75176300	-1.02656200
C	-1.55694800	-0.90401300	-3.41982300
C	-0.18789300	-1.04269500	-3.19028600
C	0.29948600	-2.09983800	-2.32219200

C	-0.60135600	-2.97989700	-1.71854100
C	-2.02731700	-2.83519500	-1.95478200
C	-3.67626300	-1.05901900	-2.41414600
C	-3.46791200	0.32306900	-2.81645700
C	-2.16008800	0.41832800	-3.44093200
C	-1.36694700	1.54852100	-3.23131300
C	0.05891100	1.40668700	-3.00026300
C	0.64036400	0.13409500	-2.97616500
C	1.42479600	-1.57982700	-1.56856300
C	1.61519900	-1.95838800	-0.24617300
C	0.66914400	-2.85025000	0.38437600
C	-0.41155600	-3.36643800	-0.33551200
C	-1.72122900	-3.46362000	0.28950600
C	-2.72031300	-3.13469900	-0.71256100
C	-3.85488100	-2.40460300	-0.35341400
C	-4.34290500	-1.34649500	-1.22117800
C	-3.93492200	1.36164100	-2.00948600
C	-4.62561200	1.06208700	-0.76665800
C	-4.82766600	-0.26447200	-0.38091000
C	-4.63725900	-0.65345400	1.00626200
C	-4.03677800	-1.97620100	1.02340200
C	-3.07667500	-2.29430000	1.98550900
C	-1.89548300	-3.05238800	1.61051200
C	-0.76813500	-2.52658000	2.36433500
C	0.48857900	-2.42271900	1.76191400
C	1.64203200	-0.19477100	-1.98449700
C	2.13372000	-1.00448600	0.76727800
C	-2.49565100	-1.81704000	-2.78682100
C	8.22302800	1.08930800	-0.12717600
C	6.95147300	1.52995000	0.25868000
C	5.88789500	0.63981700	0.39526300
C	6.05501800	-0.72792600	0.13193100
C	7.33058600	-1.17206200	-0.25368600
C	8.39043300	-0.27952200	-0.38146000
H	6.78810900	2.58765200	0.45248100
H	4.91061900	1.02153000	0.67798400
H	7.49641000	-2.23026000	-0.43514300
H	9.36866300	-0.65260500	-0.67682600
C	4.91854900	-1.68688400	0.26501500
N	3.98310200	-1.53084100	1.24821300
H	4.22048500	-0.73715700	1.84862000
C	9.38400600	2.04879800	-0.23721100
H	9.04095600	3.07493600	-0.40461000
H	9.98591100	2.05139700	0.68147200

H	10.05319500	1.77602000	-1.06052600
C	4.79750800	-2.76209700	-0.58801400
H	3.99862800	-3.48072600	-0.44990700
H	5.47421800	-2.90403400	-1.42228500

Energy = -2689.83431543 a.u.

The xyz coordinates for the lowest energy structure of **H-1a**

C	0.29011400	0.54650500	-3.33368100
C	-0.96670100	0.48568800	-2.62728800
C	-1.30953000	1.51097200	-1.73570100
C	-0.41888300	2.65376800	-1.56460700
C	0.78583600	2.71508000	-2.25936400
C	1.15353900	1.63922700	-3.16460800
C	0.83707000	-0.79948700	-3.39546900
C	-0.08630300	-1.69332500	-2.71827900
C	-1.20754200	-0.91384400	-2.23519600
C	-1.81391900	-1.22313300	-1.02981700
C	-1.92563500	1.22536000	-0.47861800
C	-0.47799500	3.04181000	-0.17318300
C	0.67043000	3.47924700	0.48111300
C	1.93157400	3.54372800	-0.23755500
C	1.98832900	3.16936700	-1.58153000
C	3.09930100	2.36852800	-2.06657100
C	2.58027400	1.42425700	-3.04500900
C	3.10331300	0.12942800	-3.10950200
C	2.21240300	-1.00436200	-3.29222400
C	0.40540600	-2.76429400	-1.96746600
C	1.83813400	-2.97499900	-1.85226700
C	2.72427400	-2.11245900	-2.50017300
C	3.92393800	-1.66008100	-1.82252200
C	4.15790800	-0.27374600	-2.19873100
C	4.65249400	0.63046500	-1.25694200
C	4.11082300	1.97783200	-1.18978700
C	4.05219500	2.36826600	0.20962400
C	2.98423700	3.13408300	0.67646300
C	-1.40530900	2.13496500	0.49353900
C	1.92973100	0.86050800	3.39319700
C	0.55536300	1.05968200	3.26805700
C	-0.33080900	-0.07526600	3.07837700
C	0.19477800	-1.36876700	3.03001600
C	1.62663300	-1.57834600	3.15366000
C	3.73578400	-0.42273600	2.61233200
C	3.97063800	0.96330700	2.23615500
C	2.85717100	1.75624500	2.72225500

C	2.36941800	2.82015300	1.95787200
C	0.94229300	3.03506400	1.83747600
C	0.04403200	2.16854700	2.47839200
C	-1.39415200	0.31844200	2.17742000
C	-1.90982000	-0.58373700	1.26328600
C	-1.31931700	-1.88701700	1.16956300
C	-0.31201000	-2.29876300	2.05043800
C	0.80044800	-3.09702700	1.56447100
C	2.00211500	-2.65104100	2.24719100
C	3.21395100	-2.59068900	1.55646800
C	4.09897700	-1.45456700	1.74269200
C	4.55782200	1.26154700	1.00524100
C	4.92781300	0.18938900	0.09862100
C	4.70472300	-1.14211600	0.46037600
C	4.19428900	-2.08489500	-0.51903900
C	3.27313700	-2.98082400	0.15714400
C	2.11783700	-3.41524900	-0.49543600
C	0.85702700	-3.47146400	0.22244600
C	-0.19754200	-3.06539200	-0.69146900
C	-1.26277800	-2.28001800	-0.23216300
C	-1.15595900	1.72506300	1.80917900
C	-2.48626400	-0.14906200	-0.11459700
C	2.47760900	-0.48602200	3.32995300
C	-8.94626500	0.58343600	-0.05814200
C	-7.88961900	1.36920700	0.41794900
C	-6.58909200	0.87167100	0.48071200
C	-6.29953600	-0.44081900	0.07442500
C	-7.35656700	-1.22756400	-0.40957500
C	-8.65369600	-0.72524400	-0.46678700
H	-8.08804000	2.38471000	0.75415800
H	-5.79199000	1.49416000	0.87648400
H	-7.15061200	-2.23631800	-0.75512800
H	-9.45354900	-1.35744900	-0.84656300
C	-4.91379900	-0.98711700	0.15317700
N	-3.94491400	-0.01914400	-0.14872200
H	-4.25557700	0.66499500	-0.82668500
C	-10.34908400	1.13523800	-0.15636800
H	-10.51526000	1.93881500	0.56878900
H	-10.54495200	1.55143700	-1.15387000
H	-11.09967500	0.35753000	0.02189200
C	-4.68607500	-2.25975100	0.53254100
H	-3.70526500	-2.71049300	0.55896700
H	-5.51453800	-2.87050500	0.87007000

Energy = -2689.85733891 a.u.