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Electronic Supplementary Information

Palladium-catalyzed 1,4-aminoarylation of [60]fullerene with aryl iodides, *N*-methoxysulfonamides and further transformations

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Table of Content

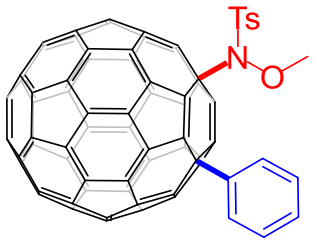
Experimental procedures and characterization data.

General information. Unless otherwise specified, NMR spectra were recorded on a 300 MHz, 400 MHz or 600 MHz (300 MHz, 400 MHz or 600 MHz for ^{1}H NMR, respectively; 75 MHz, 100 MHz or 150 MHz for ^{13}C NMR, respectively) spectrometer at room temperature. ^{1}H NMR spectra were referenced to TMS at 0.00 ppm, while ^{13}C NMR spectra were referenced to $CDCl_3$ at 77.16 ppm, DMSO-d_6 at 39.52 ppm, $C_2D_2Cl_4$ at 72.95 ppm, respectively. Data were represented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (*J*, Hz), and integration. FT-IR spectra were measured in KBr pellets from 4000 to 500 cm^{-1}. UV−vis spectra in $CHCl_3$ were recorded in a 1.0 cm quartz cuvette at 25 °C. High-resolution mass spectra (HRMS) were obtained by MALDI-TOF with trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as the matrix and in positive mode. Compounds **4a** and **4b** are known compounds, and their ^{1}H NMR data are consistent with those reported in the literature.[1,2]

Procedures for the synthesis of products 3a–j and 4a–e.

General procedure for the synthesis of products 3a–j.

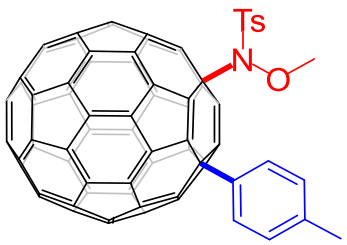
To a 35 mL tube containing a solution of C_{60} (36.0 mg, 0.05 mmol) in 1,2-$C_6H_4Cl_2$ (4 mL) were added aryl iodides **1** (0.10 mmol), *N*-methoxyl sulfonamides **2** (0.10 mmol), Ag(TFA) (22.1 mg, 0.10 mmol), TFA (100 μL) and $Pd(OAc)_2$ (1.7 mg, 0.0075 mmol), then sealed tightly in air and stirred in an oil bath. After being stirred at 100 °C for 2 h (5 h for **3f**). The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60}, subsequent elution with carbon disulfide/dichloromethane (4/1, v/v) afforded compounds **3**.



3a

Compound 3a: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with iodobenzene **1a** (20.4 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (14.9 mg, 41%) and then **3a** (16.4 mg, 33%) as an amorphous black solid: mp >300 °C. Spectral data of **3a**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.16 (d, J = 7.5 Hz, 2H), 8.01 (d, J = 8.0 Hz, 2H), 7.58 (t, J = 7.4 Hz, 2H), 7.48 (t, J = 7.2 Hz, 1H), 7.27 (d, J = 8.0

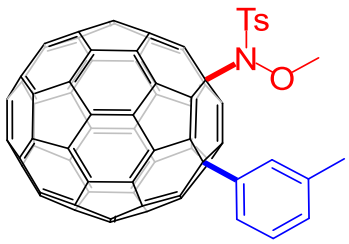
Hz, 2H), 3.80 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with Cr(acac)$_3$ as relaxation reagent) δ 154.95, 152.32, 150.03, 148.51, 148.11, 147.34, 147.16, 146.75, 146.71, 146.61, 146.60, 146.55, 146.46, 146.24, 145.34, 145.26, 145.15, 144.93, 144.71, 144.61, 144.53, 144.38, 144.13, 144.07, 144.00, 143.96, 143.81, 143.70, 143.65, 143.38, 143.27, 143.13, 143.09, 143.00, 142.86, 142.70, 142.56, 142.52, 142.49, 142.30, 142.14, 142.08, 142.02, 141.94, 141.85, 141.80, 140.63, 140.03, 139.64, 139.26, 138.87, 137.54, 137.09, 133.28, 130.05, 128.94, 128.82, 128.03, 127.43, 70.65, 65.51, 61.23, 21.56; ^{1}H NMR (600 MHz, 340 K, $C_2D_2Cl_4$) δ 8.14 (d, J = 7.4 Hz, 2H), 7.98 (d, J = 8.2 Hz, 2H), 7.58 (t, J = 7.7 Hz, 2H), 7.49 (t, J = 7.4 Hz, 1H), 7.27 (d, J = 8.2 Hz, 2H), 3.77 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, 340 K, $C_2D_2Cl_4$ with Cr(acac)$_3$ as relaxation reagent) δ 154.37, 151.69, 149.49, 147.76, 147.35, 146.58, 146.45, 146.25, 146.01, 145.93, 145.87, 145.81, 145.75, 145.73, 145.70, 145.47, 145.35, 144.56, 144.47, 144.43, 144.36, 144.10, 143.78, 143.76, 143.59, 143.33, 143.27, 143.20, 143.18, 143.04, 142.93, 142.89, 142.62, 142.53, 142.35, 142.29, 142.22, 142.08, 141.92, 141.84, 141.71, 141.48, 141.36, 141.28, 141.22, 141.14, 141.09, 141.02, 139.80, 139.29, 139.06, 138.53, 138.06, 136.77, 136.22, 132.48, 129.11, 128.20, 127.30, 126.52, 70.11, 64.94, 60.53, 20.68; ^{1}H NMR (400 MHz, 240 K, CS_2/$CDCl_3$) δ 8.21 (d, J = 7.2 Hz, 1H), 8.09–7.99 (m, 3H), 7.65–7.55 (m, 2H), 7.55–7.47 (m, 1H), 7.38–7.29 (m, 2H), 3.80 (s, 2H), 3.77 (s, 1H), 2.48 (s, 2H), 2.44 (s, 1H); ^{13}C NMR (100 MHz, 240 K, CS_2/$CDCl_3$ with Cr(acac)$_3$ as relaxation reagent) δ 155.00, 154.27, 152.56, 152.07, 150.39, 149.64, 148.41, 148.01, 147.98, 147.37, 147.20, 147.05, 146.85, 146.82, 146.61, 146.49, 146.38, 146.32, 146.26, 146.13, 145.79, 145.22, 145.13, 145.05, 144.78, 144.49, 144.45, 144.34, 144.28, 144.24, 144.19, 144.05, 143.99, 143.94, 143.84, 143.76, 143.73, 143.61, 143.59, 143.50, 143.40, 143.33, 143.22, 143.07, 143.03, 142.96, 142.90, 142.85, 142.75, 142.63, 142.55, 142.52, 142.41, 142.37, 142.01, 141.95, 141.88, 141.82, 141.73, 141.58, 140.62, 140.47, 140.23, 140.01, 139.68, 139.28, 139.20, 139.16, 138.62, 138.31, 137.43, 137.27, 137.17, 136.96, 132.39, 132.33, 130.03, 129.86, 129.01, 128.95, 128.86, 128.10, 127.96, 127.39, 127.33, 70.40, 65.67, 65.53, 61.12, 60.93, 21.73; FT-IR ν/cm^{-1} (KBr) 2924, 1593, 1427, 1356, 1164, 1084, 1006, 809, 734, 673, 561, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.99), 322 (4.47), 445 (3.75); MALDI-TOF MS m/z calcd. for $C_{66}H_5$ [M-TsNOCH$_3$]$^+$ 797.0386, found 797.0385.



3b

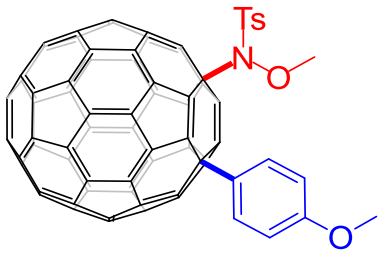
Compound 3b: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-iodo-4-methylbenzene **1b** (21.8 mg, 0.10 mmol) and *N*-methoxy-4-

methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (13.8 mg, 38%) and then **3b** (16.2 mg, 32%) as an amorphous black solid: mp >300 °C. Spectral data of **3b**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.09 (d, J = 7.6 Hz, 2H), 8.05 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 7.9 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 3.88 (s, 3H), 2.53 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 148.43, 148.01, 147.30, 147.05, 146.67, 146.63, 146.51, 146.37, 146.16, 145.25, 145.17, 145.06, 144.87, 144.52, 144.45, 144.31, 144.07, 143.97, 143.94, 143.88, 143.75, 143.67, 143.64, 143.56, 143.29, 143.24, 143.05, 142.99, 142.92, 142.75, 142.63, 142.44, 142.40, 142.18, 142.05, 141.95, 141.88, 141.80, 141.73, 140.53, 139.88, 139.20, 138.71, 137.51, 137.38, 136.97, 136.64, 133.37, 129.99, 129.55, 128.69, 127.33, 70.53, 65.46, 60.99, 21.51, 21.10; FT-IR ν/cm^{-1} (KBr) 2922, 1594, 1506, 1427, 1357, 1164, 1083, 1009, 809, 673, 563, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.99), 322 (4.49), 445 (3.78); MALDI-TOF MS m/z calcd. for $C_{67}H_7$ [M-$TsNOCH_3$]$^+$ 811.0542, found 811.0538.



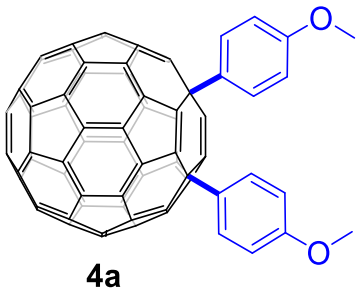
3c

Compound 3c: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-iodo-3-methylbenzene **1c** (21.8 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (15.2 mg, 42%) and then **3c** (14.9 mg, 29%) as an amorphous black solid: mp >300 °C. Spectral data of **3c**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.14 (s, 1H), 8.07 (d, J = 8.1 Hz, 2H), 8.02 (d, J = 7.3 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.35 (d, J = 7.6 Hz, 1H), 7.31 (d, J = 8.1 Hz, 2H), 3.92 (s, 3H), 2.60 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 154.94, 152.52, 150.15, 148.54, 148.12, 147.43, 147.13, 146.78, 146.73, 146.69, 146.63, 146.58, 146.48, 146.26, 145.36, 145.27, 145.16, 144.90, 144.70, 144.64, 144.40, 144.16, 144.07, 144.05, 143.98, 143.84, 143.76, 143.73, 143.66, 143.39, 143.15, 143.10, 143.03, 142.85, 142.73, 142.54, 142.50, 142.26, 142.15, 142.13, 142.05, 141.95, 141.89, 141.83, 140.63, 139.98, 139.58, 139.34, 138.76, 138.67, 137.48, 137.22, 133.34, 130.01, 128.87, 128.84, 128.78, 128.30, 124.55, 70.69, 65.63, 61.36, 21.55, 21.48; FT-IR ν/cm^{-1} (KBr) 2920, 1597, 1428, 1356, 1166, 1086, 1009, 811, 761, 674, 563, 528; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 257 (4.99), 322 (4.49), 445 (3.77); MALDI-TOF MS m/z calcd. for $C_{67}H_7$ [M-$TsNOCH_3$]$^+$ 811.0542, found 811.0541.



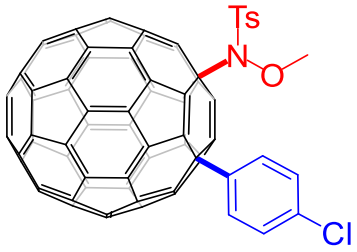
3d

Compounds 3d and 4a: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-iodo-4-methoxybenzene **1d** (23.4 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (7.8 mg, 22%), then **3d** (13.1 mg, 25%) and **4a** (4.6 mg, 10%) as amorphous black solids: mp >300 °C. Spectral data of **3d**: ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 8.15 (d, J = 8.1 Hz, 2H), 8.08 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.2 Hz, 2H), 7.16 (d, J = 8.7 Hz, 2H), 3.96 (s, 3H), 3.91 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CS_2/CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 158.89, 154.76, 148.18, 147.76, 147.08, 146.69, 146.42, 146.37, 146.27, 146.25, 146.22, 146.12, 145.90, 145.00, 144.92, 144.81, 144.34, 144.25, 144.03, 143.81, 143.70, 143.64, 143.50, 143.46, 143.42, 143.29, 143.03, 142.79, 142.67, 142.49, 142.37, 142.18, 142.15, 141.91, 141.79, 141.69, 141.63, 141.55, 141.46, 140.26, 139.62, 138.93, 138.40, 137.10, 136.67, 132.98, 131.39, 129.72, 128.52, 128.28, 113.96, 70.27, 65.36, 60.37, 54.77, 21.29; FT-IR ν/cm^{-1} (KBr) 2927, 1602, 1508, 1458, 1432, 1358, 1300, 1253, 1169, 1086, 1031, 1012, 814, 678, 564, 529; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 260 (4.98), 322 (4.51), 444 (3.79); MALDI-TOF MS m/z calcd. for $C_{67}H_7O$ $[M\text{-}TsNOCH_3]^+$ 827.0491, found 827.0493.



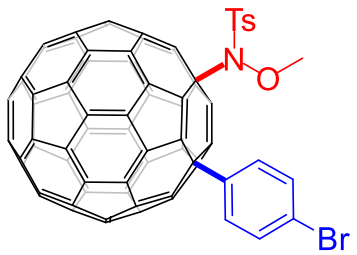
4a

Spectral data of **4a**:[1] ^{1}H NMR (400 MHz, $CS_2/CDCl_3$) δ 7.97 (d, J = 7.9 Hz, 4H), 7.00 (d, J = 7.9 Hz, 4H), 3.85 (s, 6H).



3e

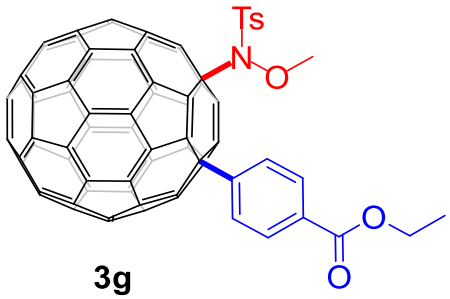
Compound 3e: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-chloro-4-iodobenzene **1e** (23.8 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (21.4 mg, 59%) and then **3e** (12.0 mg, 23%) as an amorphous black solid: mp >300 °C. Spectral data of **3e**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.16 (d, J = 7.8 Hz, 2H), 8.06 (d, J = 8.3 Hz, 2H), 7.59 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.3 Hz, 2H), 3.88 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 154.21, 148.49, 148.12, 147.22, 146.89, 146.71, 146.70, 146.60, 146.45, 146.34, 146.24, 145.34, 145.26, 145.11, 144.85, 144.64, 144.37, 144.31, 144.06, 143.92, 143.73, 143.71, 143.64, 143.55, 143.33, 143.09, 143.02, 142.98, 142.87, 142.65, 142.51, 142.35, 142.10, 142.03, 142.00, 141.89, 141.76, 140.68, 140.00, 139.11, 139.06, 138.16, 137.64, 137.12, 134.10, 133.06, 130.01, 129.01 128.83, 128.77, 70.57, 65.58, 60.38, 21.53; FT-IR ν/cm^{-1} (KBr) 2922, 1594 1487, 1429, 1358, 1167, 1089, 1012, 813, 674, 563, 529; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (4.99), 323 (4.51), 445 (3.79); MALDI-TOF MS m/z calcd. for $C_{66}H_4{}^{35}Cl$ [M-TsNOCH$_3$]$^+$ 830.9996, found 830.9995.



3f

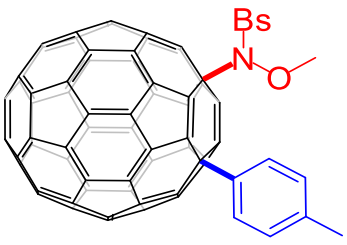
Compound 3f: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-bromo-4-iodobenzene **1f** (28.3 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (20.7 mg, 58%) and then **3f** (11.7 mg, 22%) as an amorphous black solid: mp >300 °C. Spectral data of **3f**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.14 (d, J = 7.1 Hz, 2H), 8.09 (d, J = 8.1 Hz, 2H), 7.79 (d, J = 8.5 Hz, 2H), 7.38 (d, J = 8.1 Hz, 2H), 3.92 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 153.94, 151.59, 149.05, 148.29, 147.93, 147.03, 146.70, 146.51, 146.40, 146.25, 146.14, 146.04, 145.15, 145.07, 144.91, 144.64, 144.45, 144.16, 144.12, 143.87, 143.72, 143.51, 143.46, 143.35, 143.13, 142.90, 142.83, 142.79, 142.68, 142.46, 142.31,

142.15, 141.91, 141.83, 141.80, 141.70, 141.56, 140.48, 139.80, 138.93, 138.86, 138.49, 137.45, 136.94, 132.90, 131.80, 129.83, 128.91, 128.65, 122.17, 70.37, 65.40, 60.24, 21.38. FT-IR ν/cm^{-1} (KBr) 2964, 2922, 1513, 1485, 1430, 1385, 1355, 1262, 1166, 1088, 1010, 897, 809, 732, 679, 563, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (4.99), 323 (4.51), 445 (3.79); MALDI-TOF MS *m/z* calcd. for $C_{66}H_4{}^{79}Br$ [M-$TsNOCH_3$]$^+$ 874.9491, found 874.9489.



3g

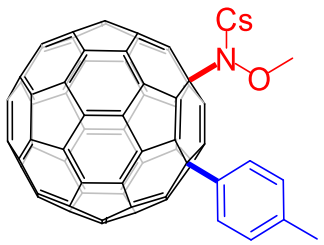
Compound 3g: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with ethyl 4-iodobenzoate **1g** (27.6 mg, 0.10 mmol), *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol) afforded first recovered C_{60} (15.9 mg, 44%) and then **3g** (10.2 mg, 19%) as an amorphous black solid: mp >300 °C. Spectral data of **3g**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.24 (bs, 4H), 8.00 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 4.43 (q, J = 7.1 Hz, 2H), 3.79 (s, 3H), 2.45 (s, 3H), 1.46 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 165.41 (*C*=O), 148.45, 148.09, 147.15, 146.96, 146.67, 146.56, 146.41, 146.32, 146.20, 145.30, 145.22, 145.07, 144.90, 144.61, 144.29, 144.28, 144.03, 144.01, 143.87, 143.67, 143.65, 143.61, 143.49, 143.29, 143.05, 142.93, 142.84, 142.61, 142.57, 142.53, 142.46, 142.06, 141.94, 141.85, 141.70, 140.64, 140.00, 139.12, 139.03, 137.63, 137.14, 132.91, 130.03, 129.96, 128.82, 127.28, 70.56, 65.53, 60.87, 60.79, 21.48, 14.11; FT-IR ν/cm^{-1} (KBr) 2923, 2853, 1715, 1605, 1455, 1431, 1359, 1272, 1166, 1104, 1018, 809, 745, 675, 562, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.98), 322 (4.74), 444 (3.74); MALDI-TOF MS *m/z* calcd. for $C_{69}H_9O_2$ [M-$TsNOCH_3$]$^+$ 869.0597, found 869.0601.



3h

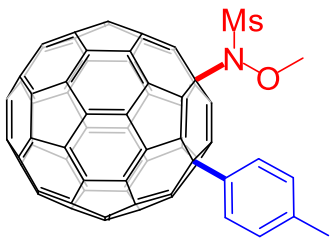
Compound 3h: According to the general procedure, the reaction of C_{60} (36.0 mg,

0.05 mmol) with 1-iodo-4-methylbenzene **1b** (21.8 mg, 0.10 mmol) and *N*-methoxybenzenesulfonamide **2b** (18.7 mg, 0.10 mmol) afforded first recovered C_{60} (15.6 mg, 43%) and then **3h** (15.3 mg, 31%) as an amorphous black solid: mp >300 °C. Spectral data of **3h**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.15 (d, J = 7.8 Hz, 2H), 8.08–8.00 (m, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.49 (t, J = 7.7 Hz, 2H), 7.39 (d, J = 7.7 Hz, 2H), 3.86 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 148.49, 148.06, 147.28, 147.10, 146.72, 146.68, 146.57, 146.55, 146.50, 146.42, 146.20, 145.31, 145.22, 145.11, 144.53, 144.51, 144.32, 144.09, 144.00, 143.96, 143.93, 143.80, 143.72, 143.69, 143.58, 143.32, 143.08, 143.04, 142.97, 142.80, 142.67, 142.48, 142.45, 142.21, 142.10, 142.06, 141.98, 141.92, 141.83, 141.76, 140.57, 139.95, 139.30, 137.64, 137.38, 136.94, 136.70, 136.23, 133.72, 129.93, 129.59, 128.18, 127.27, 70.61, 65.69, 61.03, 21.06; FT-IR ν/cm^{-1} (KBr) 2920, 2849, 1507, 1429, 1359, 1171, 1086, 1012, 755, 725, 686, 564, 528; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.99), 328 (4.50), 443 (3.74); MALDI-TOF MS m/z calcd. for $C_{67}H_7$ [M-$BsNOCH_3$]$^+$ 811.0542, found 811.0536.



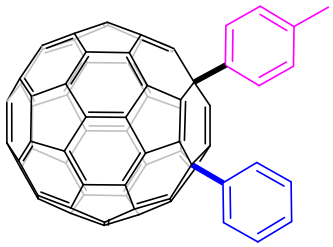
3i

Compound 3i: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-iodo-4-methylbenzene **1b** (21.8 mg, 0.10 mmol) and *N*-methoxy-4-chlorobenzenesulfonamide **2c** (22.2 mg, 0.10 mmol) afforded first recovered C_{60} (14.3 mg, 40%) and then **3i** (16.5 mg, 32%) as an amorphous black solid: mp >300 °C. Spectral data of **3i:** ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.09 (d, J = 8.5 Hz, 2H), 8.09–8.01 (m, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 3.96 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 155.22, 148.62, 148.17, 147.25, 146.83, 146.80, 146.67, 146.66, 146.55, 146.51, 146.43, 146.32, 145.43, 145.33, 145.28, 144.62, 144.55, 144.40, 144.18, 144.13, 144.05, 143.92, 143.84, 143.82, 143.76, 143.67, 143.42, 143.18, 143.10, 142.93, 142.78, 142.61, 142.59, 142.54, 142.22, 142.12, 142.09, 142.07, 141.92, 141.85, 140.75, 140.63, 140.13, 139.50, 137.82, 137.41, 136.95, 136.75, 134.58, 131.38, 129.70, 128.47, 127.24, 70.73, 65.89, 61.10, 21.14; FT-IR ν/cm^{-1} (KBr) 2922, 1577, 1506, 1468, 1428, 1363, 1171, 1086, 1010, 822, 756, 651, 564, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 256 (4.99), 328 (4.48), 441 (3.72); MALDI-TOF MS m/z calcd. for $C_{67}H_7$ [M-$CsNOCH_3$]$^+$ 811.0542, found 811.0537.



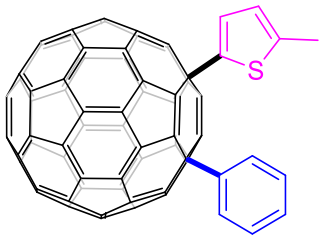
3j

Compound 3j: According to the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with 1-iodo-4-methylbenzene **1b** (21.8 mg, 0.10 mmol) and *N*-methoxymethanesulfonamide **2d** (12.5 mg, 0.10 mmol) afforded first recovered C_{60} (17.3 mg, 48%) and then **3j** (13.9 mg, 30%) as an amorphous black solid: mp >300 °C. Spectral data of **3j**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.15 (d, J =7.7 Hz, 2H), 7.40 (d, J = 7.7 Hz, 2H), 3.95 (s, 3H), 3.36 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 148.70, 148.21, 147.39, 147.33, 146.88, 146.70, 146.61, 146.54, 146.40, 145.46, 145.38, 144.66, 144.39, 144.23, 144.13, 144.08, 143.98, 143.95, 143.80, 143.68, 143.57, 143.25, 143.20, 143.17, 142.96, 142.83, 142.72, 142.69, 142.67, 142.28, 142.19, 142.14, 142.12, 142.05, 141.86, 140.81, 140.60, 139.60, 137.94, 136.95, 136.77, 129.86, 127.19, 70.77, 66.01, 61.25, 36.12, 21.11; FT-IR ν/cm^{-1} (KBr) 2920, 2849, 1507, 1429, 1359, 1171, 1086, 1012, 755, 725, 686, 641, 564, 528; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 259 (4.98), 318 (4.49), 445 (3.75); MALDI-TOF MS m/z calcd. for $C_{67}H_7$ [M-MsNOCH$_3$]$^+$ 811.0542, found 811.0539.



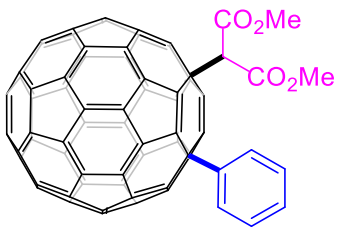
4b

Compound 4b: To a solution of **3a** (20.0 mg, 0.02 mmol) in 4 mL of toluene was added $FeCl_3$ (3.2 mg, 0.02 mmol). The reaction mixture was stirred at 80 °C for 0.5 h. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give compound **4b** (16.4 mg, 92%) as an amorphous black solid: mp >300 °C. Spectral data of **4b**:[2] ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.07 (d, J = 7.2 Hz, 2H), 7.92 (d, J = 8.0 Hz, 2H), 7.48 (t, J = 7.4 Hz, 2H), 7.41 (t, J = 7.3 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 2.43 (s, 3H).



4c

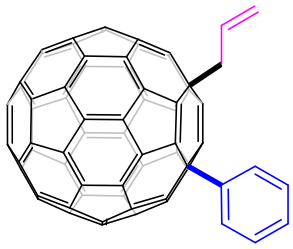
Compound 4c: To a solution of **3a** (20.0 mg, 0.02 mmol) and 2-methylthiophene (3.9 mg, 0.04 mmol) in 4 mL of 1,2-$C_6H_4Cl_2$ was added $FeCl_3$ (3.2 mg, 0.02 mmol). The reaction mixture was stirred at 80 ℃ for 0.5 h. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give compound **4c** (17.0 mg, 95%) as an amorphous black solid: mp >300 ℃. Spectral data of **4c**: ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) δ 8.13 (d, J = 7.4 Hz, 2H), 7.54 (t, J = 7.5 Hz, 2H), 7.45 (t, J = 7.3 Hz, 1H), 7.22 (d, J = 3.2 Hz, 1H), 6.75 (d, J = 3.2 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent) δ 155.52, 154.74, 149.77, 149.37, 147.54, 147.51, 147.40, 146.86, 146.00, 145.99, 145.88, 145.84, 145.71, 145.69, 145.67, 145.48, 144.44, 144.43, 144.23, 144.05, 143.93, 143.63, 143.60, 143.29, 143.24, 143.18, 143.15, 143.10, 143.09, 143.01, 142.96, 142.91, 142.84, 142.80, 142.78, 142.74, 142.12, 142.06, 142.04, 142.03, 141.89, 141.61, 141.48, 141.46, 141.40, 141.19, 141.15, 140.94, 140.26, 139.95, 139.23, 138.98, 137.88, 137.38, 136.20, 136.10, 128.49, 127.45, 126.51, 125.05, 124.77, 60.50, 56.38, 14.73; FT-IR ν/cm^{-1} (KBr) 2919, 2850, 1490, 1428, 1262, 1226, 1185, 859, 795, 761, 733, 692, 587, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 260 (4.99), 324 (4.45), 445 (3.75); MALDI-TOF MS m/z calcd for $C_{71}H_{10}S$ $[M]^+$ 894.0498, found 894.0501.



4d

Compound 4d: To a solution of **3a** (20.0 mg, 0.02 mmol) and dimethyl malonate (5.3 mg, 0.04 mmol) in 4 mL of 1,2-$C_6H_4Cl_2$ was added $FeCl_3$ (6.5 mg, 0.04 mmol). The reaction mixture was stirred at 80 ℃ for 2 h. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide/dichloromethane (4/1, v/v) as the eluent to give compound **4d** (13.0 mg, 70%) as an amorphous black solid: mp >300 ℃. Spectral data of **4d**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) δ 8.31 (d, J = 7.2 Hz, 2H), 7.67 (t, J = 7.7 Hz, 2H), 7.54 (t, J = 7.4, 1H), 4.83 (s, 1H), 3.79 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, CS_2/DMSO-d_6 with Cr(acac)$_3$ as relaxation reagent) δ

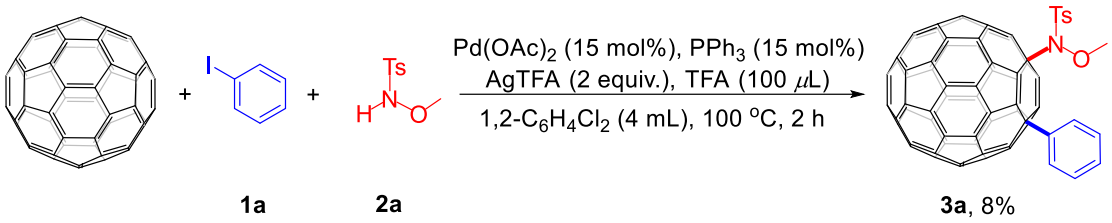
166.55 (*C*=O), 166.39 (*C*=O), 157.00, 152.21, 150.41, 148.77, 148.75, 148.57, 148.34, 148.10, 147.94, 147.22, 147.02, 146.98, 146.79, 146.59, 146.41, 145.62, 145.59, 145.56, 145.29, 144.96, 144.72, 144.71, 144.65, 144.45, 144.44, 144.42, 144.26, 144.25, 144.09, 144.05, 143.98, 143.88, 143.86, 143.43, 143.39, 143.37, 143.34, 143.31, 143.19, 143.16, 143.10, 142.84, 142.74, 142.56, 142.55, 142.34, 142.23, 142.15, 142.12, 141.19, 140.99, 140.77, 140.39, 139.14, 139.06, 136.66, 129.75, 128.45, 127.08, 61.55, 60.85, 56.06, 52.95, 52.92; FT-IR ν/cm^{-1} (KBr) 2960, 2920, 1759, 1737, 1492, 1431, 1310, 1261, 1214, 1150, 1097, 1022, 802, 735, 695, 584, 527; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 260 (5.00), 328 (4.46), 445 (3.78); MALDI-TOF MS *m*/*z* calcd for $C_{71}H_{12}O_4$ $[M]^+$ 928.0730 found 928.0733.



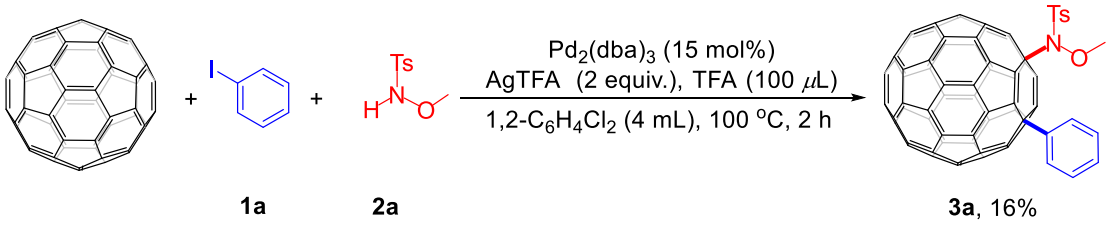
4e

Compound 4e: To a solution of **3a** (20.0 mg, 0.02 mmol) and allyltrimethylsilane (4.6 mg, 0.04 mmol) in 4 mL of 1,2-$C_6H_4Cl_2$ was added $FeCl_3$ (3.2 mg, 0.02 mmol). The reaction mixture was stirred at 80 ℃ for 0.5 h. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give compound **4e** (13.1 mg, 78%) as an amorphous black solid: mp >300 ℃. Spectral data of **4e**: ^{1}H NMR (400 MHz, CS_2/$CDCl_3$) 8.28 (d, J = 7.3 Hz, 2H), 7.64 (t, J = 7.7 Hz, 2H), 7.51 (t, J = 7.4 Hz, 1H), 6.48-6.35 (m, 1H), 5.43 (d, J = 16.8 Hz, 1H), 5.25 (d, J = 9.9 Hz, 1H), 3.72 (dd, J = 13.4, 7.4 Hz, 1H), 3.65 (dd, J = 13.4, 7.4 Hz, 1H); ^{13}C NMR (100 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) δ 156.21, 155.43, 150.19, 149.71, 147.52, 147.47, 147.46, 147.37, 146.31, 146.07, 145.92, 145.83, 145.77, 145.73, 145.69, 145.57, 144.86, 144.40, 144.34, 144.03, 143.94, 143.93, 143.75, 143.72, 143.58, 143.46, 143.25, 143.23, 143.21, 143.19, 143.11, 143.05, 142.94, 142.92, 142.85, 142.82, 142.72, 142.65, 142.06, 142.04, 142.02, 141.98, 141.89, 141.56, 141.55, 141.45, 141.37, 141.33, 141.09, 141.05, 140.87, 139.83, 139.74, 137.98, 137.57, 137.45, 135.95, 131.59, 128.65, 127.42, 126.23, 119.15, 60.43, 57.83, 45.11; FT-IR ν/cm^{-1} (KBr) 2919, 2850, 1488, 1425, 1184, 988, 918, 732, 693, 581, 525; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 258 (4.97), 327 (4.46), 445 (3.77); MALDI-TOF MS *m*/*z* calcd for $C_{69}H_{10}$ $[M]^+$ 838.0777, found 838.0780.

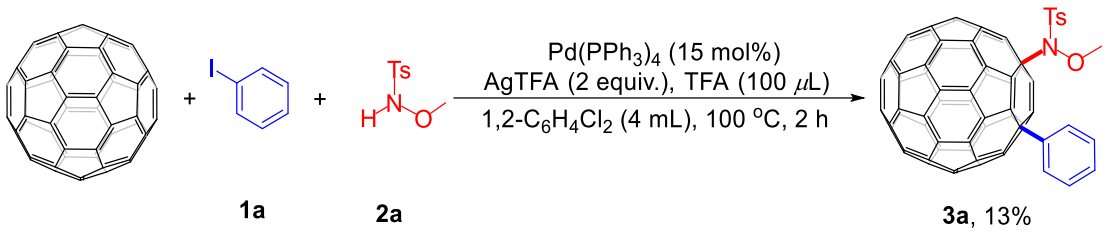
Control experiments.



To a 35 mL tube containing a solution of C_{60} (36.0 mg, 0.05 mmol) in 1,2-$C_6H_4Cl_2$ (4 mL) were added iodobenzene **1a** (20.4 mg, 0.10 mmol), *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol), Ag(TFA) (22.1 mg, 0.10 mmol), TFA (100 μL), $Pd(OAc)_2$ (1.7 mg, 0.0075 mmol) and PPh_3 (2.0 mg, 0.0075 mmol), then sealed tightly in air and stirred in an oil bath. After being stirred at 100 °C for 2 h. The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to first give recovered C_{60} (28.1 mg, 78%), and then subsequent elution with carbon disulfide/dichloromethane (4/1, v/v) to give **3a** (4.0 mg, 8%).



To a 35 mL tube containing a solution of C_{60} (36.0 mg, 0.05 mmol) in 1,2-$C_6H_4Cl_2$ (4 mL) were added iodobenzene **1a** (20.4 mg, 0.10 mmol), *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol), Ag(TFA) (22.1 mg, 0.10 mmol), TFA (100 μL) and $Pd_2(dba)_3$ (6.9 mg, 0.0075 mmol), then sealed tightly in air and stirred in an oil bath. After being stirred at 100 °C for 2 h. The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to first give recovered C_{60} (24.1 mg, 67%), and then subsequent elution with carbon disulfide/dichloromethane (4/1, v/v) to give **3a** (8.1 mg, 16%).



To a 35 mL tube containing a solution of C_{60} (36.0 mg, 0.05 mmol) in 1,2-$C_6H_4Cl_2$ (4 mL) were added iodobenzene **1a** (20.4 mg, 0.10 mmol) and *N*-methoxy-4-methylbenzenesulfonamide **2a** (20.1 mg, 0.10 mmol), Ag(TFA) (22.1 mg, 0.10 mmol), TFA (100 μL) and $Pd(PPh_3)_4$ (8.7 mg, 0.0075 mmol), then sealed tightly in air and stirred in an oil bath. After being stirred at 100 ℃ for 2 h. The reaction mixture was filtered through a silica gel plug in order to remove any insoluble material. After evaporation in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to first give recovered C_{60} (25.9 mg, 72%), and then subsequent elution with carbon disulfide/dichloromethane (4/1, v/v) to give **3a** (6.6 mg, 13%).

NMR spectra of compounds 3a–j and 4a–e

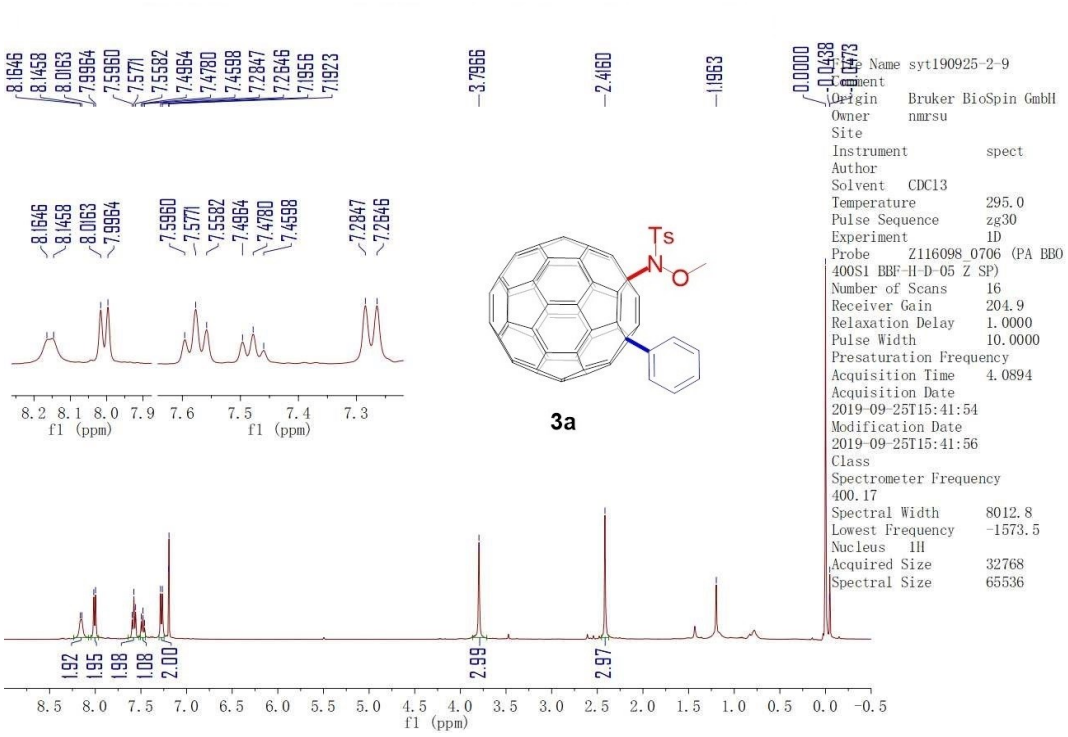


Figure S1. ^{1}H NMR spectrum (400 MHz, CS_2/$CDCl_3$) of compound **3a**.

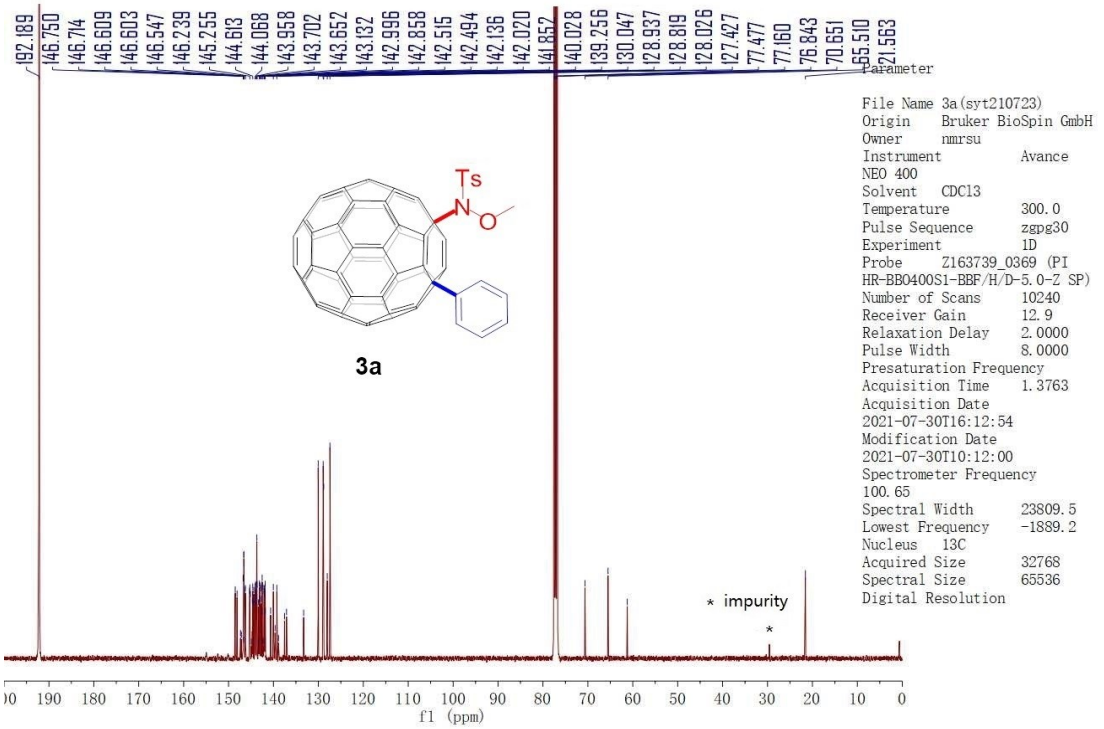


Figure S2. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3a**.

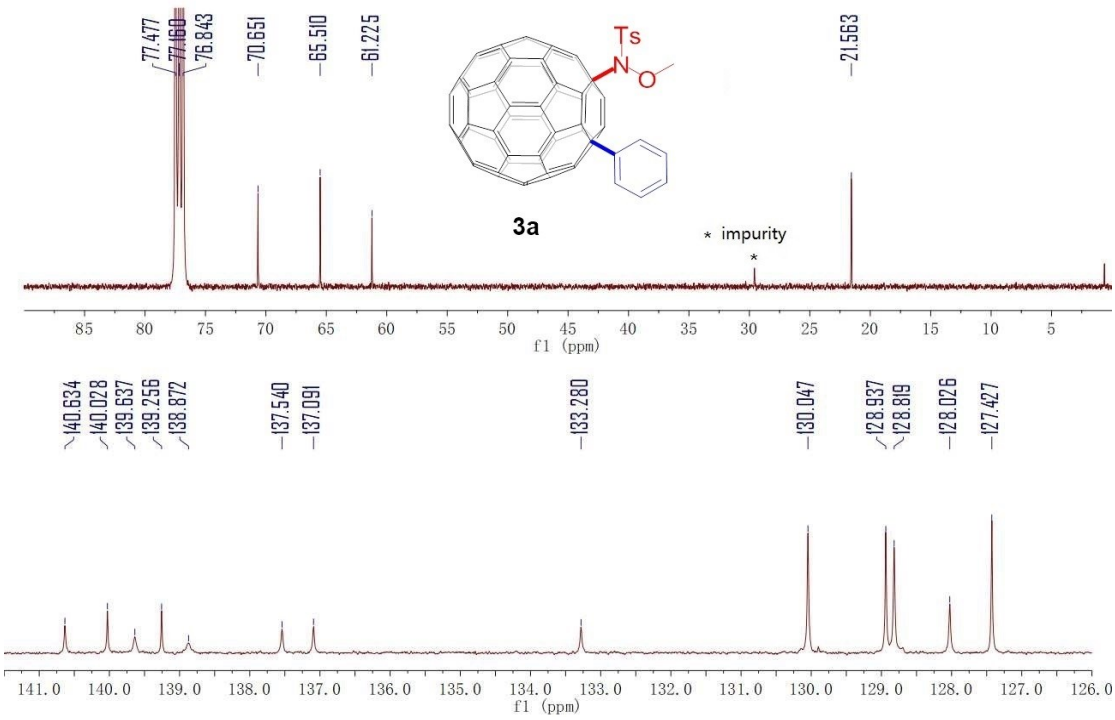


Figure S3. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3a**.

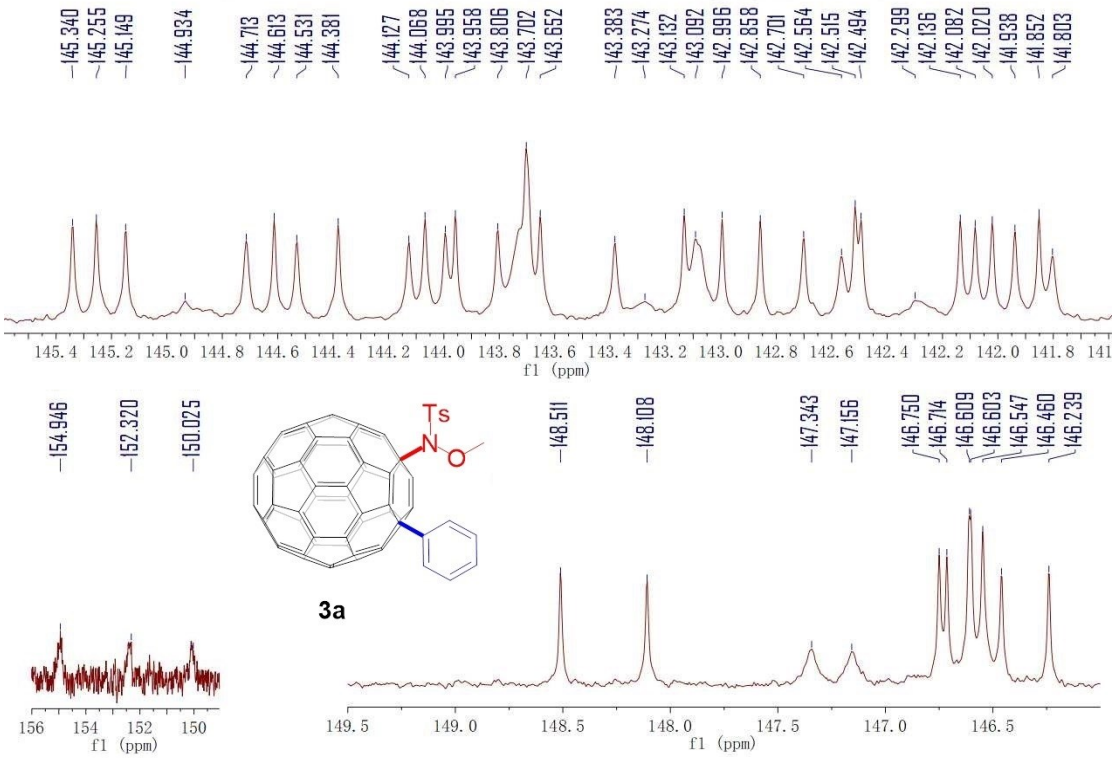


Figure S4. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3a**.

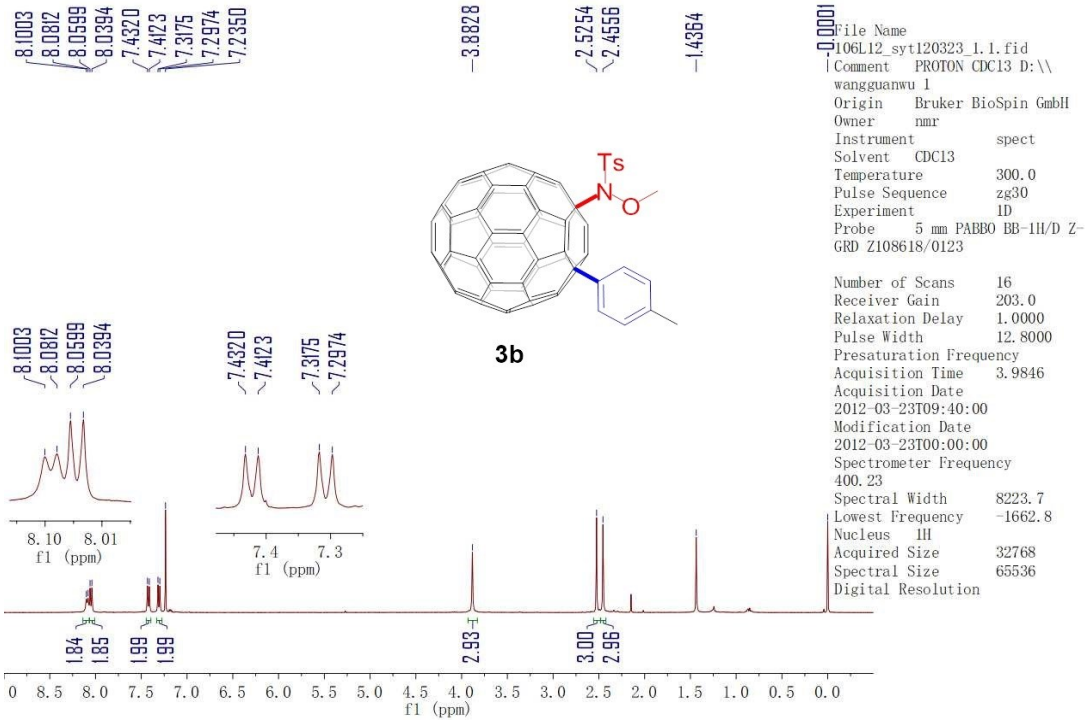


Figure S5. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3b**.

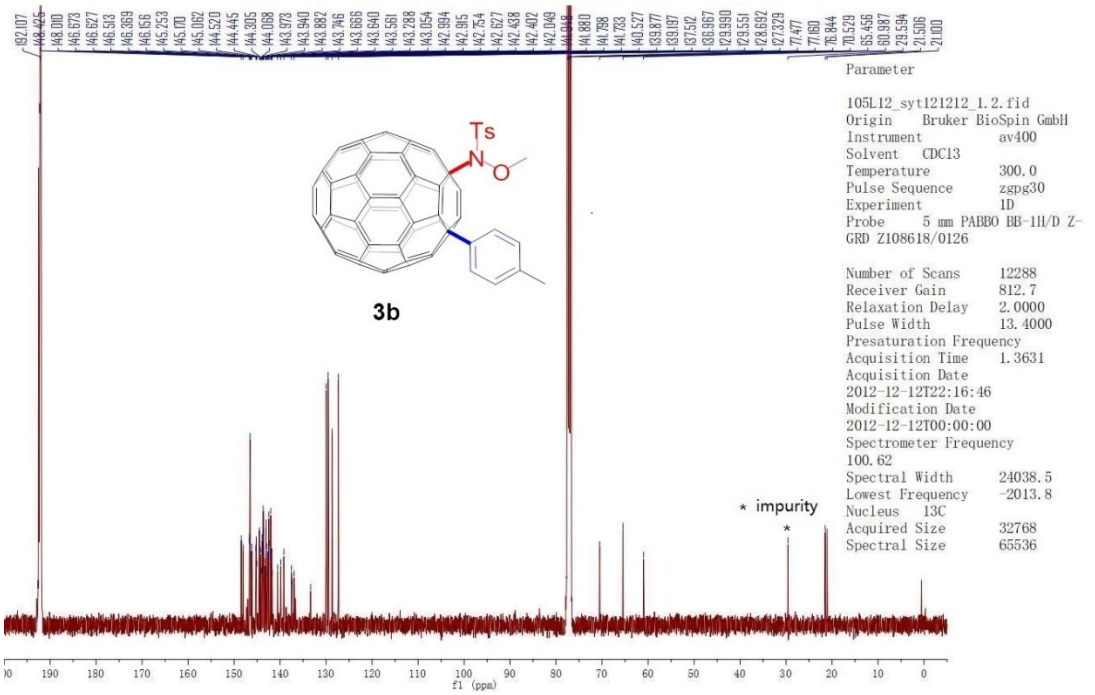


Figure S6. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3b**.

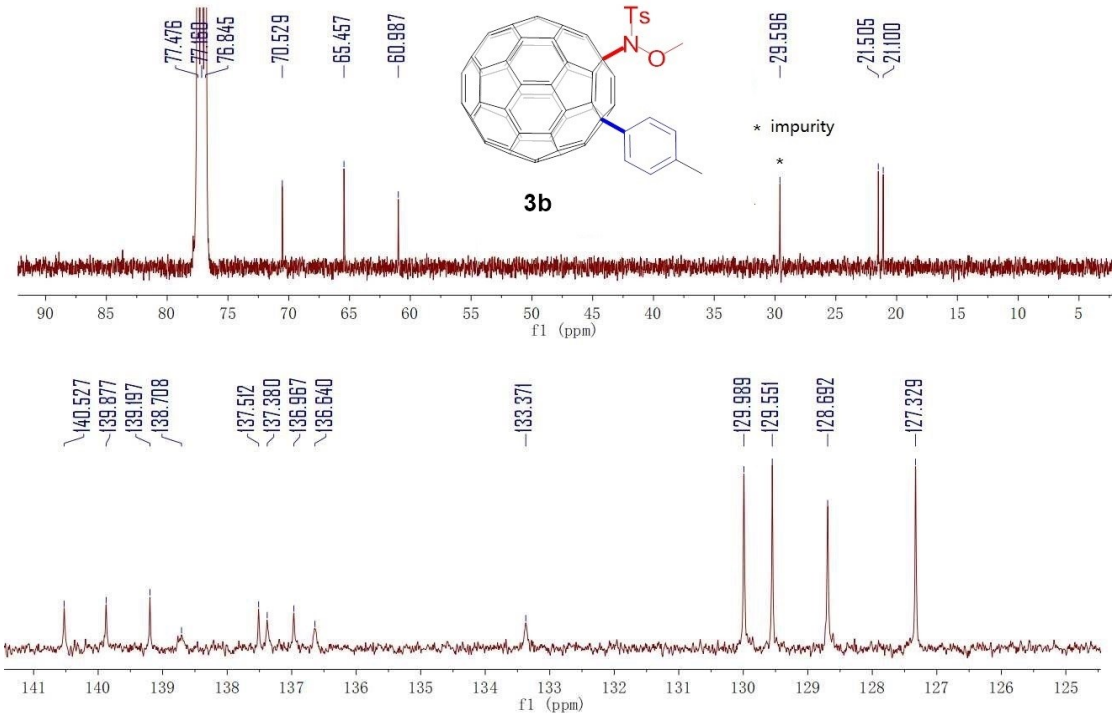


Figure S7. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3b**.

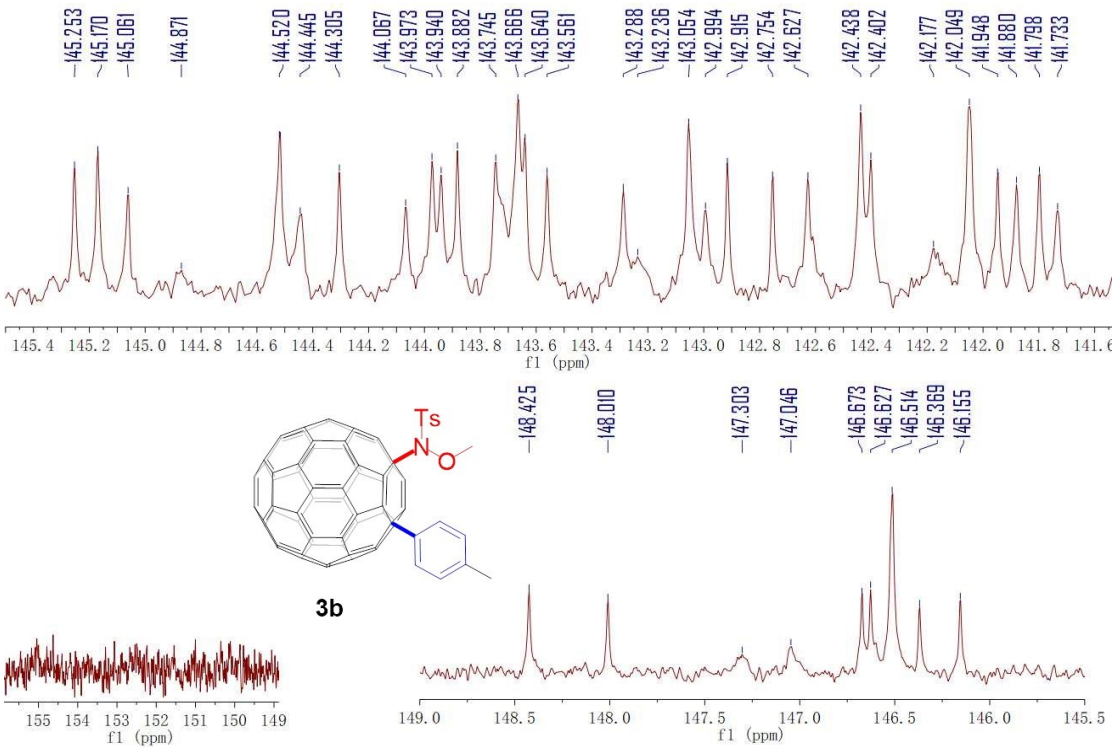


Figure S8. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3b**.

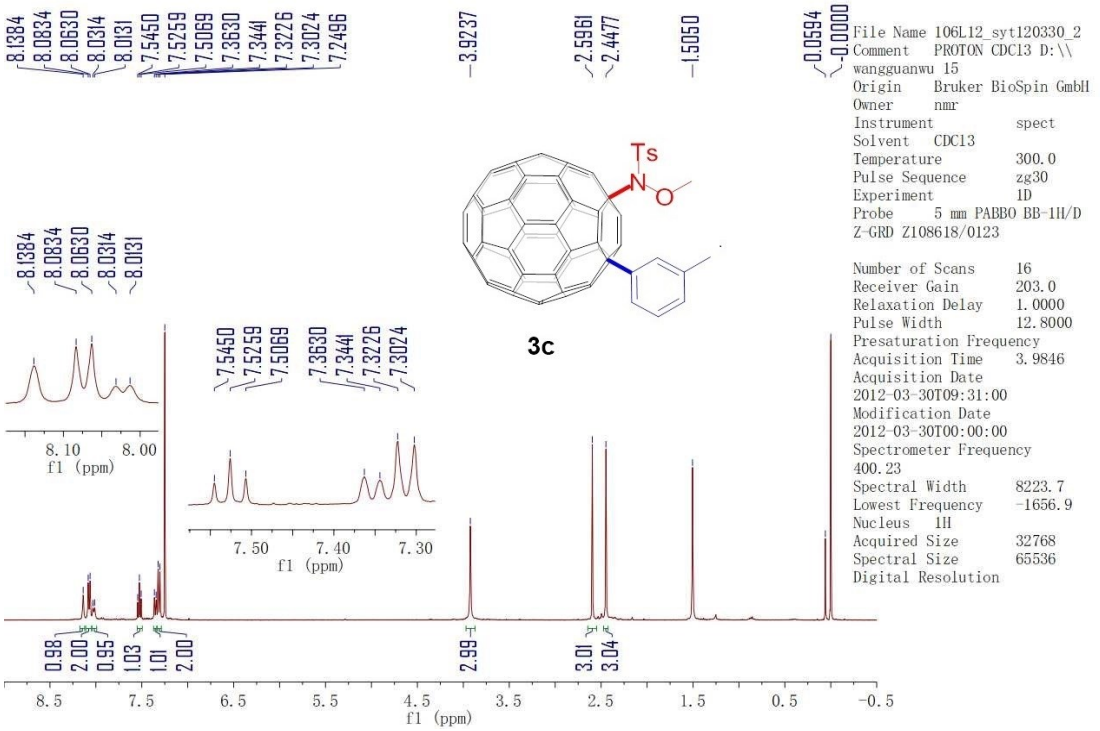


Figure S9. ^1H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3c**.

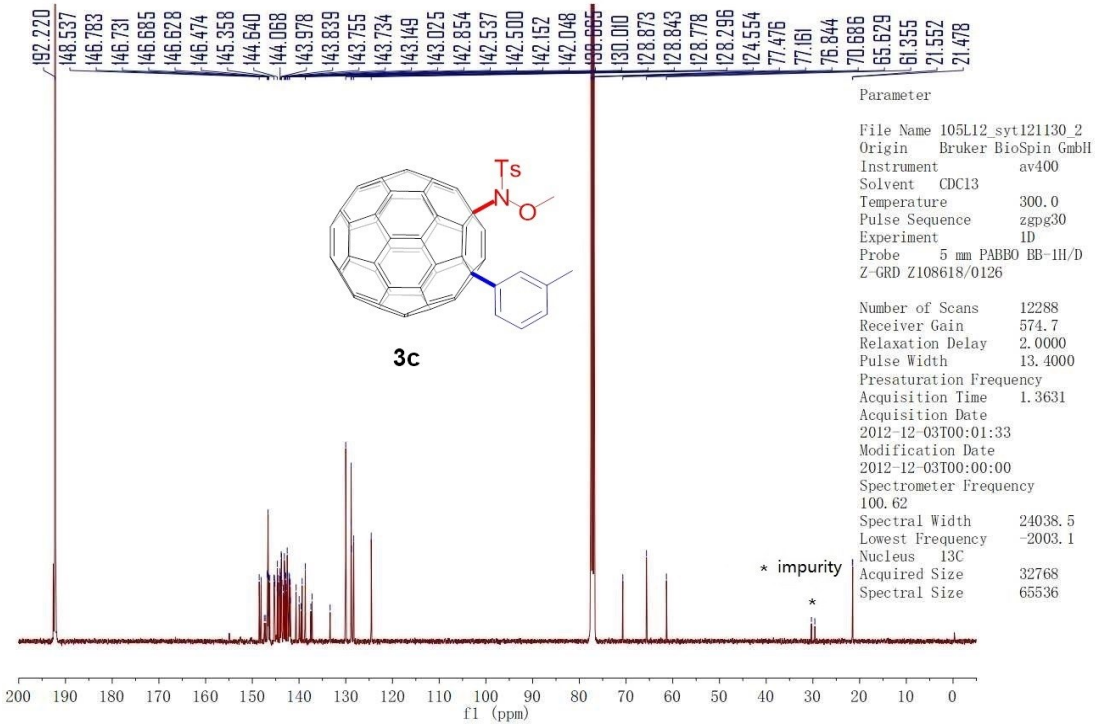


Figure S10 ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3c**.

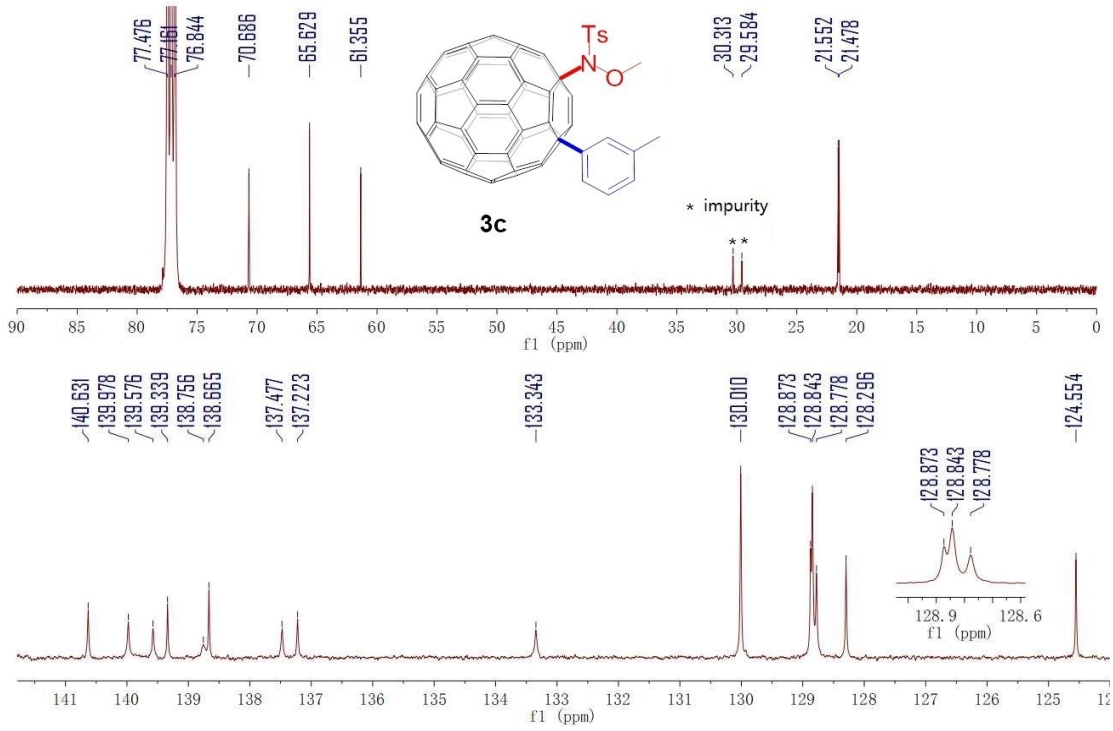


Figure S11. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3c**.

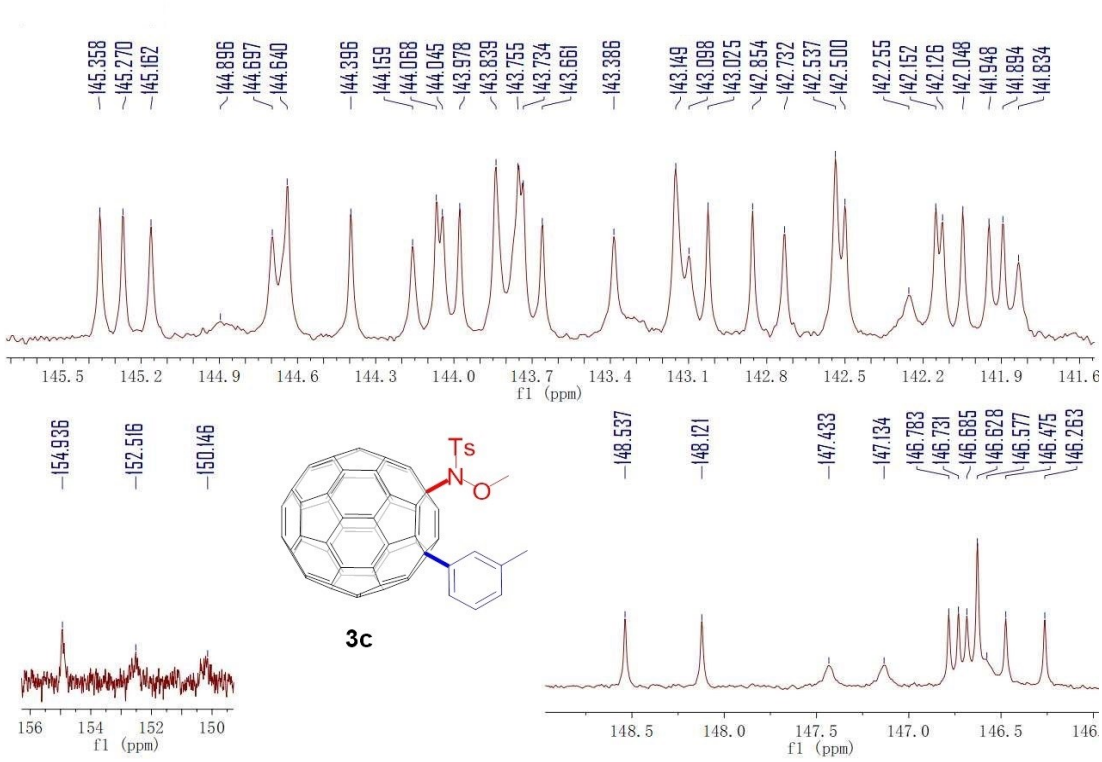


Figure S12. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3c**.

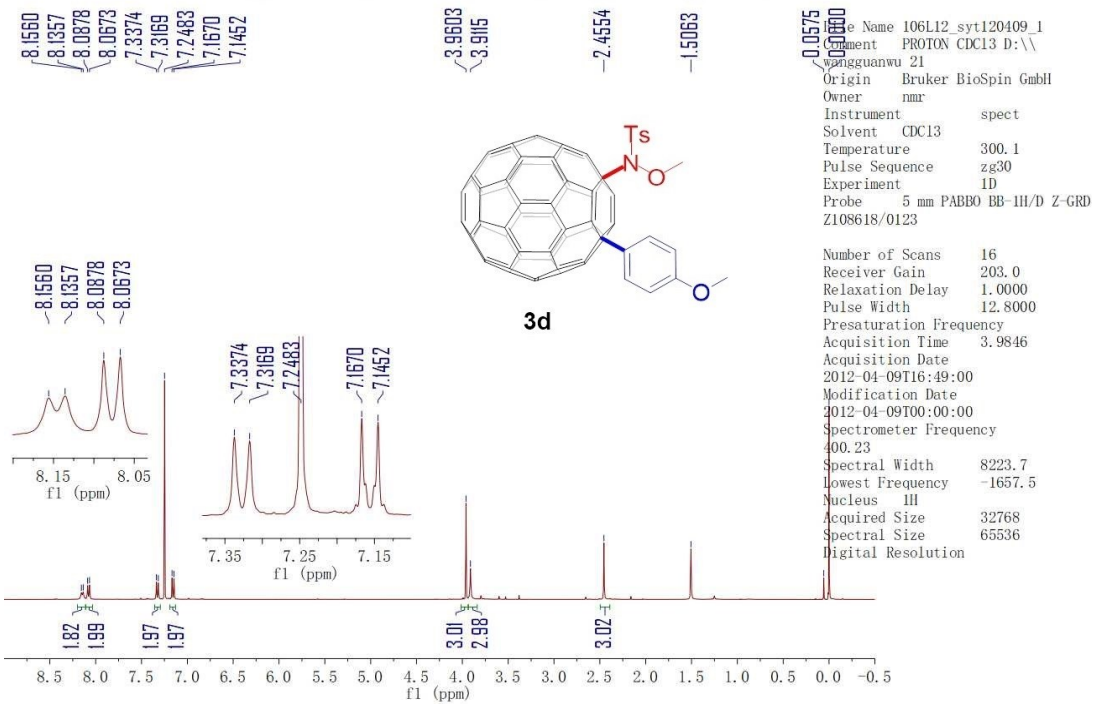


Figure S13. ^1H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3d**.

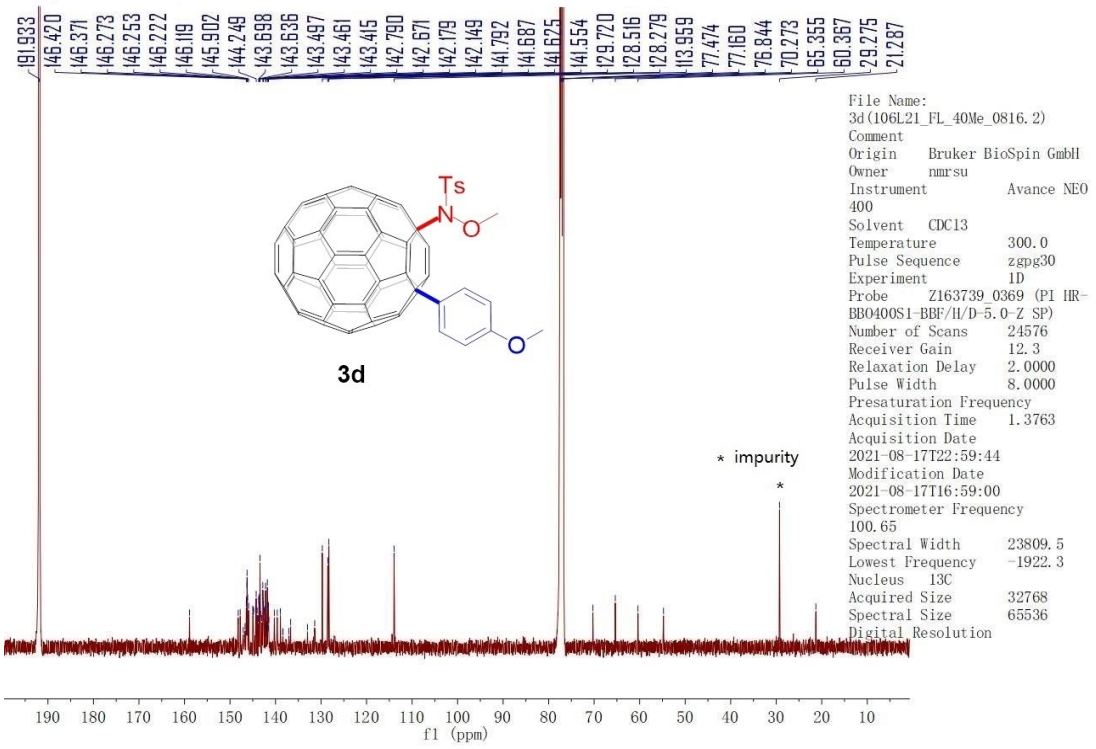


Figure S14. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3d**.

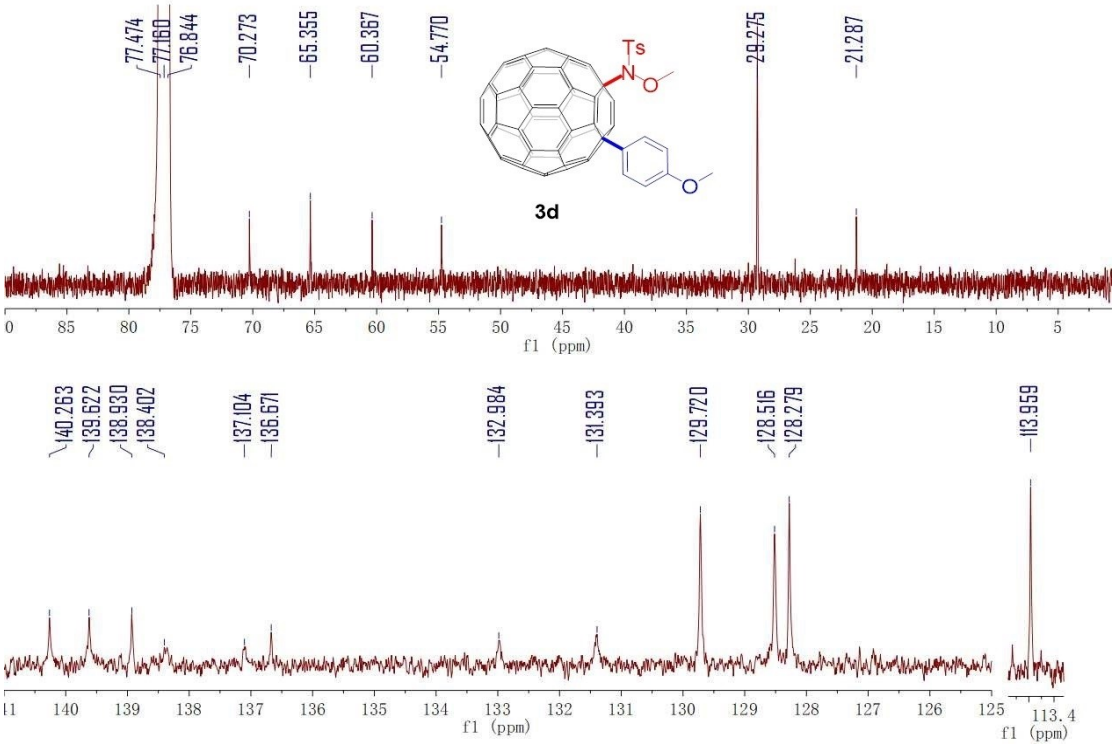


Figure S15. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3d**.

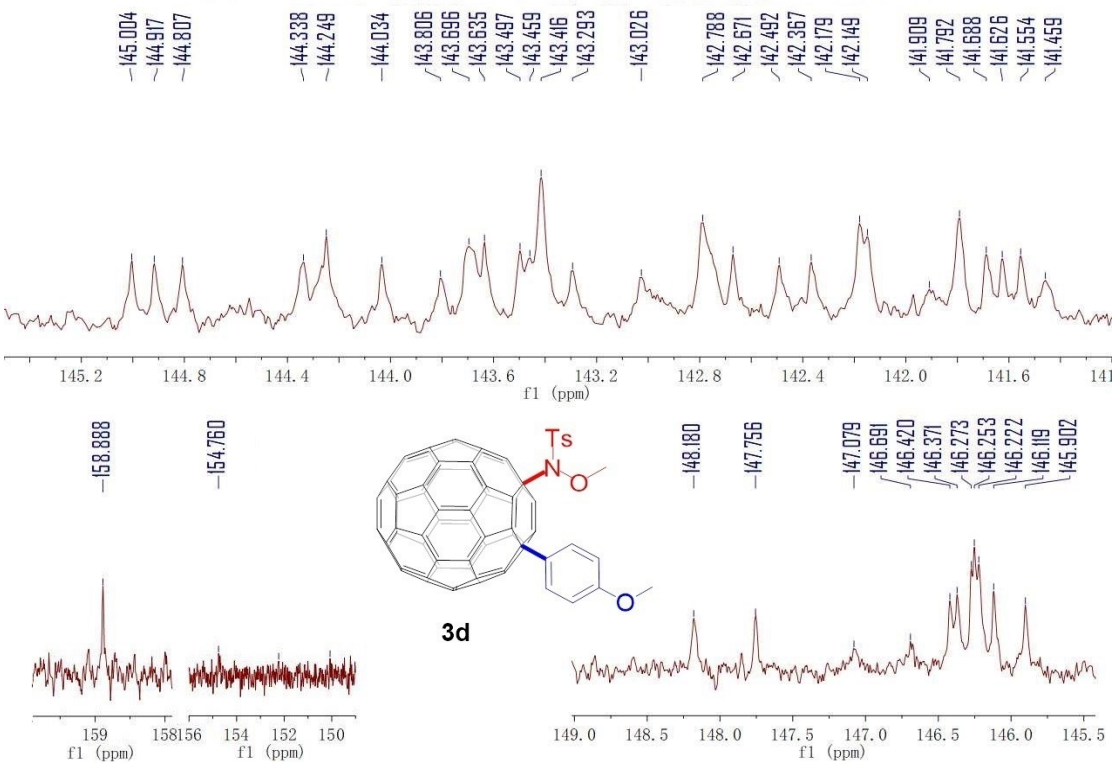


Figure S16. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3d**.

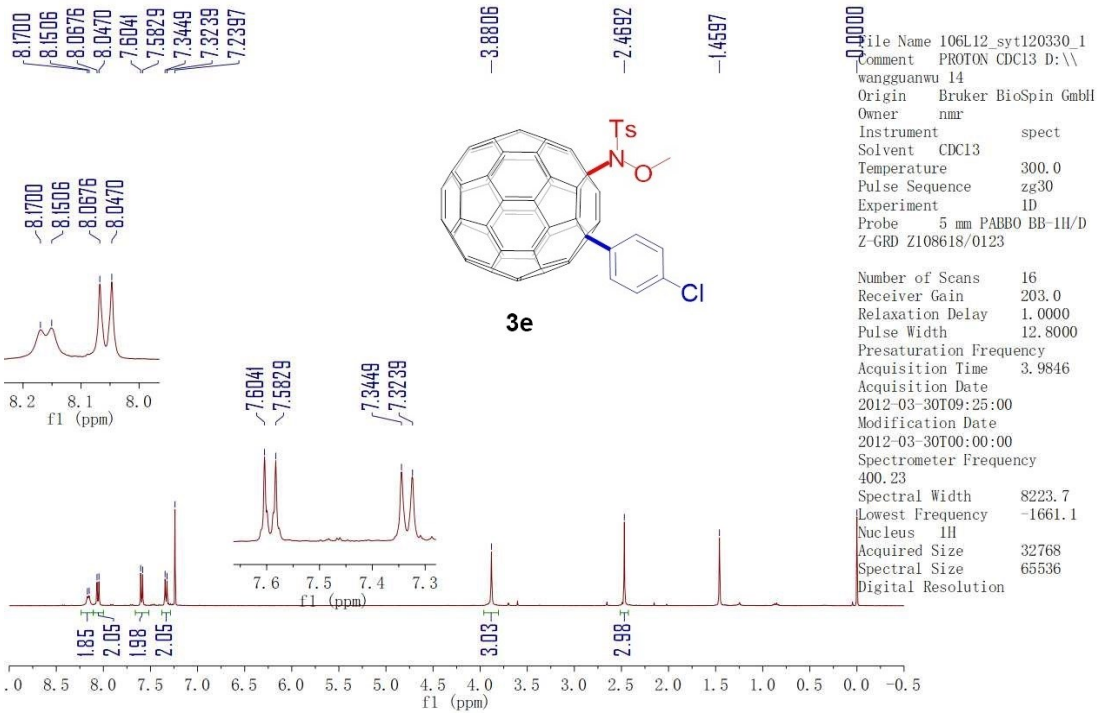


Figure S17. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3e**.

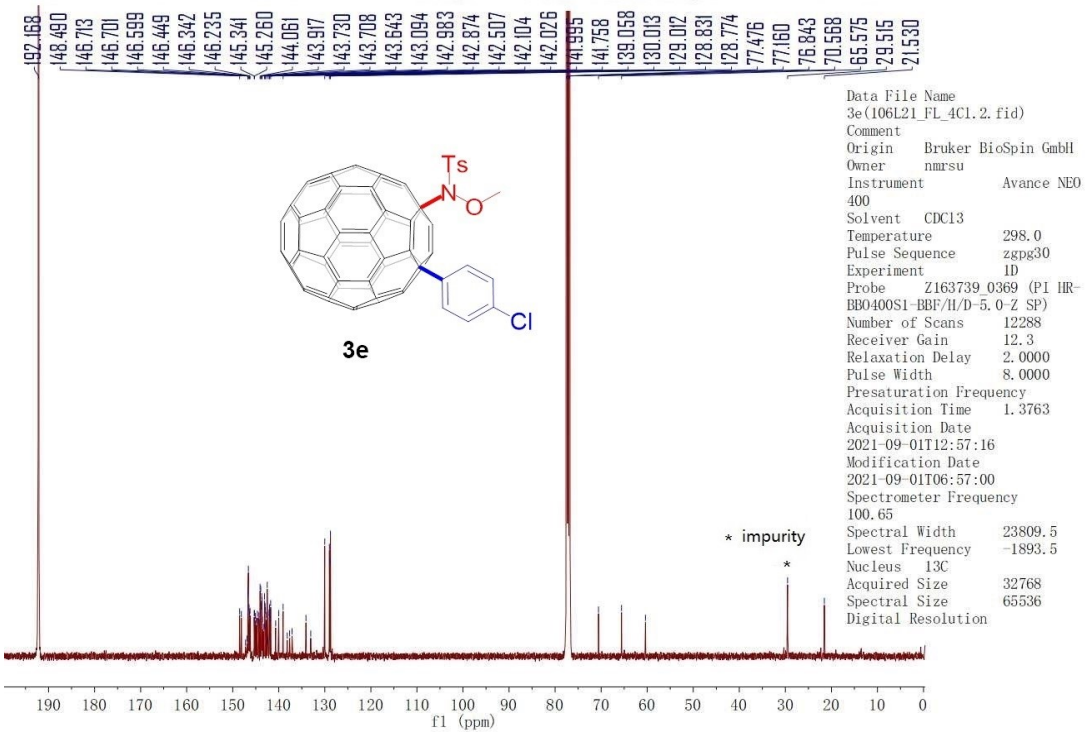


Figure S18. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3e**.

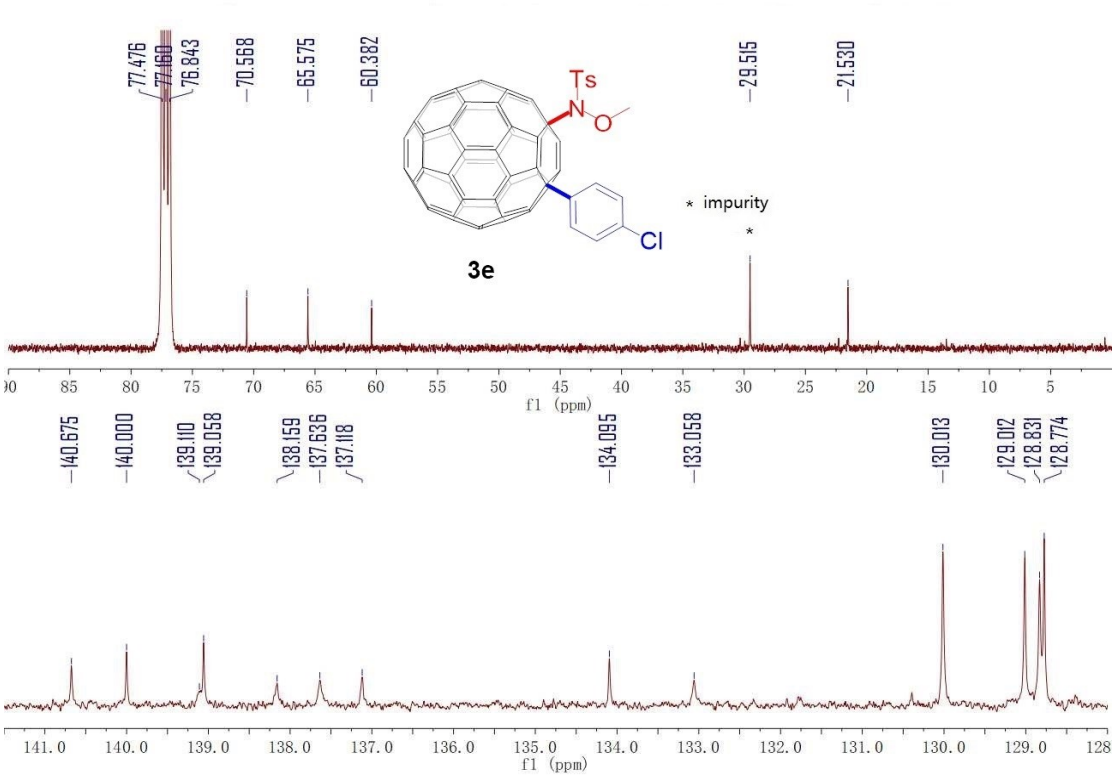


Figure S19. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3e**.

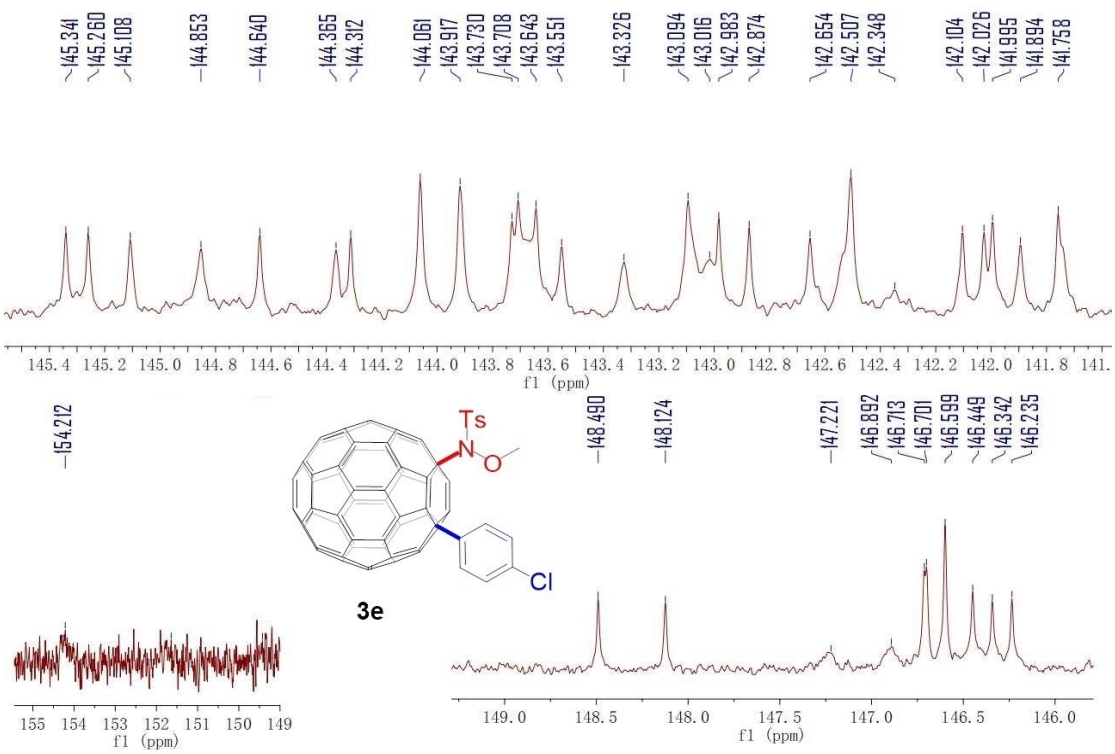


Figure S20. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3e**.

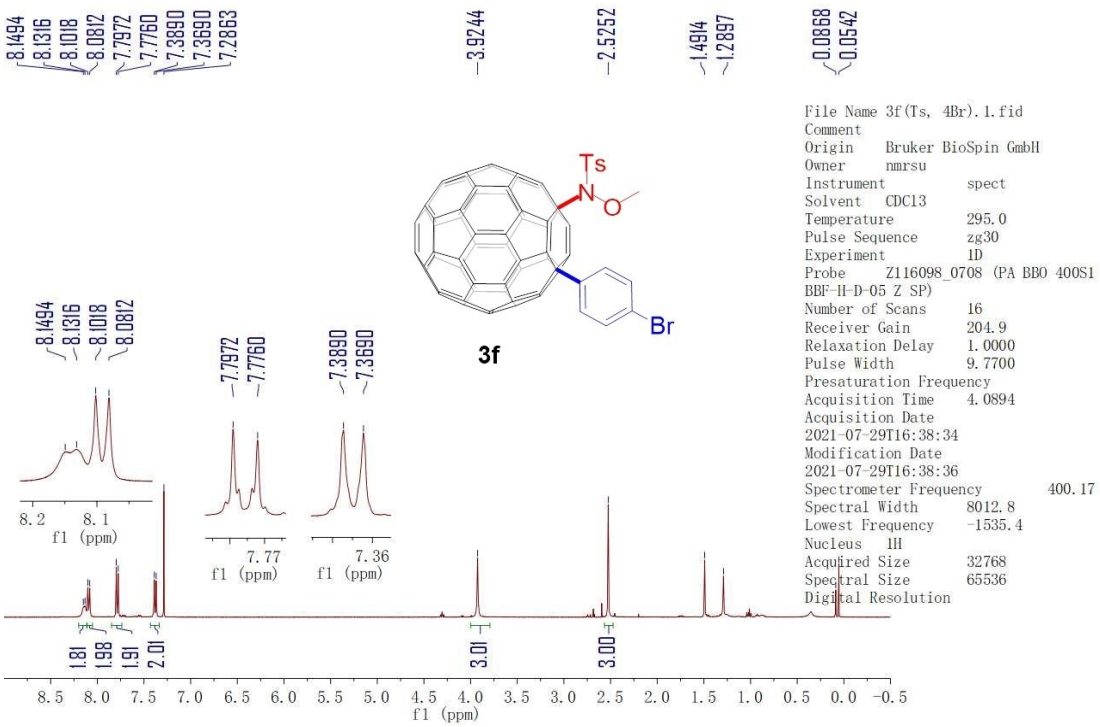


Figure S21. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3f**.

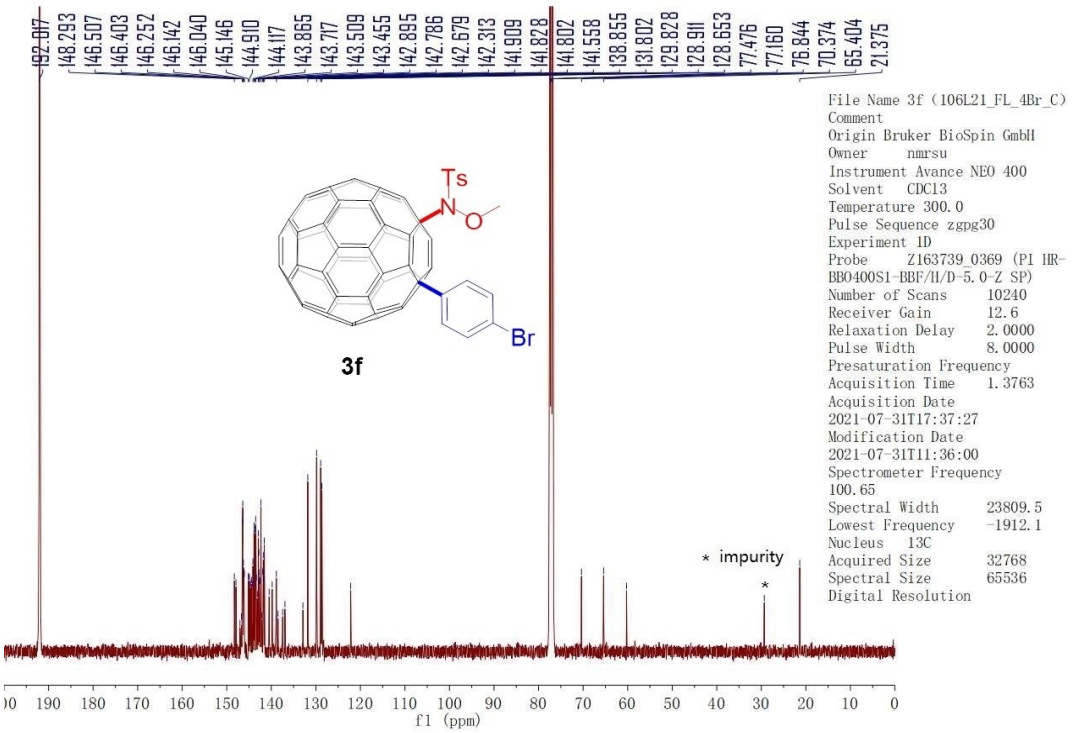


Figure S22. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3f**.

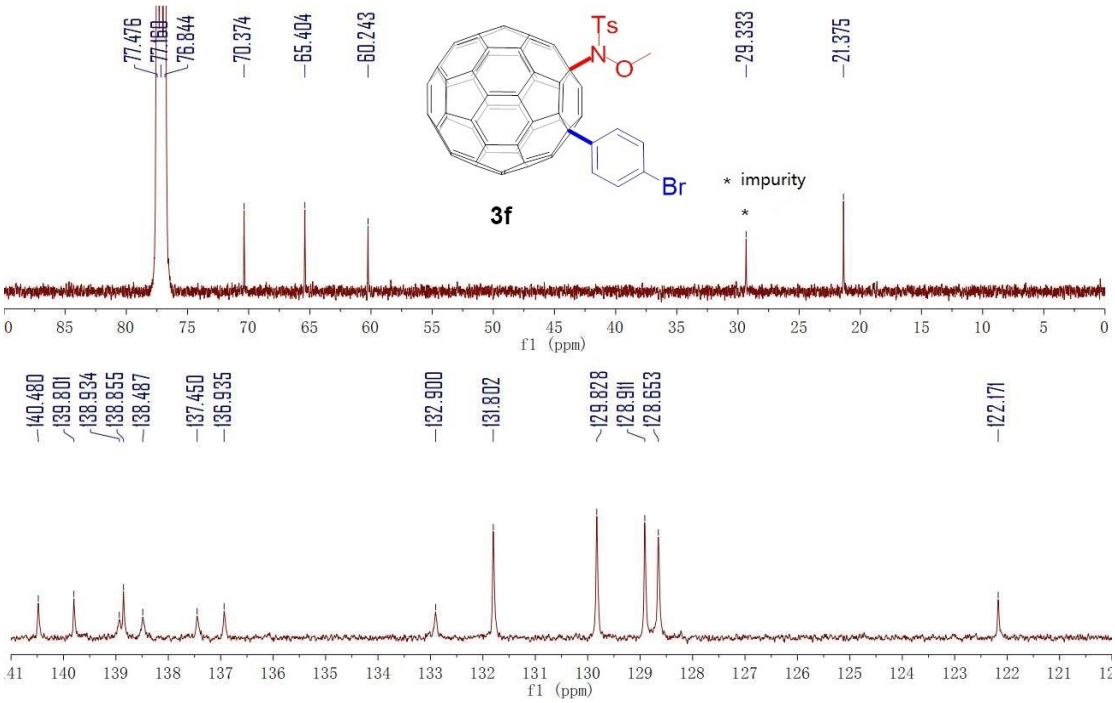


Figure S23. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3f**.

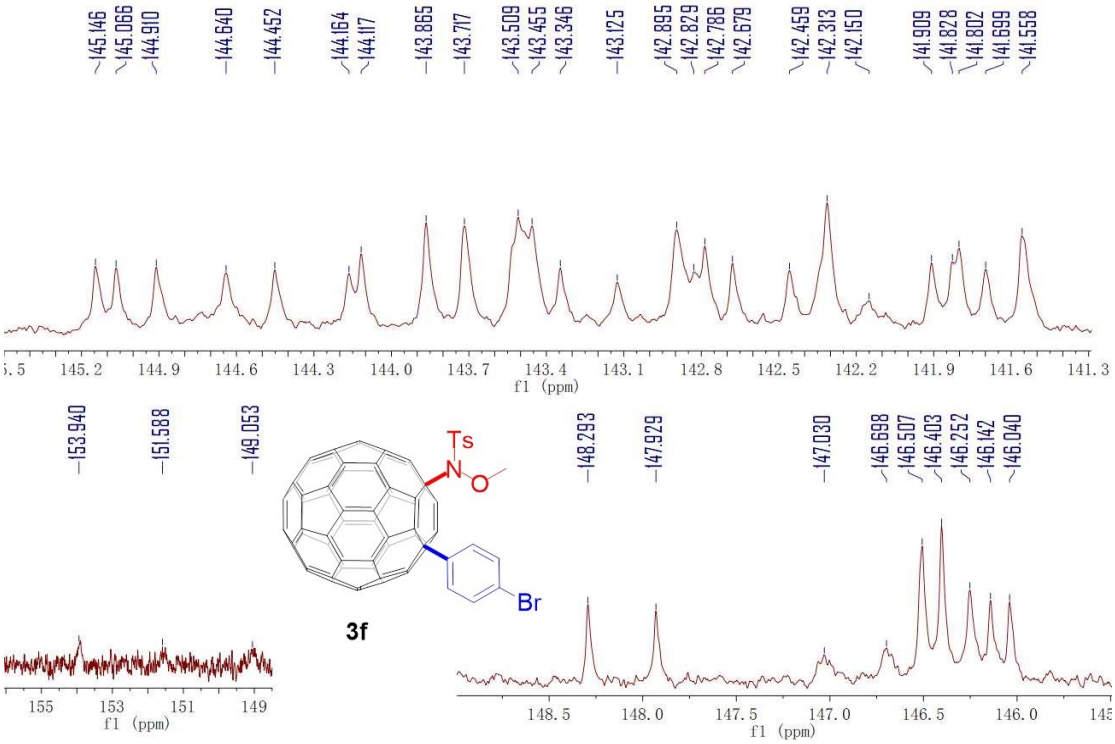


Figure S24. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3f**.

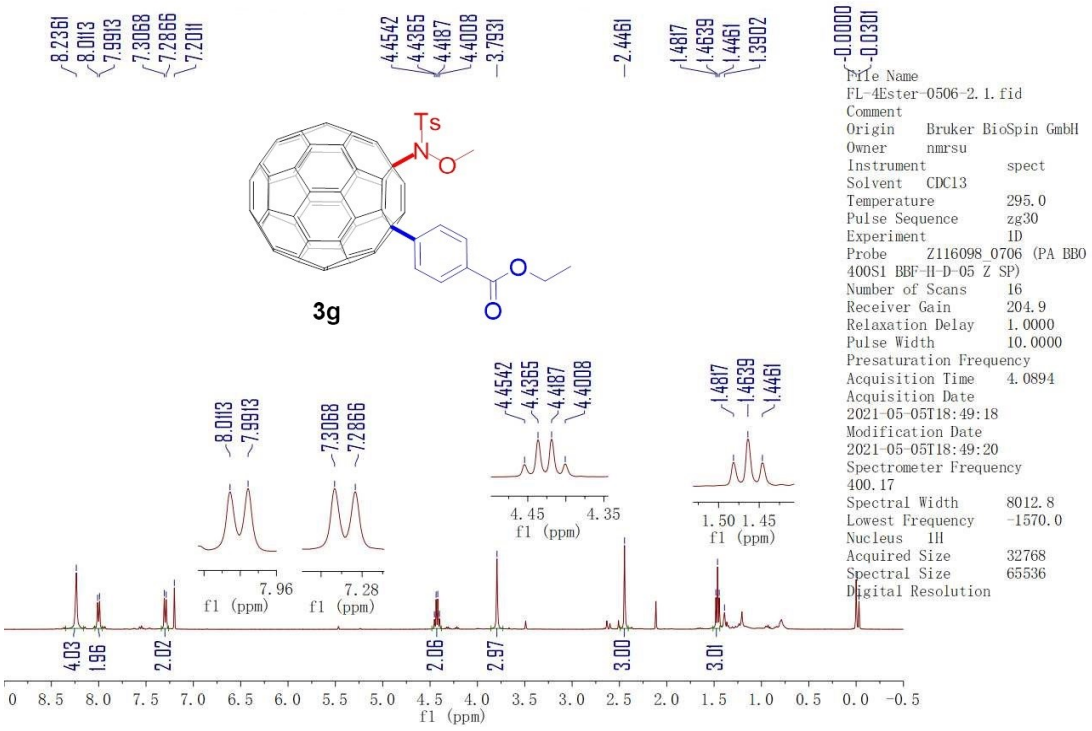


Figure S25. ^1H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3g**.

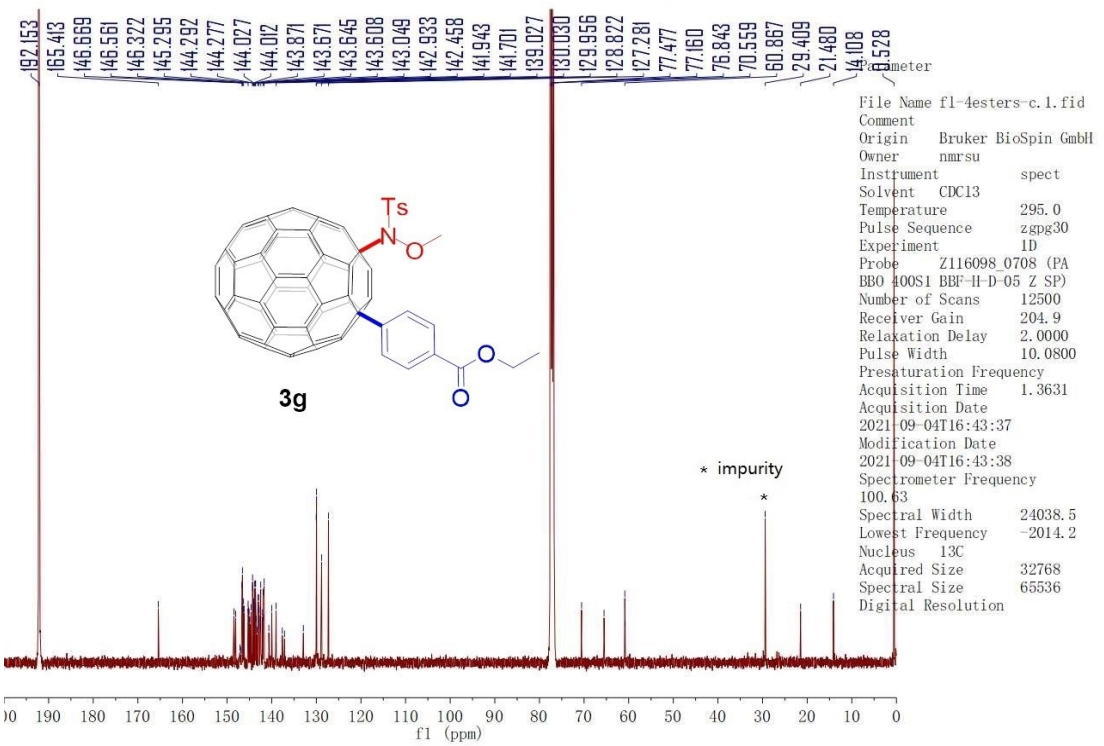


Figure S26. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3g**.

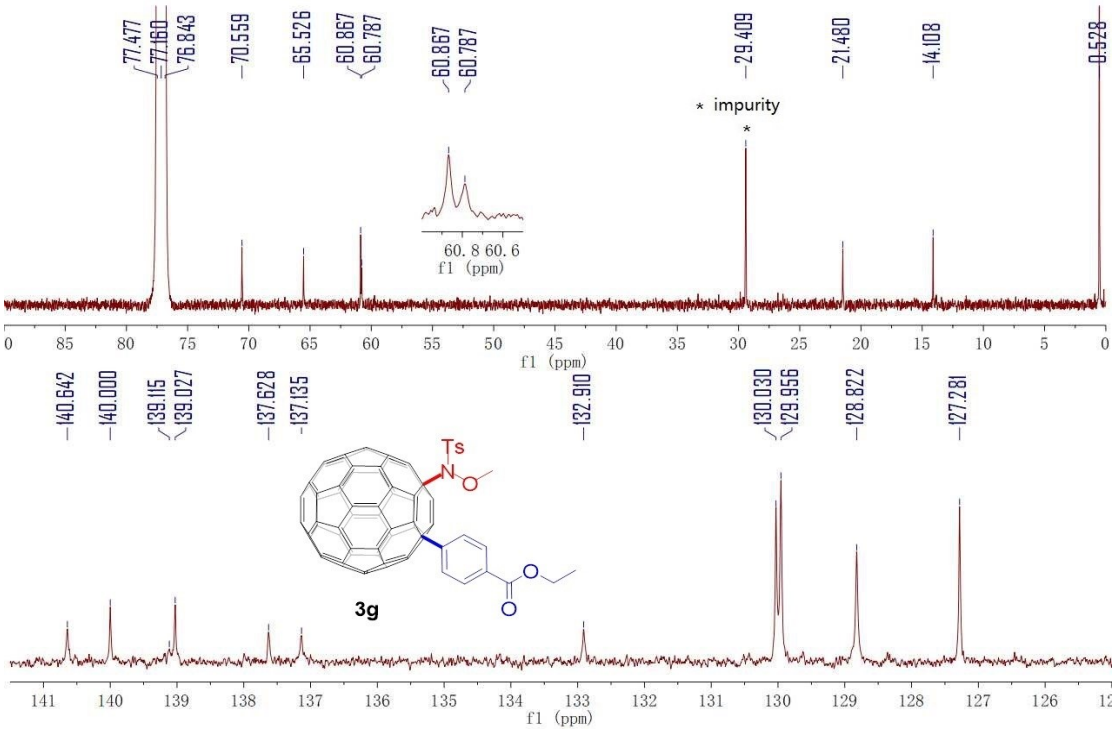


Figure S27. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3g**.

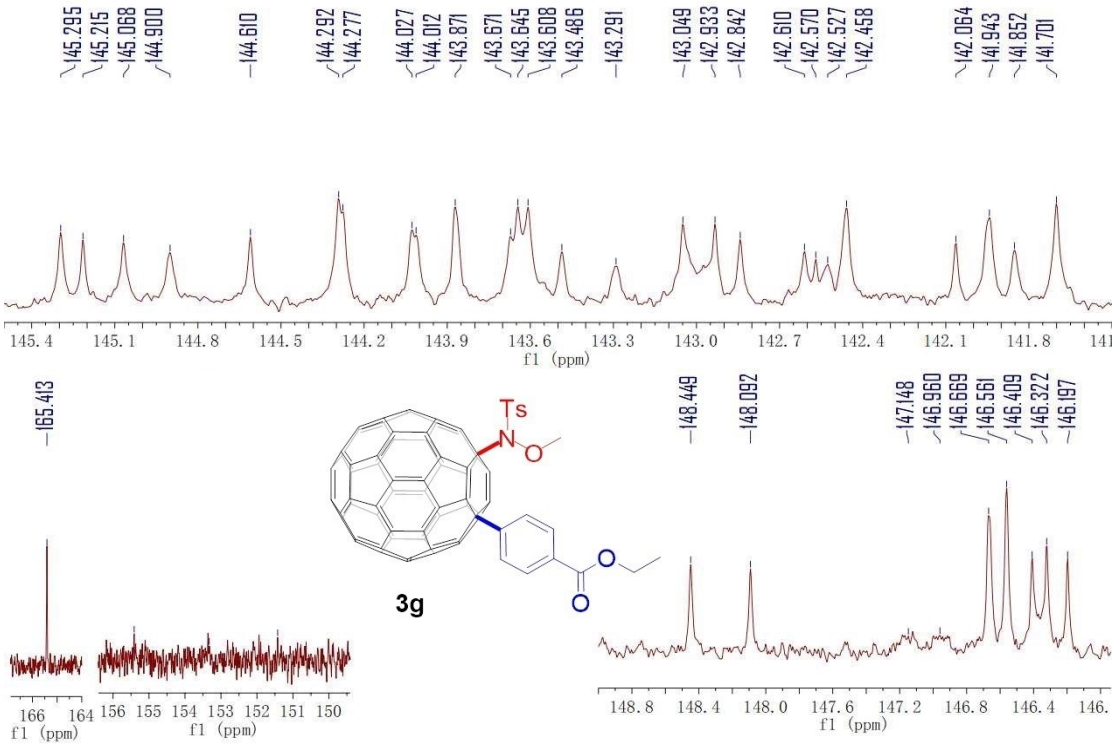


Figure S28. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3g**.

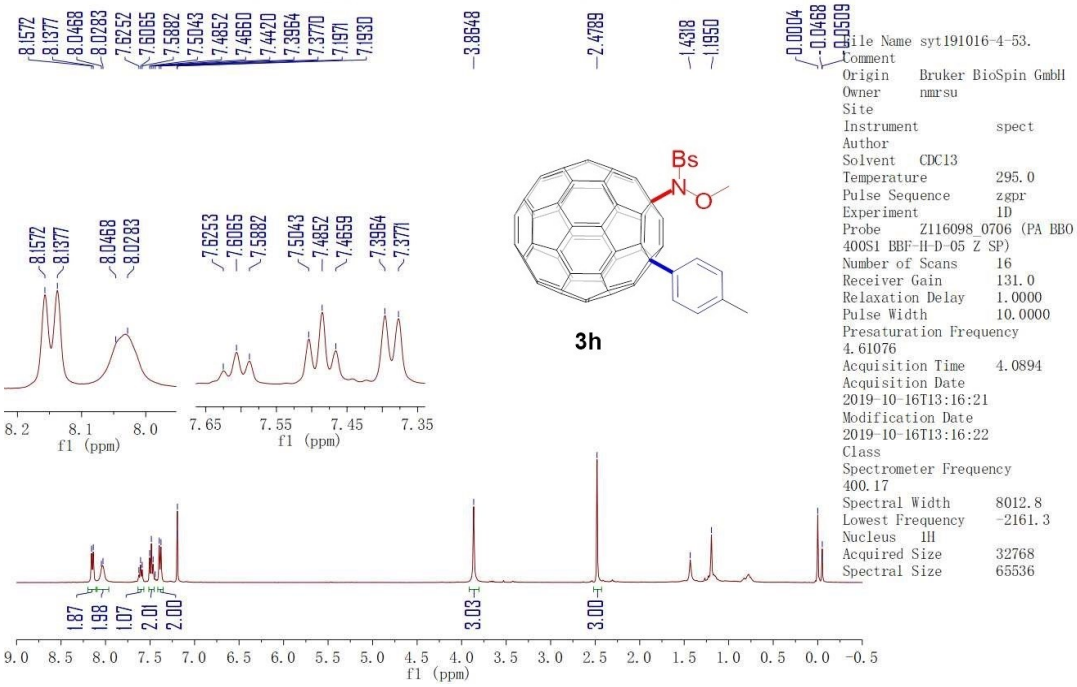


Figure S29. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3h**.

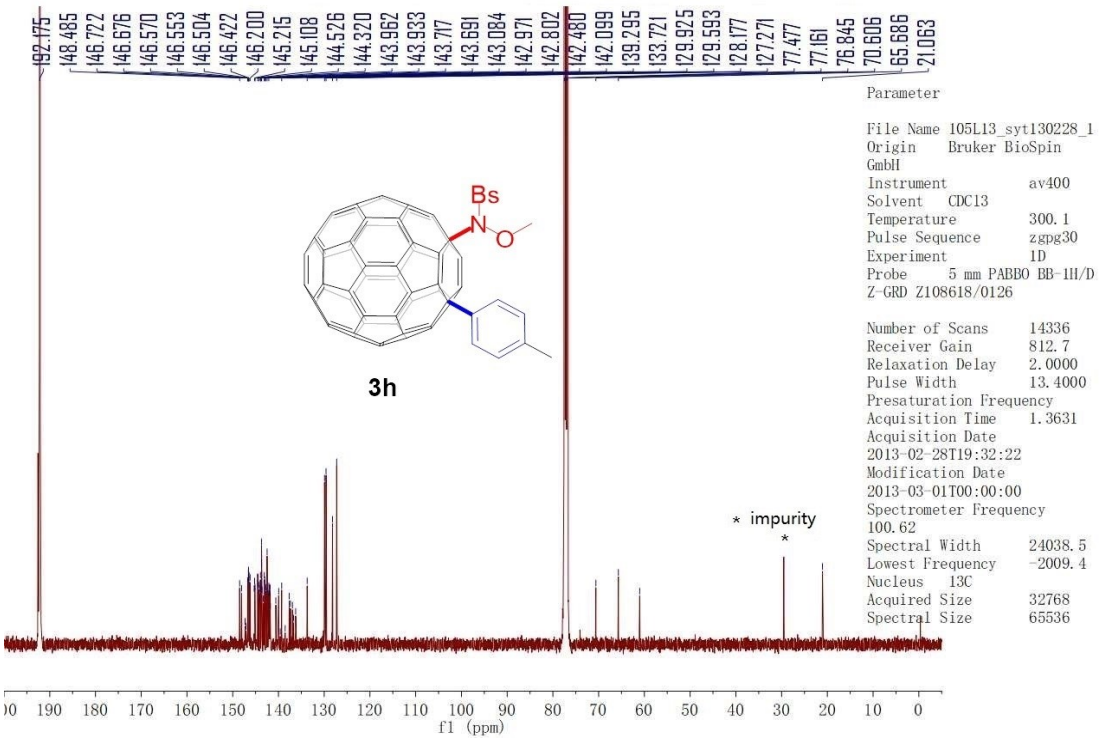


Figure S30. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3h**.

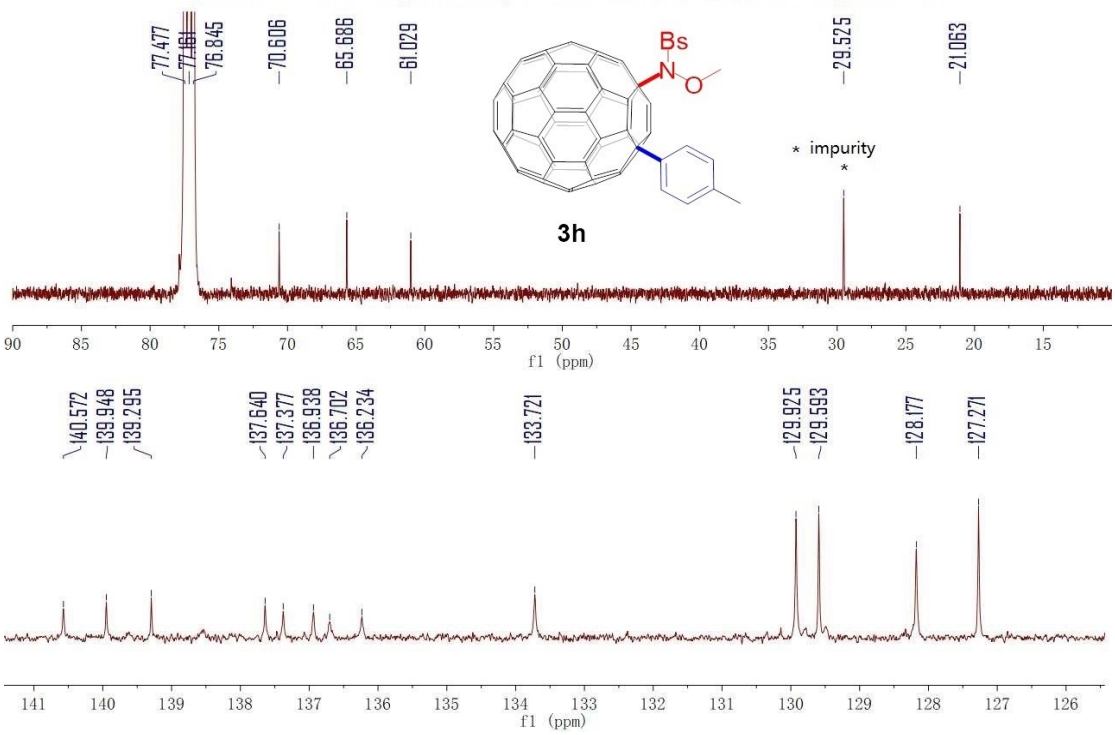


Figure S31. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3h**.

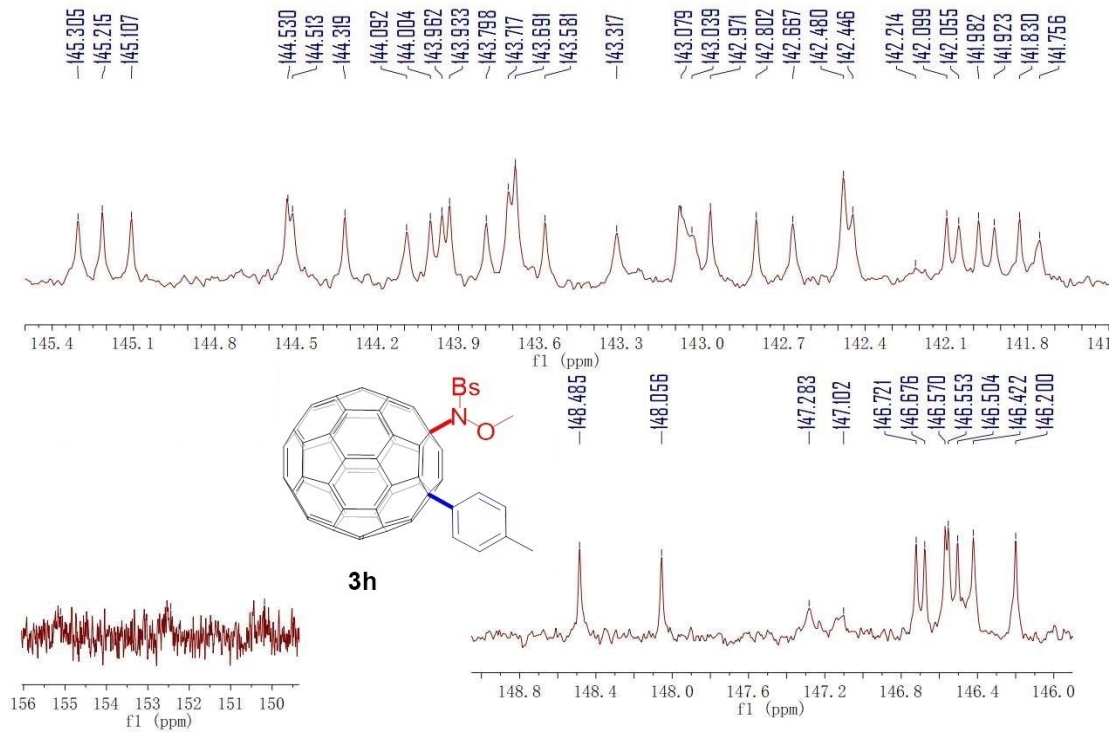


Figure S32. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3h**.

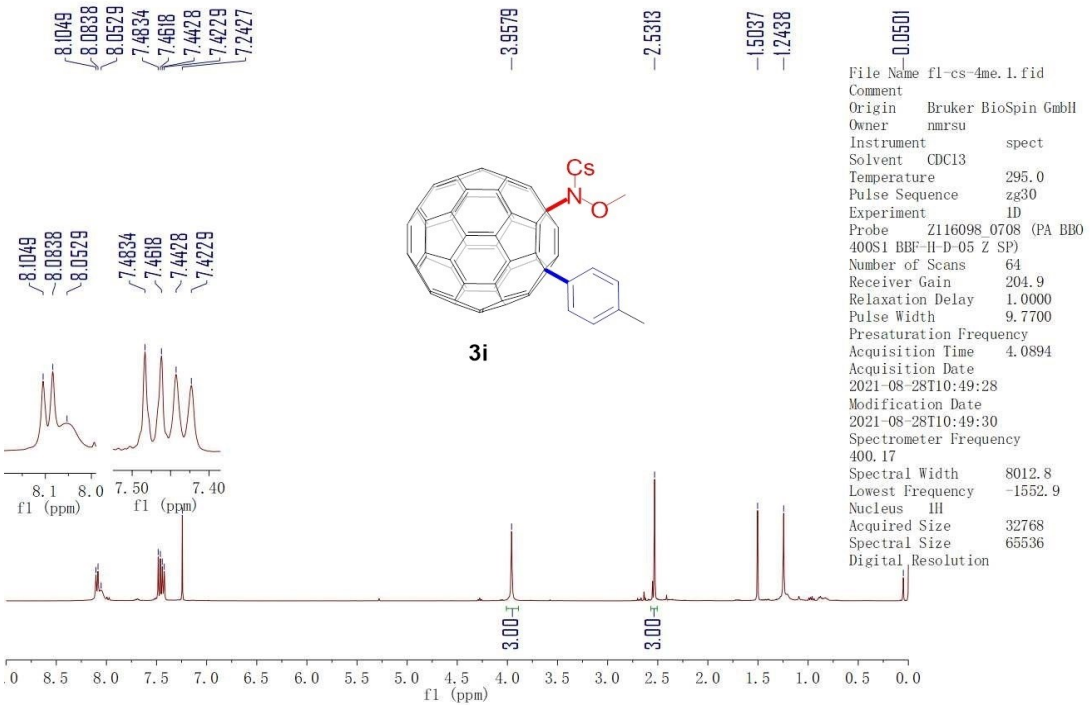


Figure S33. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3i**.

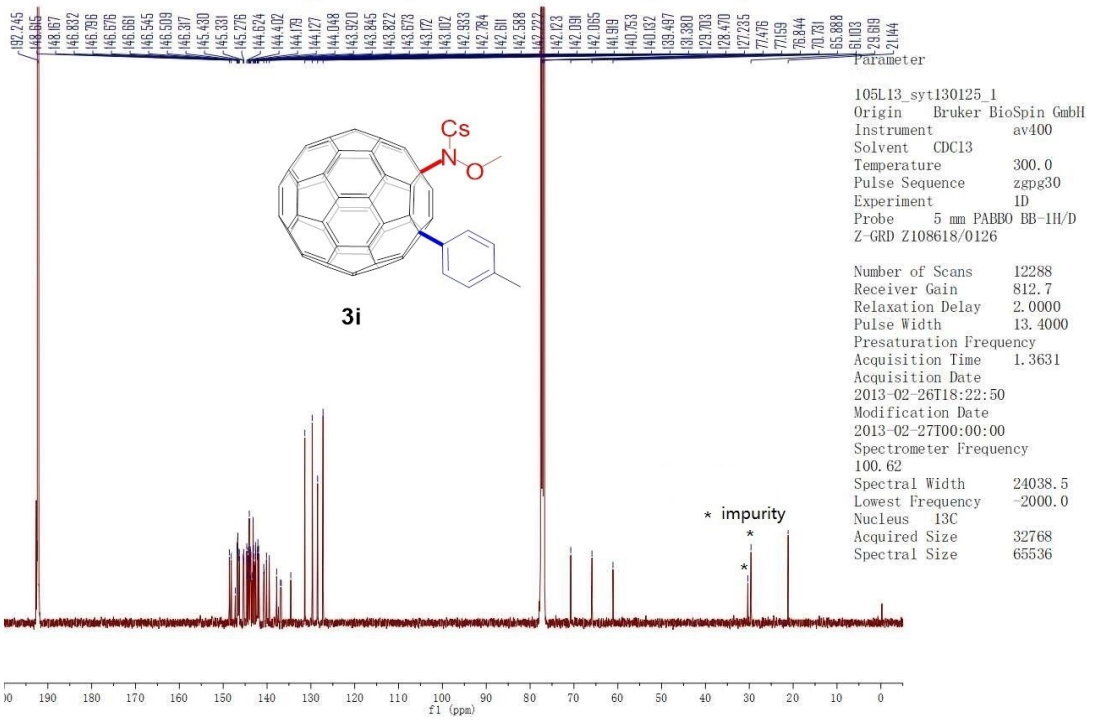


Figure S34. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3i**.

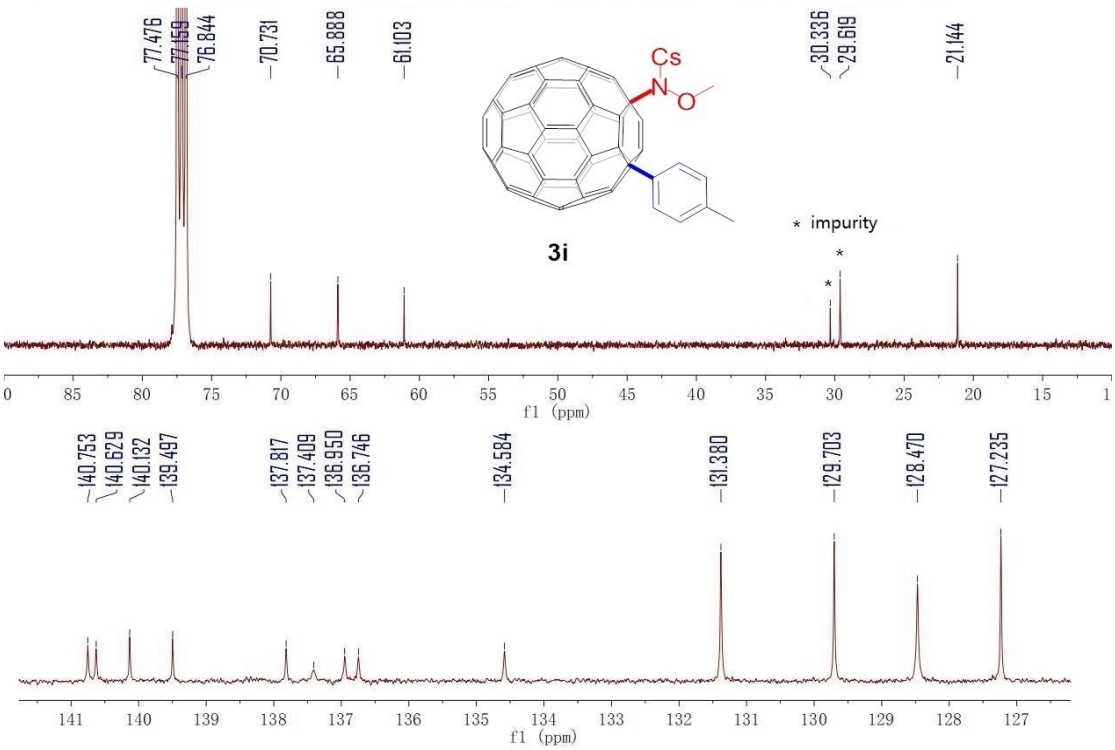


Figure S35. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3i**.

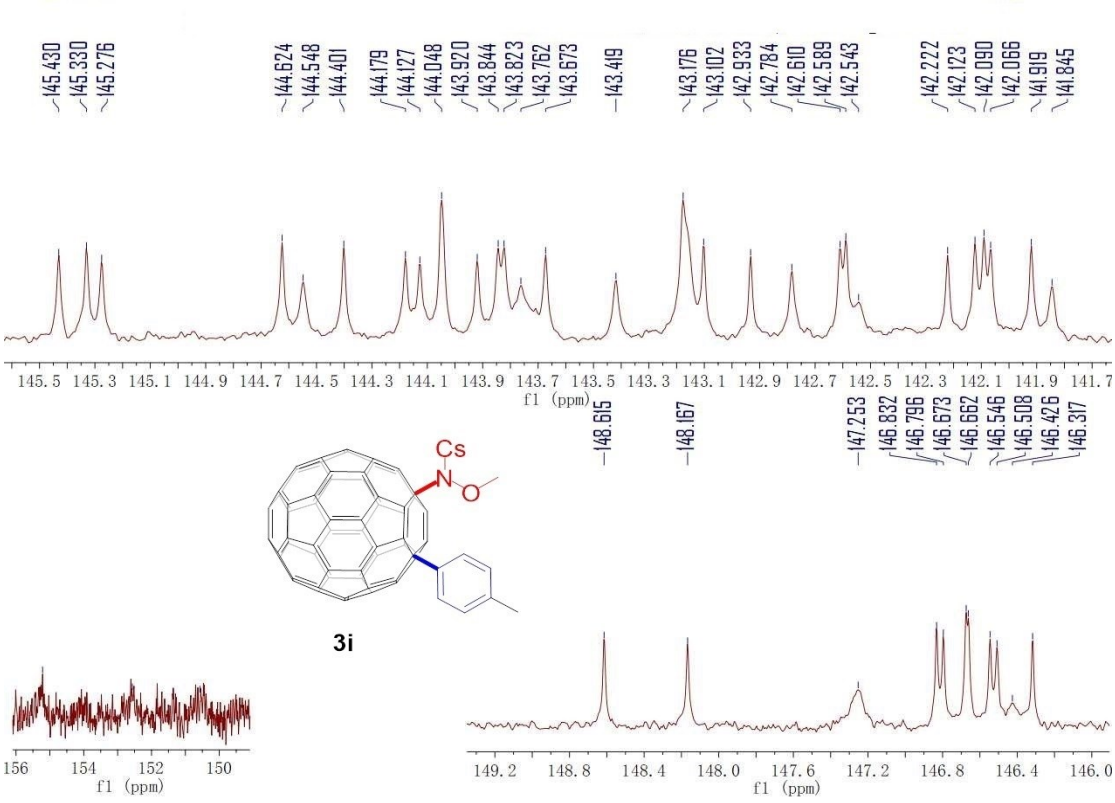


Figure S36. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3i**.

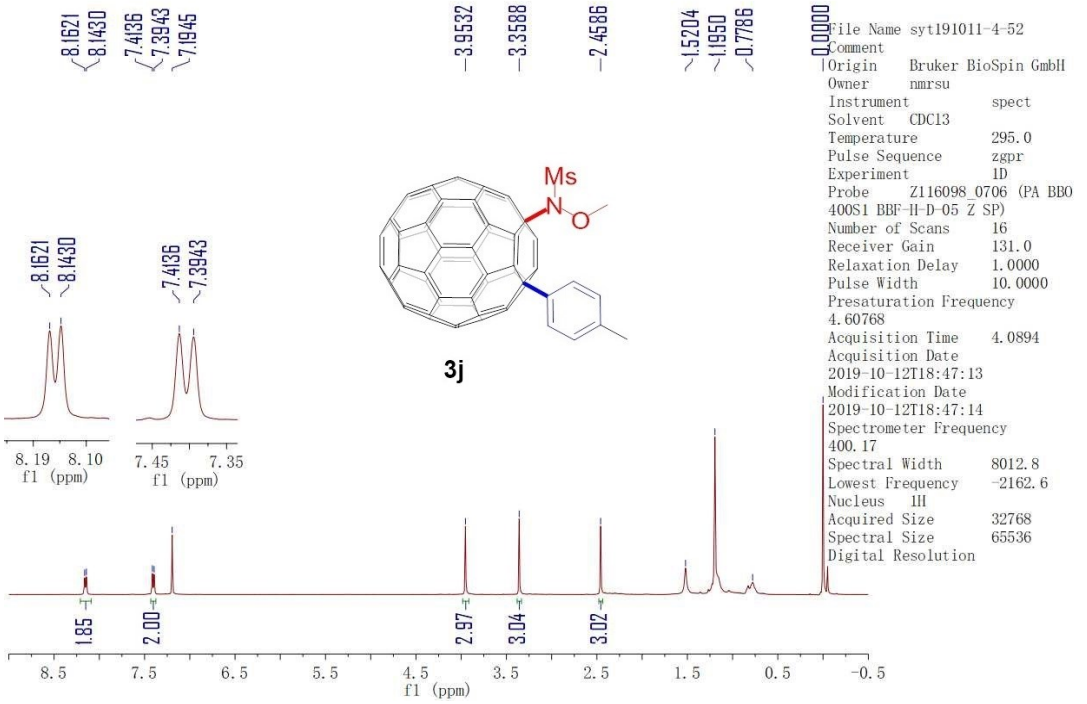


Figure S37. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **3j**.

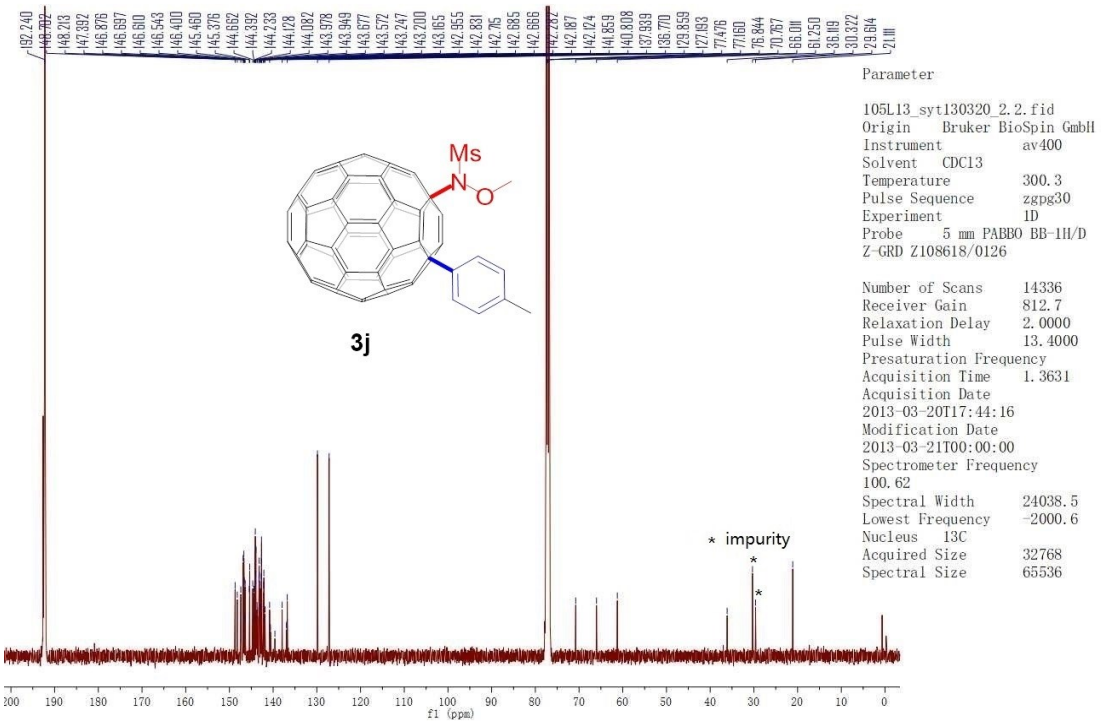


Figure S38. ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3j**.

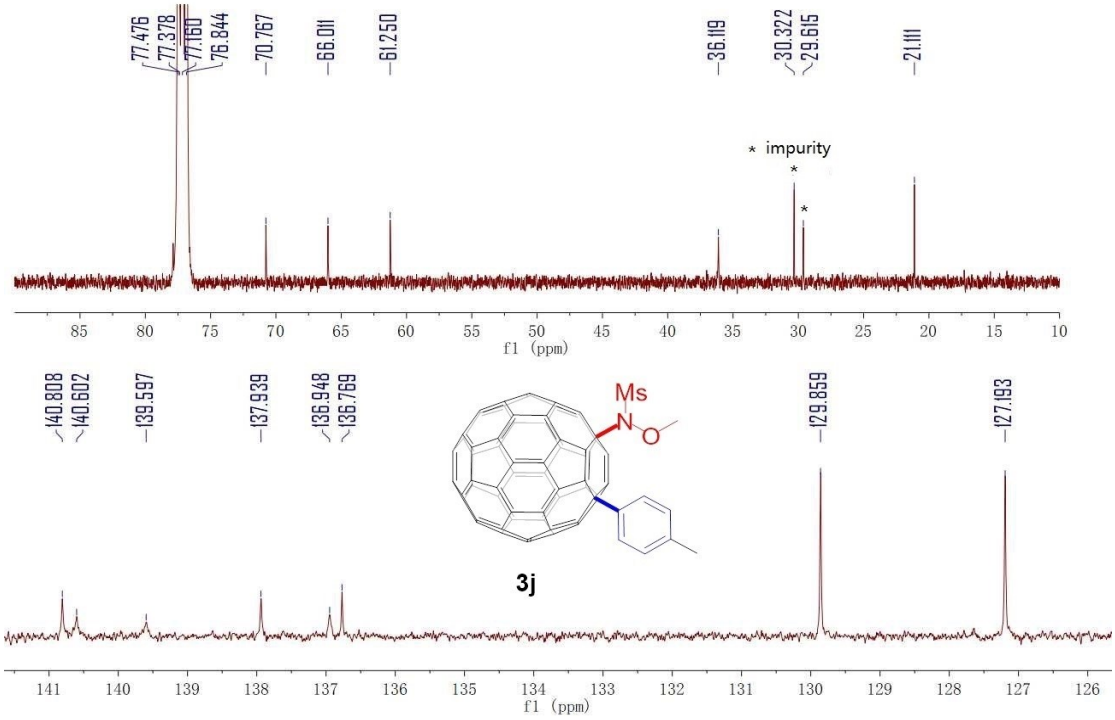


Figure S39. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3j**.

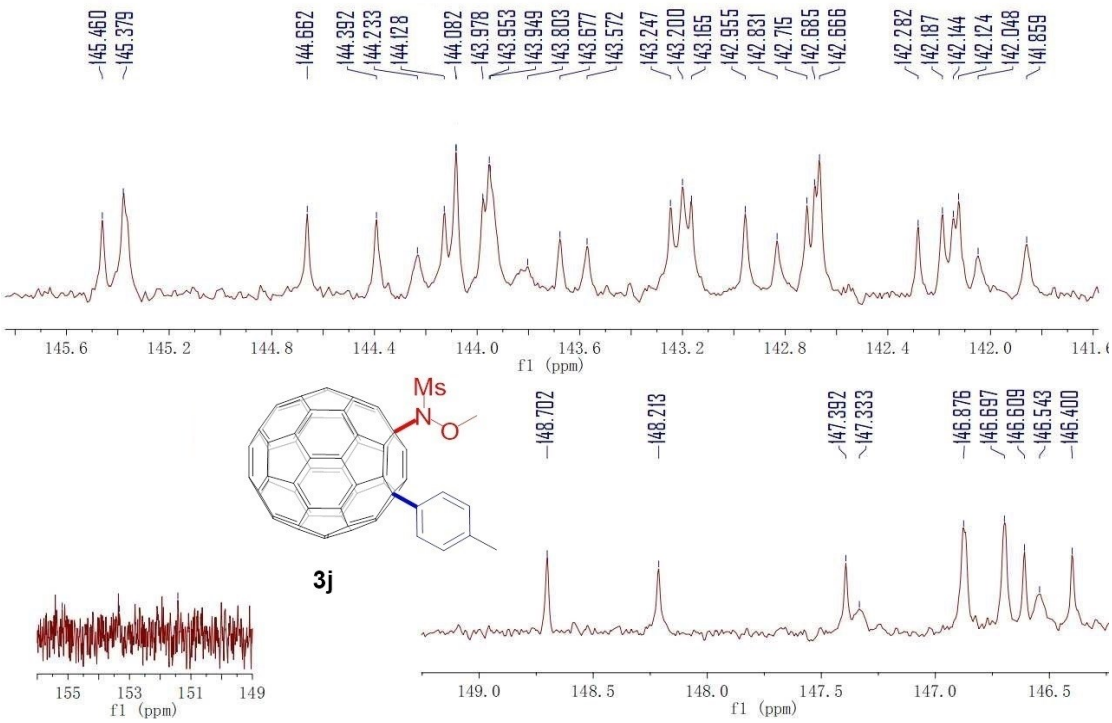


Figure S40. Expanded ^{13}C NMR spectrum (100 MHz, $CS_2/CDCl_3$) of compound **3j**.

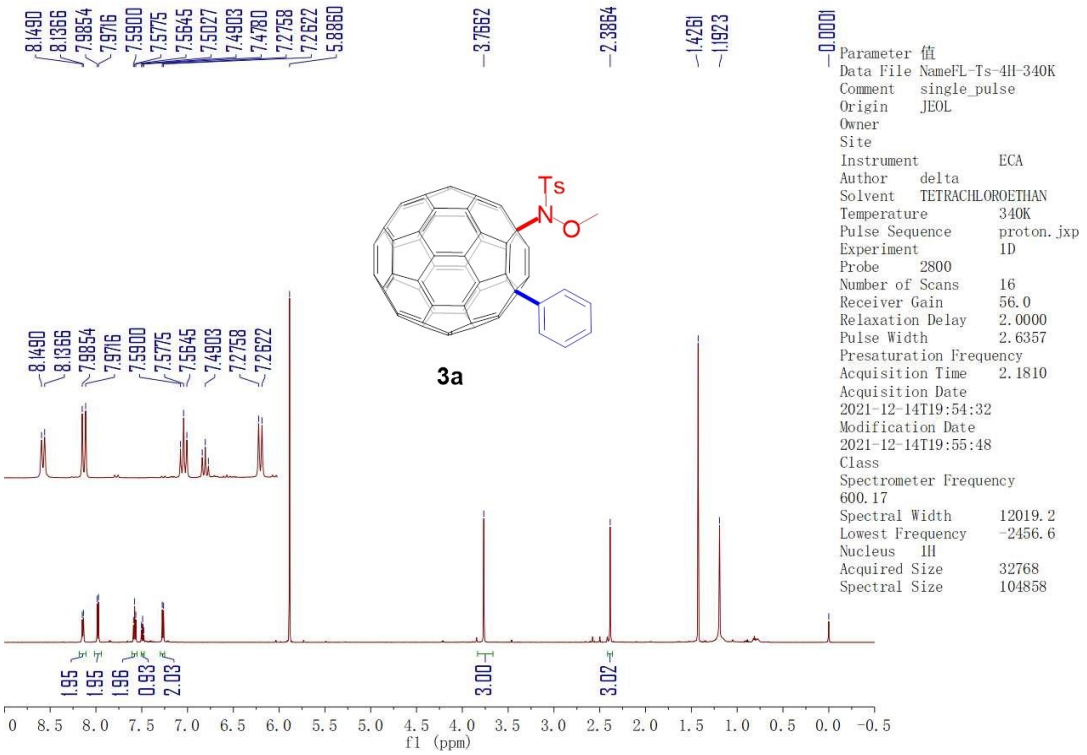


Figure S41. ^1H NMR spectrum (600 MHz, 340 K, $C_2D_2Cl_4$) of compound **3a**.

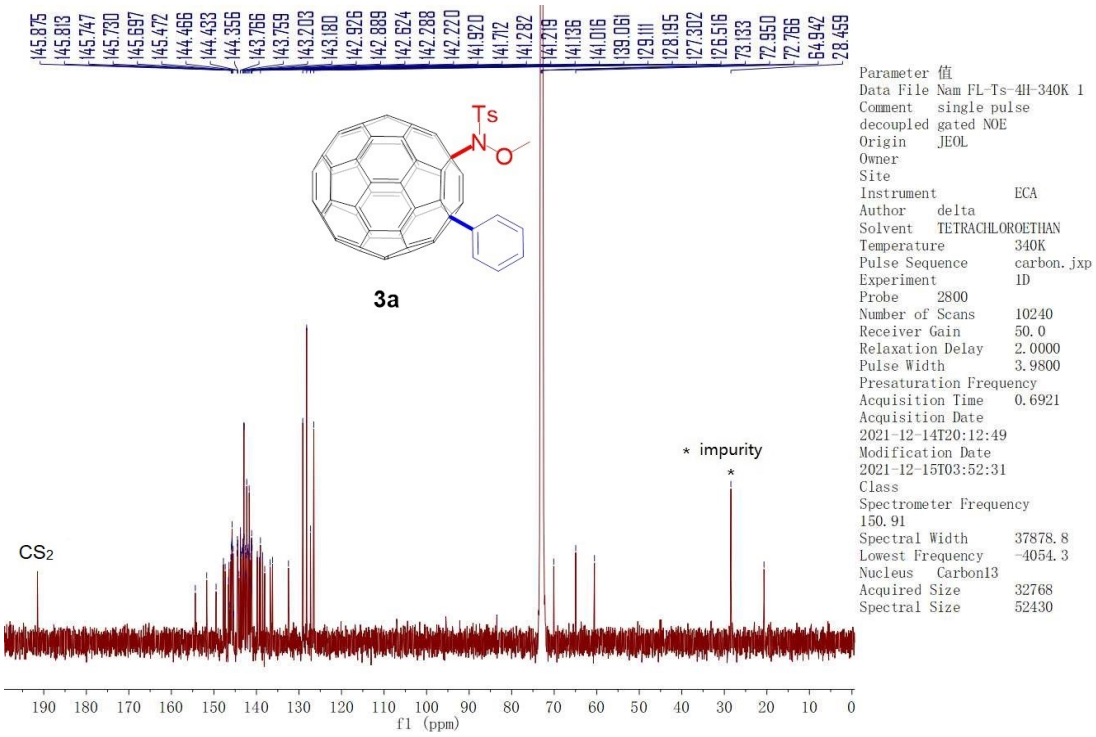


Figure S42. ^{13}C NMR spectrum (150 MHz, 340 K, $C_2D_2Cl_4$) of compound **3a**.

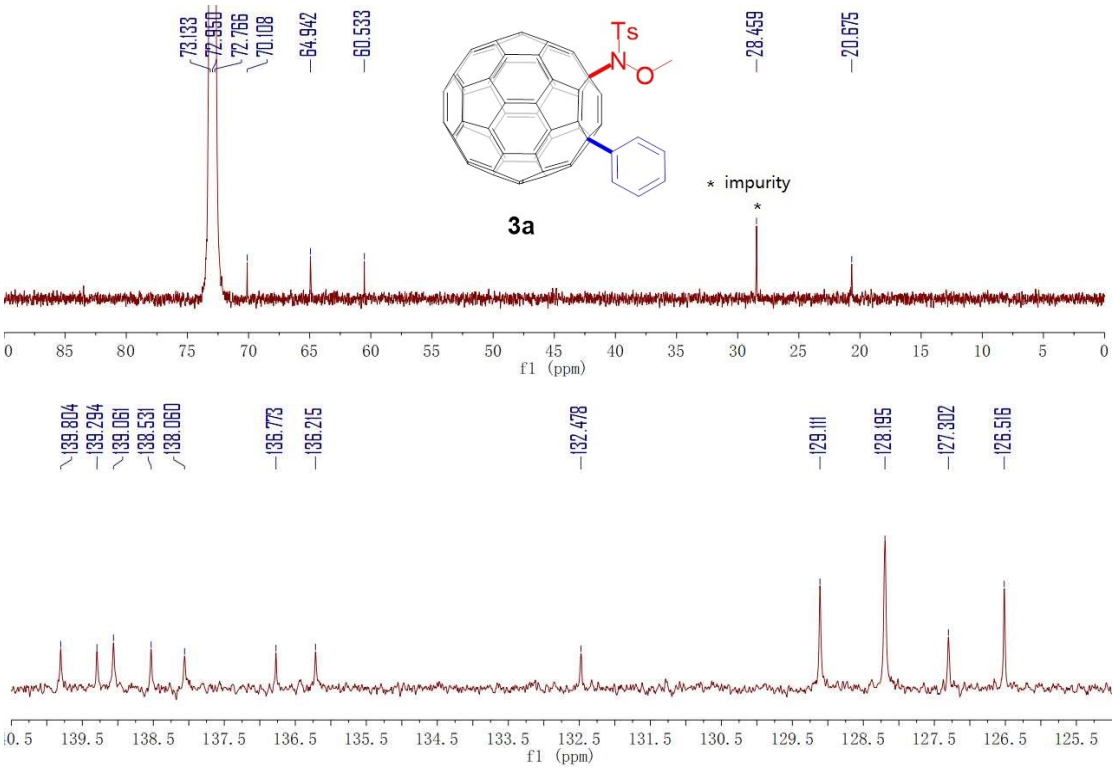


Figure S43. Expanded ^{13}C NMR spectrum (150 MHz, 340 K, $C_2D_2Cl_4$) of compound **3a**.

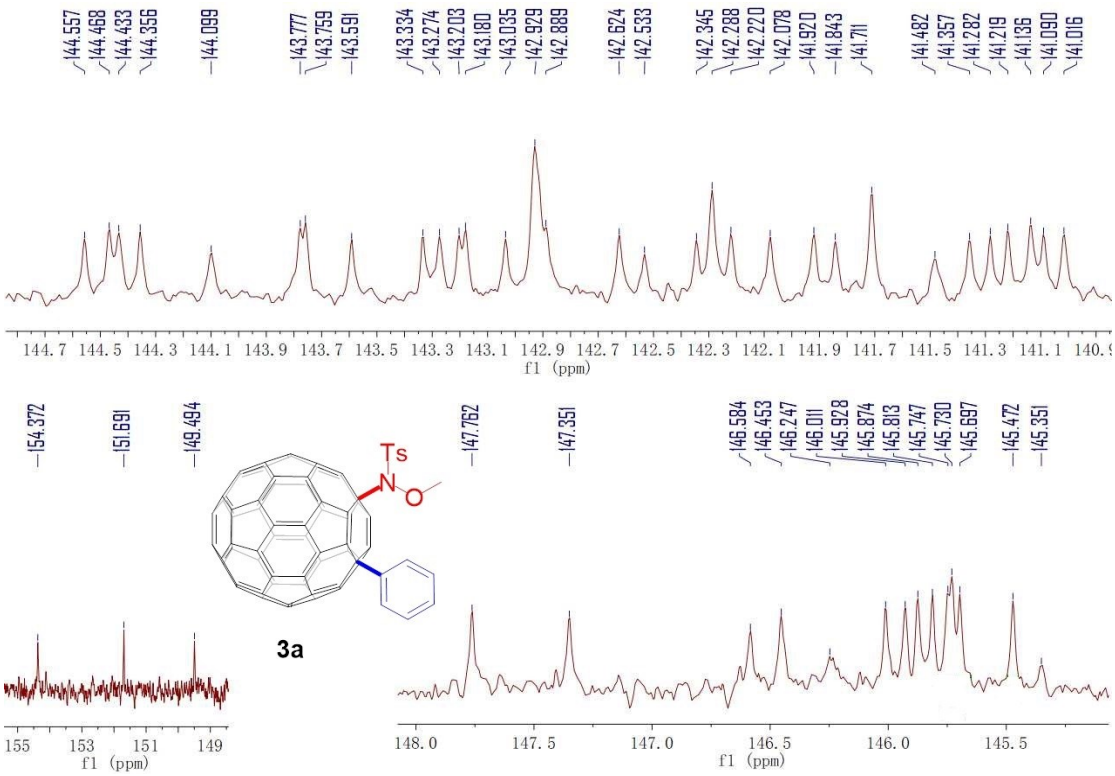


Figure S44. Expanded ^{13}C NMR spectrum (150 MHz, 340 K, $C_2D_2Cl_4$) of compound **3a**.

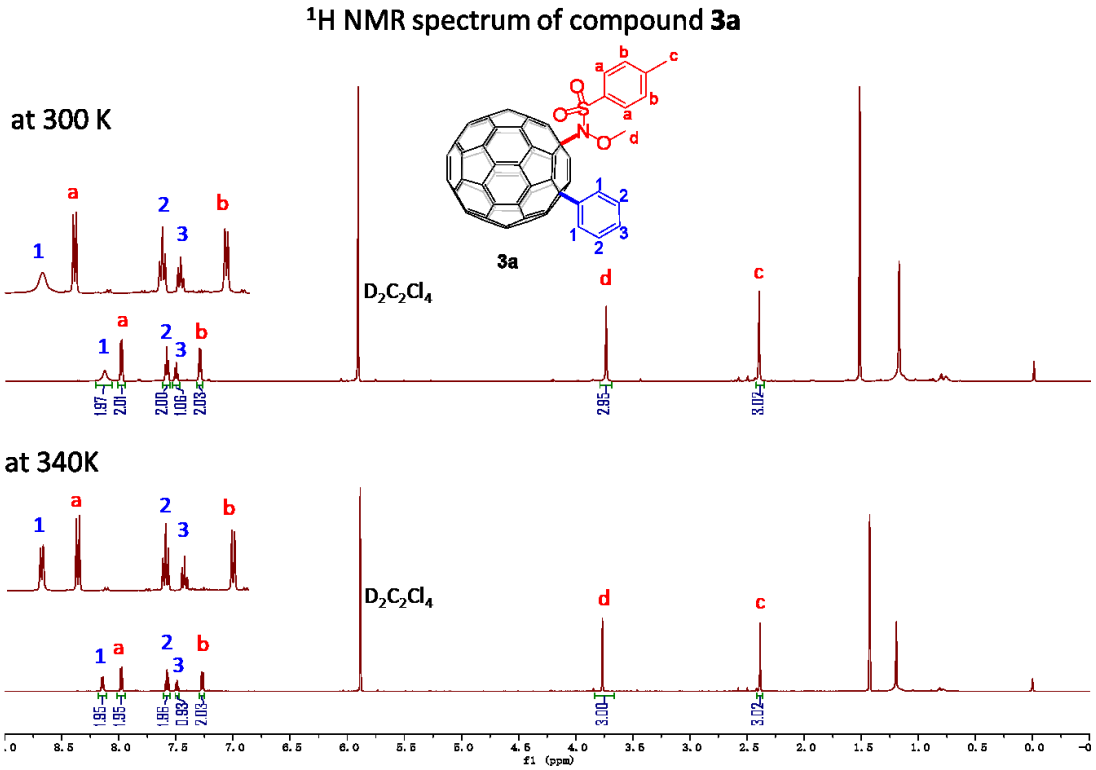


Figure S45. ^1H NMR spectra (100 MHz, $C_2D_2Cl_4$) of compound **3a** at 300 K and 340 K, respectively.

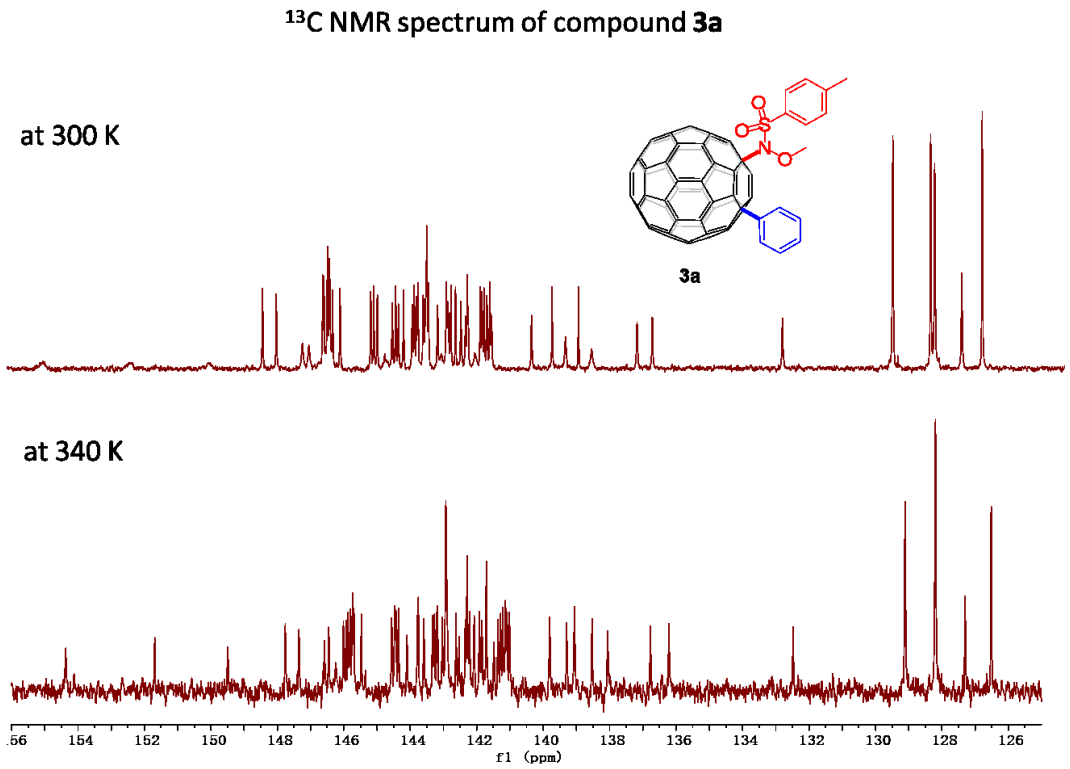


Figure S46. ^{13}C NMR spectra (100 MHz, $C_2D_2Cl_4$) of compound **3a** at 300 K and 340 K, respectively.

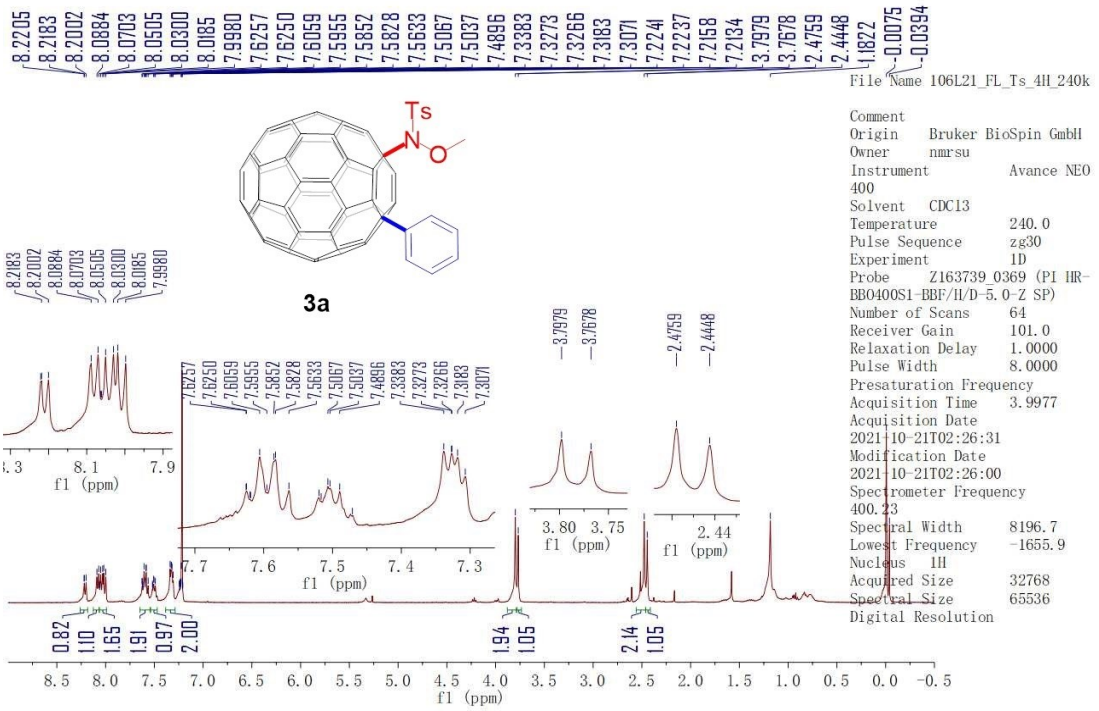


Figure S47. ^{1}H NMR spectrum (400 MHz, 240 K, $CS_2/CDCl_3$) of compound **3a**.

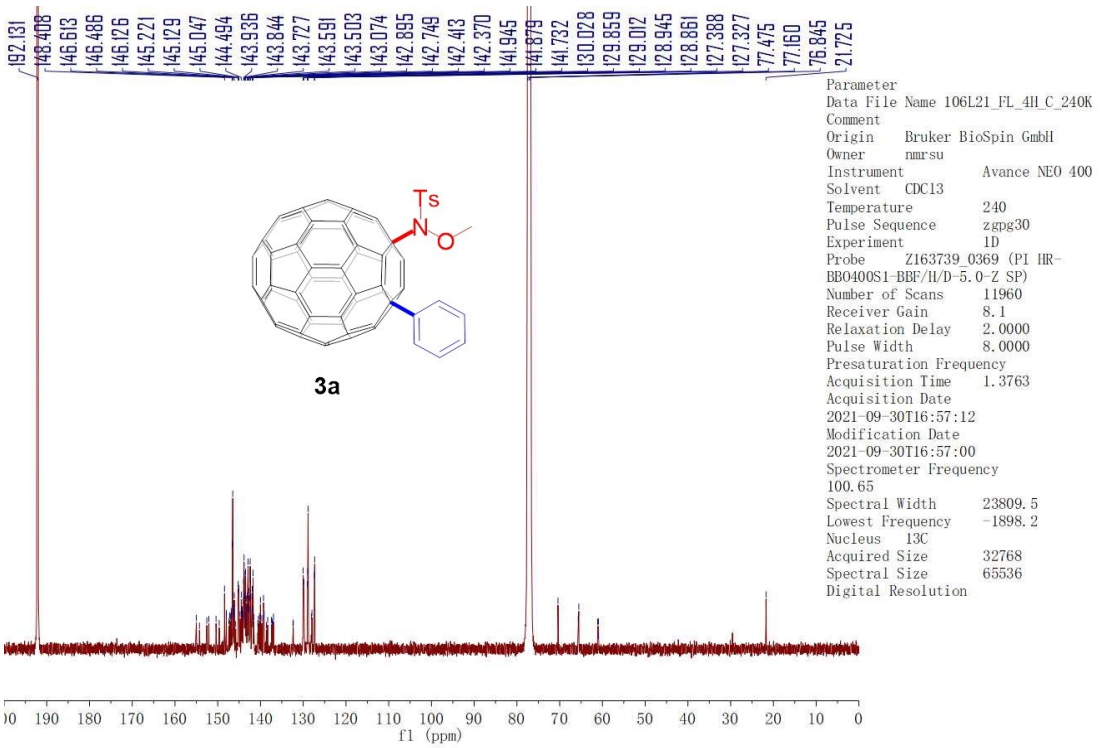


Figure S48. Expanded ^{13}C NMR spectrum (100 MHz, 240 K, $CS_2/CDCl_3$) of compound **3a**.

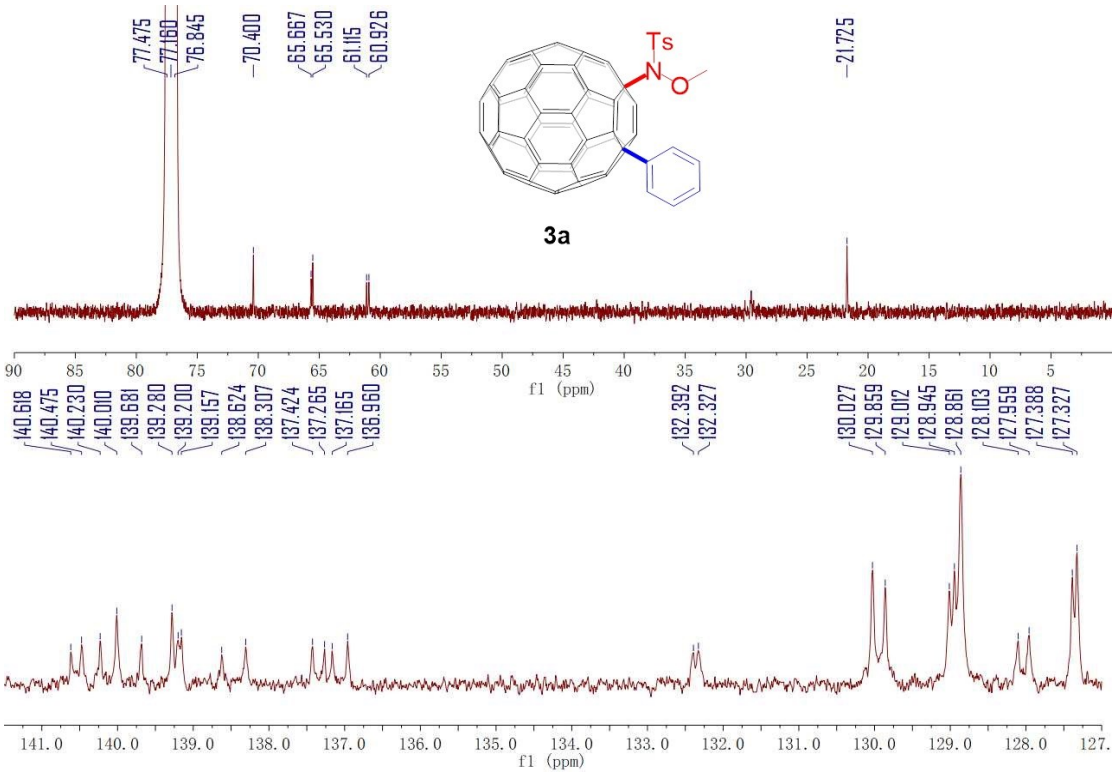


Figure S49. Expanded ^{13}C NMR spectrum (100 MHz, 240 K, $CS_2/CDCl_3$) of compound **3a**.

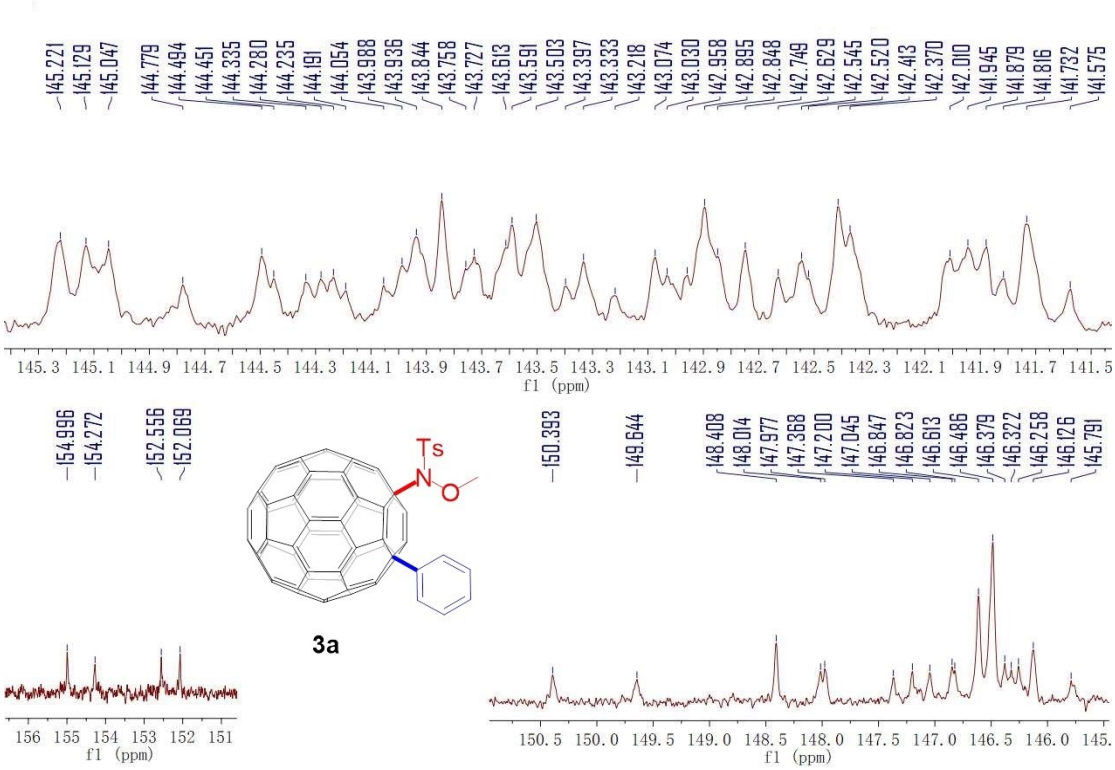


Figure S50. Expanded ^{13}C NMR spectrum (100 MHz, 240 K, $CS_2/CDCl_3$) of compound **3a**.

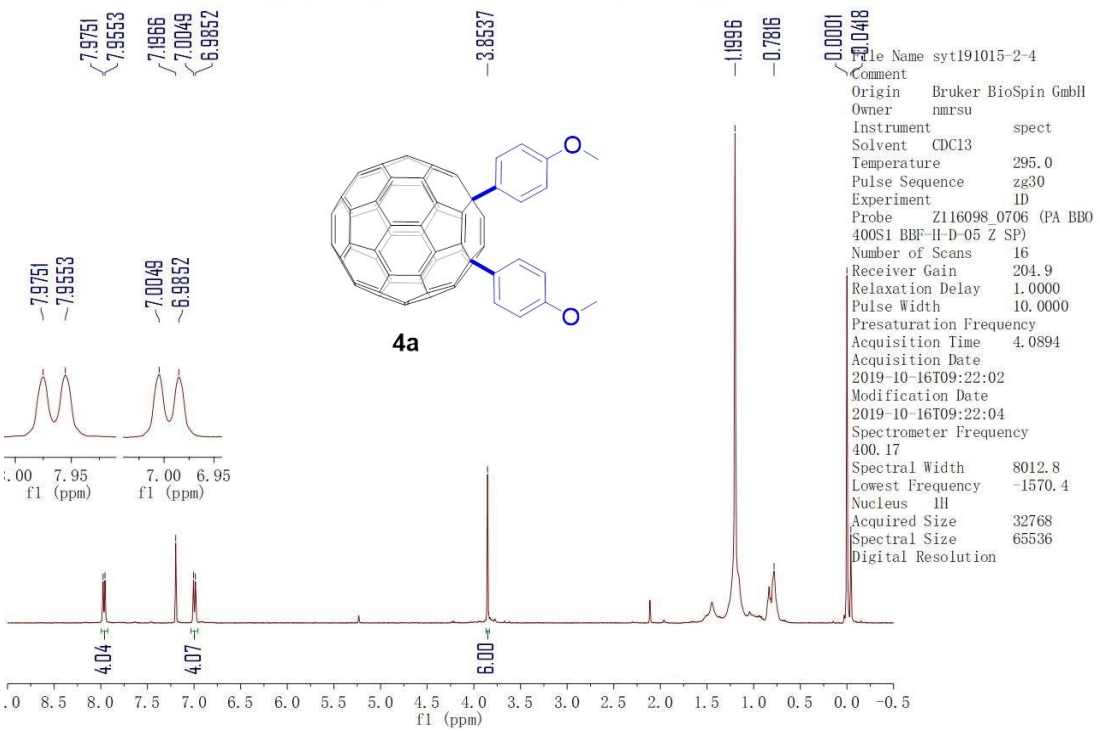


Figure S51. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **4a**.

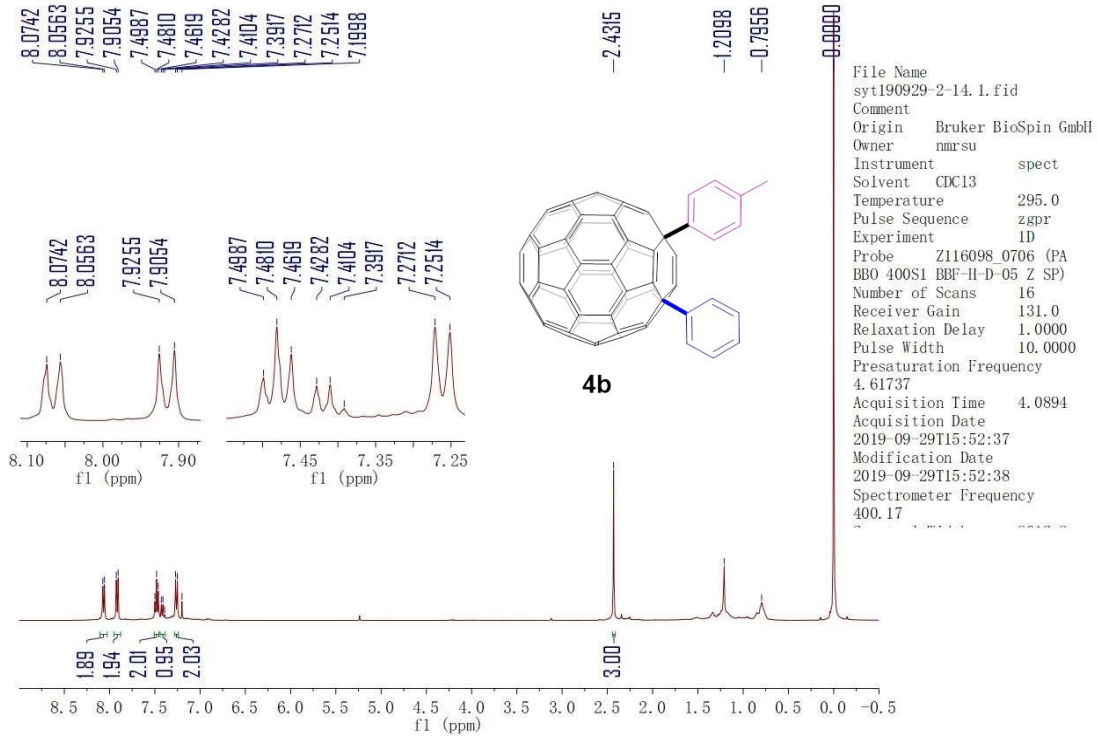


Figure S52. ^{1}H NMR spectrum (400 MHz, CS_2/$CDCl_3$) of compound **4b**.

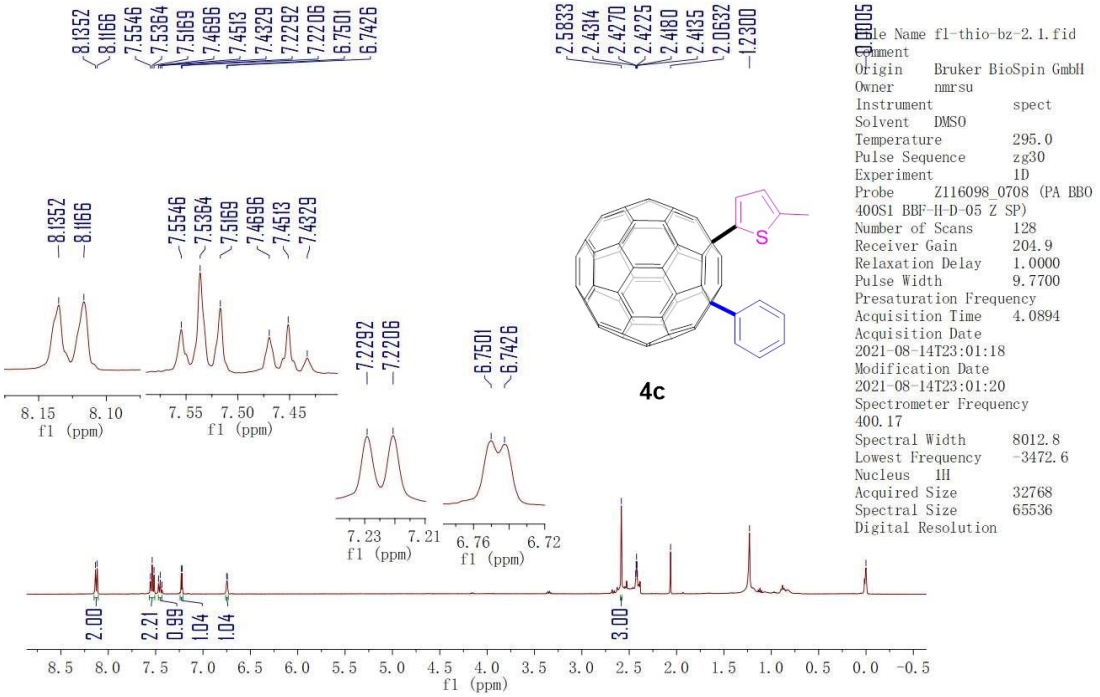


Figure S53. ^{1}H NMR spectrum (400 MHz, CS_2/DMSO-d_6) of compound **4c**.

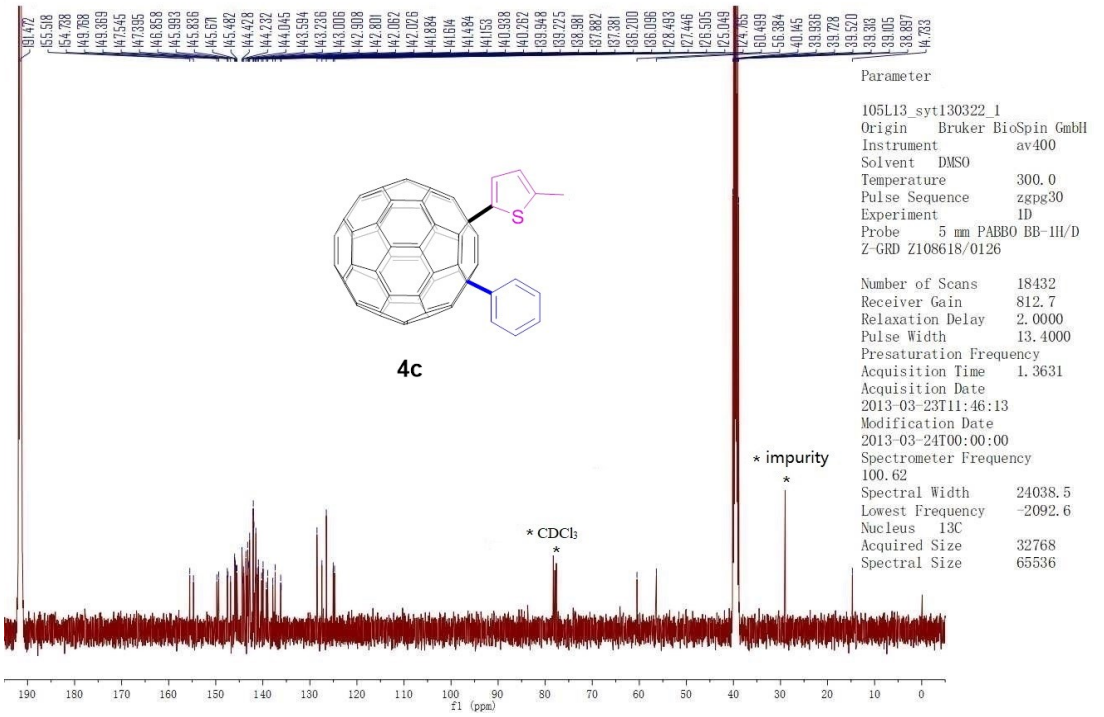


Figure S54. ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4c**.

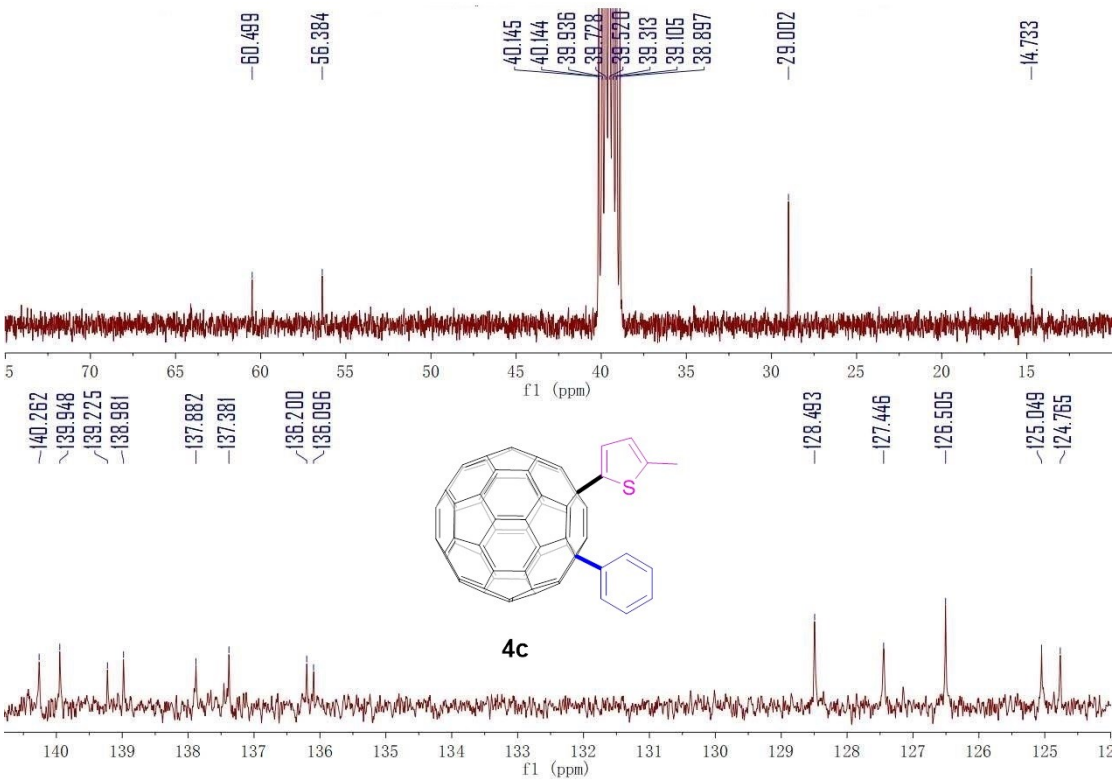


Figure S55. Expanded ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4c**.

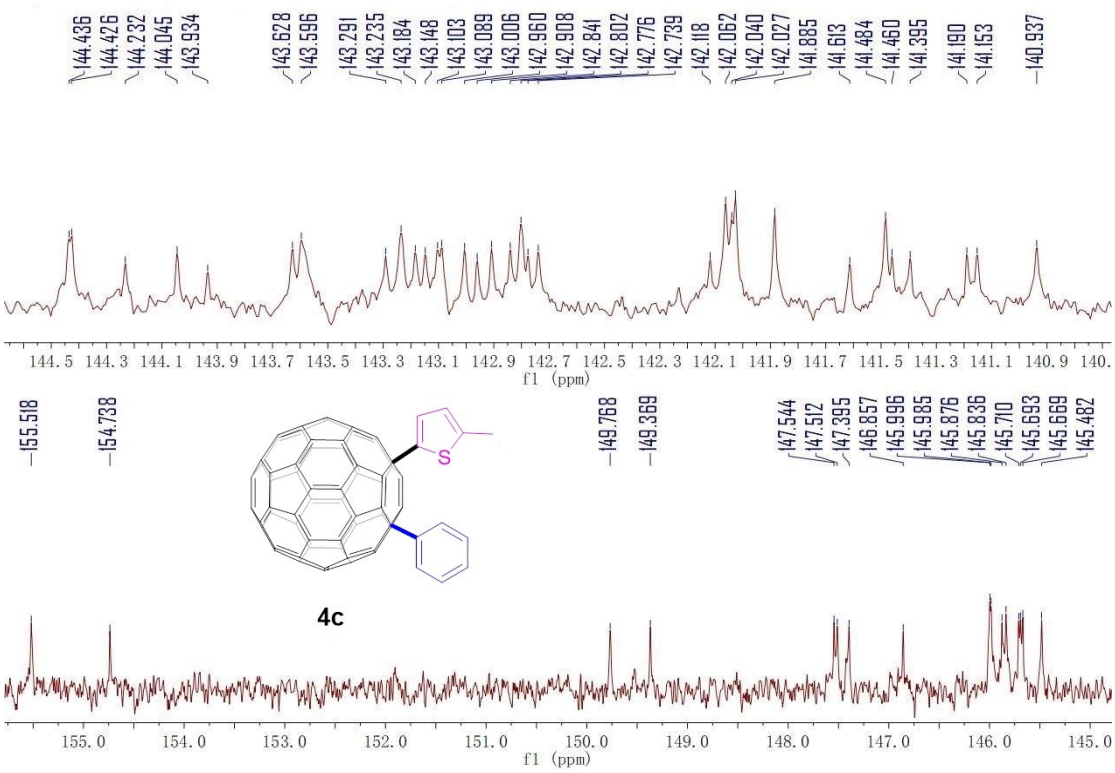


Figure S56. Expanded ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4c**.

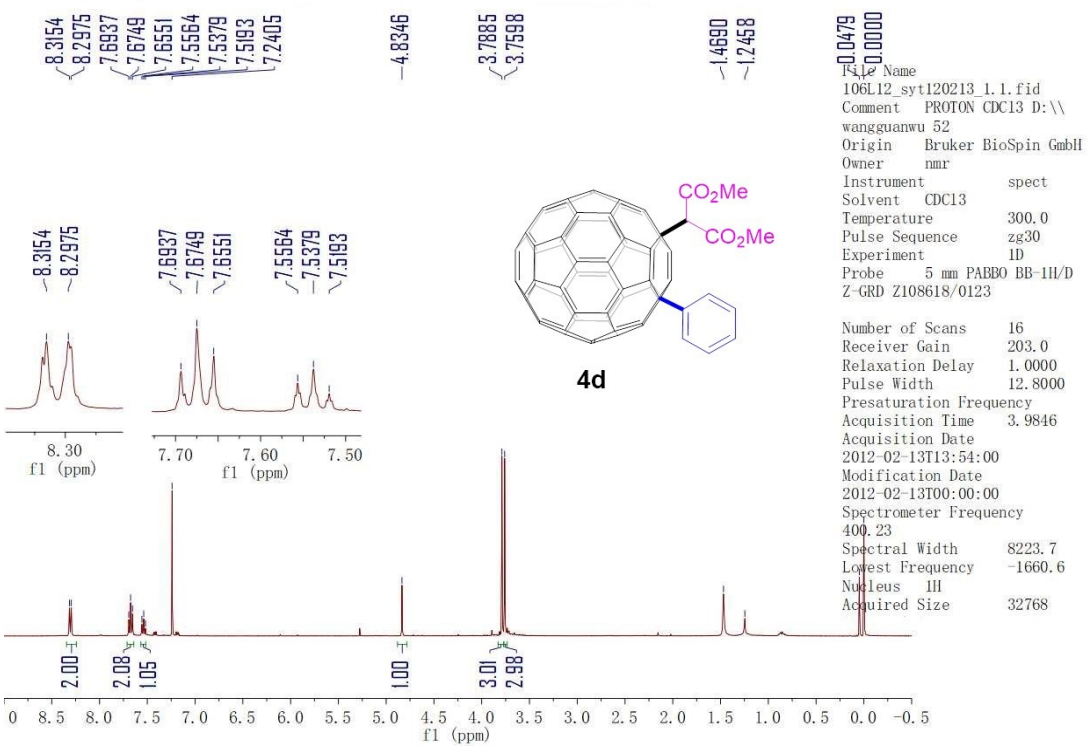


Figure S57. ^1H NMR spectrum (400 MHz, CS_2/$CDCl_3$) of compound **4d**.

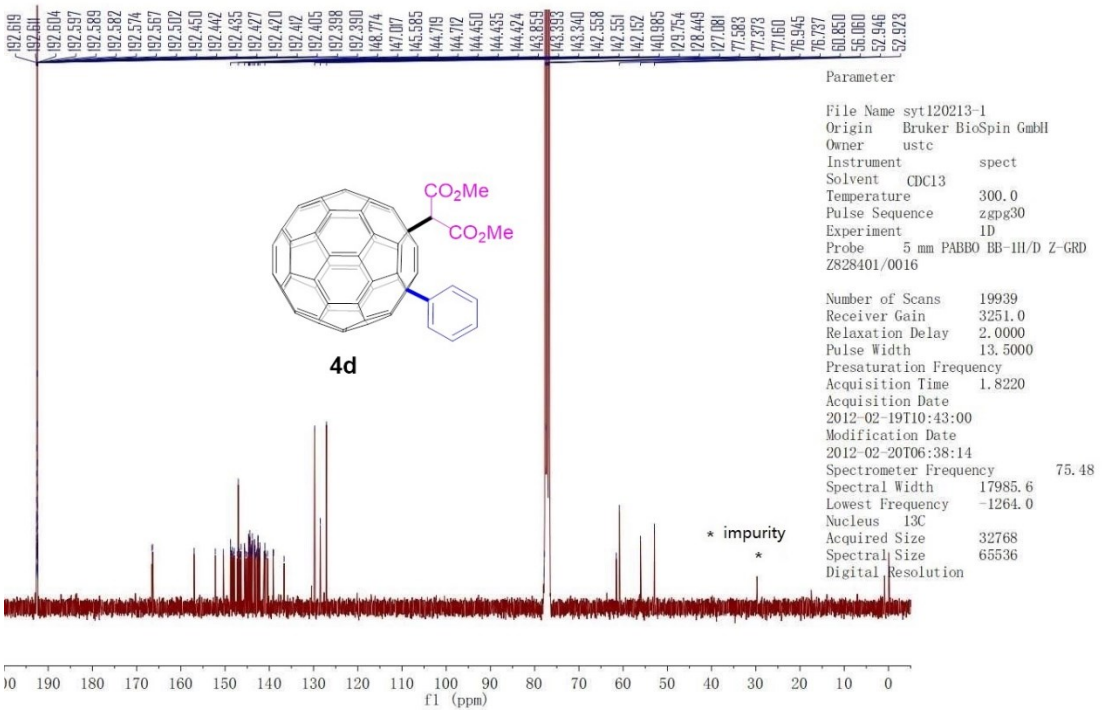


Figure S58. ^{13}C NMR spectrum (75 MHz, $CS_2/CDCl_3$) of compound **4d**.

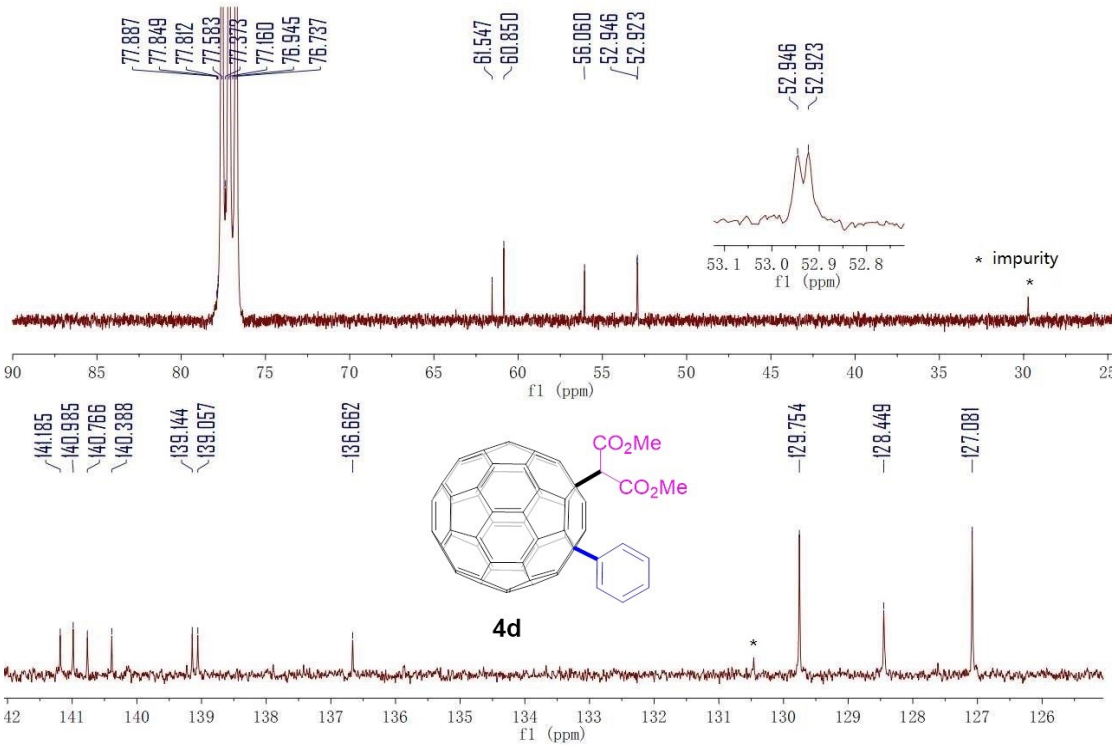


Figure S59. Expanded ^{13}C NMR spectrum (75 MHz, $CS_2/CDCl_3$) of compound **4d**.

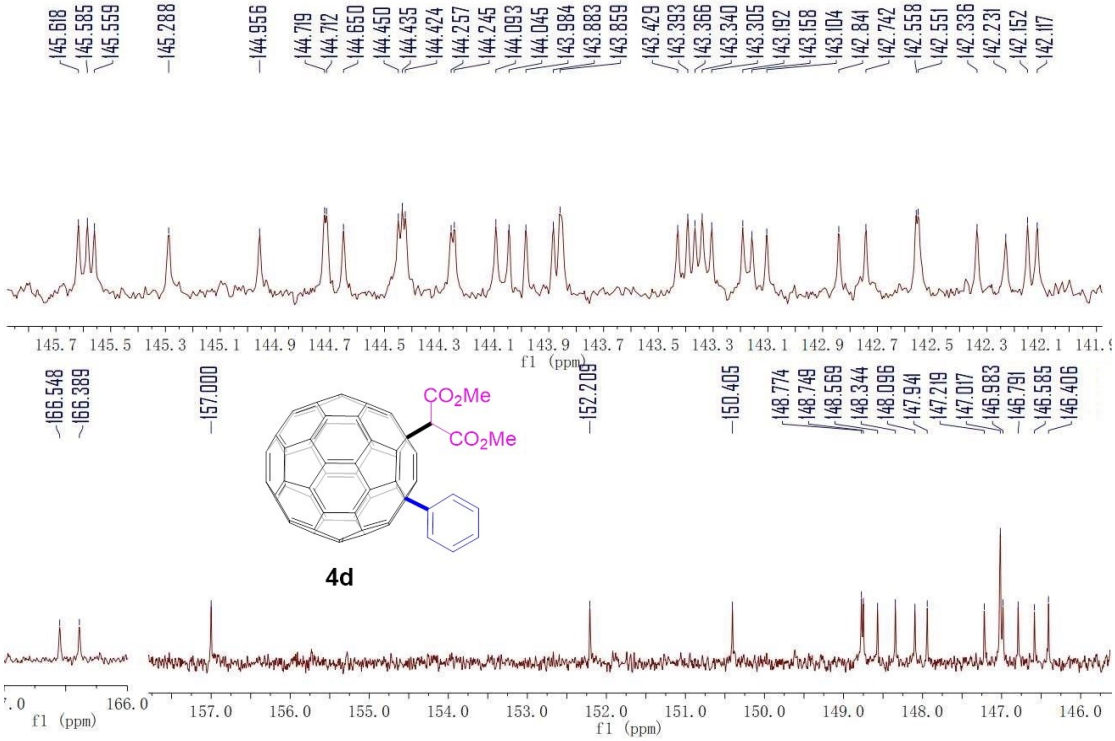


Figure S60. Expanded ^{13}C NMR spectrum (75 MHz, $CS_2/CDCl_3$) of compound **4d**.

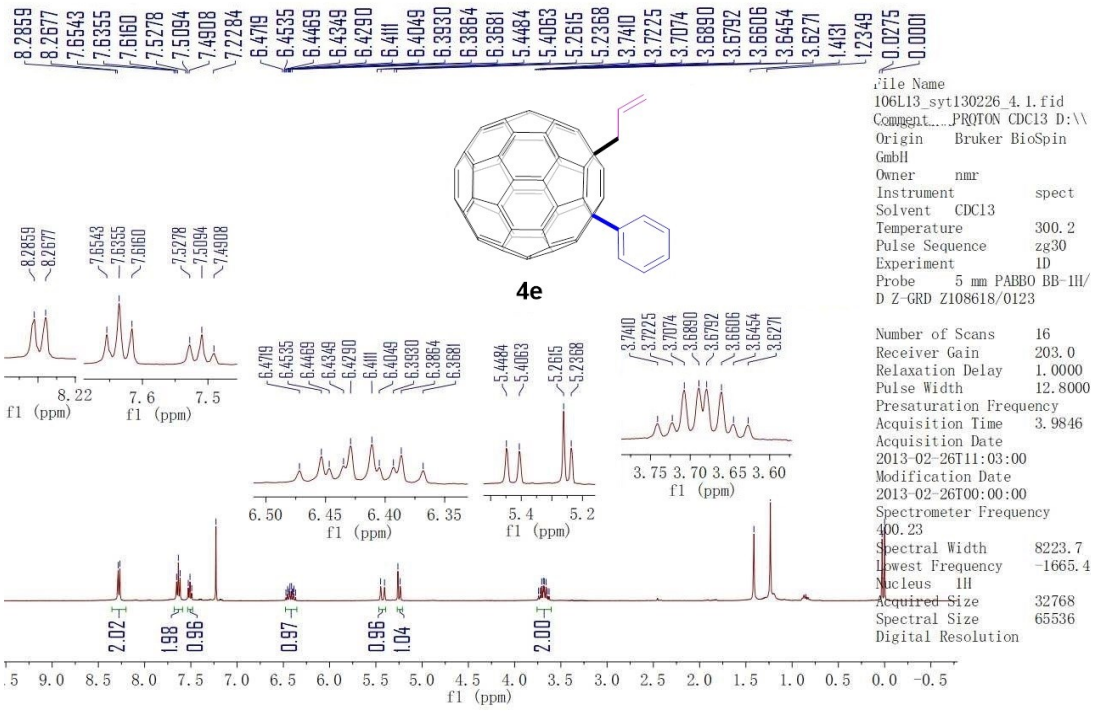


Figure S61. ^{1}H NMR spectrum (400 MHz, $CS_2/CDCl_3$) of compound **4e**.

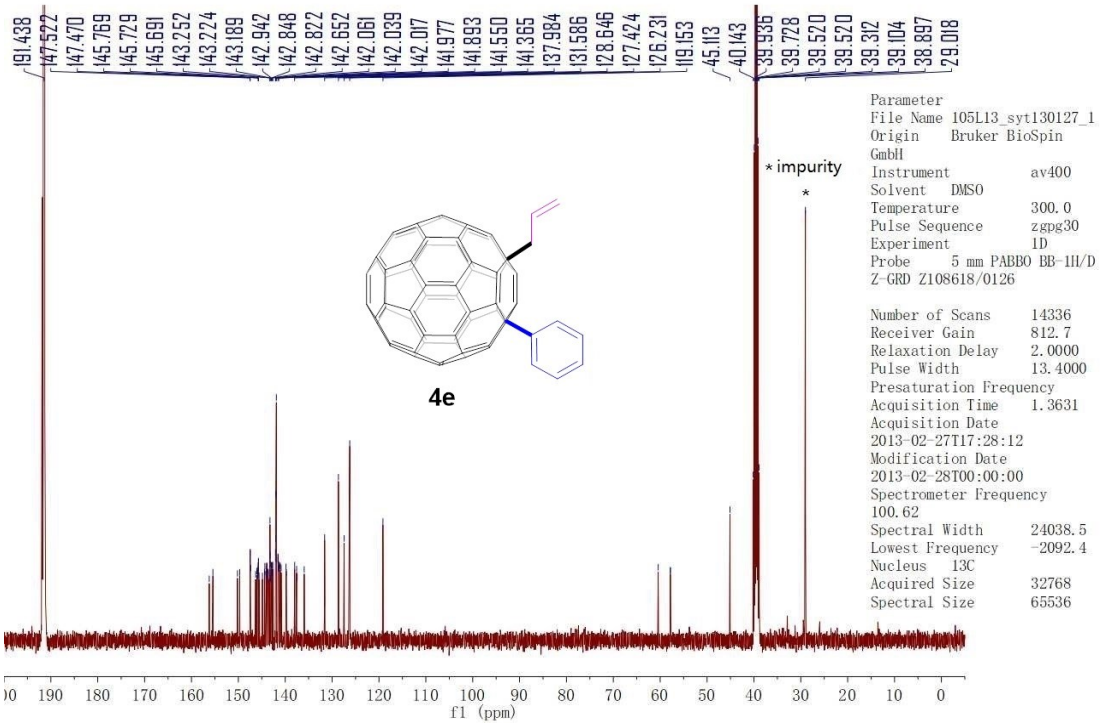


Figure S62. ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4e**.

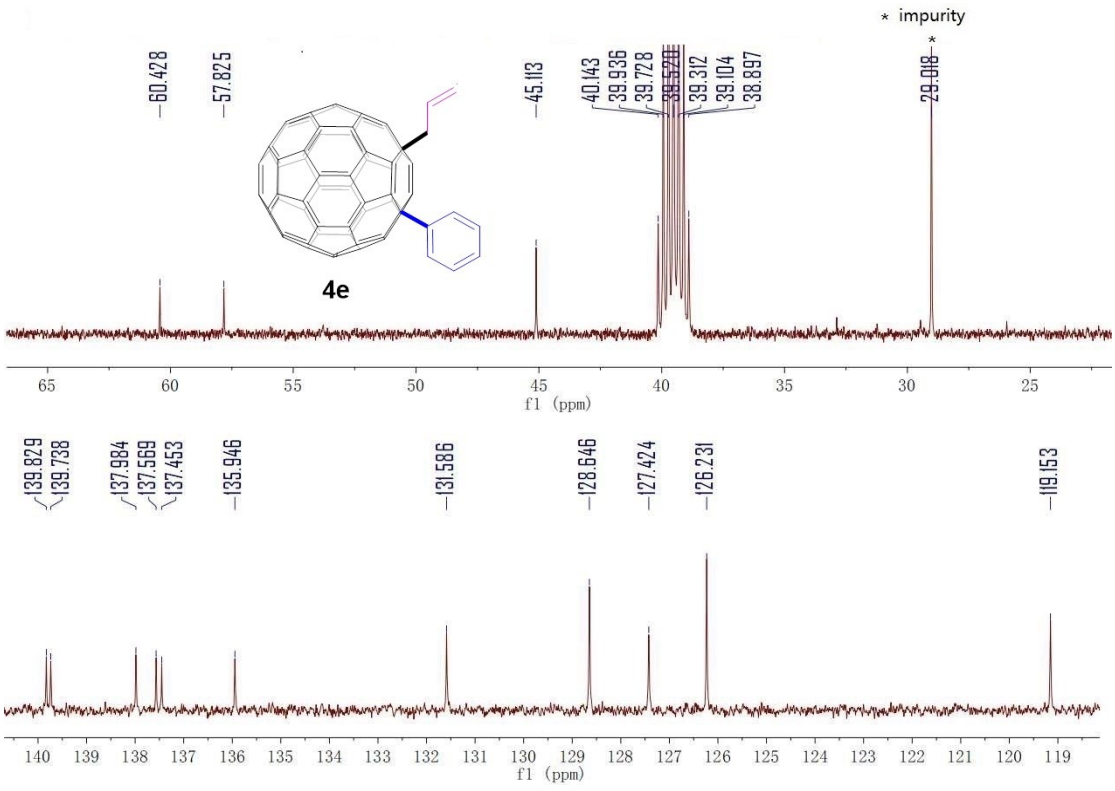


Figure S63. Expanded ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4e**.

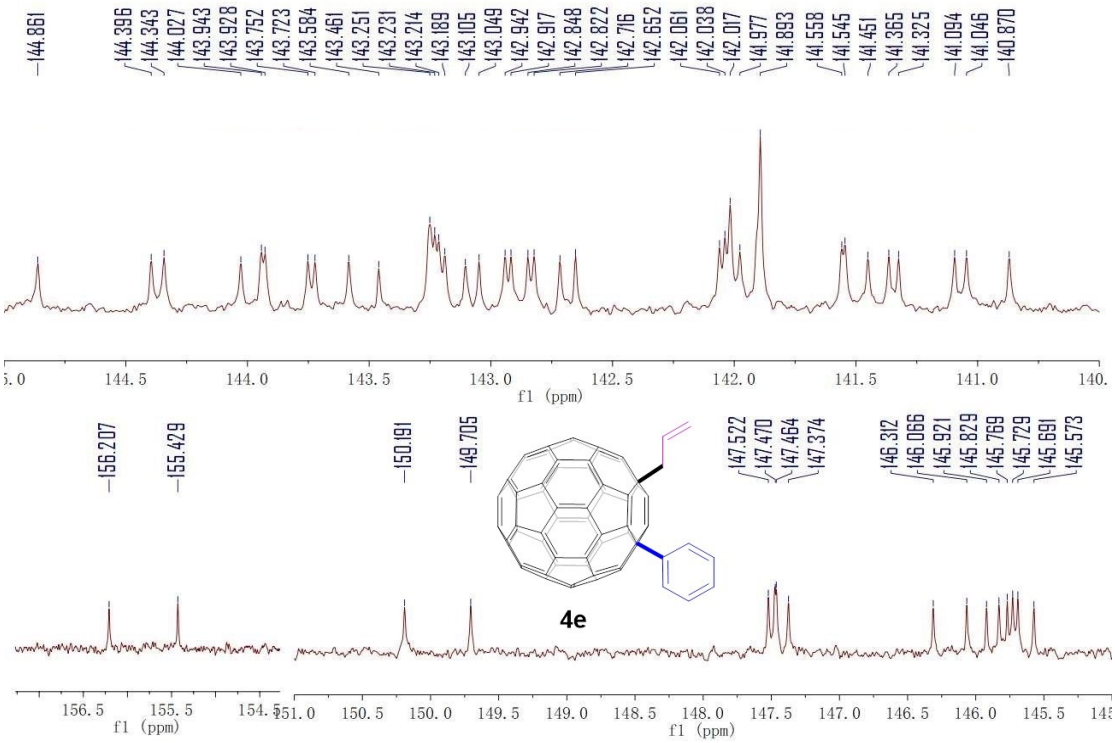


Figure S64. Expanded ^{13}C NMR spectrum (100 MHz, CS_2/DMSO-d_6) of compound **4e**.

References

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