Electronic Supplementary Material (ESI) for Chemical Communications.

Palladium-catalyzed synthesis of [60]fullerene-fused benzofurans via heteroannulation of phenols

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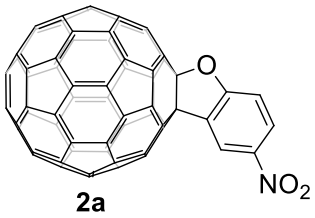
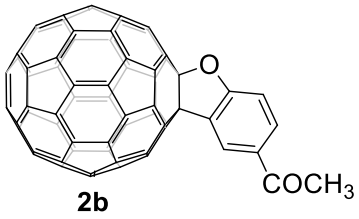
Synthesis and spectral data of product 2a



2a

C_{60} (36.2 mg, 0.05 mmol), 4-nitrophenol (35.1 mg, 0.25 mmol), $K_2S_2O_8$ (67.5 mg, 0.25 mmol), NaOAc (12.0 mg, 0.15 mmol), 1,10-phenanthroline (3.8 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 10 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was separated by a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (3.1 mg, 9%), subsequently with carbon disulfide/dichloromethane (5:1 v/v) to afford **2a** (27.3 mg, 63%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 8.77 (d, J = 2.4 Hz, 1H), 8.46 (dd, J = 8.8, 2.4 Hz, 1H), 7.55 (d, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) (all 2C unless indicated) δ 161.76 (1C, aryl C), 148.62, 147.30 (1C), 146.55 (1C), 145.52, 145.47, 145.36, 145.23, 145.15, 144.66, 144.45, 144.36, 144.25, 144.06, 143.72, 143.54, 143.40, 142.94, 142.62 (1C, aryl *C*), 142.05, 141.93, 141.88, 141.64, 141.45, 141.42, 141.33, 141.04, 140.71, 140.05, 139.02, 136.73, 134.99, 127.61 (1C, aryl *C*), 126.79 (1C, aryl *C*), 121.42 (1C, aryl *C*), 111.38 (1C, aryl *C*), 103.98 (1C, sp^3-*C* of C_{60}), 68.95 (1C, sp^3-*C* of C_{60}); FT-IR (KBr) ν 1591, 1515, 1470, 1334, 1269, 1187, 1126, 1070, 951, 918, 825, 743, 701, 564, 528 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 256 (4.59), 318 (4.27), 430 (2.85) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{66}H_3NO_3$ $[M]^-$ 857.0113, found 857.0126.

Synthesis and spectral data of product 2b

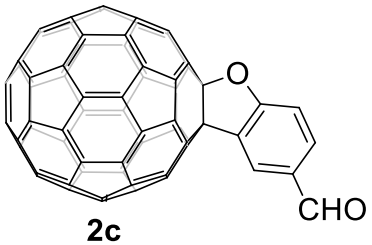


2b

C_{60} (36.0 mg, 0.05 mmol), 4-hydroxyacetophenone (34.5 mg, 0.25 mmol), $K_2S_2O_8$ (67.9 mg, 0.25 mmol), NaOAc (12.7 mg, 0.15 mmol), 1,10-phenanthroline (4.0 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was separated a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (5.3 mg, 15%), subsequently with carbon disulfide/dichloromethane (1:1 v/v) to afford **2b** (27.1 mg, 63%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 8.47 (d, J = 1.8 Hz, 1H), 8.15 (dd, J = 8.6, 1.8 Hz, 1H), 7.43 (d, J =

8.6 Hz, 1H), 2.60 (s, 3H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent) (all 2C unless indicated) δ 191.95 (1C, *C*=O), 160.20 (1C, aryl *C*), 149.28, 147.07 (1C), 146.32 (1C), 145.28, 145.21, 145.12, 145.00, 144.92, 144.35, 144.34, 144.14 (4C), 144.01, 143.74, 143.58, 143.38, 143.24, 141.85, 141.70, 141.65, 141.58, 141.25, 141.21, 141.13, 140.82, 140.61, 139.80, 138.77, 136.51, 134.64, 131.80 (1C, aryl *C*), 131.40 (1C, aryl *C*), 126.39 (1C, aryl *C*), 125.46 (1C, aryl *C*), 110.79 (1C, aryl *C*), 102.87 (1C, sp^3-*C* of C_{60}), 69.34 (1C, sp^3-*C* of C_{60}), 25.45 (1C, *C*H$_3$); FT-IR (KBr) *v* 1677, 1593, 1510, 1482, 1424, 1351, 1264, 1184, 971, 918, 815, 769, 568, 528 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 257 (4.46), 317 (4.00), 428 (2.30) nm; HRMS (MALDI-TOF-MS, negative mode), *m/z* calcd for $C_{68}H_6O_2$ [M]$^-$ 854.0368, found 854.0385.

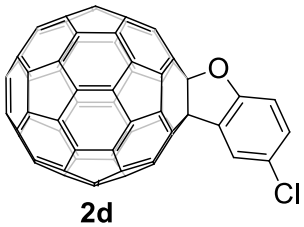
Synthesis and spectral data of product 2c



2c

C_{60} (36.0 mg, 0.05 mmol), 4-hydroxybenzaldehyde (30.4 mg, 0.25 mmol), $K_2S_2O_8$ (69.4 mg, 0.25 mmol), NaOAc (12.5 mg, 0.15 mmol), 1,10-phenanthroline (4.1 mg, 0.02 mmol), and Pd(OAc)$_2$ (1.0 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 10 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was separated by a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (12.3 mg, 34%), subsequently with carbon disulfide/dichloromethane (5:1 v/v) to afford **2c** (24.5 mg, 58%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 9.99 (s, 1H), 8.44 (d, *J* = 1.6 Hz, 1H), 8.07 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent) (all 2C unless indicated) δ 186.99 (1C, *C*=O), 161.43 (1C, aryl *C*), 149.22, 147.21 (1C), 146.46 (1C), 145.43, 145.37, 145.26, 145.15, 145.06, 144.50, 144.46, 144.28, 144.16, 144.13, 143.83, 143.51, 143.45, 143.37, 141.99, 141.85, 141.80, 141.69, 141.39, 141.36, 141.27, 140.96, 140.72, 139.99, 138.92, 136.67, 134.81, 133.10 (1C, aryl *C*), 131.70 (1C, aryl *C*), 127.31 (1C, aryl *C*), 126.27 (1C, aryl *C*), 111.53 (1C, aryl *C*), 103.21 (1C, sp^3-*C* of C_{60}), 69.17 (1C, sp^3-*C* of C_{60}); FT-IR (KBr) *v* 1691, 1594, 1482, 1433, 1267, 1180, 1143, 923, 817, 530 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 256 (4.55), 315 (4.13), 428 (2.60) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{67}H_4O_2$ [M]$^-$ 840.0211, found 840.0225.

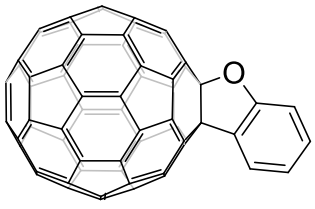
Synthesis and spectral data of product 2d



2d

C_{60} (36.4 mg, 0.05 mmol), *p*-chlorophenol (32.7 mg, 0.25 mmol), $K_2S_2O_8$ (68.9 mg, 0.25 mmol), NaOAc (12.0 mg, 0.15 mmol), 1,10-phenanthroline (3.9 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was dissolved in toluene and subjected to semi-preparative HPLC equipped with a Buckyprep column (eluent: toluene) to give unreacted C_{60} (2.7 mg, 7%) and **2d** (24.9 mg, 58%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 7.85 (d, J = 2.0 Hz, 1H), 7.46 (dd, J = 8.7, 2.0 Hz, 1H), 7.32 (d, J = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) (all 2C unless indicated) δ 155.21 (1C, aryl *C*), 149.00, 147.14 (1C), 146.40 (1C), 145.32, 145.26, 145.19, 145.07, 144.97, 144.43, 144.41, 144.19, 144.10, 144.00, 143.96, 143.83, 143.42, 143.35, 141.92, 141.75, 141.72, 141.62, 141.32, 141.29, 141.17, 140.83, 140.74, 139.88, 138.84, 136.43, 134.88, 129.92 (1C, aryl *C*), 127.32 (1C, aryl *C*), 126.53 (1C, aryl *C*), 124.89 (1C, aryl *C*), 112.19 (1C, aryl *C*), 102.40 (1C, sp^3-*C* of C_{60}), 69.72 (1C, sp^3-*C* of C_{60}); FT-IR (KBr) ν 1592, 1495, 1291, 1193, 1155, 1085, 1027, 987, 957, 820, 526 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 258 (4.55), 328 (4.05), 428 (2.92) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{66}H_3ClO$ $[M]^-$ 845.9872, found 845.9885.

Synthesis and spectral data of product 2e

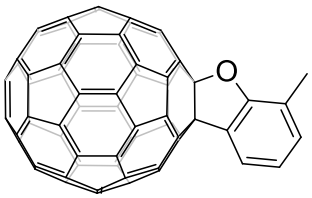


2e

C_{60} (36.3 mg, 0.05 mmol), phenol (24.3 mg, 0.25 mmol), $K_2S_2O_8$ (68.2 mg, 0.25 mmol), NaOAc (12.0 mg, 0.15 mmol), 1,10-phenanthroline (4.1 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.2 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was dissolved in toluene and subjected to semi-preparative HPLC equipped with a Buckyprep column (eluent: toluene) to give unreacted C_{60} (11.4 mg, 31%) and **2e** (18.5 mg, 43%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 7.85 (d, J = 7.6 Hz, 1H), 7.50 (t, J = 7.2 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) (all 2C unless

indicated) δ 156.55 (1C, aryl *C*), 149.74, 147.13 (1C), 146.40 (1C), 145.32, 145.24, 145.18, 145.07, 144.96, 144.53 (4C), 144.31, 144.23, 144.20, 144.08, 144.04, 143.47, 143.40, 142.08, 141.95, 141.76 (4C), 141.72, 141.35, 141.32, 141.19, 140.83 (4C), 139.85, 138.84, 136.49, 134.78, 129.97 (1C, aryl *C*), 125.28 (1C, aryl *C*), 124.81 (1C, aryl *C*), 121.79 (1C, aryl *C*), 111.23 (1C, aryl *C*), 101.74 (1C, sp^3-*C* of C_{60}), 70.19 (1C, sp^3-*C* of C_{60}); FT-IR (KBr) *v* 1463, 1424, 1210, 1106, 1077, 948, 928, 861, 762, 650, 564, 526 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 255 (4.60), 315 (4.16), 426 (3.18) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{66}H_4O$ $[M]^-$ 862.0262, found 862.0276.

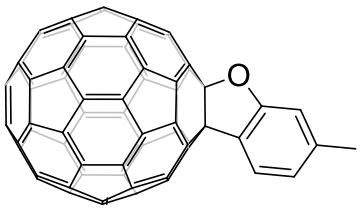
Synthesis and spectral data of product 2f



2f

C_{60} (35.8 mg, 0.05 mmol), o-cresol (26 µL, 0.25 mmol), $K_2S_2O_8$ (69.0 mg, 0.25 mmol), NaOAc (12.3 mg, 0.15 mmol), 1,10-phenanthroline (4.3 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.2 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was dissolved in toluene and subjected to semi-preparative HPLC equipped with a Buckyprep column (eluent: toluene) to give unreacted C_{60} (5.8 mg, 16%) and **2f** (22.9 mg, 56%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 7.67-7.64 (m, 1H), 7.30-7.26 (m, 1H), 7.11 (t, J = 7.4 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) (all 2C unless indicated) δ 154.83 (1C, aryl *C*), 149.85, 147.12 (1C), 146.37 (1C), 145.30, 145.21, 145.14, 145.04, 144.94, 144.74, 144.51, 144.27, 144.26, 144.18, 144.06 (4C), 143.47, 143.39, 141.94, 141.77, 141.73, 141.70, 141.34, 141.30, 141.17, 140.84, 140.81, 139.85, 138.80, 136.47, 134.69, 130.97 (1C, aryl *C*), 124.41 (1C, aryl *C*), 122.20 (1C, aryl *C*), 121.93 (1C, aryl *C*), 121.30 (1C, aryl *C*), 101.44 (1C, sp^3-*C* of C_{60}), 70.55 (1C, sp^3-*C* of C_{60}), 15.31 (1C, *C*H_3); FT-IR (KBr) *v* 1558, 1506, 1463, 1262, 1210, 1106, 948, 927, 861, 760, 648, 594, 562, 526 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 255 (4.59), 315 (4.12), 426 (2.94) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{67}H_6O$ $[M]^-$ 826.0419, found 826.0432.

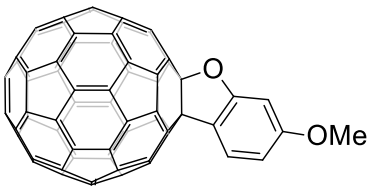
Synthesis and spectral data of product 2g



2g

C_{60} (35.8 mg, 0.05 mmol), m-cresol (27 μL, 0.25 mmol), $K_2S_2O_8$ (67.6 mg, 0.25 mmol), NaOAc (13.4 mg, 0.15 mmol), 1,10-phenanthroline (4.0 mg, 0.02 mmol), and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was dissolved in toluene and subjected to semi-preparative HPLC equipped with a Buckyprep column (eluent: toluene) to give unreacted C_{60} (20.4 mg, 57%) and **2g** (13.3 mg, 32%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 7.78 (d, J = 7.6 Hz, 1H),7.23 (s, 1H), 7.11 (d, J = 7.6 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) (all 2C unless indicated) δ 156.78 (1C, aryl *C*), 149.92, 147.11 (1C), 146.37 (1C), 145.29, 145.20, 145.13, 145.04, 144.93, 144.69, 144.52, 144.25, 144.21, 144.17, 144.04, 144.03, 143.46, 143.37, 141.92, 141.79, 141.72, 141.69, 141.32, 141.28, 141.15, 140.80 (4C), 140.06 (1C, aryl *C*), 139.81, 138.78, 136.47, 134.65, 124.33 (1C, aryl *C*), 122.61 (1C, aryl *C*), 122.52 (1C, aryl *C*), 111.66 (1C, aryl *C*), 101.97 (1C, sp^3-*C* of C_{60}), 70.05 (1C, sp^3-*C* of C_{60}), 21.19 (1C, *C*H_3); FT-IR (KBr) ν 1558, 1506, 1452, 1273, 1139, 1085, 985, 951, 949, 883, 802, 782, 622, 594, 525 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 255 (4.52), 315 (4.05), 428 (2.80) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{67}H_6O$ $[M]^-$ 826.0419, found 826.0435.

Synthesis and spectral data of product 2h

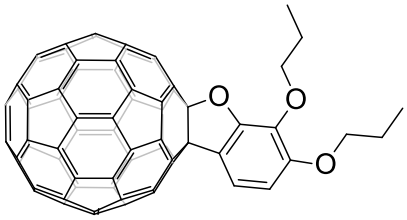


2h

C_{60} (36.1 mg, 0.05 mmol), 3-methoxyphenol (35 μL, 0.25 mmol), $K_2S_2O_8$ (67.4 mg, 0.25 mmol), NaOAc (12.4 mg, 0.15 mmol), 1,10-phenanthroline (4.4 mg, 0.02 mmol) and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 12 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was separated by a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (5.8 mg, 16%), subsequent elution with carbon disulfide/dichloromethane (5:1 v/v) affording **2h** (21.2 mg, 50%). ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 7.69 (d, J = 8.3 Hz, 1H), 6.88 (d, J = 2.0 Hz, 1H), 6.74 (dd, J = 8.3, 2.0 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as

relaxation reagent) (all 2C unless indicated) δ 161.13 (1C, aryl *C*), 157.83 (1C, aryl *C*), 149.86, 147.05 (1C), 146.32 (1C), 145.24, 145.14, 145.05, 144.98, 144.87, 144.59, 144.47, 144.17, 144.11, 144.09, 143.96, 143.92, 143.42, 143.31, 141.86, 141.80, 141.66, 141.63, 141.27, 141.23, 141.08, 140.76, 140.71, 139.74, 138.69, 136.54, 134.49, 124.79 (1C, aryl *C*), 116.98 (1C, aryl *C*), 108.20 (1C, aryl *C*), 102.53 (1C, aryl *C*), 96.85 (1C, sp^3-*C* of C_{60}), 69.67 (1C, sp^3-*C* of C_{60}), 54.79 (1C, *C*H_3); FT-IR (KBr) *v* 1619, 1589, 1499, 1431, 1287, 1194, 1152, 1084, 1028, 989, 954, 879, 819, 623, 564, 524 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 255 (4.56), 315 (4.07), 428 (2.34) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{67}H_6O_2$ $[M]^-$ 842.0368, found 842.0381.

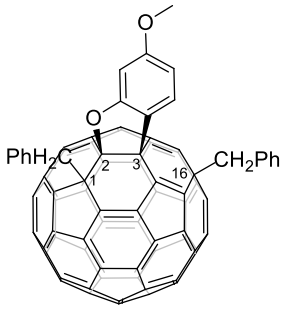
Synthesis and spectral data of product 2i



2i

C_{60} (36.1 mg, 0.05 mmol), 2,3-propoxyphenol (53.6 mg, 0.25 mmol), $K_2S_2O_8$ (67.6 mg, 0.25 mmol), NaOAc (12.3 mg, 0.15 mmol), 1,10-phenanthroline (4.2 mg, 0.02 mmol) and $Pd(OAc)_2$ (1.1 mg, 0.005 mmol) were dissolved in *o*-dichlorobenzene (3 mL). The reaction mixture was stirred at 140 °C for 15 h and then was filtered through a silica gel plug in order to remove the insoluble material. After evaporation in vacuo, the residue was separated by a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (13.3 mg, 37%), subsequently with carbon disulfide/dichloromethane (5:1 v/v) to afford **2i** (21.7 mg, 44%). ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 7.46 (d, *J* = 8.4 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 4.39 (t, *J* = 6.6 Hz, 2H), 4.10 (t, *J* = 6.4 Hz, 2H), 1.88-2.03 (m, 4H), 1.18 (t, *J* = 7.4 Hz, 3H), 1.15 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) (all 2C unless indicated) δ 153.97 (1C, aryl *C*), 151.00, 150.28 (1C, aryl *C*), 148.26 (1C), 147.51 (1C), 146.42, 146.35, 146.23, 146.15, 146.03, 145.85, 145.64, 145.30, 145.28, 145.23, 145.20, 145.13, 144.56, 144.48, 142.98, 142.89, 142.80, 142.78, 142.44, 142.40, 142.22, 141.88, 141.81, 140.86, 139.79, 137.83, 135.72, 134.29 (1C, aryl *C*), 120.78 (1C, aryl *C*), 119.16 (1C, aryl *C*), 108.46 (1C, aryl *C*), 103.93 (1C, sp^3-*C* of C_{60}), 75.28 (1C, *C*H_2), 71.44 (1C, *C*H_2), 71.01 (1C, sp^3-*C* of C_{60}), 23.78 (1C, *C*H_2), 23.00 (1C, *C*H_2), 10.82 (1C, *C*H_3), 10.74 (1C, *C*H_3); FT-IR (KBr) *v* 1592, 1496, 1455, 1385, 1325, 1281, 1255, 1233, 1182, 1161, 1108, 1081, 1038, 1023, 964, 948, 920, 848, 779, 639, 576, 526 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 255 (4.57), 315 (4.18), 428 (3.08) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{75}H_{22}O_4$ $[M]^-$ 986.1518, found 986.1529.

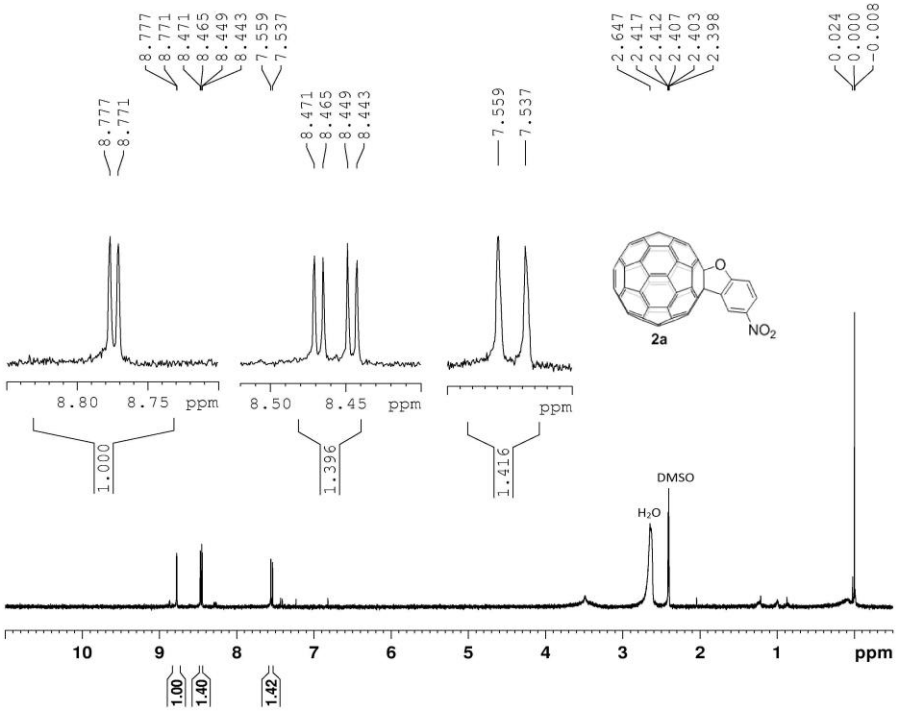
Synthesis and spectral data of product 3h



3h

25.3 mg (0.030 mmol) of **2h** was electroreduced at -1.0V vs SCE in 30 mL of ODCB containing 0.1M TBAP under argon atmosphere at room temperature. The electrolysis was terminated when the theoretical number of coulombs required for a full conversion of **2h** to $\mathbf{2h}^{2-}$ was reached. Then, the dianionic **2h** was reacted with benzyl bromide (72.0 μL, 0.60 mmol) in the presence of NaH (23.9 mg, 0.60 mmol) at 25 °C for 2 h and the reaction mixture was filtered through a silica gel flash chromatography to remove the electrolyte. After evaporation in vacuo, the residue was separated by a silica gel column with carbon disulfide as the eluent to give unreacted **2h** (7.5 mg, 30%), subsequently with carbon disulfide/dichloromethane (3:1 v/v) to afford **3h** (9.4 mg, 31%). ^{1}H NMR (400 MHz, CS_2/acetone-d_6) δ 7.09 (d, J = 8.2 Hz, 1H), 6.65 (dd, J = 7.6, 1.6 Hz, 2H), 6.57-6.49 (m, 3H), 6.41-6.33 (m, 5H), 6.11 (dd, J = 8.2, 2.4 Hz, 1H), 6.06 (d, J = 2.4 Hz, 1H), 3.81 (d, J = 12.8 Hz, 1H), 3.59 (d, J = 12.8 Hz, 1H), 3.38 (d, J = 12.8 Hz, 1H), 3.23 (s, 3H), 3.20 (d, J = 12.8 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/acetone-d_6, all 1C unless indicated) δ 162.46, 161.96, 156.21, 154.97, 152.46, 151.11, 150.43, 150.34, 148.99, 148.82, 148.46, 148.42, 148.26, 148.25, 147.47, 147.36, 147.08, 147.02, 146.92, 146.89 (2C), 146.77, 146.54, 146.30, 146.11, 146.08, 145.77, 145.67, 145.64 (2C), 145.17, 145.12, 144.78 (3C), 144.71, 144.66, 144.63, 144.23, 143.85, 143.69, 143.61, 143.41, 142.95, 142.59, 142.50, 141.65, 141.53, 141.43, 141.17, 141.12, 140.01, 138.97, 138.91, 138.74, 137.80, 136.50, 135.75, 134.51, 133.73, 132.00 (2C), 130.86 (2C), 128.75 (2C), 128.33 (2C), 127.80, 127.39, 125.47, 120.86, 109.21, 102.86 (sp^3-*C* of C_{60}), 97.46, 64.92 (sp^3-*C* of C_{60}), 62.89 (sp^3-*C* of C_{60}), 59.19 (sp^3-*C* of C_{60}), 55.71, 50.24, 46.24; FT-IR (KBr) ν 2922, 2850, 1624, 1498, 1444, 1157, 1025，947，700, 530 cm^{-1}; UV–vis ($CHCl_3$) λ_{max} (log ε) 252 (4.93), 315 (4.52), 403.5 (3.87), 703.5 (2.30) nm; HRMS (MALDI-TOF-MS, negative mode) *m/z* calcd for $C_{81}H_{20}O_2$ $[M]^-$ 1024.1463, found 1024.1472.

^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2a

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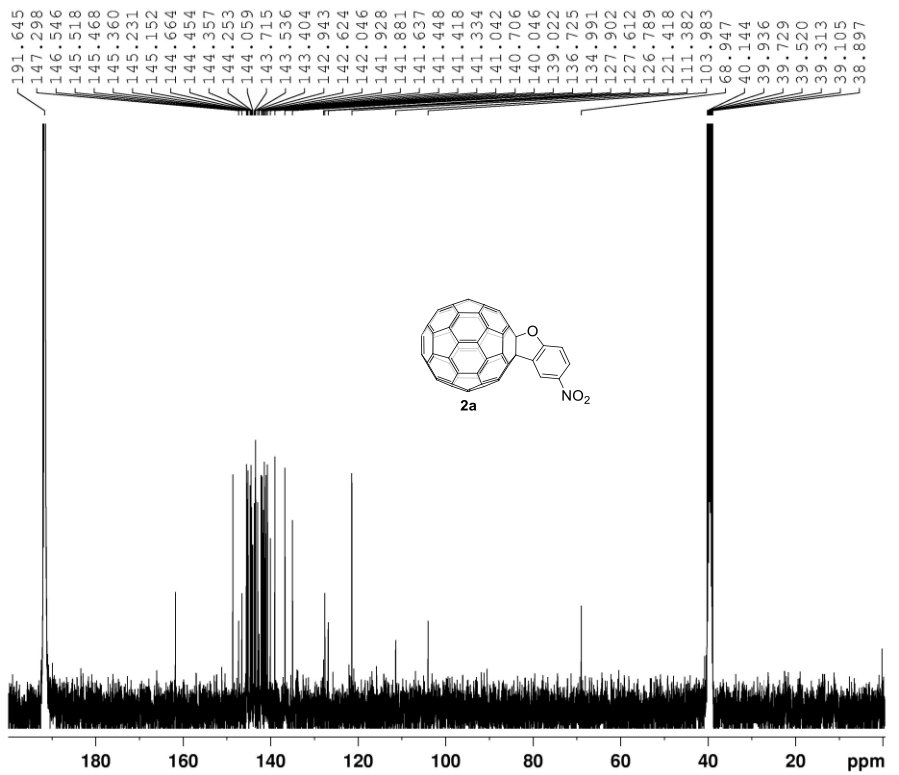
PROCNO                      1
Date_              20140402
Time                    8.20
INSTRUM                av400
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       64
DS                        2
SWH                8250.825 Hz
FIDRES             0.125898 Hz
AQ                 3.9715922 sec
RG                       362
DW                    60.600 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.80 usec
PL1                     -2.00 dB
SFO1               400.1324710 MHz
SI                       32768
SF                 400.1300415 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2a

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NAME          105L13_1fe131218_c
EXPNO                       2
PROCNO                      1
Date_              20131219
Time                   17.35
INSTRUM                av400
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                    16384
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3632196 sec
RG                       812.7
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        16

======== CHANNEL f1 ========
NUC1                      13C
P1                      13.30 usec
PL1                      2.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2              400.1316005 MHz
SI                       32768
SF                100.6128761 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.00
```
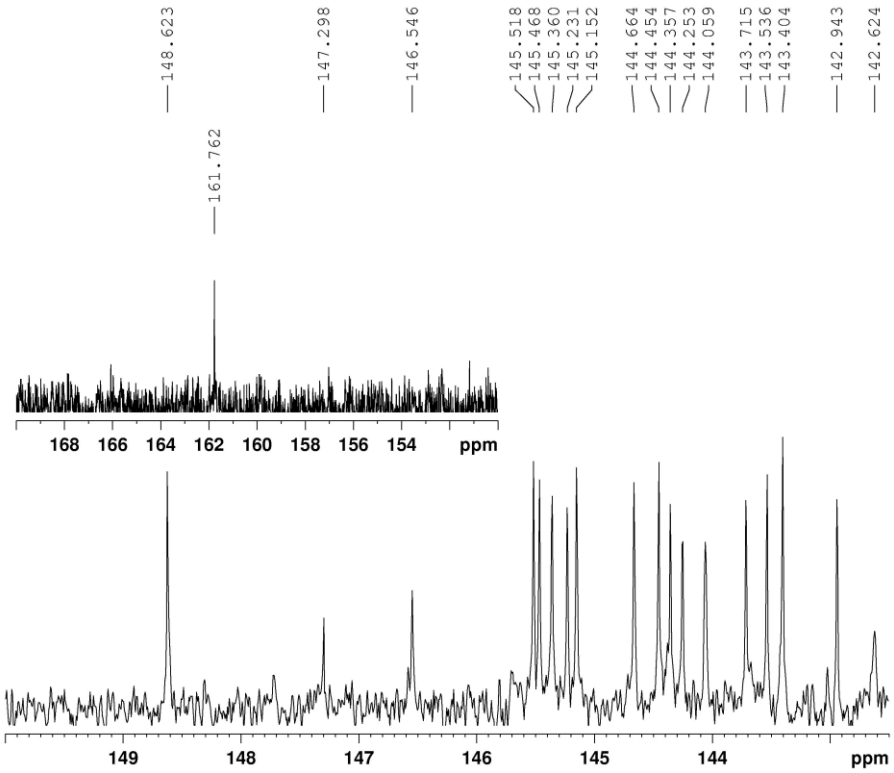

Expanded ^{13}C NMR (100MHz, CS_2/DMSO-d_6) compound 2a

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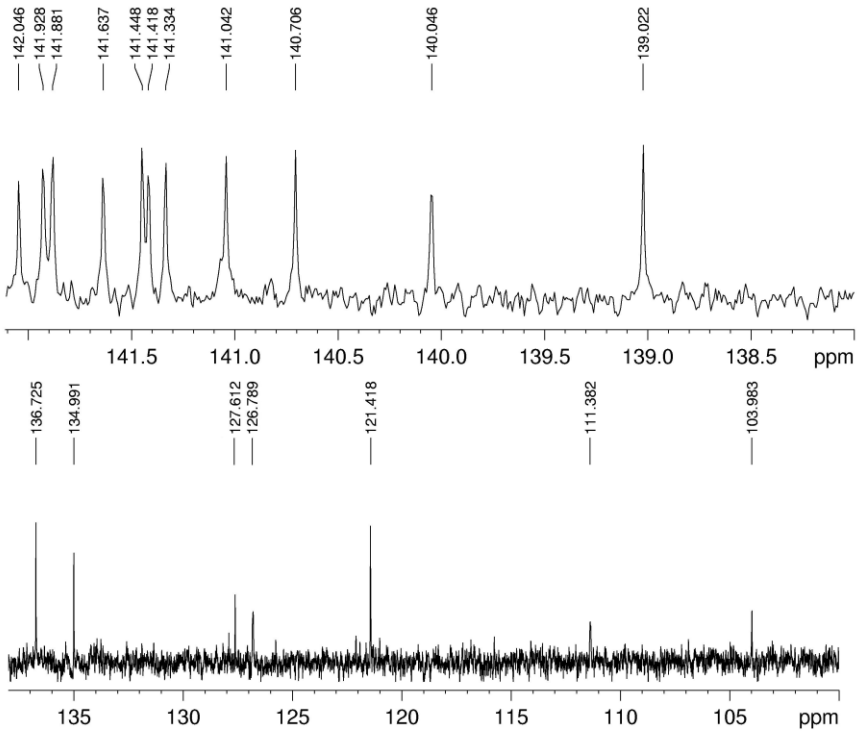
NAME          105L13_1fe131218_c
EXPNO                          2
PROCNO                         1
Date_                   20131219
Time                       17.35
INSTRUM                   av400
PROBHD        5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                        16384
DS                            4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                   1.3632196 sec
RG                        812.7
DW                       20.800 usec
DE                        6.50 usec
TE                       300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           16

======== CHANNEL f1 ========
NUC1                         13C
P1                        13.30 usec
PL1                        2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      13.92 dB
PL13                      13.92 dB
SFO2                400.1316005 MHz
SI                        32768
SF                  100.6128761 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2a

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NAME          105L13_1fe131218_c
EXPNO                          2
PROCNO                         1
Date_                   20131219
Time                       17.35
INSTRUM                   av400
PROBHD        5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                        16384
DS                            4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                   1.3632196 sec
RG                        812.7
DW                       20.800 usec
DE                        6.50 usec
TE                       300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           16

======== CHANNEL f1 ========
NUC1                         13C
P1                        13.30 usec
PL1                        2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      13.92 dB
PL13                      13.92 dB
SFO2                400.1316005 MHz
SI                        32768
SF                  100.6128761 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```
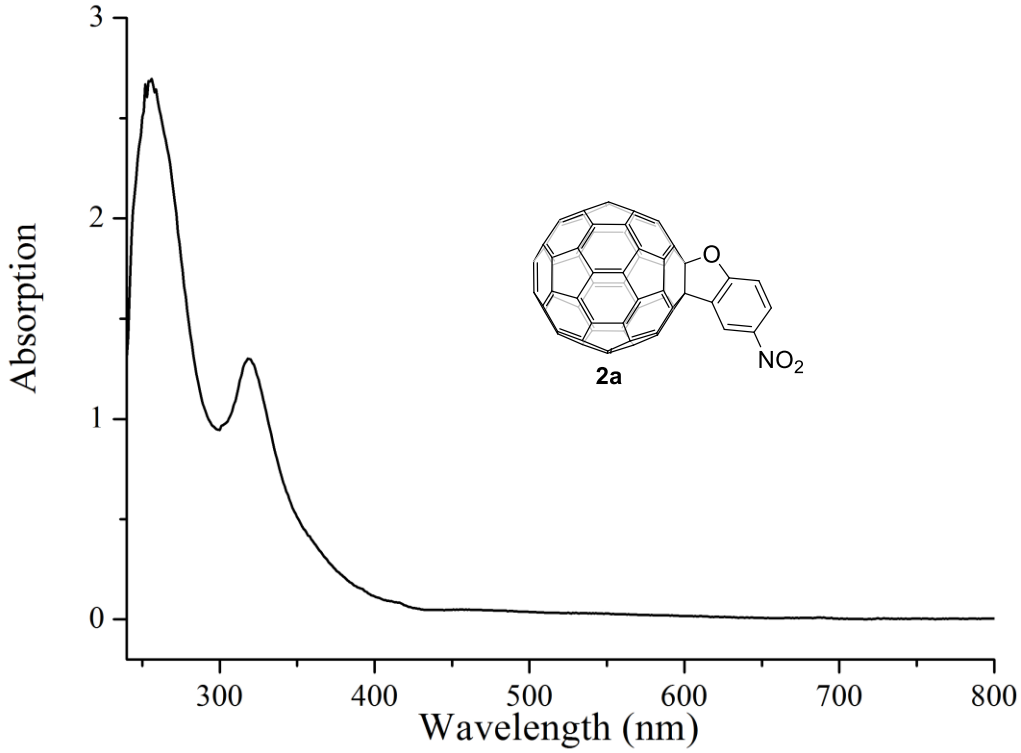
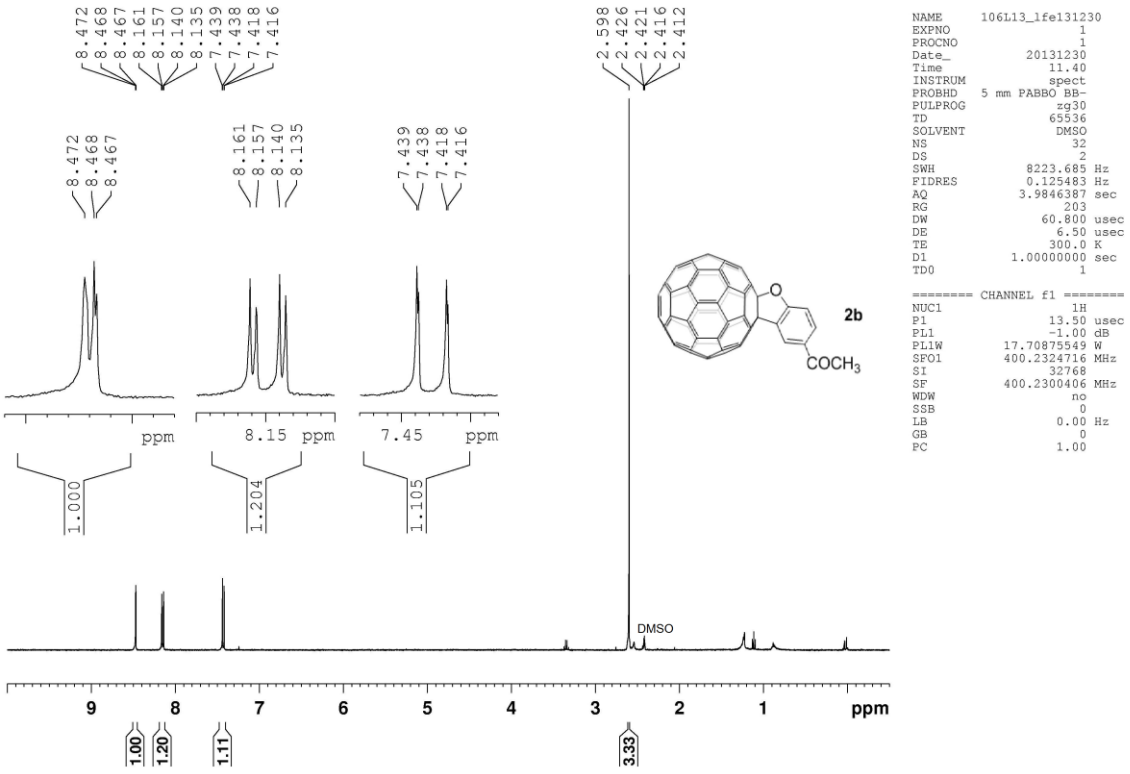

UV-vis absorption of compound 2a

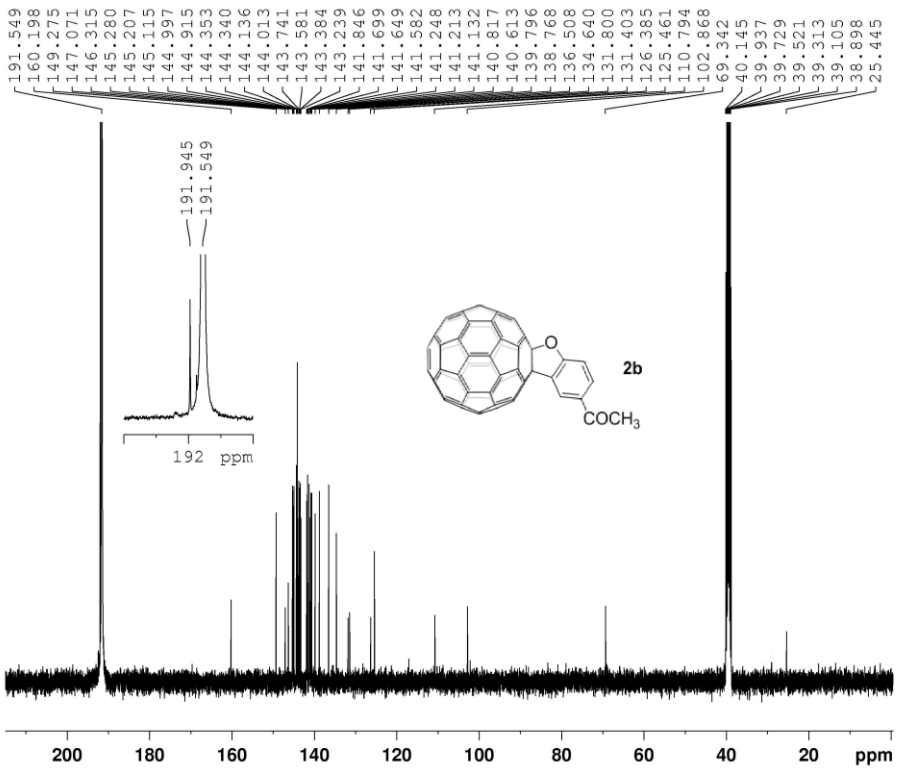


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2b



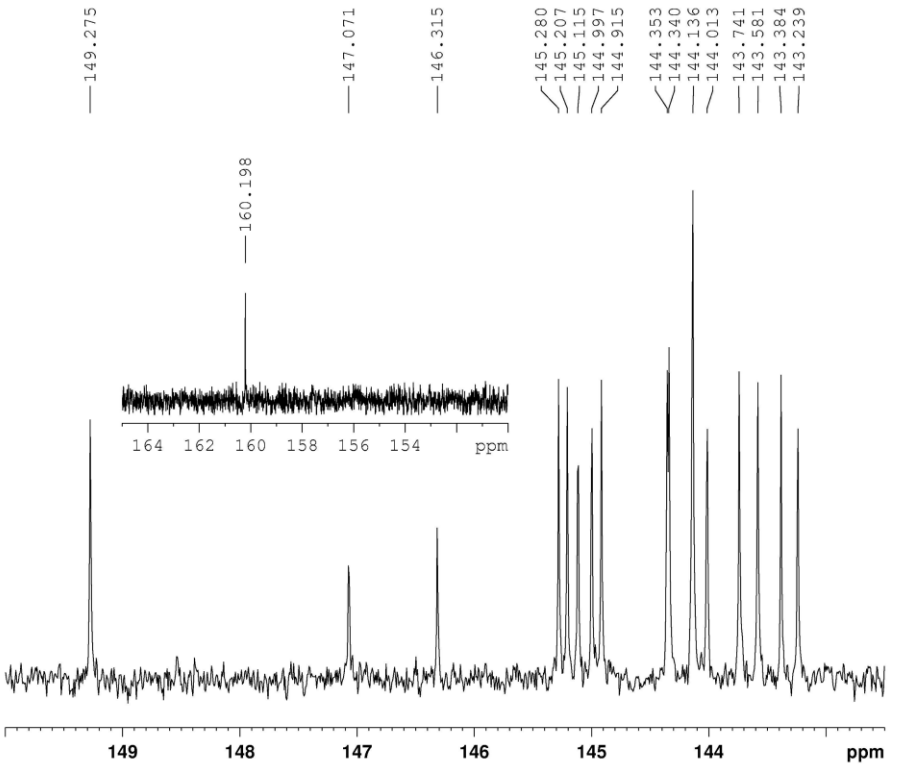

```
NAME          106L13_1fe131230
EXPNO                       1
PROCNO                      1
Date_                20131230
Time                    11.40
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        32
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                        203
DW                     60.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.50 usec
PL1                     -1.00 dB
PL1W               17.70875549 W
SFO1               400.2324716 MHz
SI                       32768
SF                 400.2300406 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2b



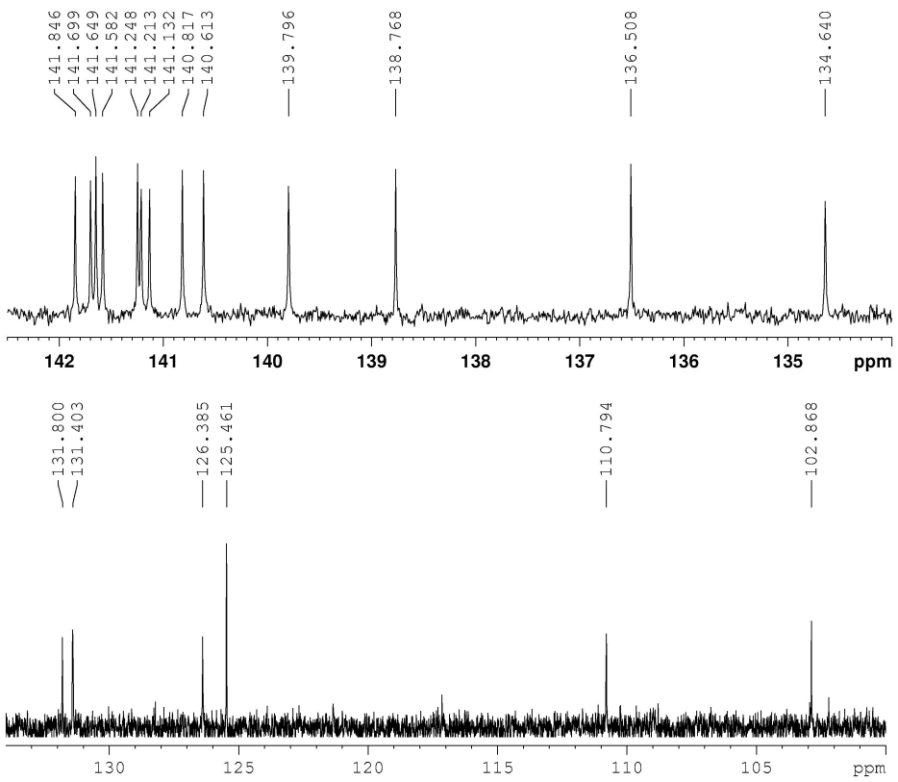

```
NAME          105L13_1fe131231
EXPNO                       2
PROCNO                      1
Date_                20131231
Time                    17.50
INSTRUM                 av400
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3632196 sec
RG                       812.7
DW                      20.800 usec
DE                       6.50 usec
TE                      300.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                      13.30 usec
PL1                      2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6128942 MHz
WDW                         EM
SSB                          0
LB                       0.50 Hz
GB                           0
PC                       1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2b



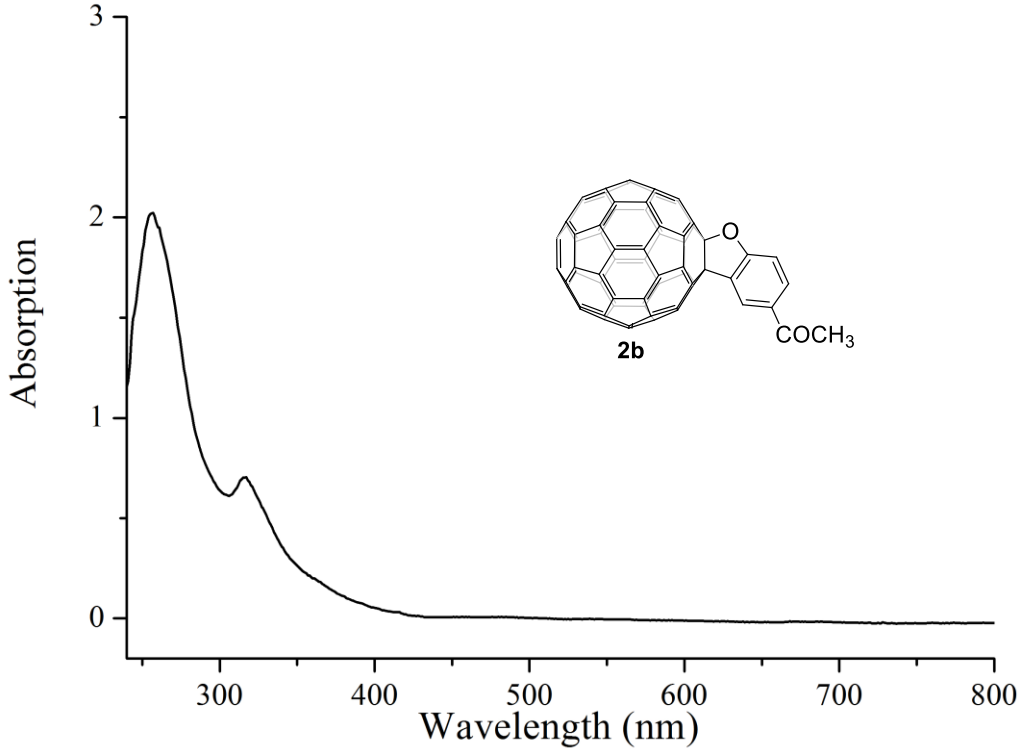

```
NAME          105L13_1fe131231
EXPNO                       2
PROCNO                      1
Date_                20131231
Time                    17.50
INSTRUM                 av400
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3632196 sec
RG                       812.7
DW                      20.800 usec
DE                       6.50 usec
TE                      300.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                      13.30 usec
PL1                      2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6128942 MHz
WDW                         EM
SSB                          0
LB                       0.50 Hz
GB                           0
PC                       1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2b

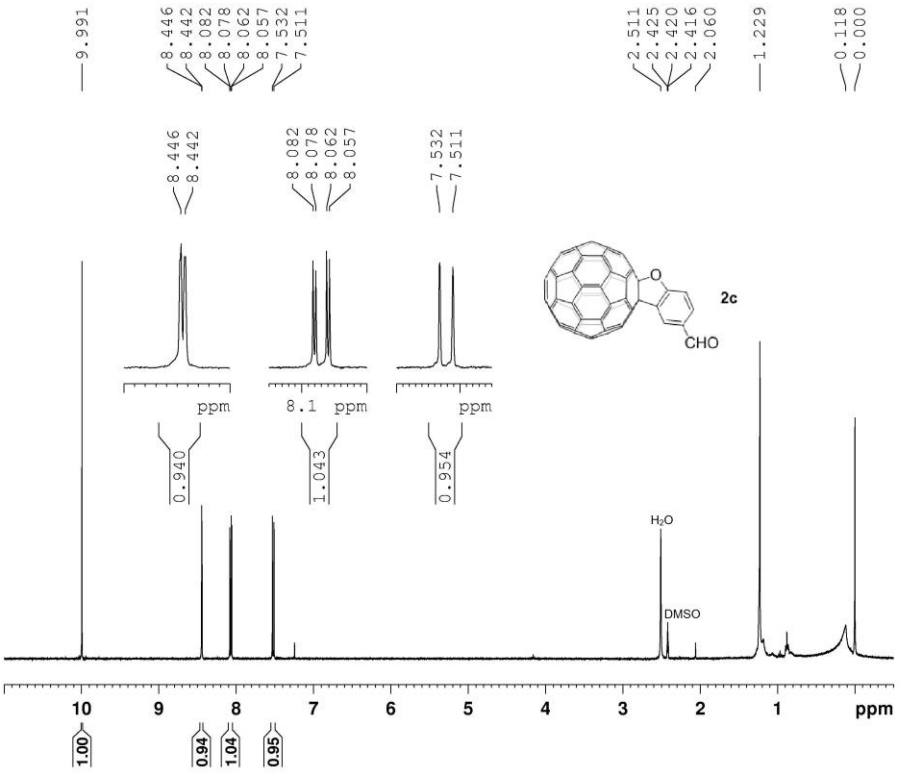



```
NAME          105L13_1fe131231
EXPNO                       2
PROCNO                      1
Date_                20131231
Time                    17.50
INSTRUM                 av400
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                      16384
DS                          4
SWH                 24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3632196 sec
RG                      812.7
DW                     20.800 usec
DE                      6.50 usec
TE                     300.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        16

======== CHANNEL f1 ========
NUC1                       13C
P1                      13.30 usec
PL1                      2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6128942 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```

UV-vis absorption of compound 2b

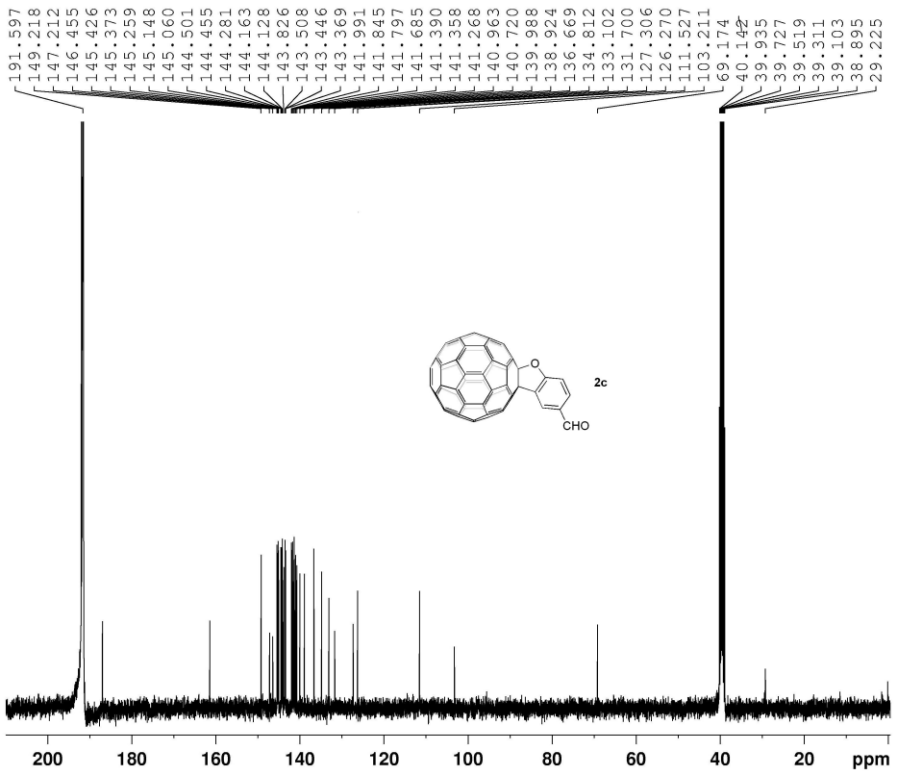


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2c



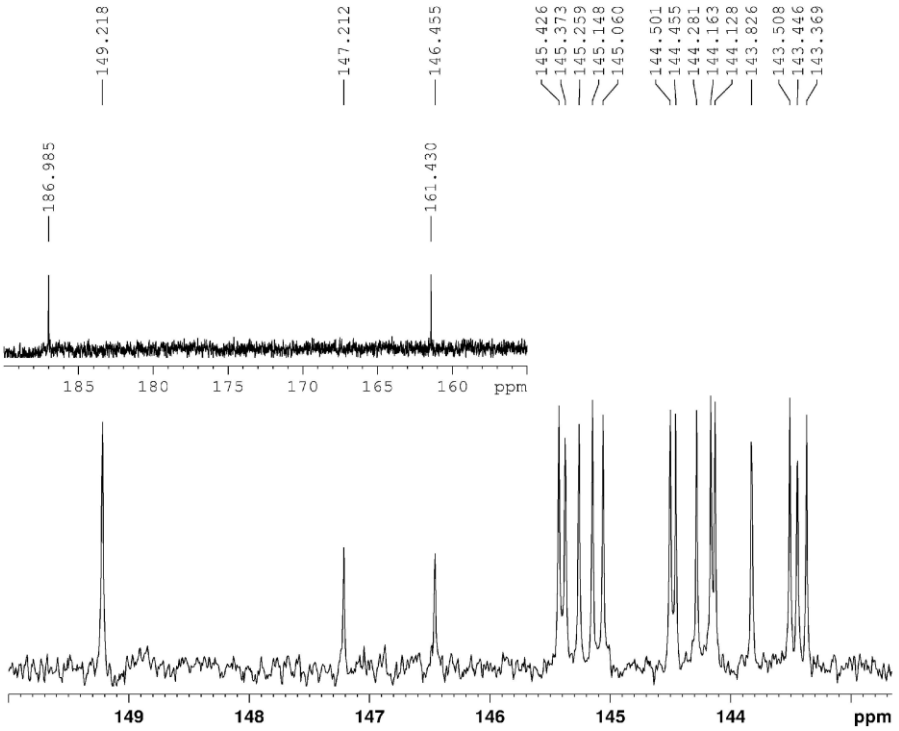

```
NAME          105L14_1fe140224
EXPNO                       1
PROCNO                      1
Date_              20140224
Time                   10.08
INSTRUM                av400
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       32
DS                        2
SWH               8250.825 Hz
FIDRES               0.125898 Hz
AQ                3.9715922 sec
RG                      362
DW                   60.600 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    12.80 usec
PL1                   -2.00 dB
SFO1          400.1324710 MHz
SI                    32768
SF            400.1300365 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2c



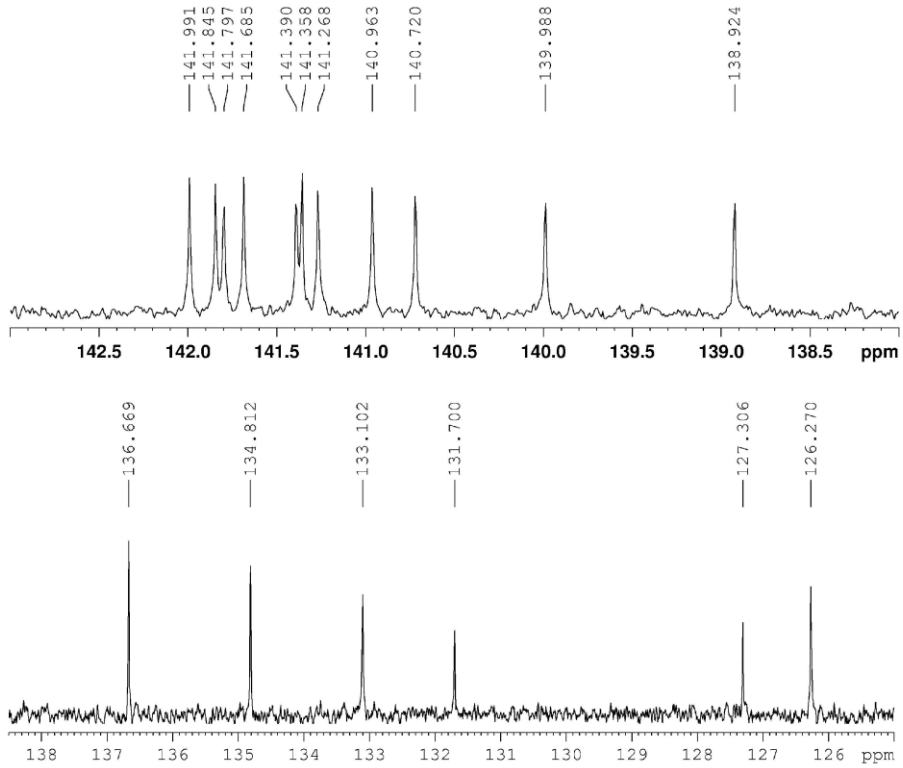

```
NAME          105L14_1fe140225
EXPNO                       2
PROCNO                      1
Date_              20140225
Time                   17.35
INSTRUM                av400
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                    16384
DS                        4
SWH              24038.461 Hz
FIDRES               0.366798 Hz
AQ                1.3632196 sec
RG                   1149.4
DW                   20.800 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      16

======== CHANNEL f1 ========
NUC1                    13C
P1                    13.30 usec
PL1                    2.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -2.00 dB
PL12                  13.92 dB
PL13                  13.92 dB
SFO2          400.1316005 MHz
SI                    32768
SF            100.6128810 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2c



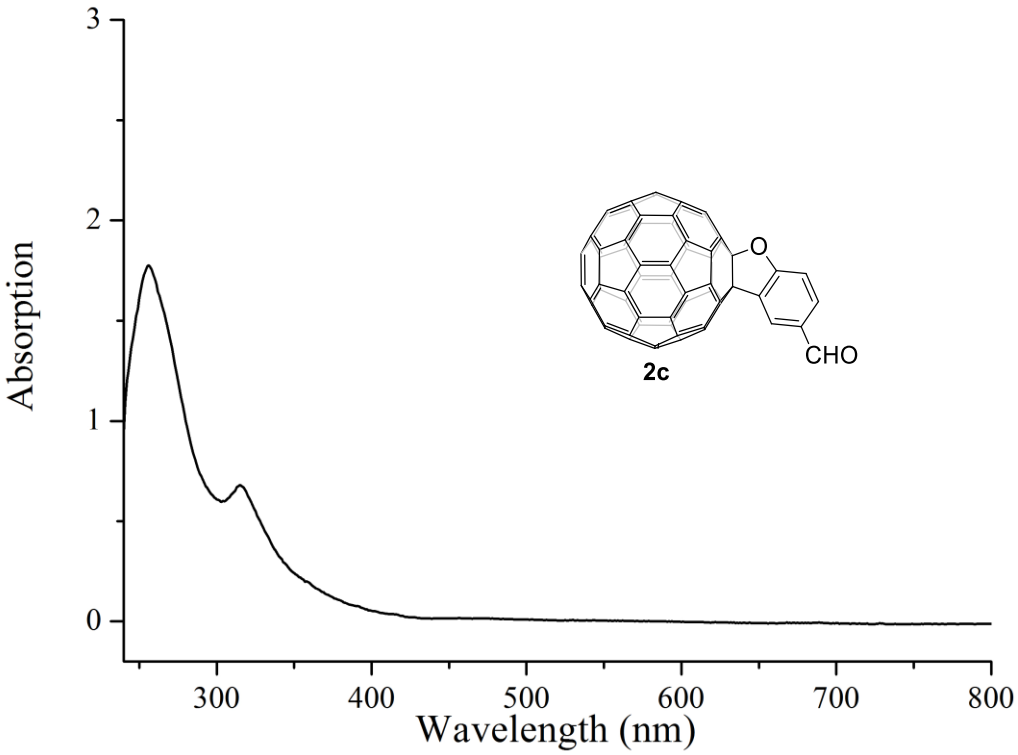

```
NAME          105L14_1fe140225
EXPNO                        2
PROCNO                       1
Date_                 20140225
Time                     17.35
INSTRUM                  av400
PROBHD       5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                      16384
DS                          4
SWH                 24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3632196 sec
RG                     1149.4
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                       13.30 usec
PL1                       2.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2              400.1316005 MHz
SI                       32768
SF                100.6128810 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2c

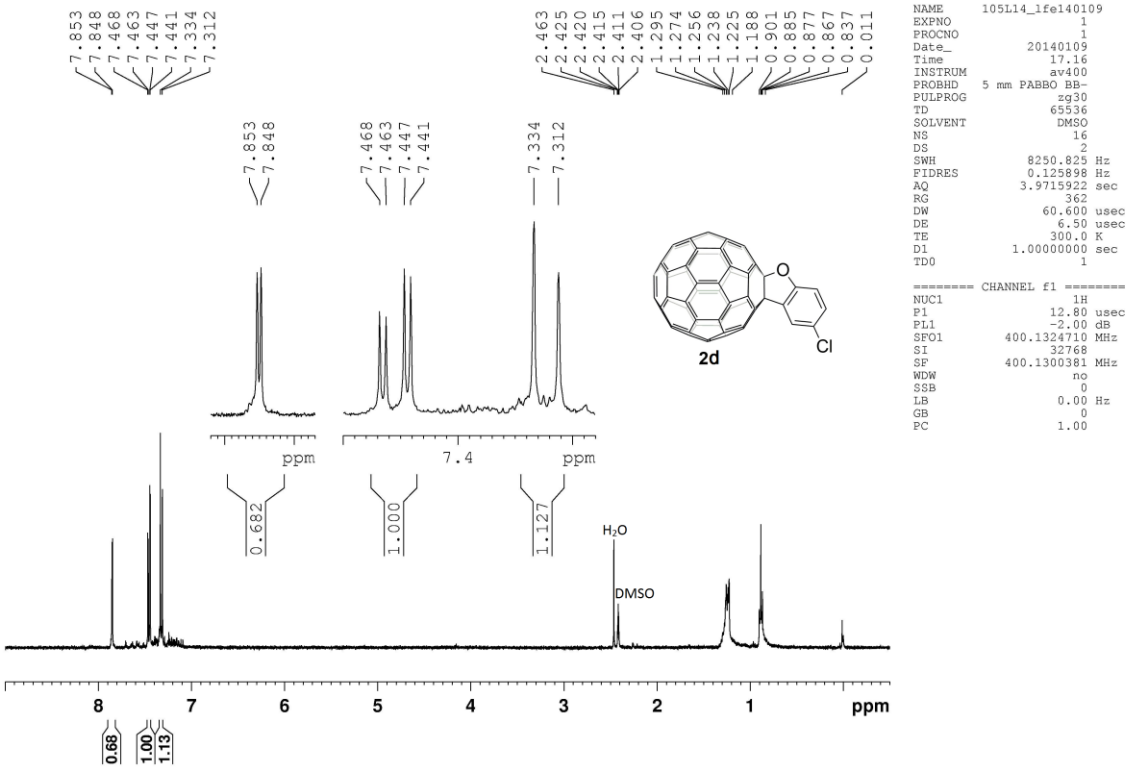



```
NAME          105L14_1fe140225
EXPNO                        2
PROCNO                       1
Date_                 20140225
Time                     17.35
INSTRUM                  av400
PROBHD       5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                      16384
DS                          4
SWH                 24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3632196 sec
RG                     1149.4
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                       13.30 usec
PL1                       2.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.92 dB
PL13                    13.92 dB
SFO2              400.1316005 MHz
SI                       32768
SF                100.6128810 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.00
```

UV-vis absorption of compound 2c

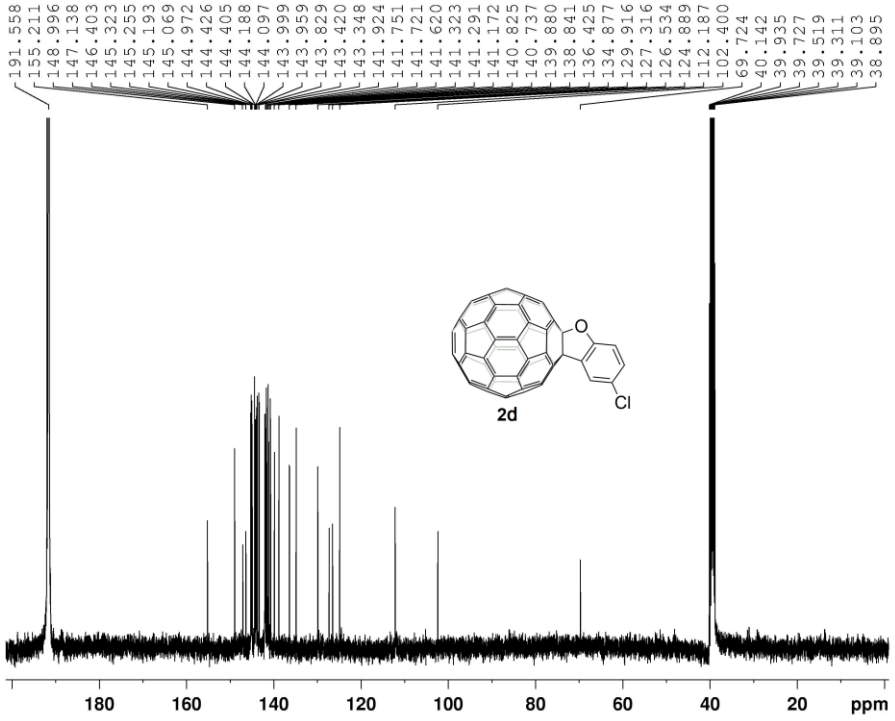


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2d



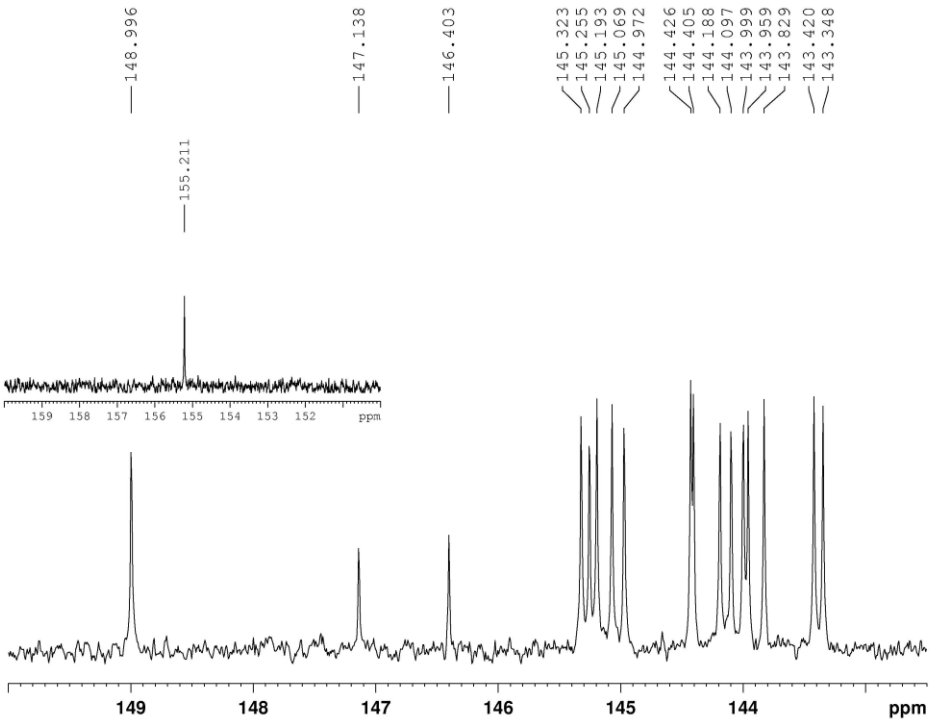

```
NAME          105L14_1fe140109
EXPNO                       1
PROCNO                      1
Date_              20140109
Time                   17.16
INSTRUM                av400
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8250.825 Hz
FIDRES              0.125898 Hz
AQ                  3.9715922 sec
RG                       362
DW                    60.600 usec
DE                     6.50 usec
TE                     300.0 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     12.80 usec
PL1                    -2.00 dB
SFO1           400.1324710 MHz
SI                       32768
SF             400.1300381 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2d



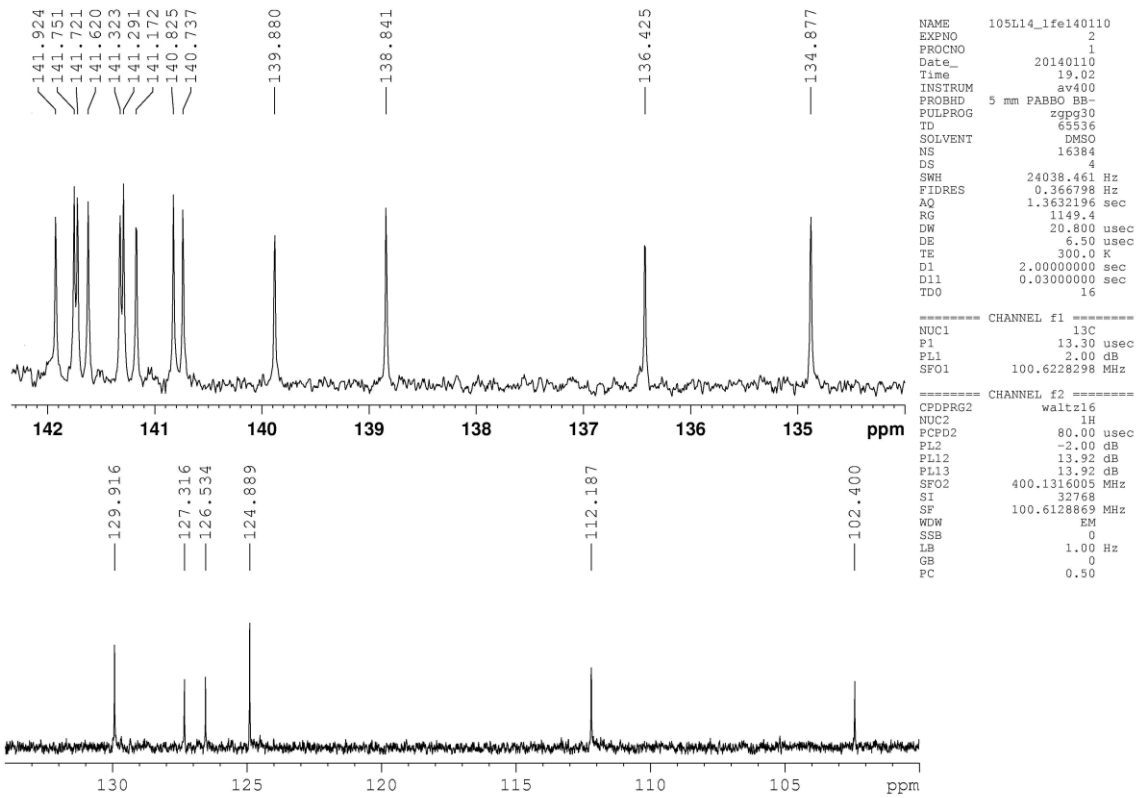

```
NAME          105L14_1fe140110
EXPNO                       2
PROCNO                      1
Date_              20140110
Time                    19.02
INSTRUM                av400
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                      16384
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3632196 sec
RG                     1149.4
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        16

======== CHANNEL f1 ========
NUC1                      13C
P1                     13.30 usec
PL1                     2.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.92 dB
PL13                   13.92 dB
SFO2              400.1316005 MHz
SI                      32768
SF                100.6128869 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      0.50
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2d

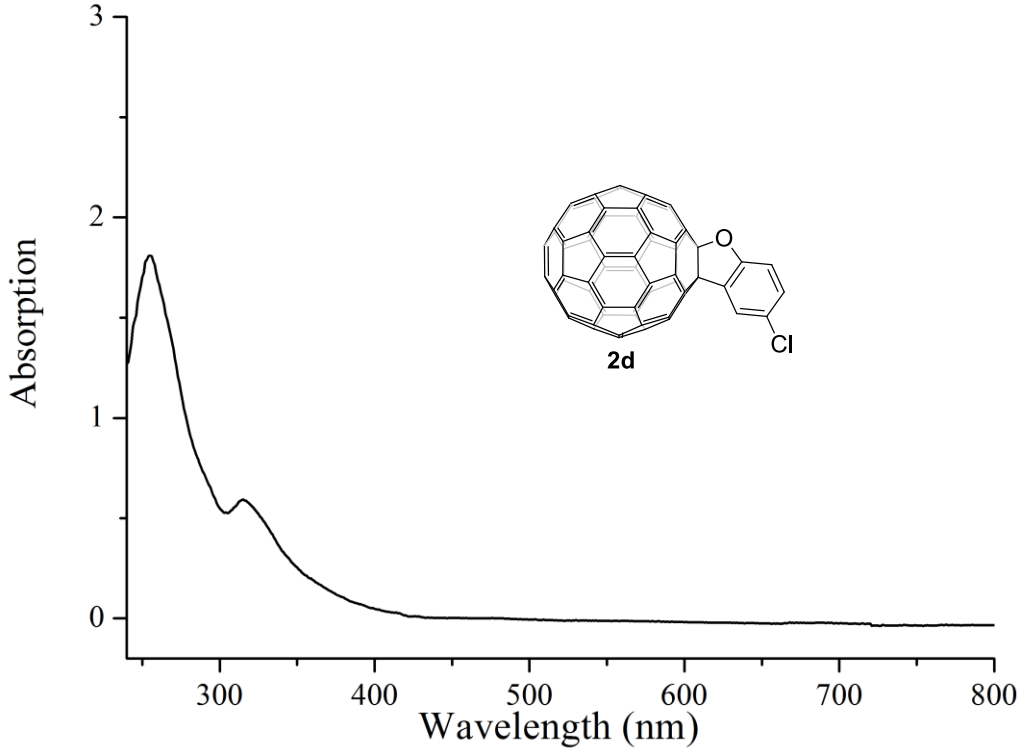



```
NAME          105L14_1fe140110
EXPNO                       2
PROCNO                      1
Date_              20140110
Time                    19.02
INSTRUM                av400
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                      16384
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3632196 sec
RG                     1149.4
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        16

======== CHANNEL f1 ========
NUC1                      13C
P1                     13.30 usec
PL1                     2.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -2.00 dB
PL12                   13.92 dB
PL13                   13.92 dB
SFO2              400.1316005 MHz
SI                      32768
SF                100.6128869 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      0.50
```

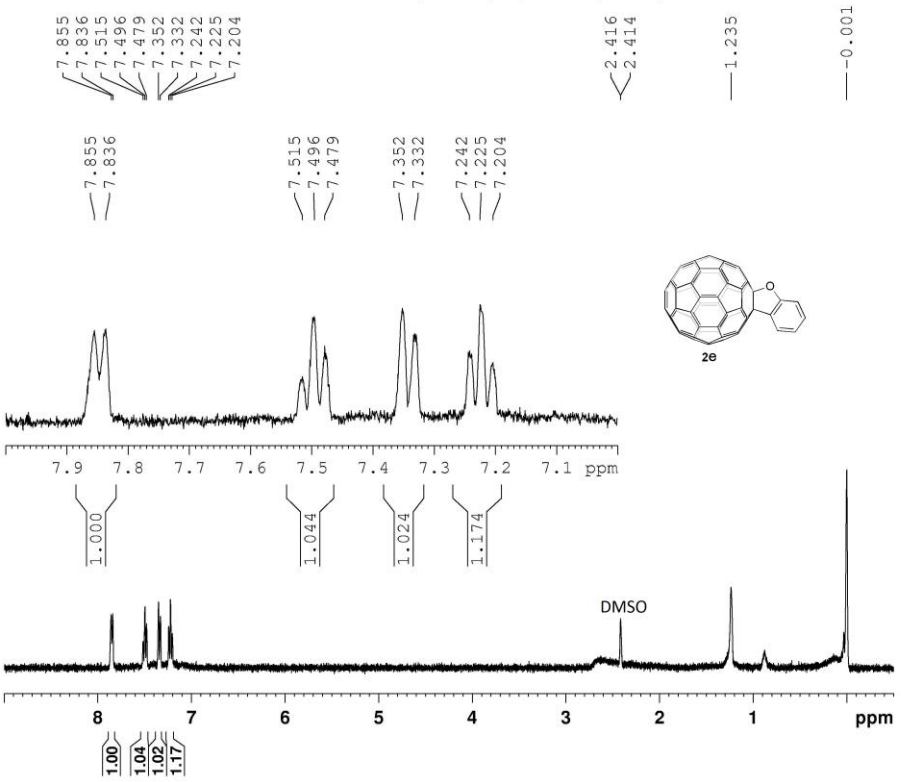
Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2d



UV-vis absorption of compound 2d

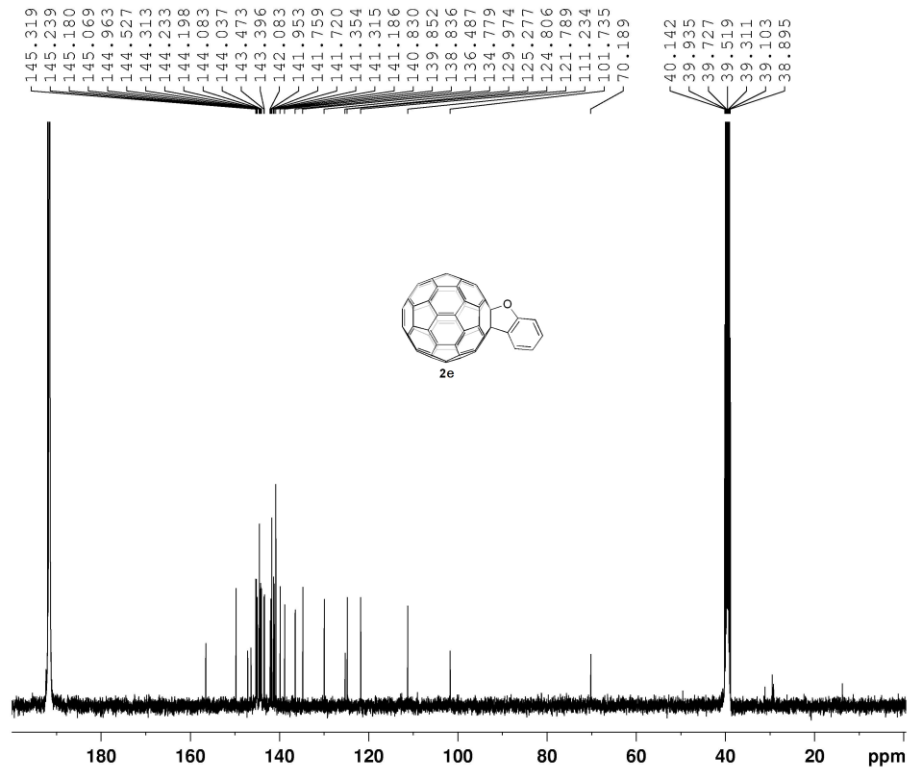


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2e



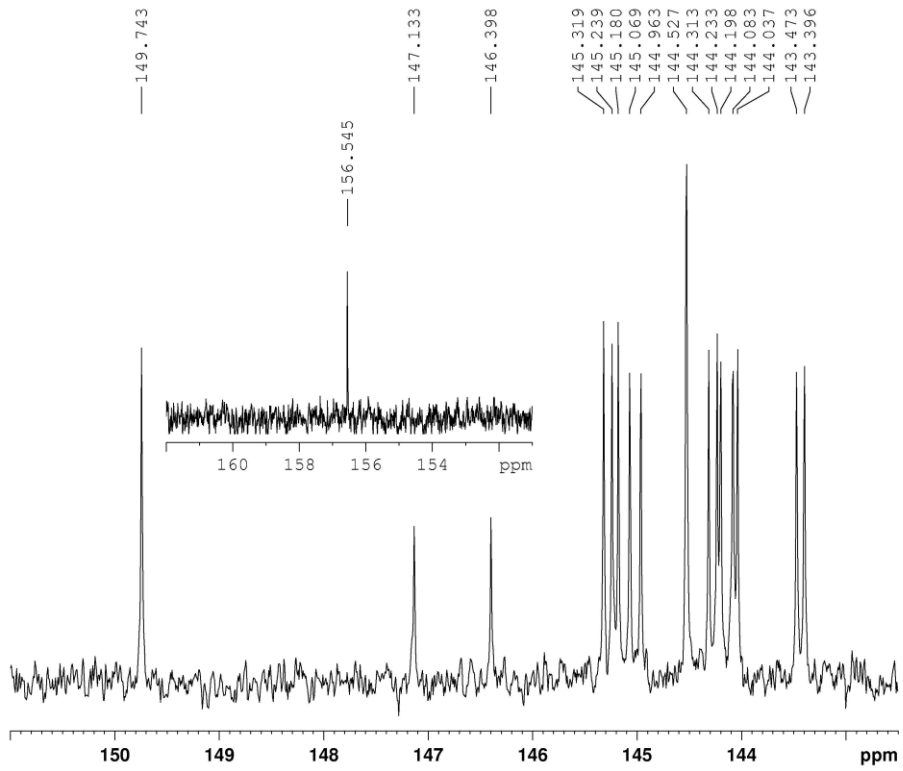

```
NAME        105L14_1fe140518_1
EXPNO                        1
PROCNO                       1
Date_                 20140528
Time                     17.21
INSTRUM                  av400
PROBHD   5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                         32
DS                          2
SWH                 8250.825 Hz
FIDRES                0.125898 Hz
AQ                    3.9715922 sec
RG                        362
DW                     60.600 usec
DE                      6.50 usec
TE                     300.0 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      13.40 usec
PL1                      0.00 dB
SFO1             400.1324710 MHz
SI                       32768
SF               400.1300378 MHz
WDW                         no
SSB                          0
LB                       0.00 Hz
GB                           0
PC                        1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2e



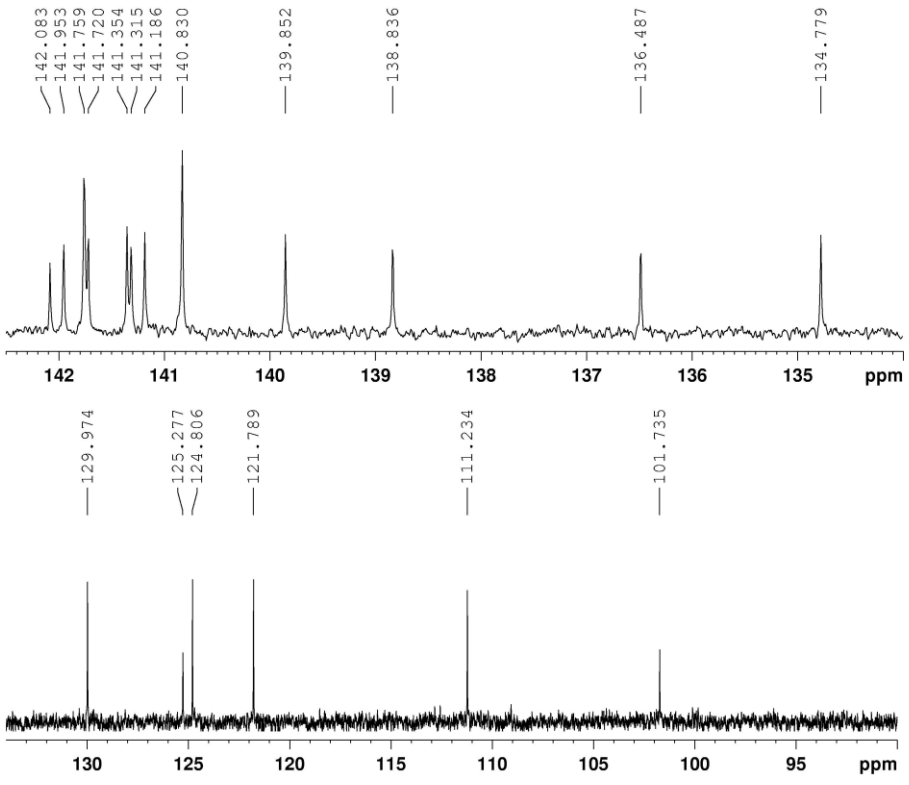

```
NAME        106L13_1fe131226_1
EXPNO                        2
PROCNO                       1
Date_                 20131226
Time                     16.37
INSTRUM                  spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                      12.30 usec
PL1                      3.00 dB
PL1W               41.92221451 W
SFO1             100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   90.00 usec
PL2                     -1.00 dB
PL12                    15.48 dB
PL13                    17.00 dB
PL2W               17.70875549 W
PL12W               0.39827961 W
PL13W               0.28066486 W
SFO2             400.2316009 MHz
SI                       32768
SF               100.6380290 MHz
WDW                         EM
SSB                          0
LB                       1.00 Hz
GB                           0
PC                        1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2e



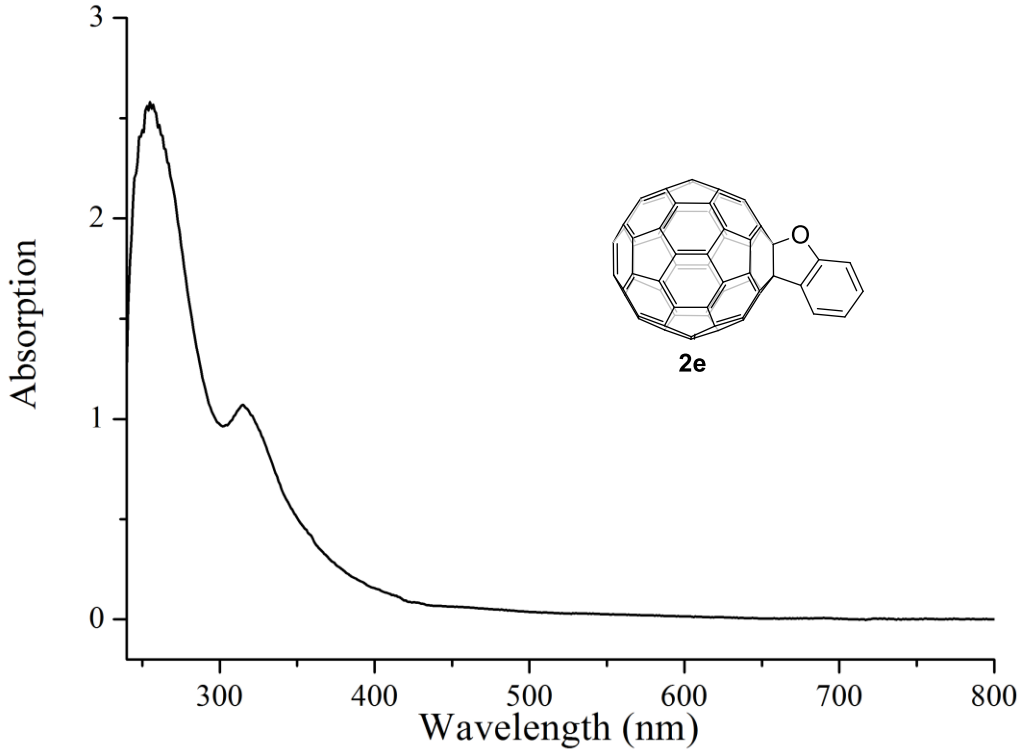

```
NAME          106L13_1fe131226_1
EXPNO                         2
PROCNO                        1
Date_                  20131226
Time                      16.37
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                      20.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          16

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.30 usec
PL1                       3.00 dB
PL1W                41.92221451 W
SFO1               100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                      -1.00 dB
PL12                     15.48 dB
PL13                     17.00 dB
PL2W                17.70875549 W
PL12W                0.39827961 W
PL13W                0.28066486 W
SFO2               400.2316009 MHz
SI                         32768
SF                 100.6380290 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                        1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2e

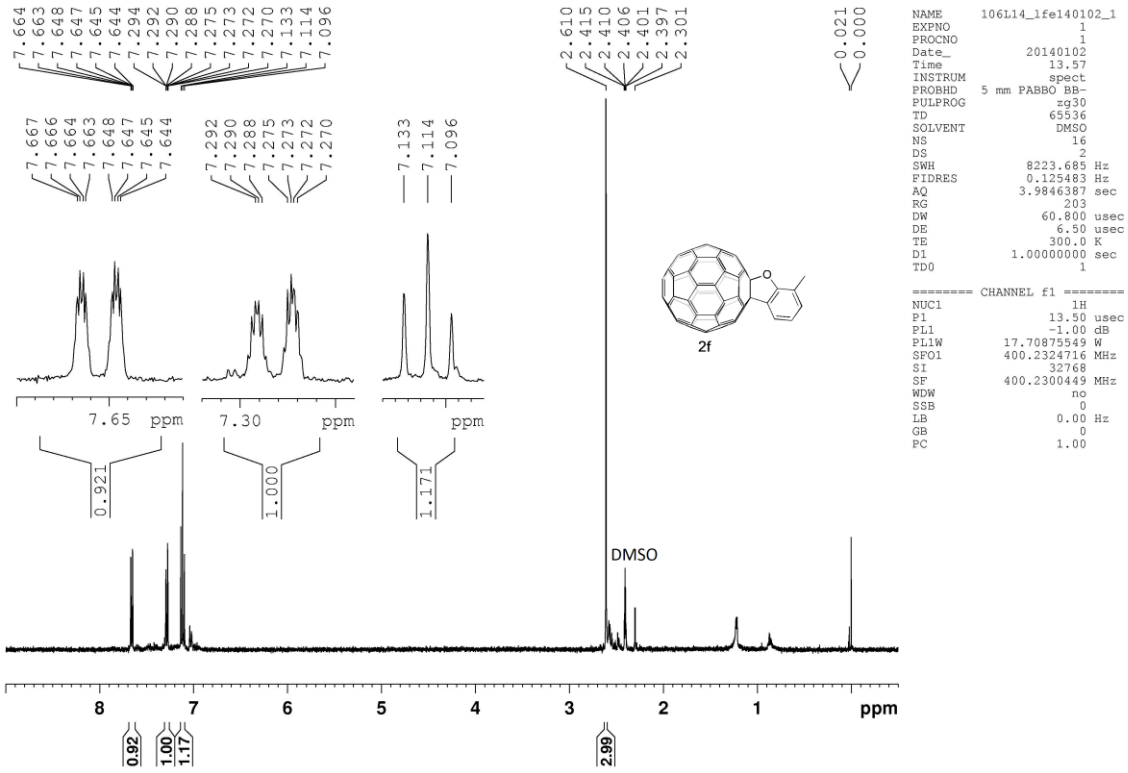



```
NAME          106L13_1fe131226_1
EXPNO                         2
PROCNO                        1
Date_                  20131226
Time                      16.37
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                      20.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          16

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.30 usec
PL1                       3.00 dB
PL1W                41.92221451 W
SFO1               100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                      -1.00 dB
PL12                     15.48 dB
PL13                     17.00 dB
PL2W                17.70875549 W
PL12W                0.39827961 W
PL13W                0.28066486 W
SFO2               400.2316009 MHz
SI                         32768
SF                 100.6380290 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                        1.00
```

UV-vis absorption of compound 2e

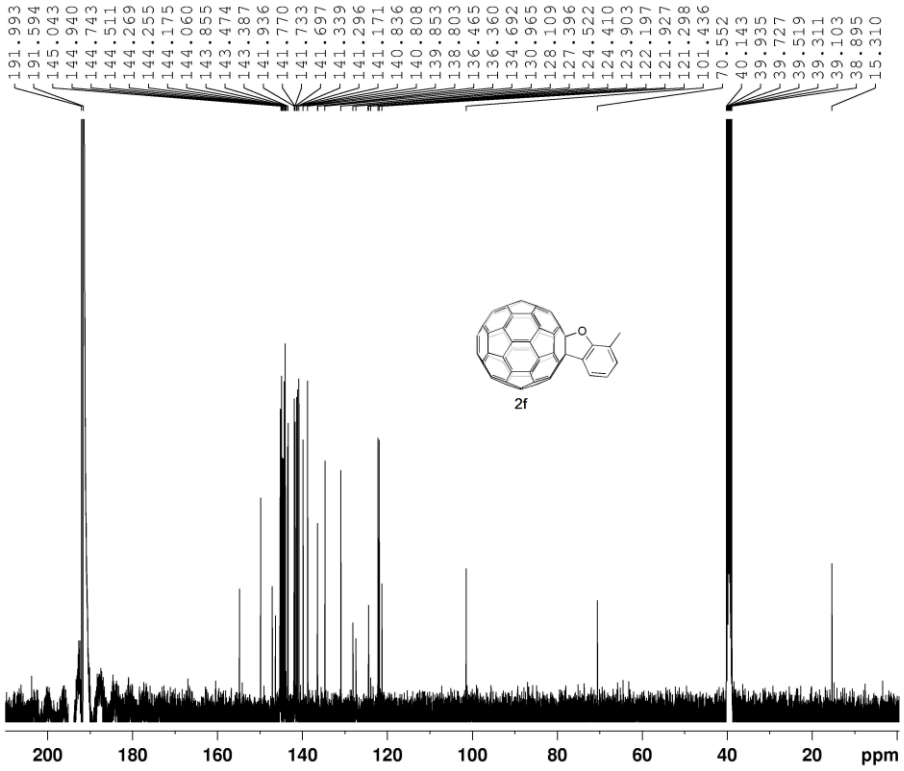


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2f



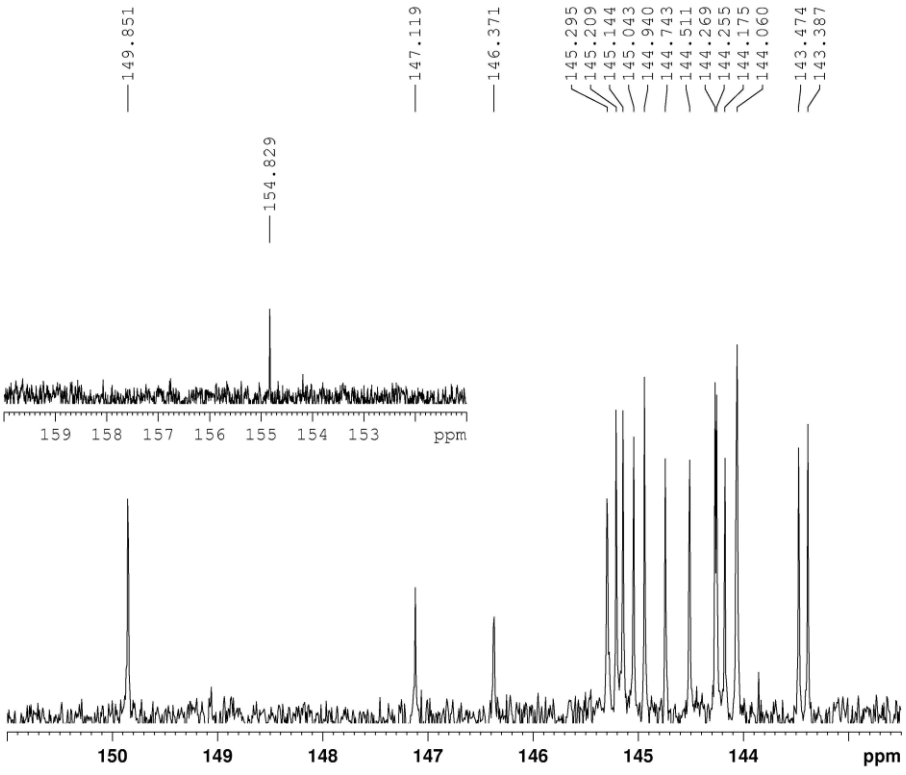

```
NAME          106L14_1fe140102_1
EXPNO                          1
PROCNO                         1
Date_                   20140102
Time                       13.57
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                     DMSO
NS                            16
DS                             2
SWH                     8223.685 Hz
FIDRES                  0.125483 Hz
AQ                      3.9846387 sec
RG                           203
DW                        60.800 usec
DE                         6.50 usec
TE                        300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        13.50 usec
PL1                       -1.00 dB
PL1W                17.70875549 W
SFO1                400.2324716 MHz
SI                         32768
SF                  400.2300449 MHz
WDW                           no
SSB                            0
LB                         0.00 Hz
GB                             0
PC                         1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2f



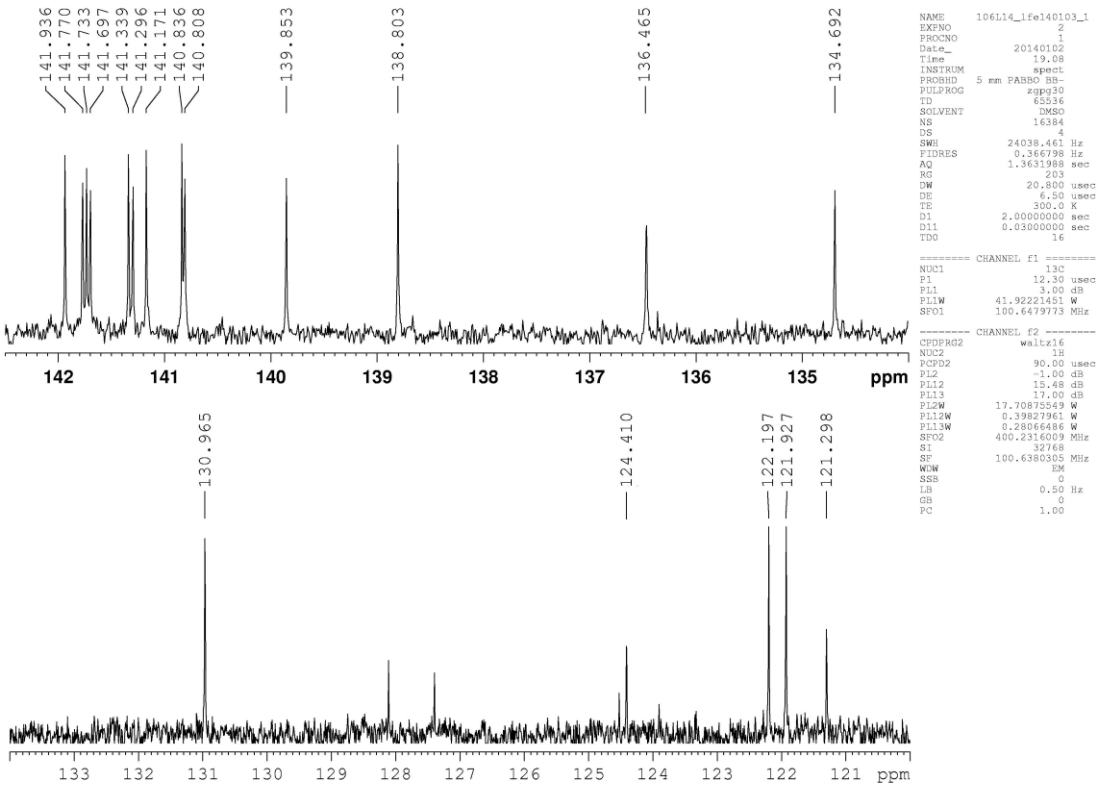

```
NAME          106L14_1fe140103_1
EXPNO                          2
PROCNO                         1
Date_               20140102
Time                      19.08
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                         203
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                      13C
P1                     12.30 usec
PL1                     3.00 dB
PL1W              41.92221451 W
SFO1              100.6479773 MHz

-------- CHANNEL f2 --------
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  90.00 usec
PL2                    -1.00 dB
PL12                   15.48 dB
PL13                   17.00 dB
PL2W              17.70875549 W
PL12W              0.39827961 W
PL13W              0.28066486 W
SFO2              400.2316009 MHz
SI                       32768
SF                100.6380305 MHz
WDW                         EM
SSB                          0
LB                      0.50 Hz
GB                           0
PC                        1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2f

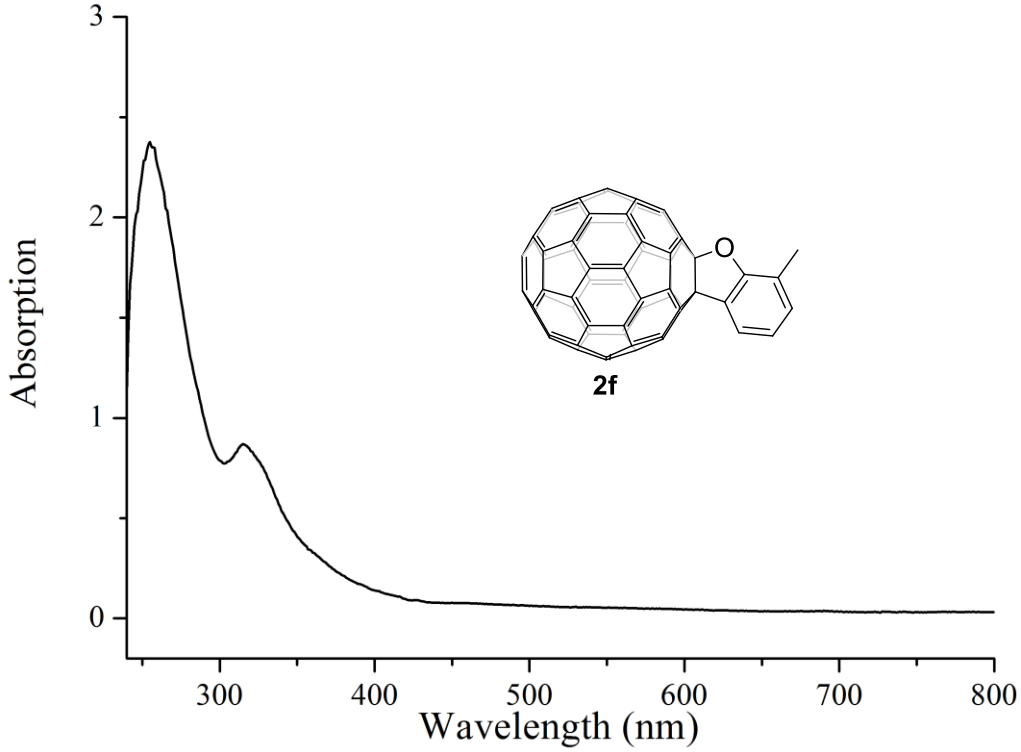



```
NAME          106L14_1fe140103_1
EXPNO                          2
PROCNO                         1
Date_               20140102
Time                      19.08
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       16384
DS                           4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                         203
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                      13C
P1                     12.30 usec
PL1                     3.00 dB
PL1W              41.92221451 W
SFO1              100.6479773 MHz

-------- CHANNEL f2 --------
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  90.00 usec
PL2                    -1.00 dB
PL12                   15.48 dB
PL13                   17.00 dB
PL2W              17.70875549 W
PL12W              0.39827961 W
PL13W              0.28066486 W
SFO2              400.2316009 MHz
SI                       32768
SF                100.6380305 MHz
WDW                         EM
SSB                          0
LB                      0.50 Hz
GB                           0
PC                        1.00
```

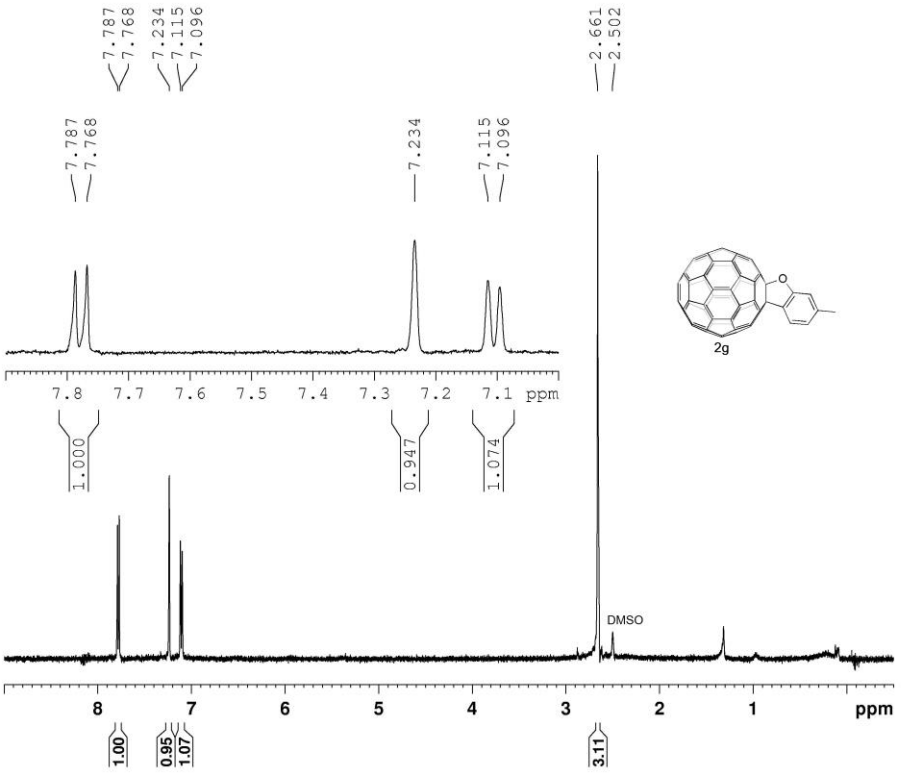
Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2f



UV-vis absorption of compound 2f

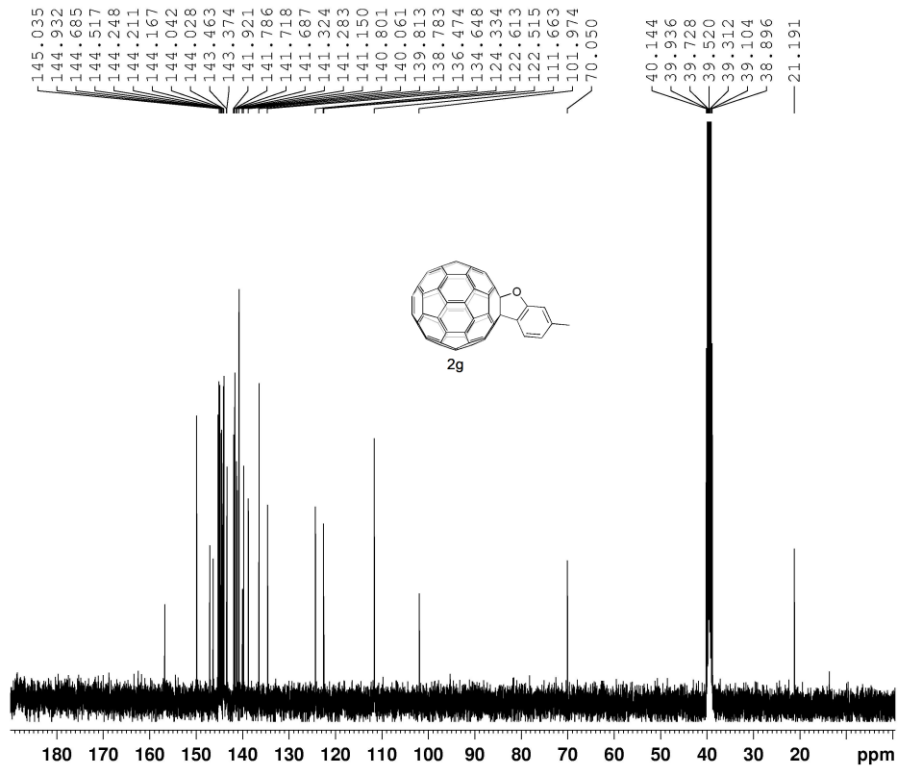


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2g



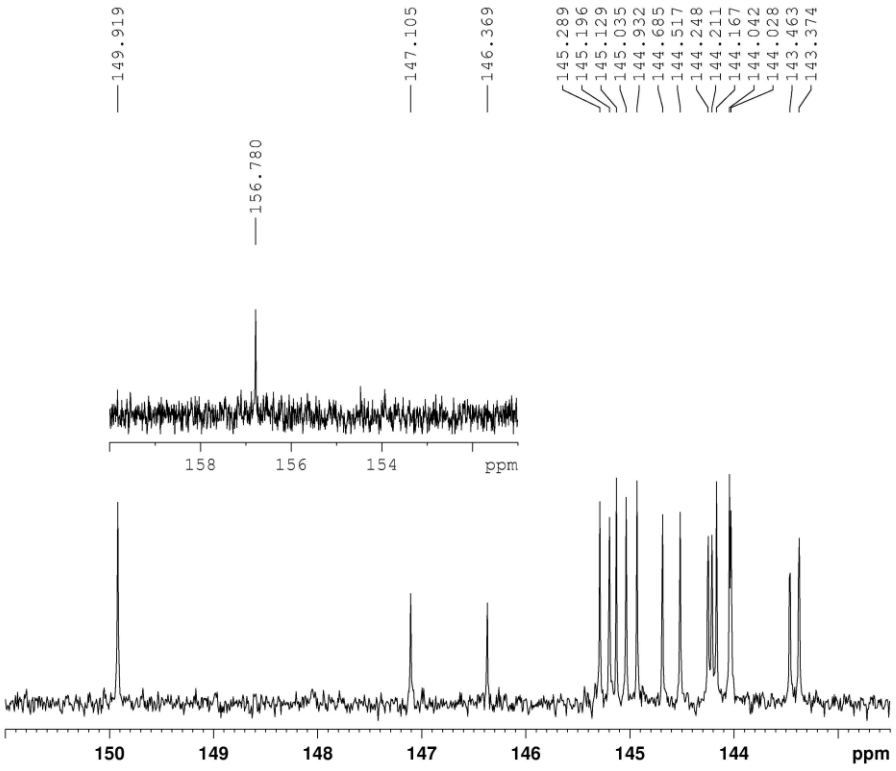

```
NAME          105L14_1fe140518_2
EXPNO                          1
PROCNO                         1
Date_                   20140528
Time                       17.40
INSTRUM                    av400
PROBHD     5 mm BBO BB-1H
PULPROG                     zg30
TD                         65536
SOLVENT                     DMSO
NS                            32
DS                             2
SWH                     8250.825 Hz
FIDRES                  0.125898 Hz
AQ                      3.9715922 sec
RG                           362
DW                        60.600 usec
DE                         6.50 usec
TE                        300.0 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        13.40 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz
SI                         32768
SF                  400.1300042 MHz
WDW                           no
SSB                            0
LB                         0.00 Hz
GB                             0
PC                         1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2g



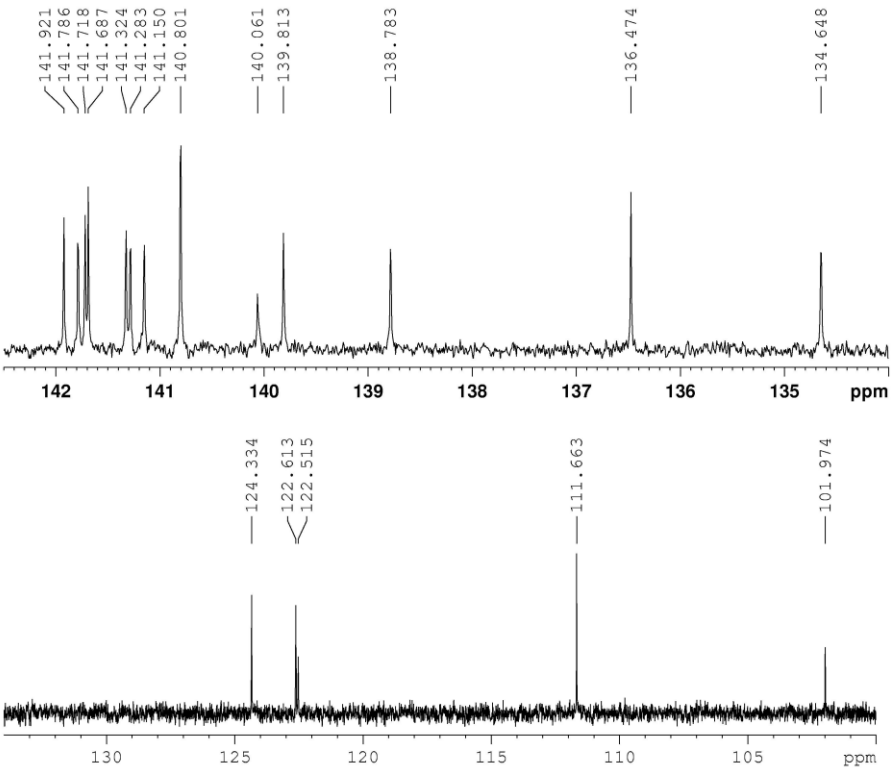

```
NAME          105L13_1fe131226_2
EXPNO                          2
PROCNO                         1
Date_                   20131227
Time                       19.17
INSTRUM                    av400
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                         65536
SOLVENT                     DMSO
NS                         16384
DS                             4
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                      1.3632196 sec
RG                         812.7
DW                        20.800 usec
DE                         6.50 usec
TE                        300.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                           16

======== CHANNEL f1 ========
NUC1                          13C
P1                        13.30 usec
PL1                        2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                          1H
PCPD2                     80.00 usec
PL2                       -2.00 dB
PL12                      13.92 dB
PL13                      13.92 dB
SFO2                400.1316005 MHz
SI                         32768
SF                  100.6128852 MHz
WDW                           EM
SSB                            0
LB                         0.50 Hz
GB                             0
PC                         1.20
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2g



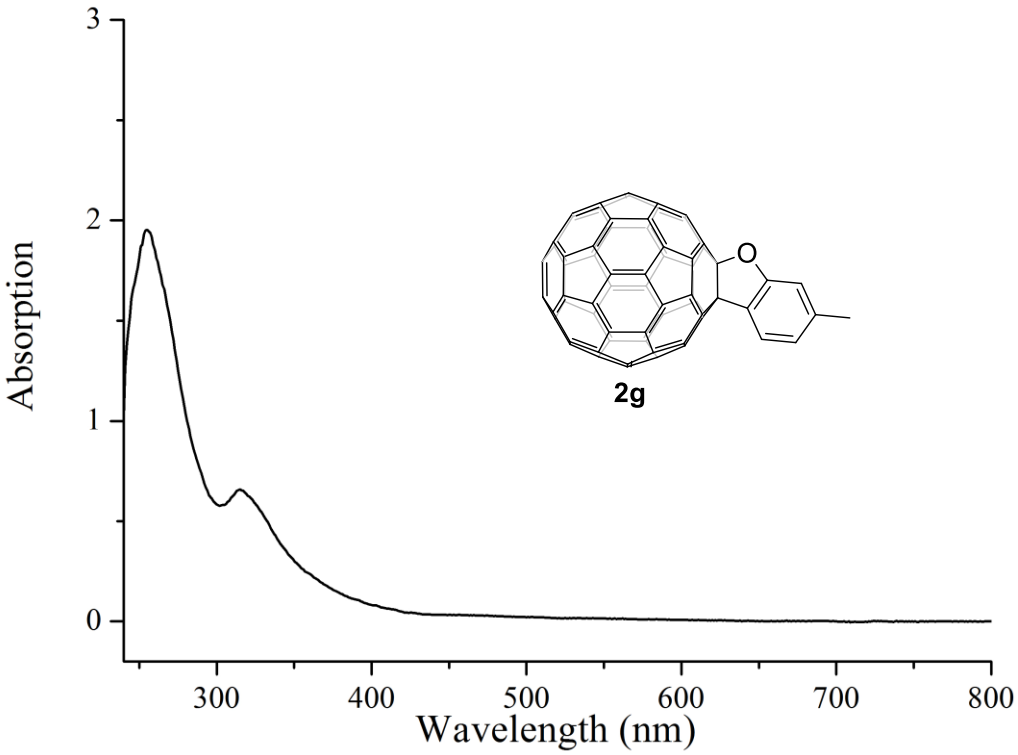

```
NAME          105L13_1fe131226_2
EXPNO                          2
PROCNO                         1
Date_                   20131227
Time                       19.17
INSTRUM                    av400
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                       16384
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                   1.3632196 sec
RG                       812.7
DW                      20.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                       13.30 usec
PL1                       2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -2.00 dB
PL12                     13.92 dB
PL13                     13.92 dB
SFO2                400.1316005 MHz
SI                       32768
SF                  100.6128852 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.20
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2g

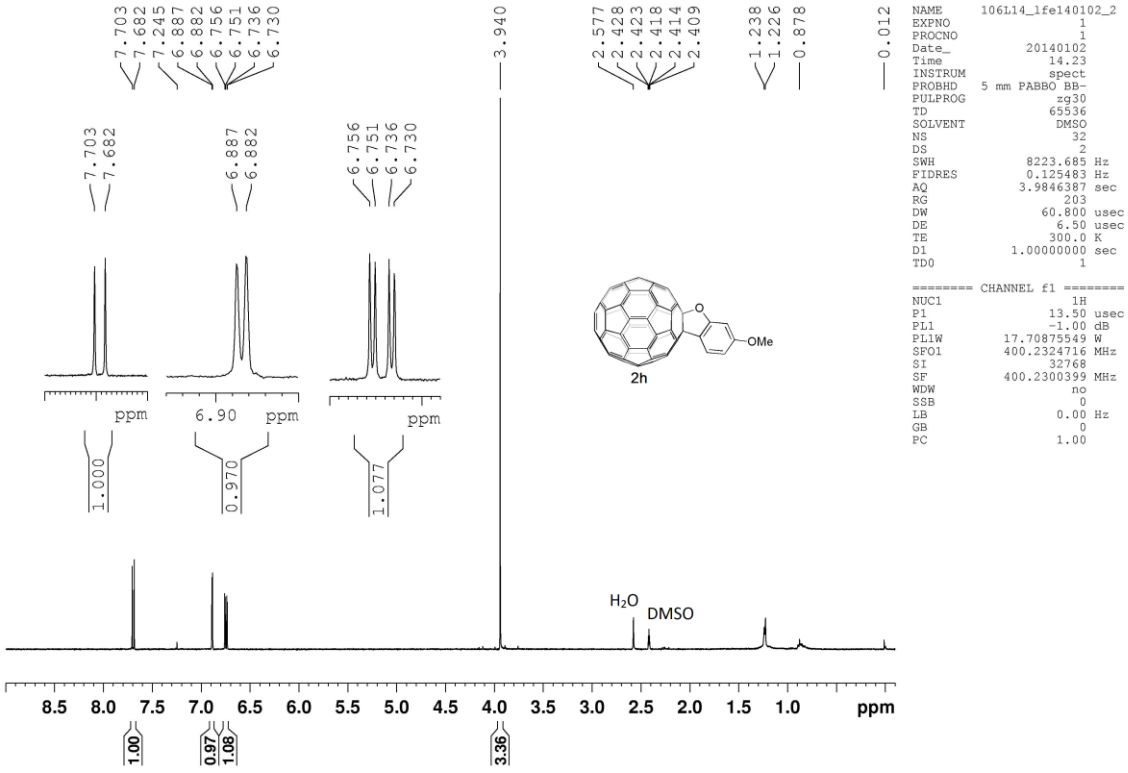



```
NAME          105L13_1fe131226_2
EXPNO                          2
PROCNO                         1
Date_                   20131227
Time                       19.17
INSTRUM                    av400
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                       16384
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                   1.3632196 sec
RG                       812.7
DW                      20.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         16

======== CHANNEL f1 ========
NUC1                       13C
P1                       13.30 usec
PL1                       2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -2.00 dB
PL12                     13.92 dB
PL13                     13.92 dB
SFO2                400.1316005 MHz
SI                       32768
SF                  100.6128852 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.20
```

UV-vis absorption of compound 2g

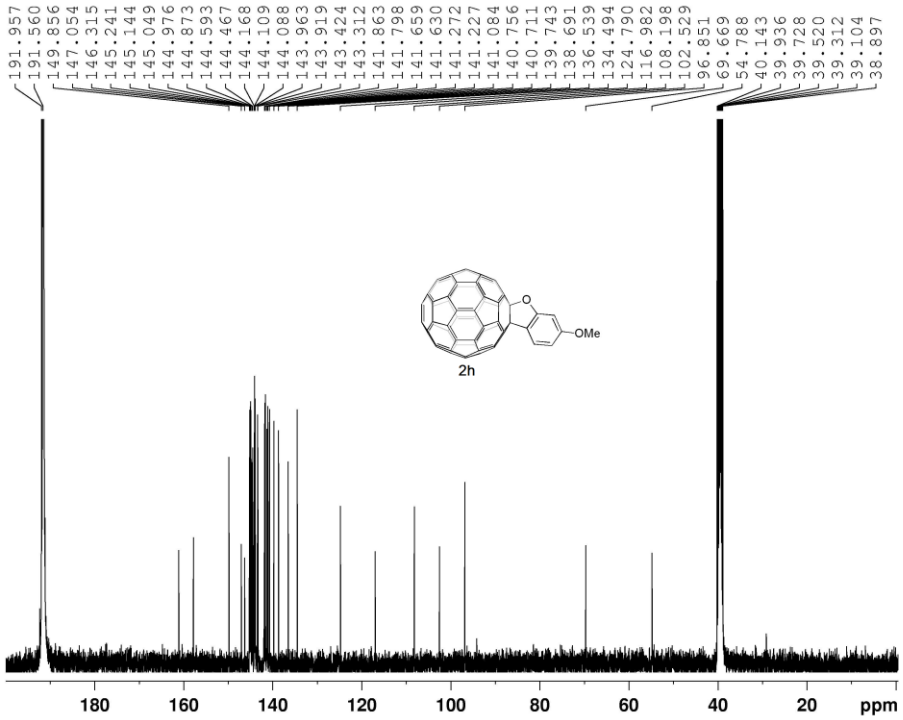


^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of compound 2h



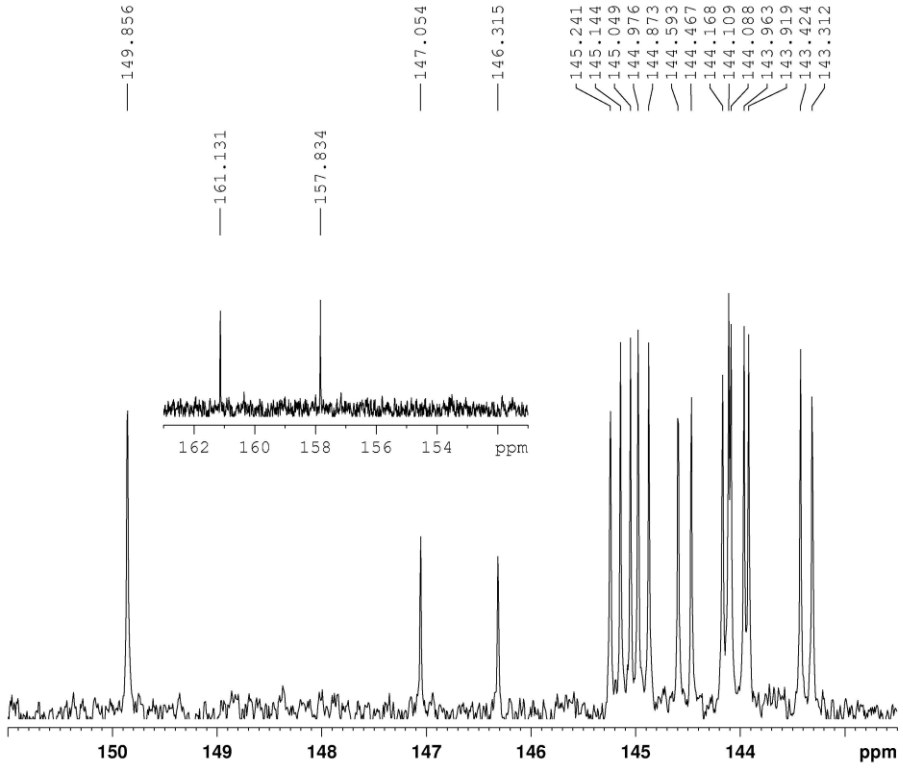

```
NAME          106L14_1fe140102_2
EXPNO                          1
PROCNO                         1
Date_                   20140102
Time                       14.23
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                           32
DS                            2
SWH                    8223.685 Hz
FIDRES                 0.125483 Hz
AQ                     3.9846387 sec
RG                           203
DW                        60.800 usec
DE                         6.50 usec
TE                        300.0 K
D1                     1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         13.50 usec
PL1                        -1.00 dB
PL1W                17.70875549 W
SFO1                400.2324716 MHz
SI                         32768
SF                  400.2300399 MHz
WDW                           no
SSB                            0
LB                          0.00 Hz
GB                             0
PC                          1.00
```

^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2h



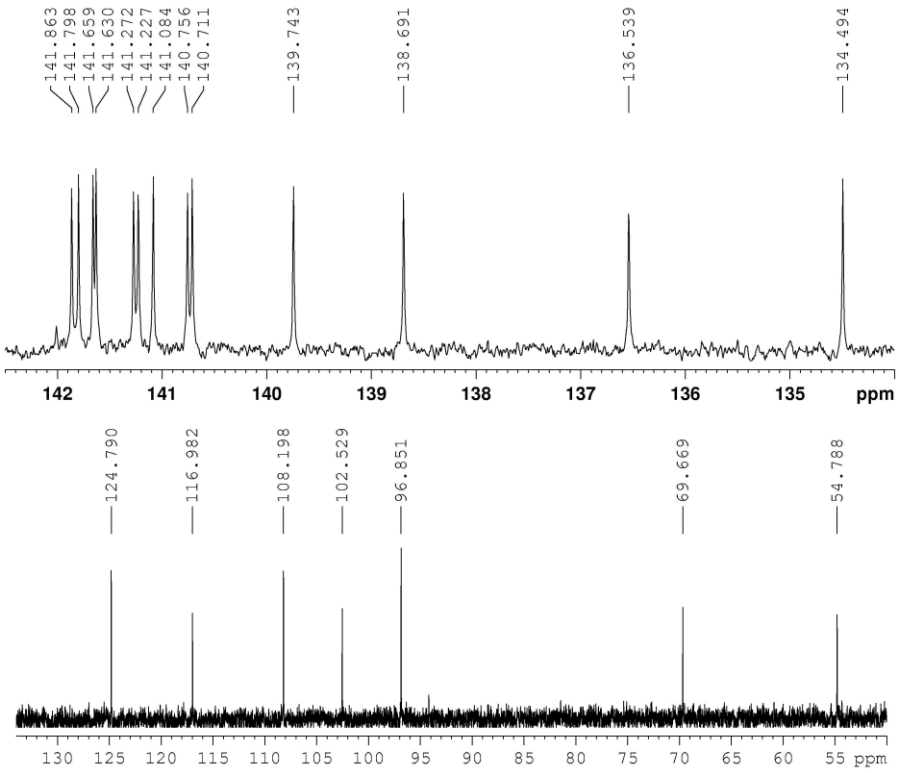

```
NAME          106L14_1fe140103_2
EXPNO                          2
PROCNO                         1
Date_                   20140104
Time                       23.32
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                        16384
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                    1.3631988 sec
RG                          203
DW                       20.800 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           16

======== CHANNEL f1 ========
NUC1                         13C
P1                         12.30 usec
PL1                         3.00 dB
PL1W                41.92221451 W
SFO1               100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     90.00 usec
PL2                       -1.00 dB
PL12                      15.48 dB
PL13                      17.00 dB
PL2W                17.70875549 W
PL12W                0.39827961 W
PL13W                0.28066486 W
SFO2               400.2316009 MHz
SI                        32768
SF                 100.6380364 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2h



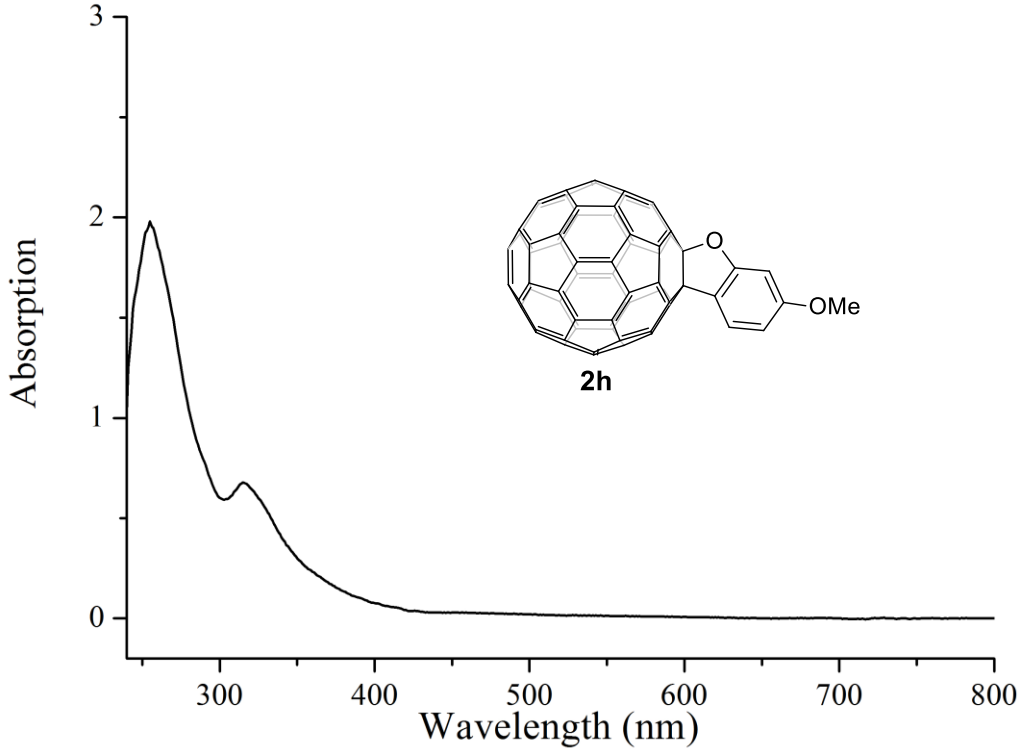

```
NAME          106L14_1fe140103_2
EXPNO                          2
PROCNO                         1
Date_                   20140104
Time                       23.32
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                        16384
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                    1.3631988 sec
RG                          203
DW                       20.800 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           16

======== CHANNEL f1 ========
NUC1                         13C
P1                         12.30 usec
PL1                         3.00 dB
PL1W                41.92221451 W
SFO1               100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     90.00 usec
PL2                       -1.00 dB
PL12                      15.48 dB
PL13                      17.00 dB
PL2W                17.70875549 W
PL12W                0.39827961 W
PL13W                0.28066486 W
SFO2               400.2316009 MHz
SI                        32768
SF                 100.6380364 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```

Expanded ^{13}C NMR (100 MHz, CS_2/DMSO-d_6) of compound 2h



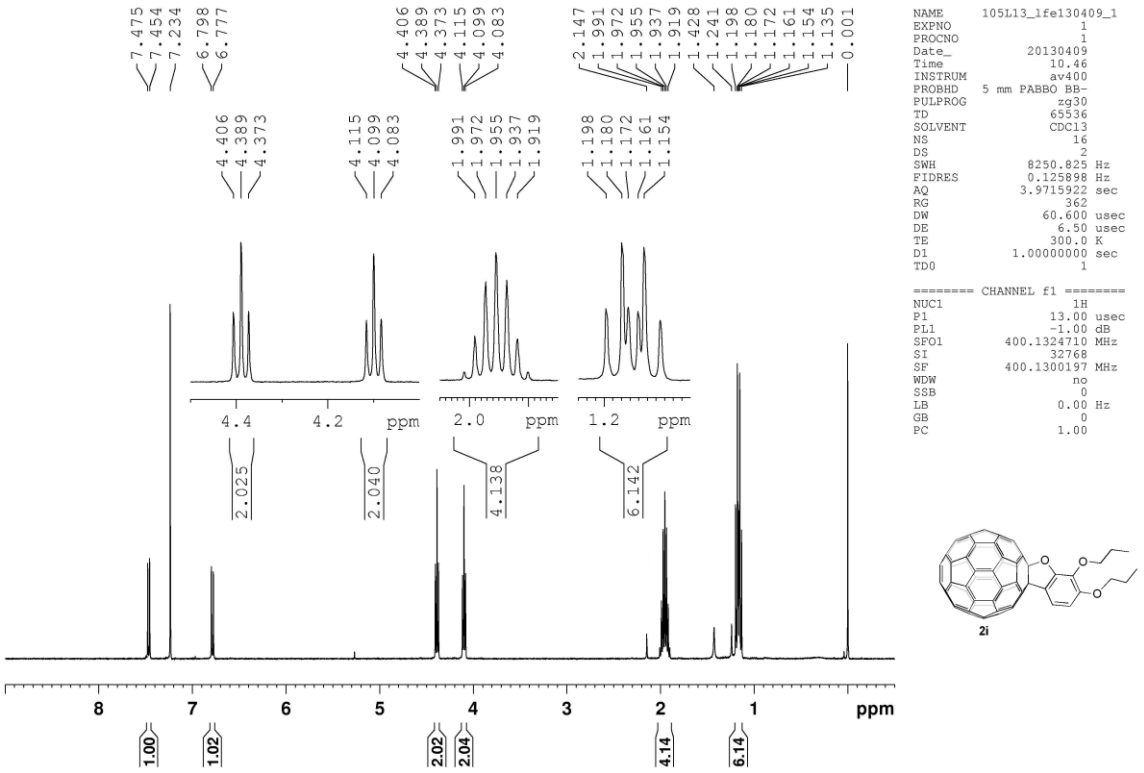

```
NAME          106L14_1fe140103_2
EXPNO                          2
PROCNO                         1
Date_                   20140104
Time                       23.32
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                       16384
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                      20.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          16

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.30 usec
PL1                       3.00 dB
PL1W                41.92221451 W
SFO1               100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                      -1.00 dB
PL12                     15.48 dB
PL13                     17.00 dB
PL2W                17.70875549 W
PL12W                0.39827961 W
PL13W                0.28066486 W
SFO2               400.2316009 MHz
SI                         32768
SF                 100.6380364 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                        1.00
```

UV-vis absorption of compound 2h



2h

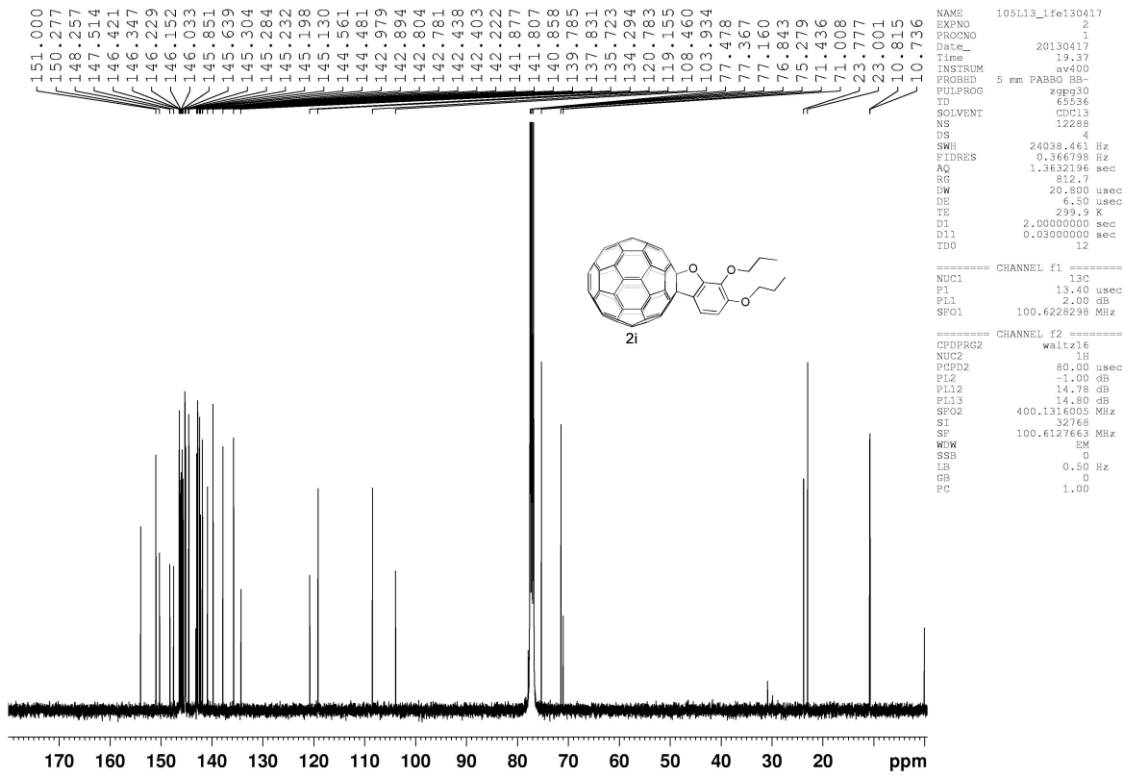
^{1}H NMR (400 MHz, CS_2/$CDCl_3$) of compound 2i



NAME 105L13_1fe130409_1
EXPNO 1
PROCNO 1
Date_ 20130409
Time 10.46
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 362
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300197 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

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

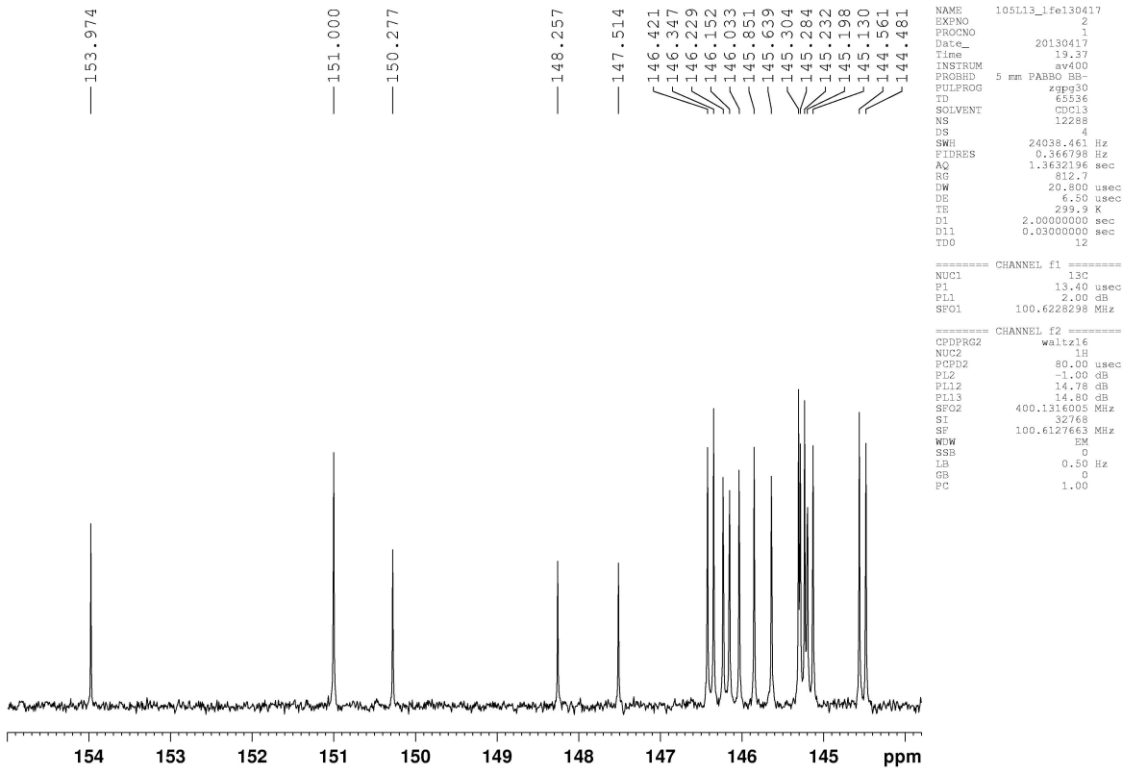


NAME 105L13_1fe130417
EXPNO 2
PROCNO 1
Date_ 20130417
Time 19.37
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12288
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 812.7
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 12

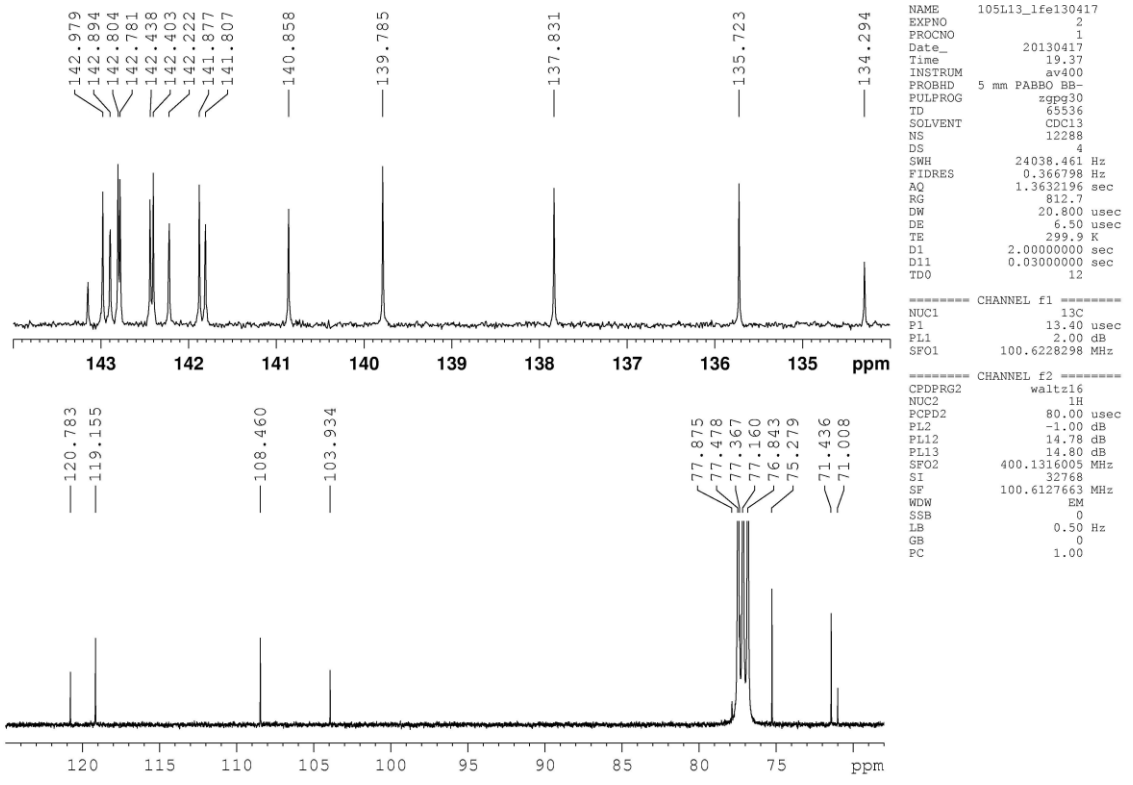
======== CHANNEL f1 ========
NUC1 13C
P1 13.40 usec
PL1 2.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.78 dB
PL13 14.80 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127663 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

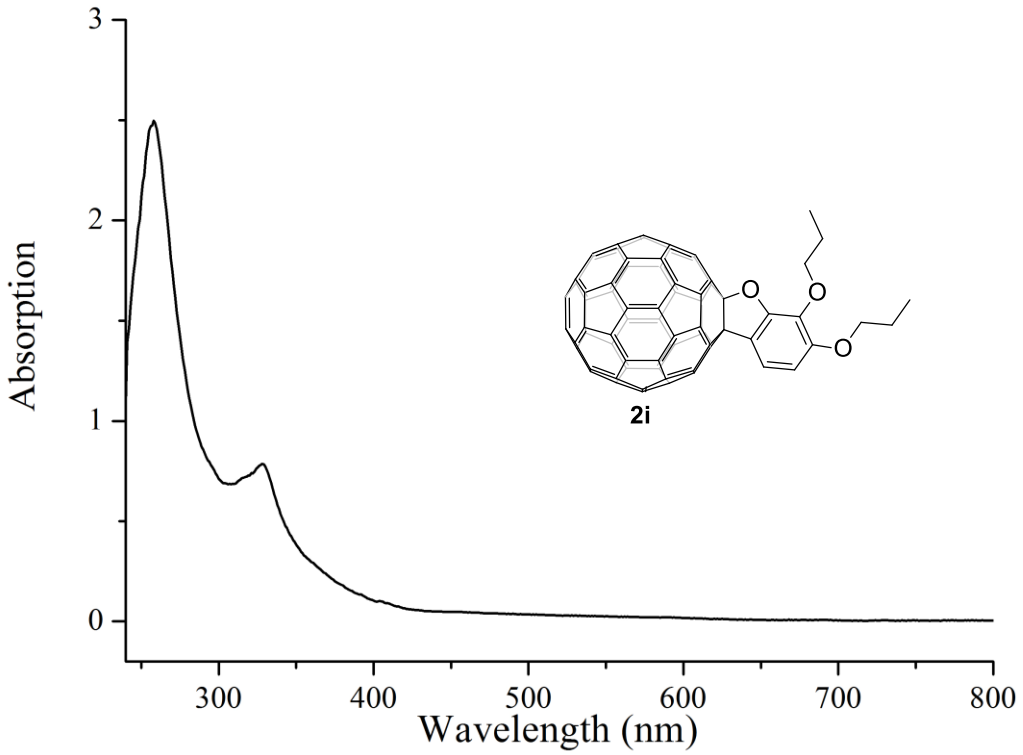
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2i



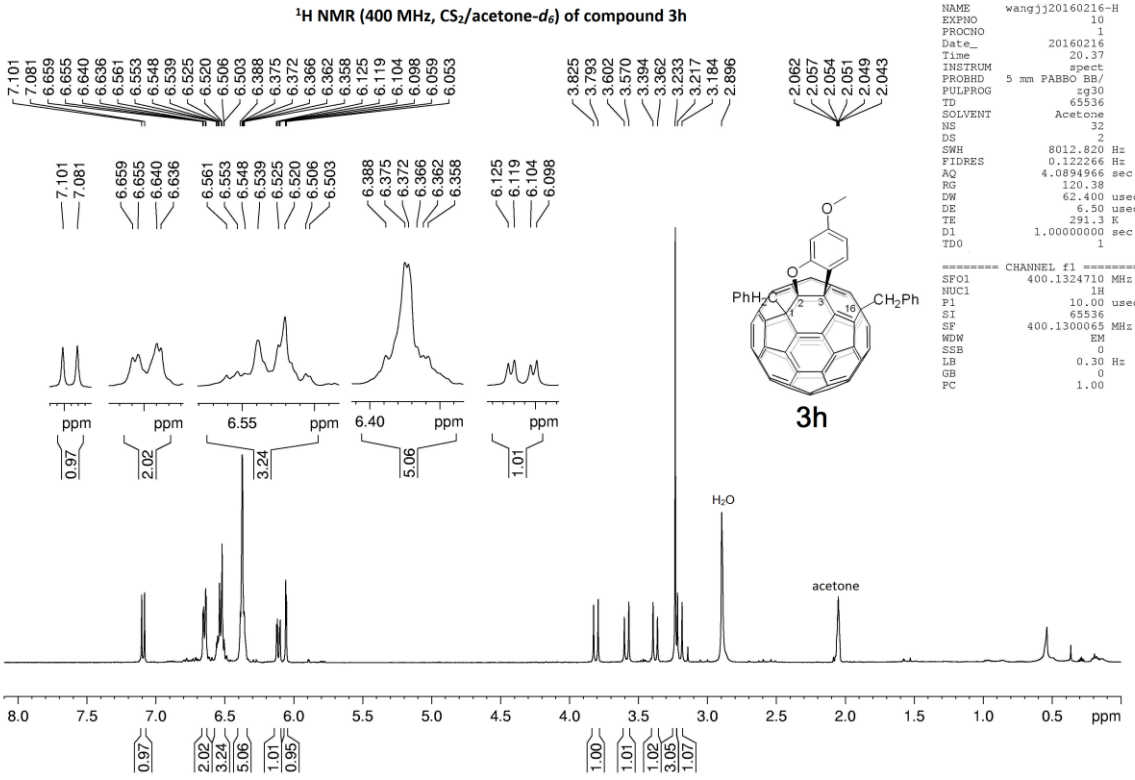
Expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$) of compound 2i



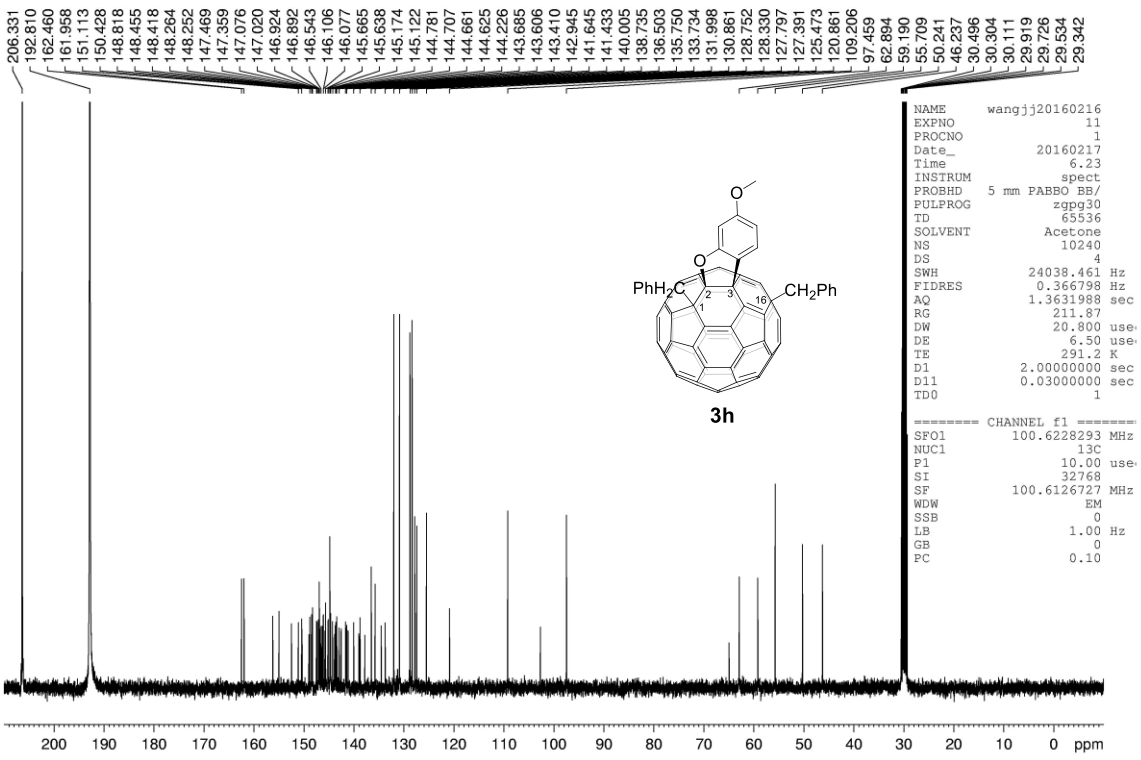
UV-vis absorption of compound 2i



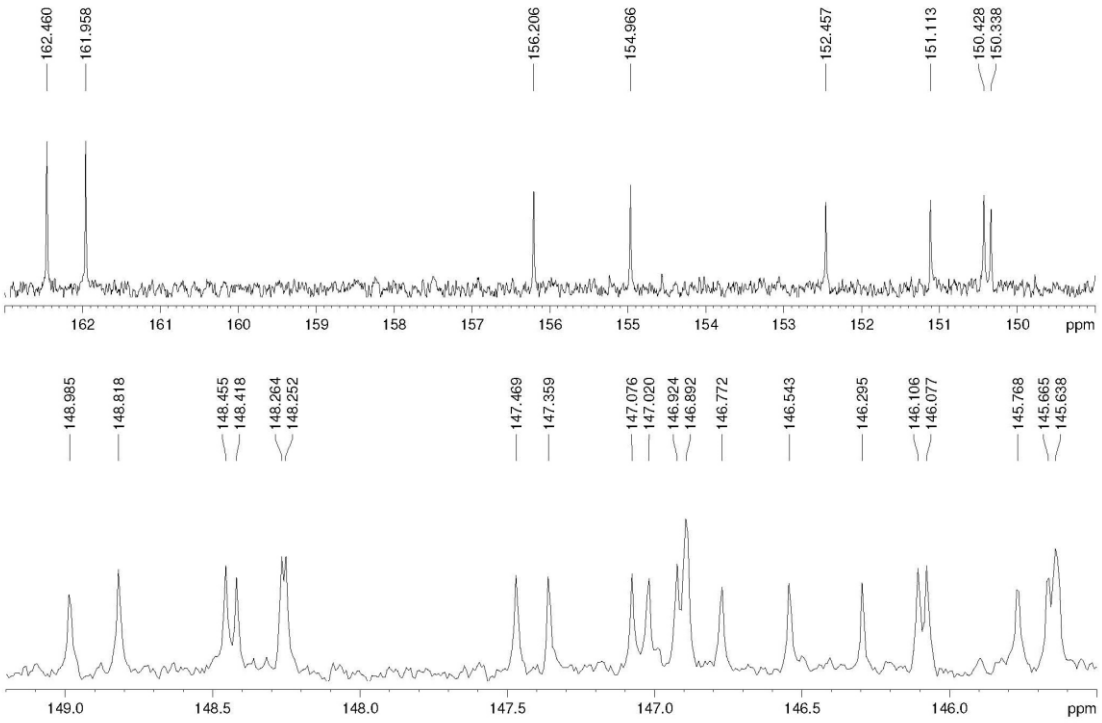
^{1}H NMR (400 MHz, CS_2/acetone-d_6) of compound 3h



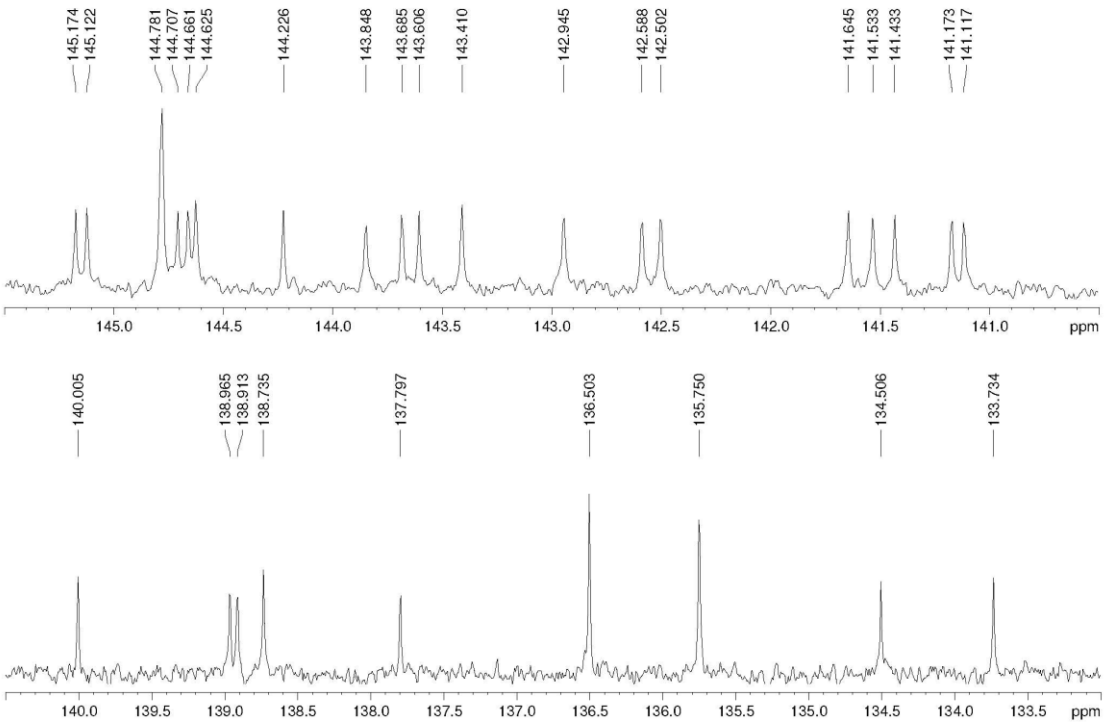
^{13}C NMR (100 MHz, CS_2/actone-d_6) of compound 3h



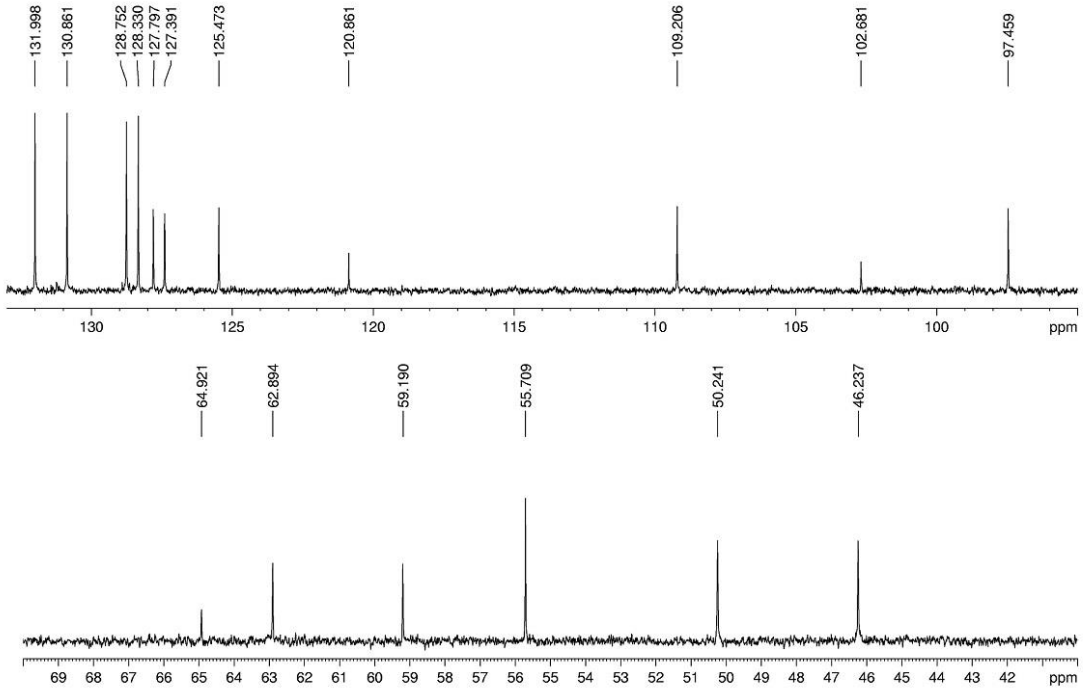
Expanded ^{13}C NMR (100 MHz, CS_2/acetone-d_6) of compound 3h

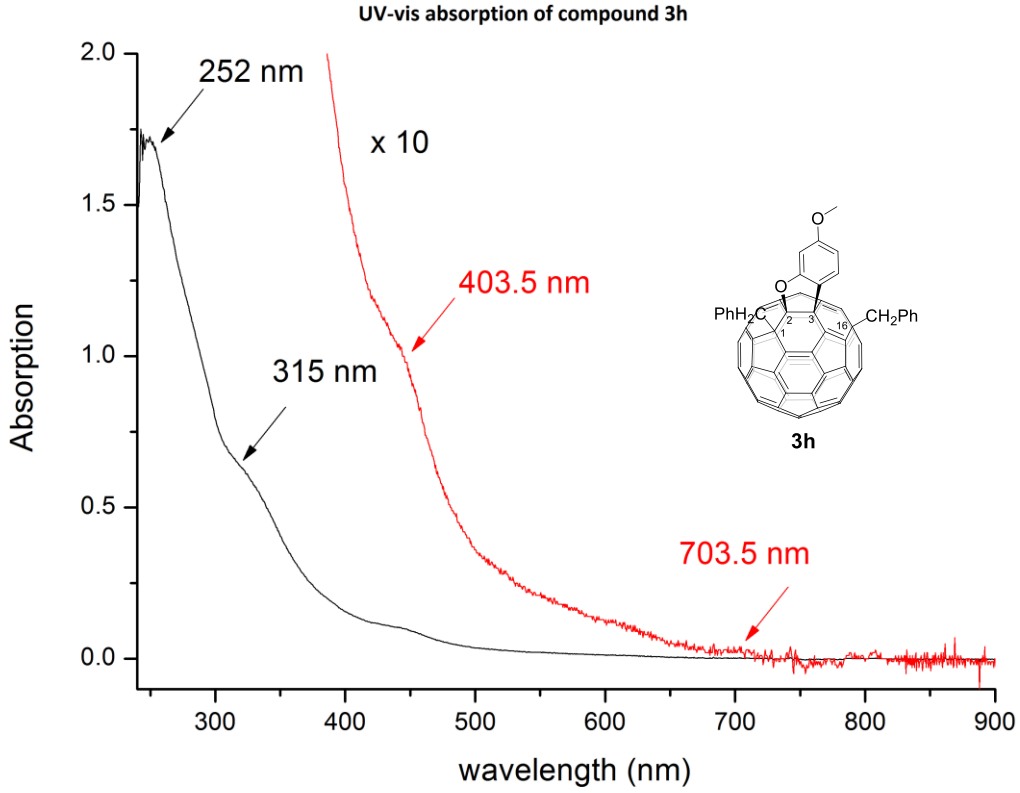


Expanded ^{13}C NMR (100 MHz, CS_2/acetone-d_6) of compound 3h

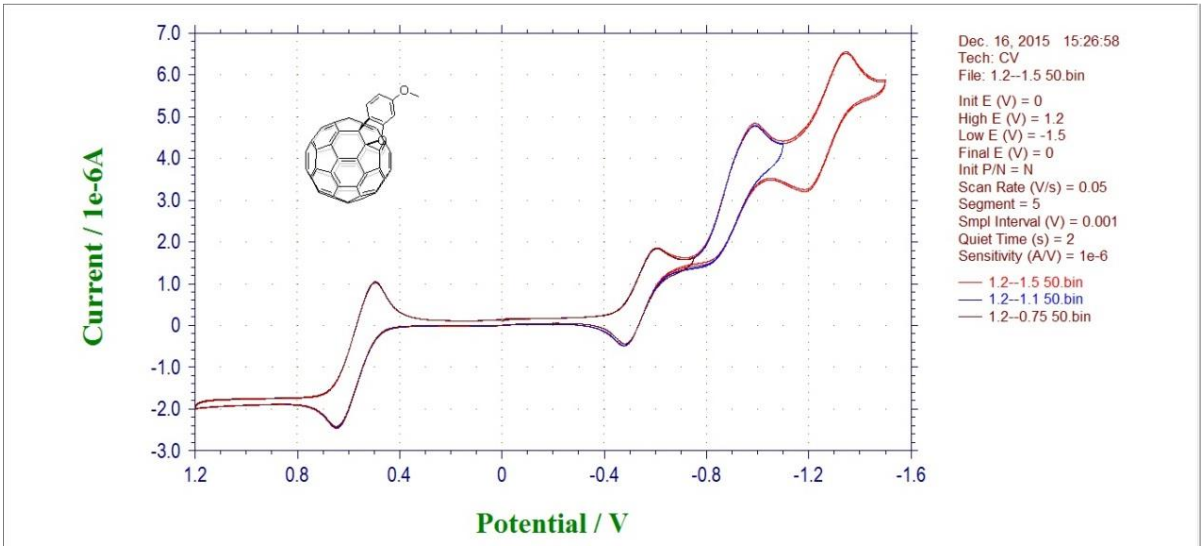


Expanded ^{13}C NMR (100 MHz, CS_2/acetone-d_6) of compound 3h




UV-vis absorption of compound 3h
252 nm
x 10
403.5 nm
315 nm
703.5 nm
Absorption
wavelength (nm)
3h

CV of **2h**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Potential / V
Dec. 16, 2015 15:26:58
Tech: CV
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High E (V) = 1.2
Low E (V) = -1.5
Final E (V) = 0
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Scan Rate (V/s) = 0.05
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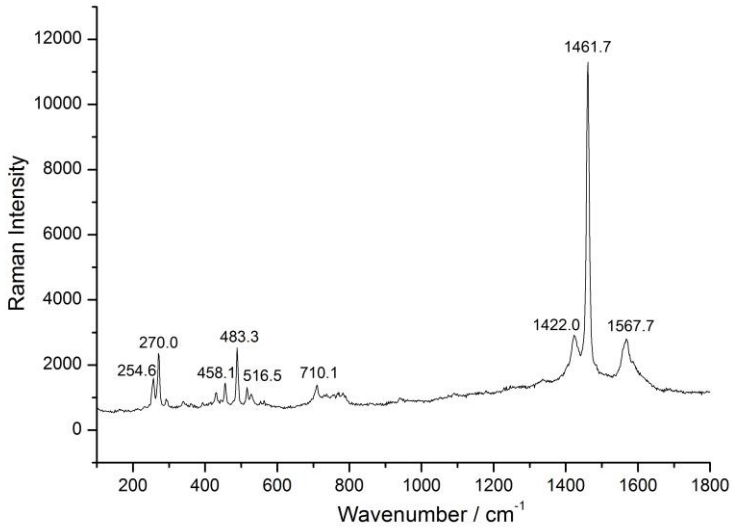
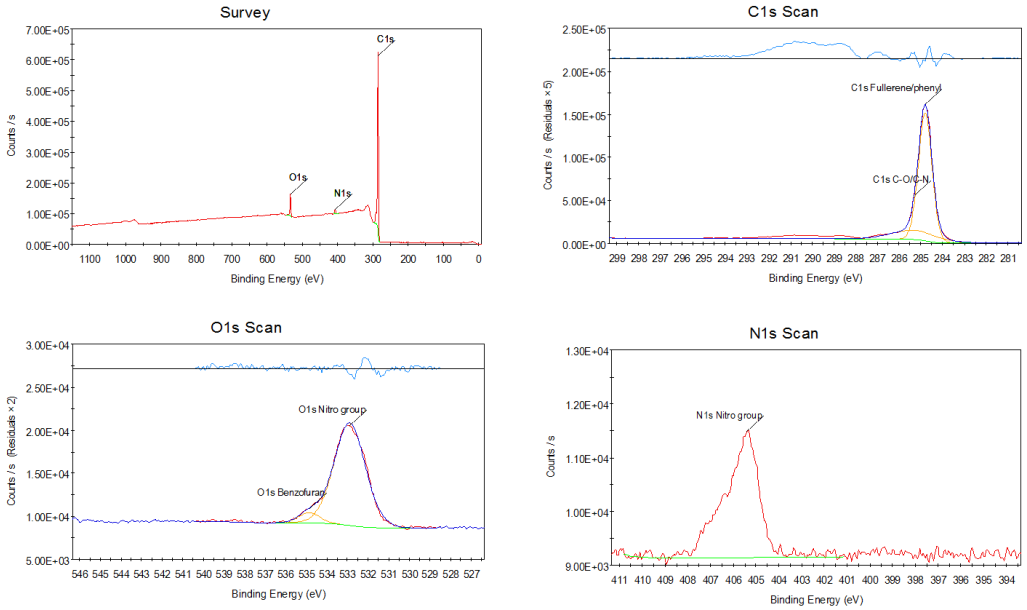
Smpl Interval (V) = 0.001
Quiet Time (s) = 2
Sensitivity (A/V) = 1e-6
1.2--1.5 50.bin
1.2--1.1 50.bin
1.2--0.75 50.bin

Raman spectrum of **2a**



XPS spectrum and peak table of **2a**



Peak Table						
Name	Start BE	Peak BE	End BE	Height CPS	FWHM eV	Area (P) CPS.eV
C1s Fullerene/phenyl	299.37	284.8	280.37	149649.58	0.73	117714.71
C1s C–O/C–N	299.37	285.32	280.37	11103.09	2.4	28832.24
N1s Nitro group	410.8	405.4	401.15	2292.96	1.62	4356.84
O1s Nitro group	540.4	532.89	528.55	11921.59	1.78	22943.62
O1s Benzofuran	540.4	534.85	528.55	1233.78	1.17	1566.9