Electronic Supplementary Information

Silver(I)-Mediated Three-Component Annulation Reaction of [60]Fullerene, Sulfonylhydrazones, and Nitriles: Leading to Diverse Disubstituted [60]Fullerene-Fused Dihydropyrroles

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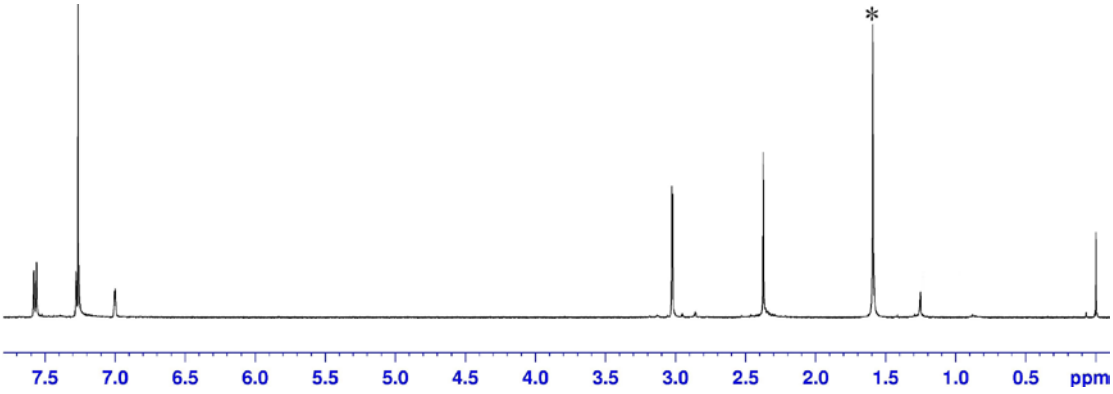
1. General information

Ag_2CO_3 and Cs_2CO_3 were purchased from Sigma-Alderich. *o*-Dichlorobenzene (ODCB) and CH_3CN were treated with CaH_2. ^1H NMR (400 MHz) and ^{13}C NMR (100 and 150 MHz) were registered on Bruker 400 and 600 M spectrometers with tetramethylsilane (TMS) as internal standard. HSQC, HMBC and NOESY spectra were recorded on Bruker 600 M spectrometers. HRMS were measured on Thermo Fisher Scientific LTQ FT Ultra with Pierce LTQ ESI Positive Ion Calibration Solution as external standard, and Bruker Apex IV FTMS with tunemix (from the instrument itself) as external standard. Geometries were optimized by the three-paramater hyrid exchange functional and Lee–Yang–Parr correlation functional (B3LYP) method with the 6–31G* basis set applied for C, H, and N elements. The ^1H and ^{13}C NMR spectra of isomers were calculated using the B3LYP functional and the 6–311+g(2d,p) basis set. All calculations were performed by Gaussian 09 program.[1] The Cartesian coordinates of optimized structures were listed at S73-S87.

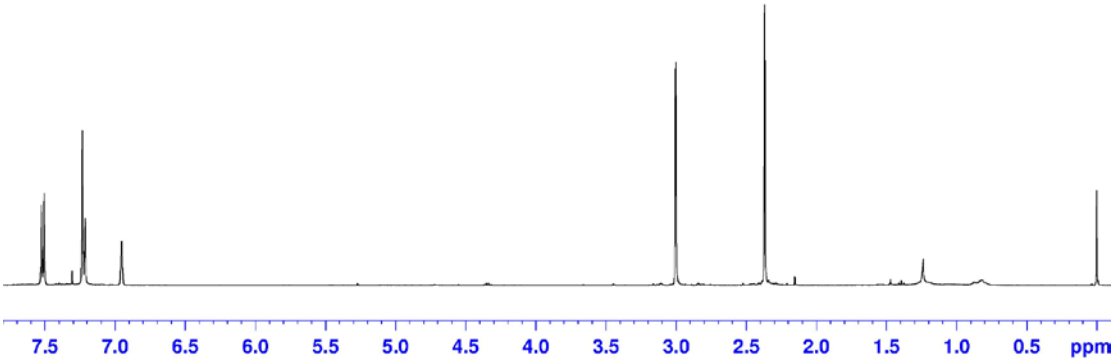
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision D.01*, Gaussian, Inc., Wallingford CT, 2009.

2. Determination of structure of 4aa

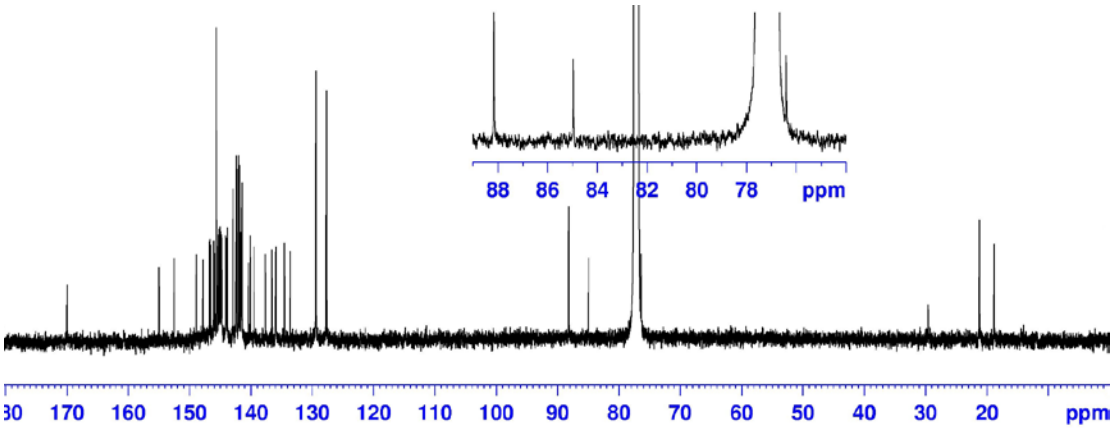
(1) 400 MHz ^{1}H NMR spectrum of product measured in $CDCl_3/CS_2$



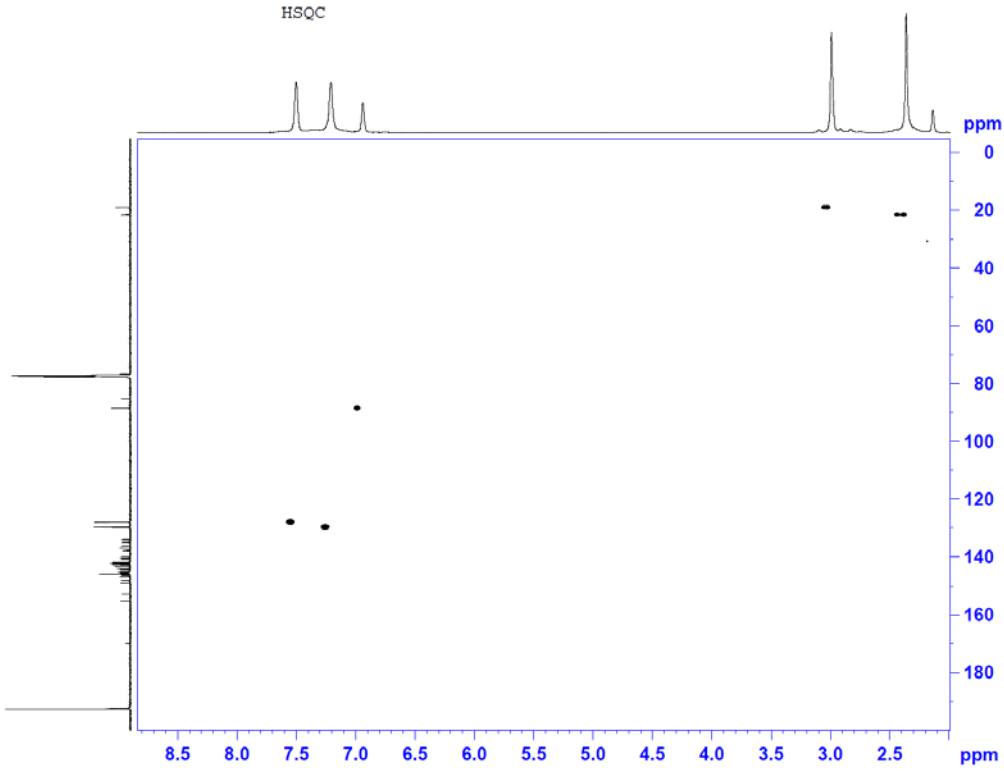
(2) D_2O Exchange Experiment



(3) 100 MHz ^{13}C NMR spectrum of product measured in $CDCl_3/CS_2$

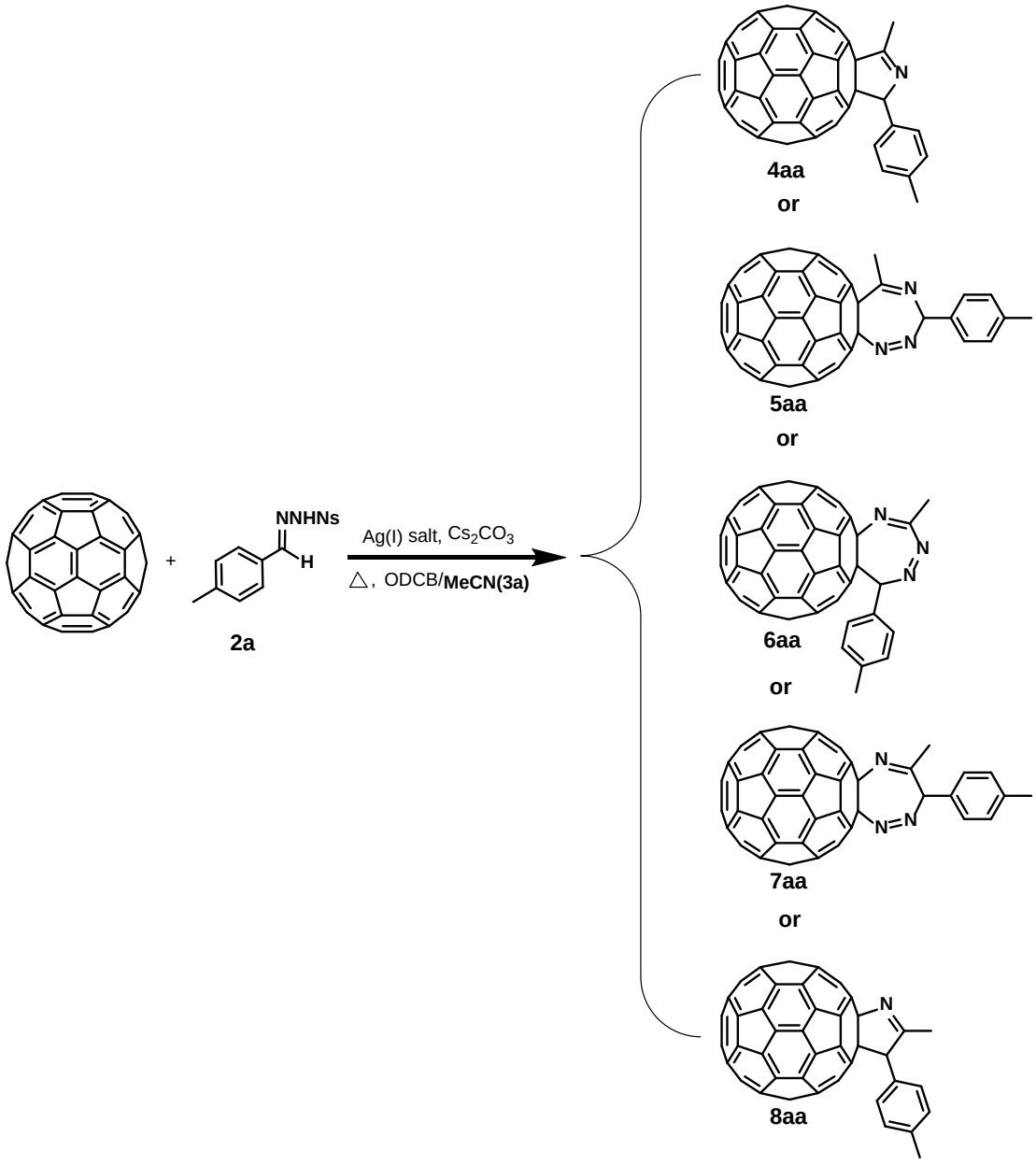


(4) HSQC spectrum of product measured in $CDCl_3/CS_2$ at 298 K

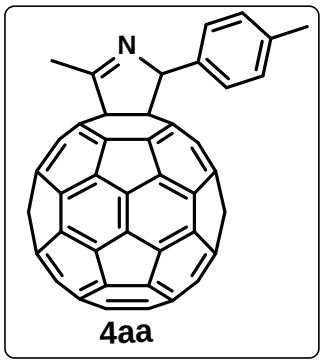


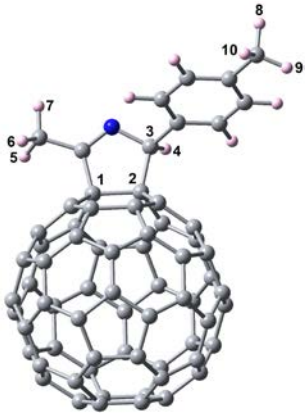
The combination of HSQC, ^{1}H and ^{13}C spectra allows easy assignment of the ***4-CH$_3$-C$_6$H$_4$-CH*** and ***CH$_3$-C=N*** substructures.

(5) Possible Structure **4aa**, **5aa**, **6aa**, **7aa** and **8aa**

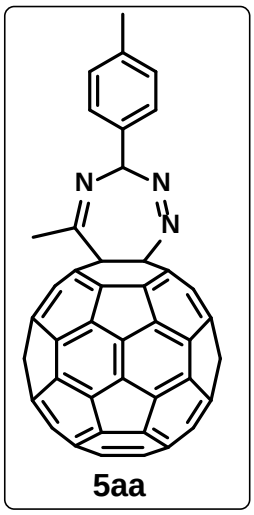


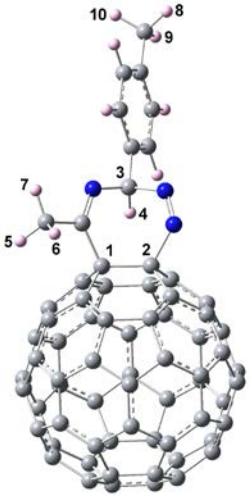
(6) Optimized structures and relative energies of **4aa, 5aa, 6aa, 7aa** and **8aa**



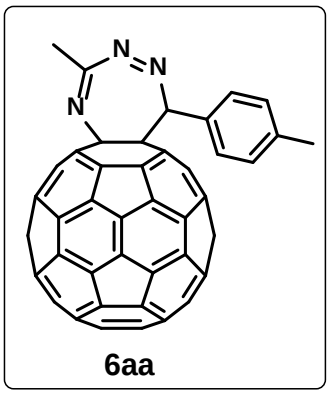


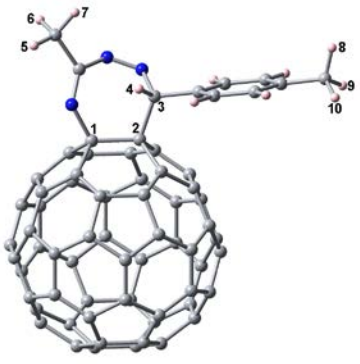
4aa

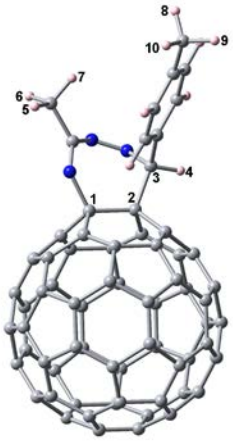




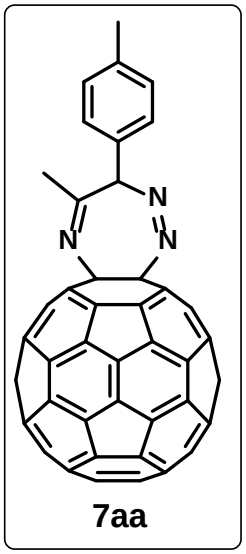
5aa



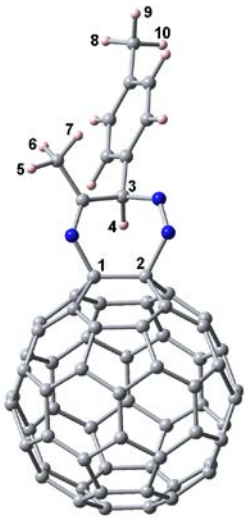




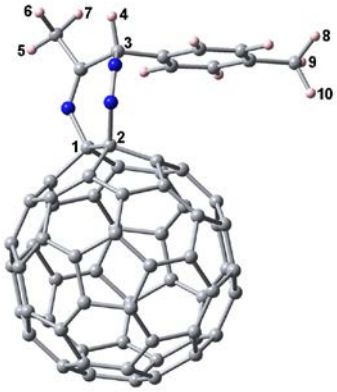
6aa (i) [E = -2838.699 a.u.] **6aa (ii)**



7aa

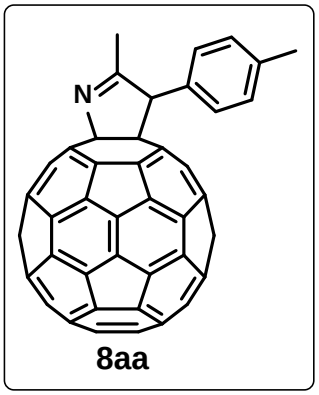


0.00 kcal/mol

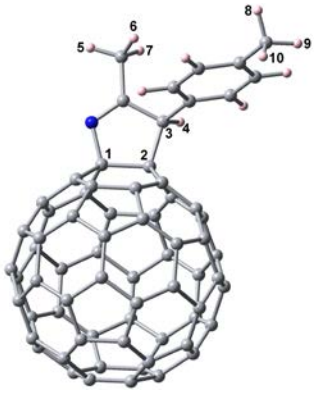


8.41 kcal/mol

7aa (i) [E = -2838.689 a.u.] 7aa (ii)



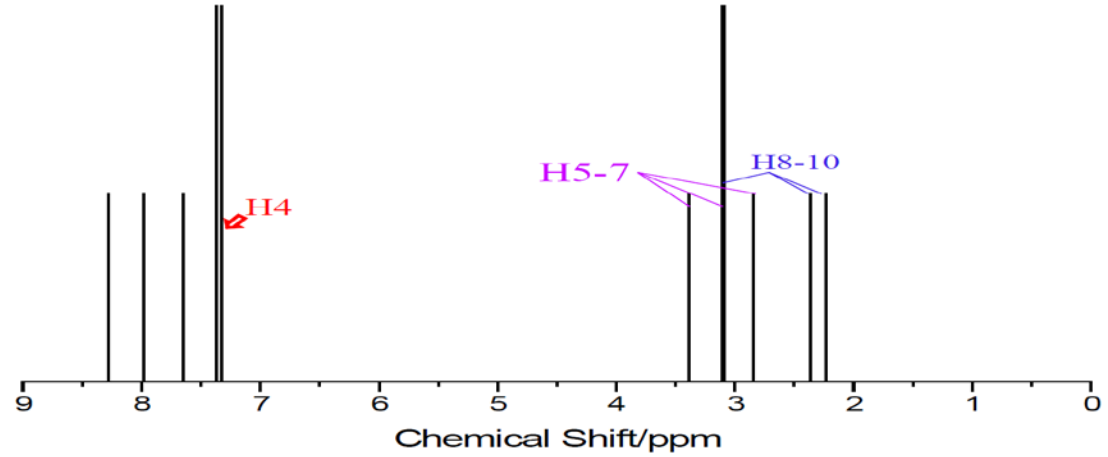
8aa



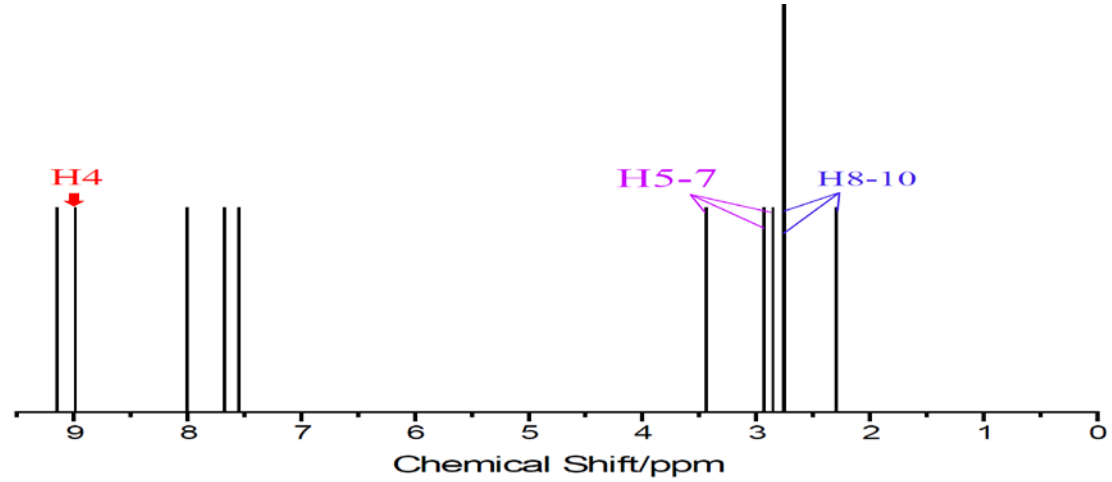
8aa

(7) Calculated ^{1}H NMR spectra of **4aa**, **5aa**, **6aa (i)**, **7aa (i)** and **8aa**

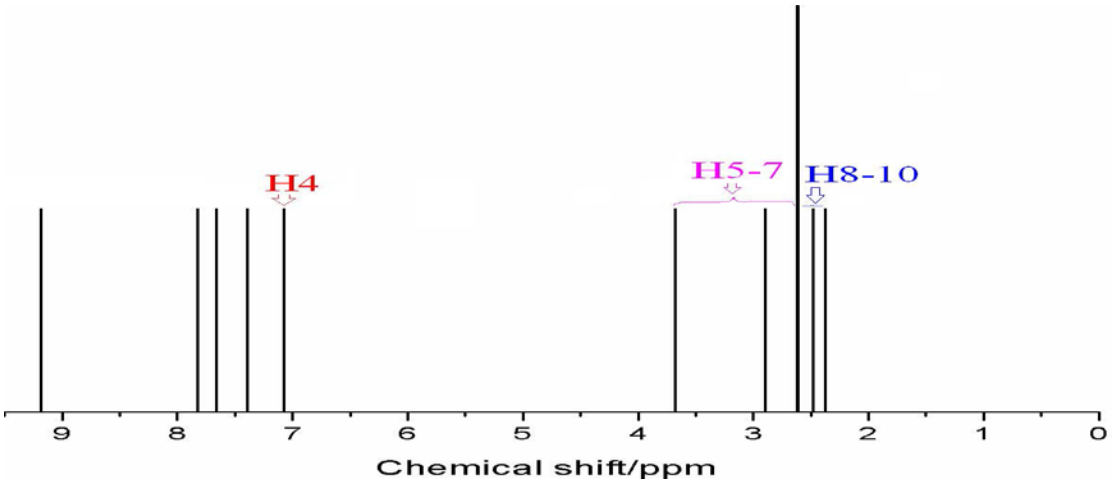
4aa



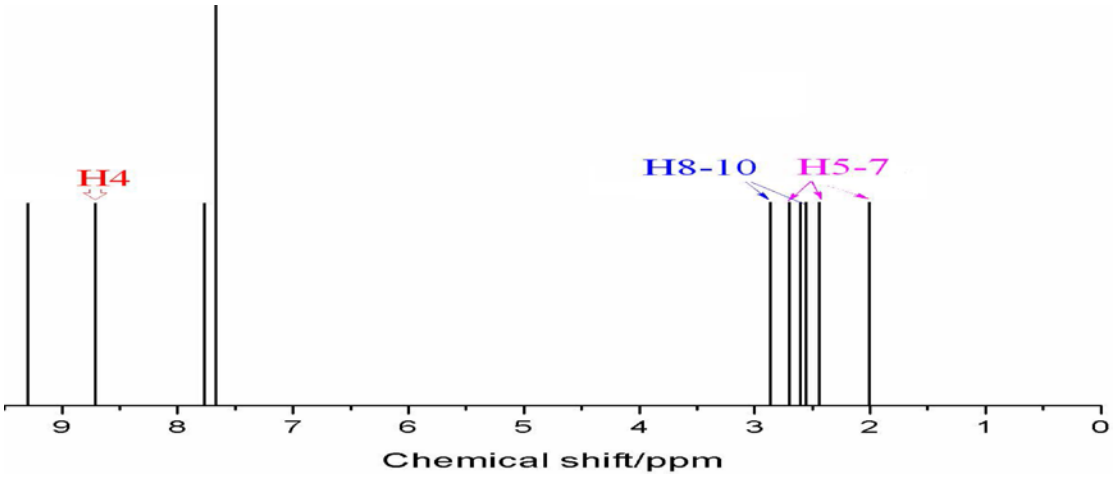
5aa



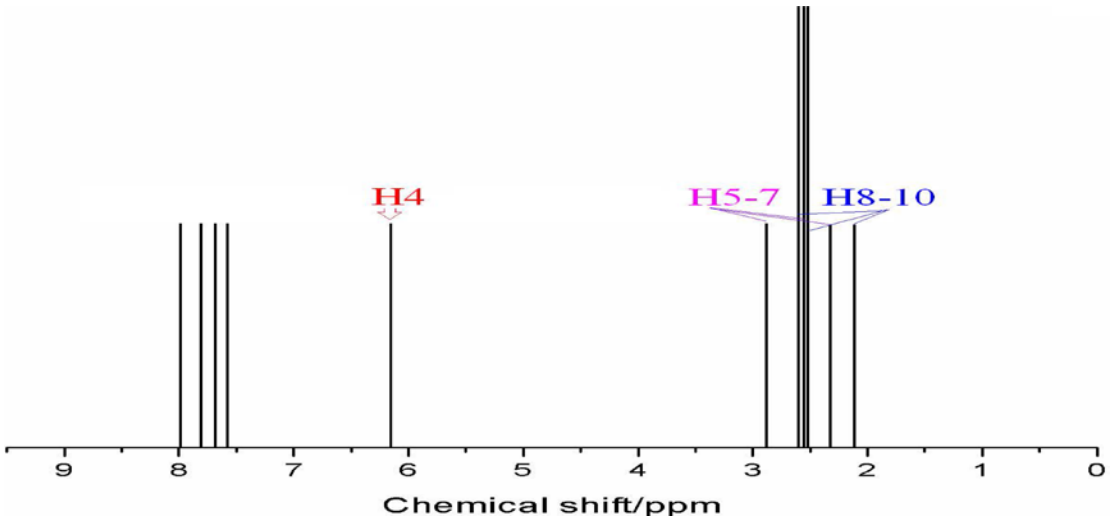
6aa (i)



7aa (i)

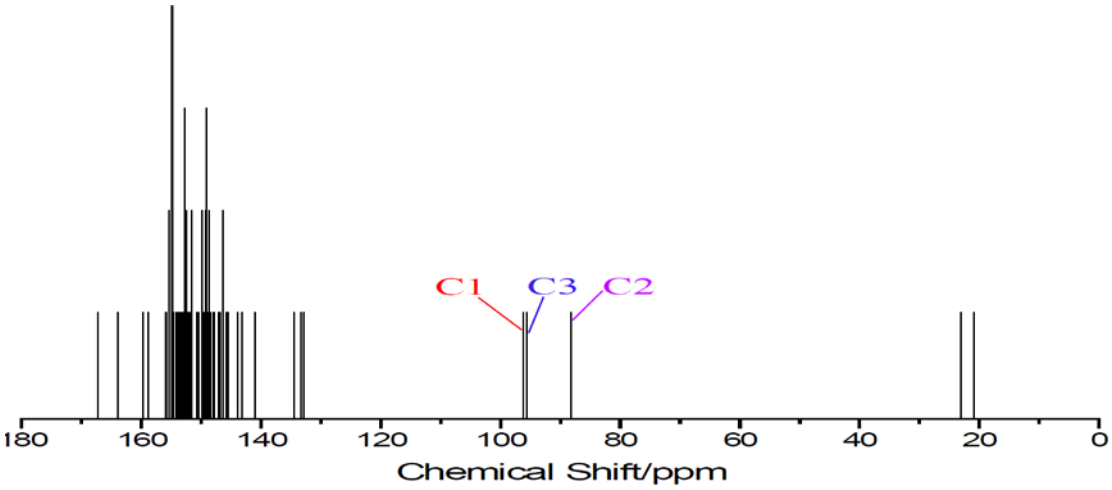

H4
H8-10
H5-7
9
8
7
6
5
4
3
2
1
0
Chemical shift/ppm

8aa

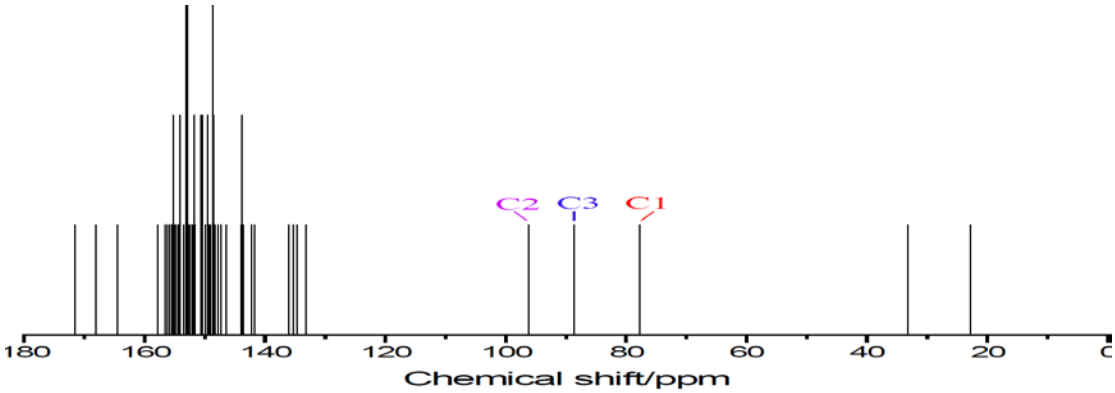

H4
H5-7
H8-10
9
8
7
6
5
4
3
2
1
0
Chemical shift/ppm

(8) Calculated ^{13}C NMR spectra of **4aa, 5aa, 6aa (i), 7aa (i)** and **8aa**

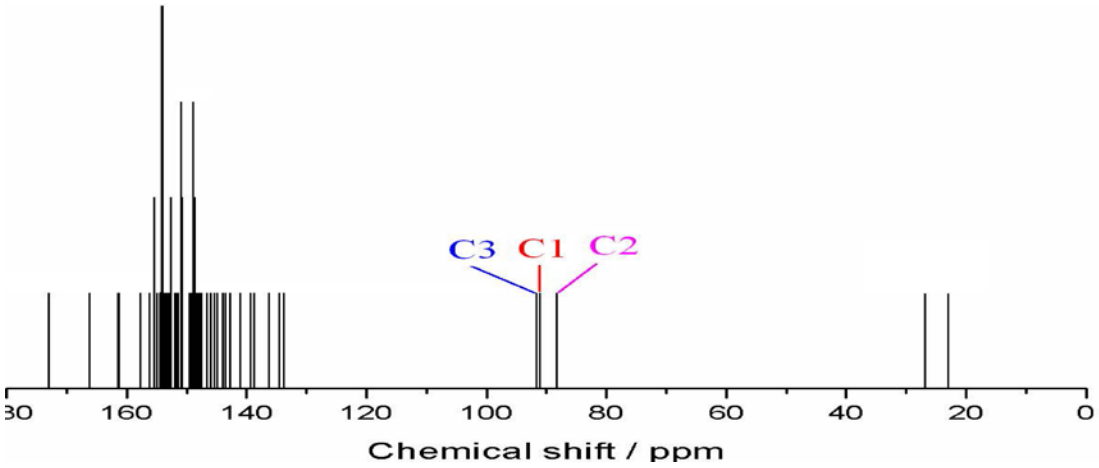
4aa



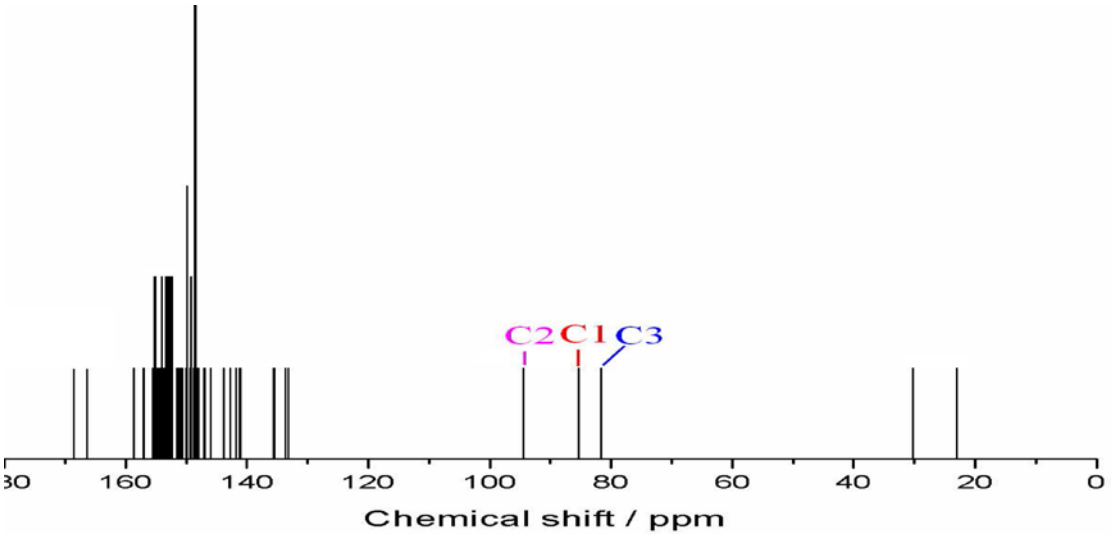
5aa



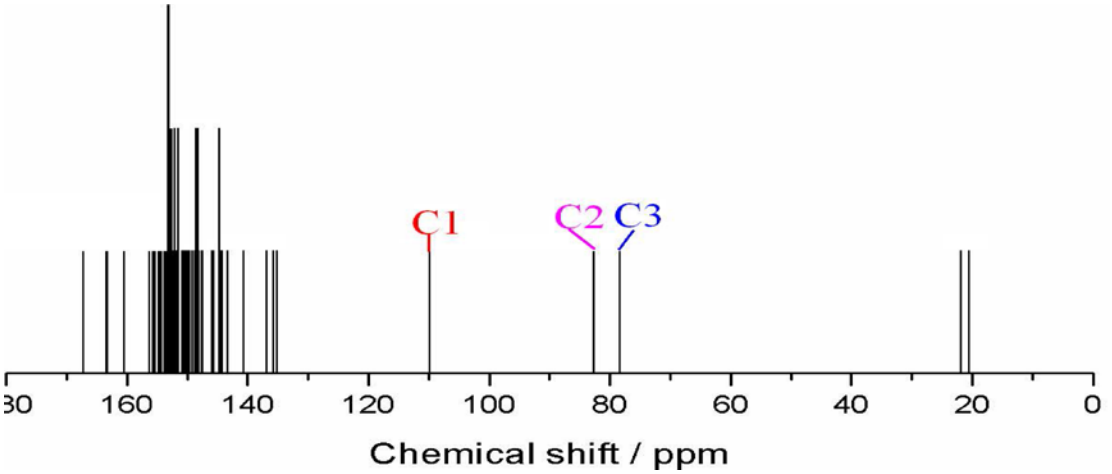
6aa (i)



7aa (i)

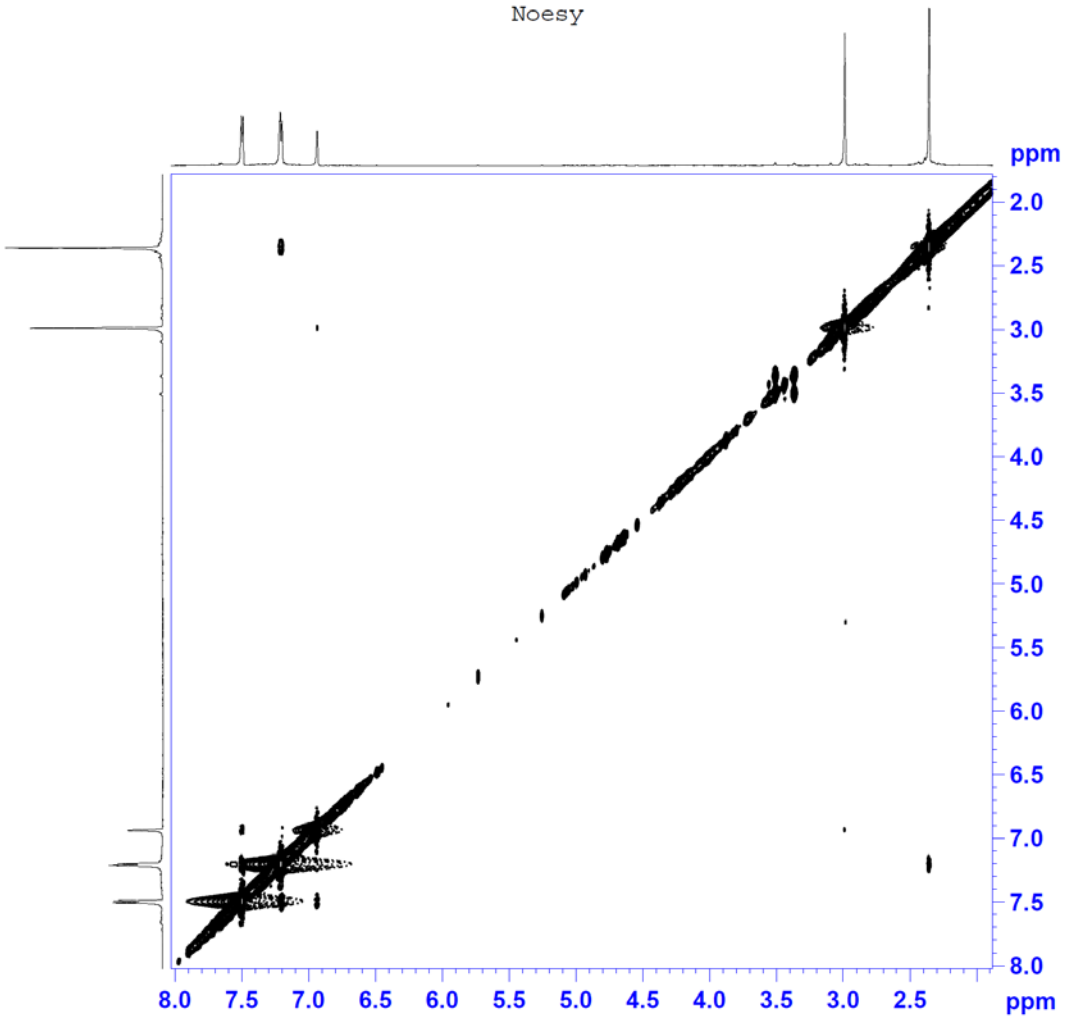


8aa



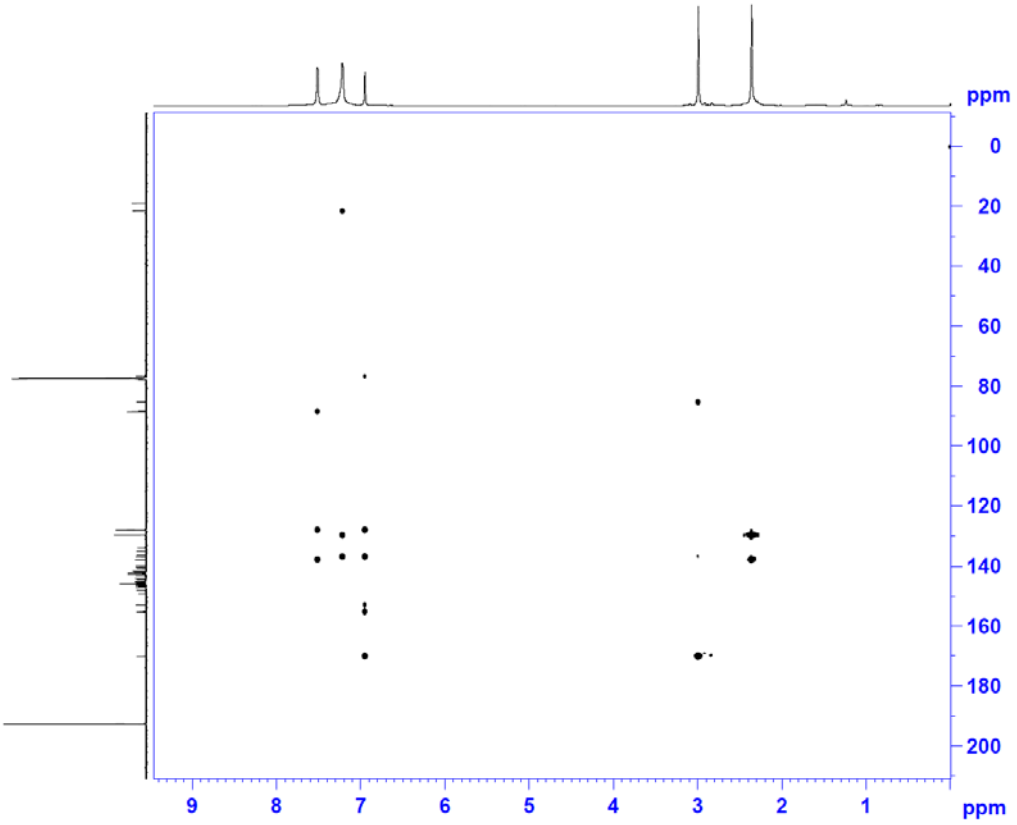
Compared **measured** ^{1}H and ^{13}C spectra of product with **calculated** ^{1}H and ^{13}C spectra of possible structures, *one of **4aa** and **6aa** should be the final structure of product, while other structures **5aa, 7aa** and **8aa** could be excluded.*

(9) NOESY spectrum of product measured in $CDCl_3/CS_2$ at 298 K



The shortest distance of ***H*$_3$**-C-C=N between ***H(4)***-C(3) and ***H***-Ar in optimized five structures is about 4.47 and 4.03 Å (for **4aa**); 4.45 and 3.82 Å (for **5aa**); 3.36 and 5.23 Å (for **6aa**); 3.60 and 2.89 Å (for **7aa**); 2.78 and 2.90 Å (for **8aa**) respectively. In NOESY spectrum, only the correlation between ***H*$_3$**-C-C=N and ***H(4)***-C(3) occurred, no the correlation between ***H*$_3$**-C-C=N and ***H***-Ar was observed. *Thus, the structures **7aa** and **8aa** could be excluded.*

(10) HMBC spectrum of product measured in $CDCl_3/CS_2$ at 298 K



In the HMBC spectrum:

(i) The methyl protons at 3.02 ppm (***H*$_3$**-C-C=N) show a strong cross-peak with the carbon signal at 84.97 ppm (sp^3-*C* of C_{60}). In the structure **4aa**, this correlation would result from a 3J coupling, while other structures **6aa**, **7aa** and **8aa** would give an unusually large 4J coupling.

(ii) Similarly, if the structure **5aa** is assigned, an unusually large 4J coupling would also happen between the methine proton (4-CH_3-C_6H_4-C***H***, at 7.00 ppm) and the other fullerene carbon (sp^3-*C* of C_{60}, at 76.40 ppm).

(iii) The structure **4aa** would also give the reason that the expected 3J correlation of the proton at 7.00 ppm (4-CH_3-C_6H_4-C***H***) with the fullerene carbon at 84.97 ppm (sp^3-*C* of C_{60}) is missing: in this rigid structure, a dihedral angle of 110° leads to null the 3J coupling.

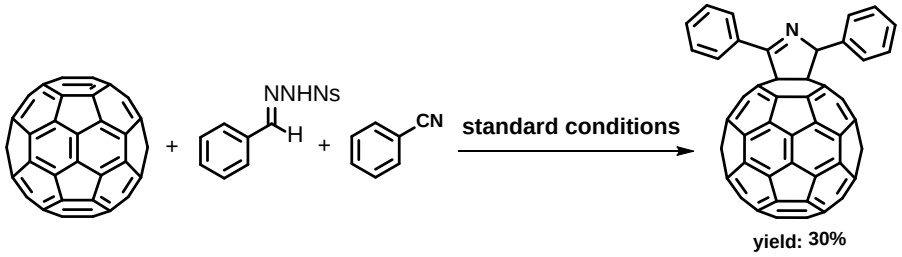
(iv) There is a scalar coupling of 2 Hz between the proton at 7.00 ppm (4-CH_3-C_6H_4-C***H***) and the methyl group at 3.02 ppm (***H*$_3$**-C-C=N). This long-range coupling would result from a 5J homoallylic coupling in the structure **4aa** (well

known to produce this size of coupling constants) again a very unusual 6J coupling in structure **6aa**.

(v) Likewise, the strong cross-peak between the carbon signal at 169.95 ppm (CH_3-***C***=N) and the proton at 7.00 ppm (4-CH_3-C_6H_4-C***H***) corresponds to an expected 3J coupling in the structure **4aa** as opposed to an unusual 4J coupling in structure **6aa**.

Thus, HMBC spectrum is consistent with the structure 4aa assignment.

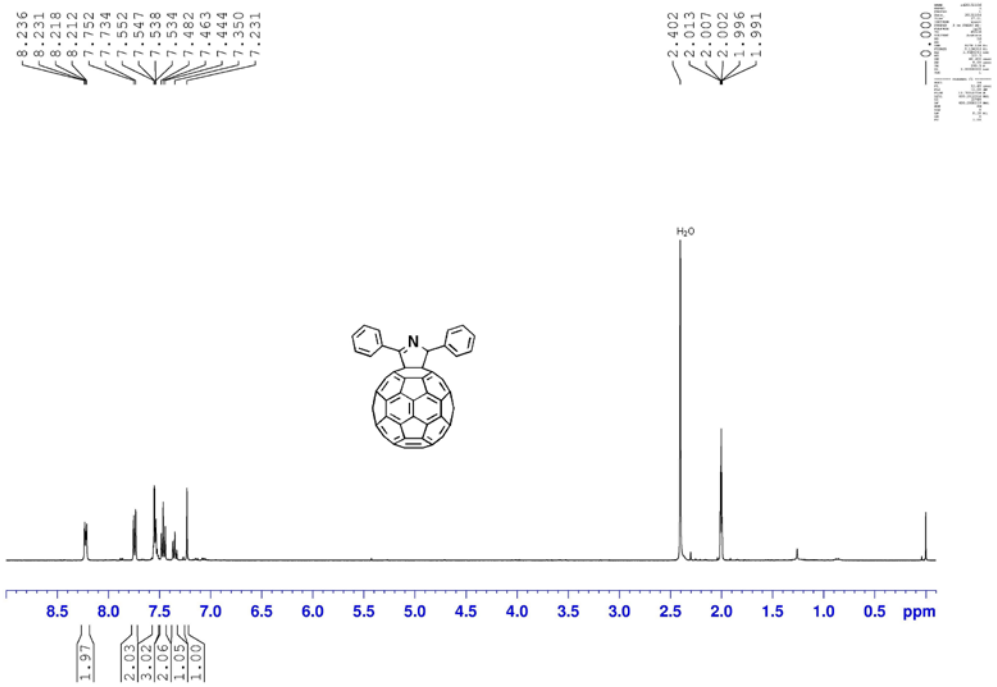
In addition, to further confirm the structure of product, we carried out the following reaction in the standard conditions. The identity of obtained product was determined by comparison of its spectral data with reported in the literature.[2]



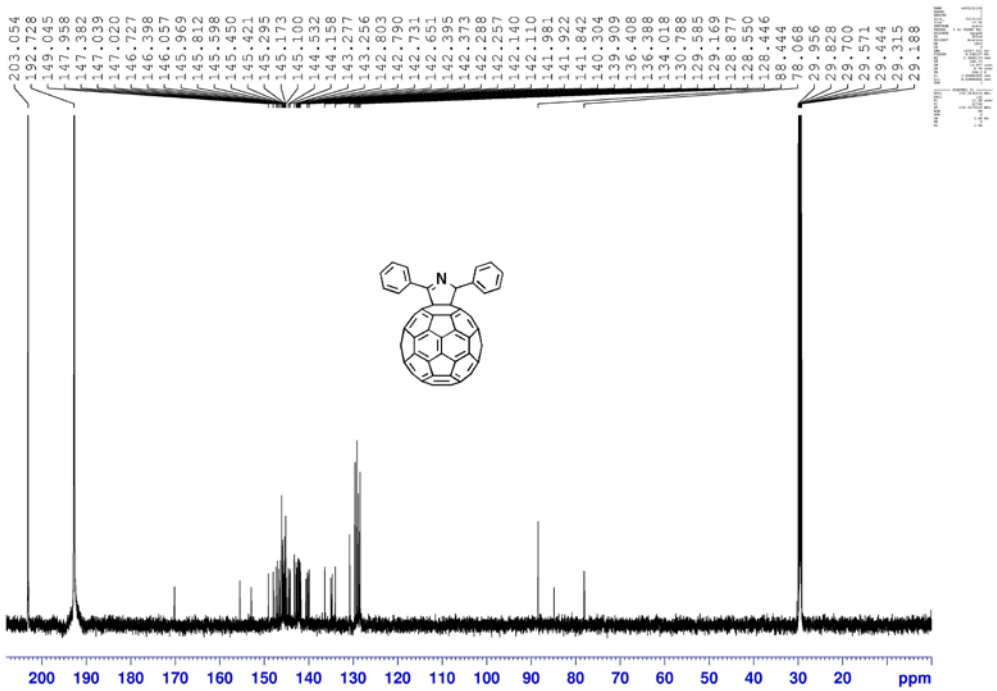
Spectral data[2]: ^{1}H NMR (400 MHz, CD_3COCD_3/CS_2) δ 8.24–8.21 (m, 2H), 7.75–7.73 (m, 2H), 7.55–7.53 (m, 3H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.23 (s, 1H). ^{13}C NMR (150 MHz, CD_3COCD_3/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.15, 155.48, 152.93, 149.05, 147.96, 147.38, 147.04, 147.02, 146.73, 146.46, 146.40, 146.06 (3C), 145.97 (2C), 145.87, 145.81 (2C), 145.72, 145.60, 145.45 (2C), 145.42, 145.30, 145.17 (2C), 145.10, 145.00, 144.53, 144.45, 144.16, 144.13, 143.28, 143.26, 142.85, 142.80, 142.79, 142.73, 142.65, 142.40, 142.37, 142.29 (2C), 142.26, 142.14, 142.11, 141.98, 141.92, 141.84, 141.74, 140.63, 140.30, 140.20, 139.91, 139.88, 136.41, 136.39, 134.99, 134.73, 134.02, 130.79, 129.59 (2C), 129.17 (2C), 128.88 (2C), 128.55, 128.45 (2C), 88.44, 84.85, 78.07.

[2] J. Averdung, E. Albrecht, J. Lauterwein, H. Luftmann, J. Mattay, H. W. H. Müller, and H.-U. ter Meer, *Chem. Ber*., 1994, **127**, 787.

^{1}H NMR (400 MHz, CD_3COCD_3/CS_2) of compound

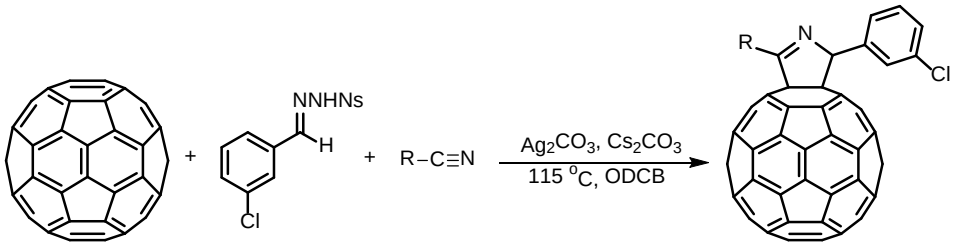


^{13}C NMR (150 MHz, CD_3COCD_3/CS_2) of compound



3. Screening for dosage of nitriles

Table 1. Optimization of Reaction Conditions[a,b]



2e **3b-3e** **4eb-4ee**

entry	substrate	molar ratio	yield (%)
1	**3b**	1:2:5:0.3:1	34
2	**3b**	1:2:10:0.3:1	39
3	**3b**	1:2:15:0.3:1	40
4	**3b**	1:2:20:0.3:1	47
5	**3c**	1:2:10:0.3:1	38
6	**3c**	1:2:15:0.3:1	39
7	**3c**	1:2:20:0.3:1	46
8	**3d**	1:2:10:0.3:1	7
9	**3d**	1:2:20:0.3:1	35
10	**3e**	1:2:10:0.3:1	14
11	**3e**	1:2:20:0.3:1	32

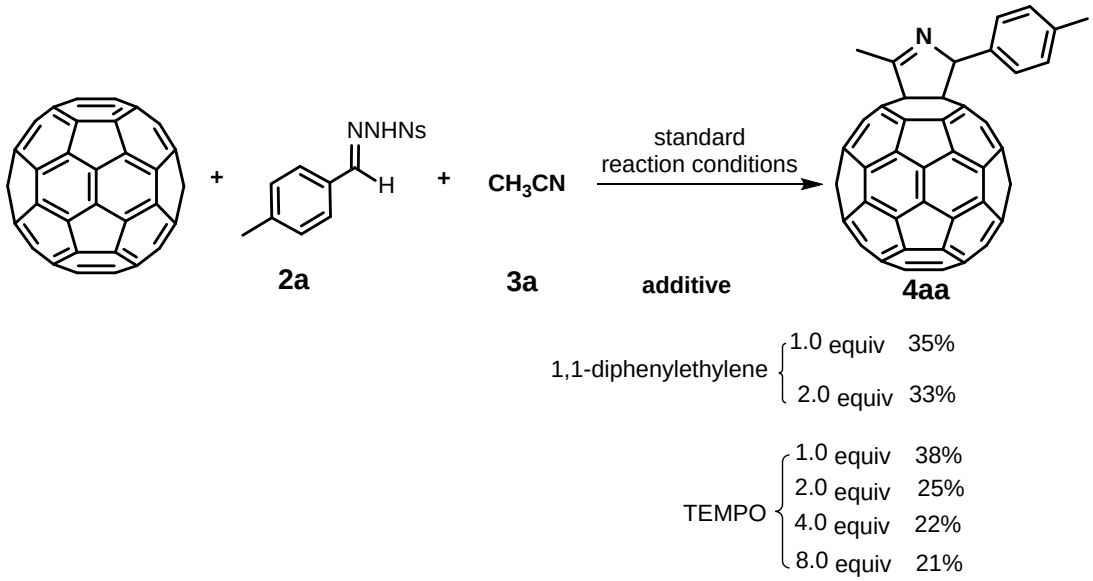
[a]All reactions were performed with a molar ratio of C_{60}/**2e**/**3**/Ag_2CO_3/Cs_2CO_3 in anhydrous *o*-dichlorobenzene (6 mL) at 115 °C for 2 h. [b]Isolated yield.

4. Experimental Procedures

*General Procedure for the Synthesis of Products **4aa–4sa** from Ag_2CO_3-Mediated Reaction of C_{60} with Substrates **2a–2s** and acetonitrile **3a***. To a dry 25-mL tube equipped with a magnetic stirrer was charged with C_{60} (36.0 mg, 0.05 mmol), **2a** (**2b**–**2s**, 0.10 mmol), Ag_2CO_3 (4.1 mg, 0.015 mmol), and Cs_2CO_3 (16.3 mg, 0.05 mmol). After they were dissolved in a mixture solvent of anhydrous **acetonitrile** (1 mL) and *o*-dichlorobenzene (7 mL) by sonication, and then the sealed mixture was heated with stirring in an oil bath preset at a designated temperature (115 ^{o}C) for a desired time (monitored by TLC). The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent was evaporated in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60}, then with CS_2/DCM as the eluent to give product **4aa** (**4ba**−**4la** and **4na**−**4qa**; for **4ma**, with CS_2/EtOAc as the eluent)..

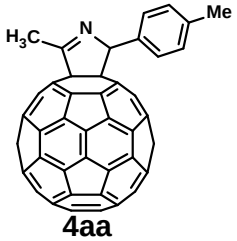
*General Procedure for the Synthesis of Products **4eb–4en** from Ag_2CO_3-Mediated Reaction of C_{60} with **2e** and Substrates **3b**–**3n***. To a dry 25-mL tube equipped with a magnetic stirrer was charged with C_{60} (36.0 mg, 0.05 mmol), **2e** (33.8 mg, 0.10 mmol), **3b** (**3c**–**3n**, 1.0 mmol), Ag_2CO_3 (4.1 mg, 0.015 mmol), and Cs_2CO_3 (16.3 mg, 0.05 mmol). After they were dissolved in a mixture solvent of anhydrous *o*-dichlorobenzene (6 mL) by sonication, and then the sealed mixture was heated with stirring in an oil bath preset at a designated temperature (115^{o}C) for a desired time (monitored by TLC). The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent was evaporated in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60}, then with CS_2/DCM as the eluent to give product **4eb** (**4ec**–**4en**).

Probe Reaction Mechanism:



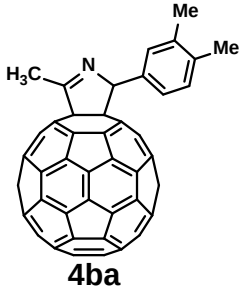
A mixture of C_{60} (36.0 mg, 0.05 mmol), **2a** (31.8 mg, 0.10 mmol), Ag_2CO_3 (4.1 mg, 0.015 mmol), Cs_2CO_3 (16.3 mg, 0.05 mmol), and 1,1-diphenylethylene (0.05, 0.01 mmol) or TEMPO (0.05−0.40 mmol) was dissolved in a mixture solvent of anhydrous **acetonitrile** (1 mL) and *o*-dichlorobenzene (7 mL) by sonication, and then the sealed mixture was heated with stirring in an oil bath at 115^{o}C for 2 h. The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent was evaporated in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60}, then with CS_2/DCM = 3/1 as the eluent to give product **4aa**. The results confirmed that 1,1-diphenylethylene and TEMPO could retarded the formation of **4aa**.

5. Spectral data for Compounds:



4aa

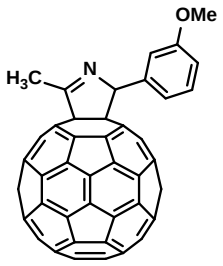
Spectral data of **4aa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 2.0 Hz, 1H), 3.02 (d, *J* =2.0 Hz, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 169.95, 154.95, 152.53, 148.89, 147.79, 146.76, 146.72, 146.56, 146.08, 146.03, 145.93, 145.67 (4C), 145.62, 145.58, 145.56, 145.35, 145.28, 145.24, 145.14, 145.10, 145.07, 144.98, 144.96, 144.85, 144.76, 144.70, 144.15, 144.06, 143.83 (2C), 142.92 (2C), 142.46, 142.39 (2C), 142.33 (2C), 142.00 (2C), 141.97, 141.83 (2C), 141.68, 141.61, 141.59, 141.52, 141.49 (2C), 140.41, 140.11, 140.08, 139.49, 137.64, 136.57, 136.02, 135.91, 134.58, 133.62, 129.42 (2C), 127.70 (2C), 88.16, 84.97 (sp^3-*C* of C_{60}), 76.40 (sp^3-*C* of C_{60}), 21.20, 18.81. FT-IR ν/cm^{-1} (KBr) 2917, 1735, 1667, 1512, 1426, 1370, 1259, 1211, 1193, 1044, 995, 931, 817, 805, 773, 731, 706, 643, 596, 566, 554, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429,693. MALDI-FT MS *m/z* calcd for $C_{70}H_{12}N$ $[M+H]^+$ 866.0964, found 866.0957.



4ba

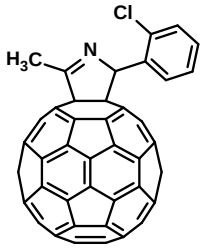
Spectral data of **4ba**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.38 (s, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 2.0 Hz, 1H), 3.01 (d, *J* =2.0 Hz, 3H), 2.31 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 169.47, 155.08, 152.64, 148.95, 147.85, 146.74, 146.71, 146.59, 146.08, 146.03, 145.94, 145.66 (4C), 145.61, 145.55, 145.35,

145.29, 145.26, 145.14, 145.10, 145.06, 145.02, 144.95, 144.85, 144.76, 144.73, 144.16, 144.07, 143.85 (2C), 142.94 (2C), 142.92, 142.47, 142.39 (2C), 142.35 (2C), 142.05, 142.01, 141.98, 141.83 (2C), 141.70, 141.64, 141.60, 141.51 (3C), 140.43, 140.12, 140.09, 139.51, 136.98, 136.70, 136.20, 136.06, 135.92, 134.60, 133.59, 130.00, 128.92, 125.45, 88.25, 85.03 (sp^3-*C* of C_{60}), 76.46 (sp^3-*C* of C_{60}), 19.90, 19.54, 18.79. FT-IR ν/cm^{-1} (KBr) 2918, 1667, 1505, 1426, 1370, 1260, 1201, 1081, 1044, 936, 877, 818, 806, 774, 726, 706, 644, 573, 552, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 698. MALDI-FT MS *m/z* calcd for $C_{71}H_{14}N$ $[M+H]^+$ 880.1121, found 880.1118.



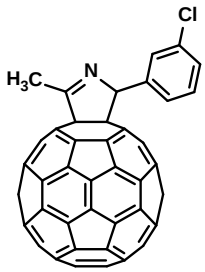
4ca

Spectral data of **4ca**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.32 (t, *J* = 8.0 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.12 (t, *J* = 2.0 Hz, 1H), 6.92 (d, *J* = 2.0 Hz, 1H), 6.82 (dd, *J* = 8.0 Hz, 2.0 Hz, 1H), 3.81 (s, 3H), 3.00 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.24, 159.74, 154.83, 152.25, 148.80, 147.74, 146.75 (2C), 146.54, 146.06 (2C), 145.91, 145.69 (4C), 145.63, 145.58 (2C), 145.36, 145.31, 145.27, 145.16, 145.13, 145.09, 144.98, 144.94, 144.91, 144.79, 144.75, 144.16, 144.08, 143.84 (2C), 142.95, 142.93, 142.49, 142.42 (2C), 142.36, 142.32, 142.00 (3C), 141.86 (2C), 141.73, 141.61 (2C), 141.52 (3C), 141.02, 140.44, 140.14 (2C), 139.45, 136.01, 135.91, 134.63, 133.69, 129.77, 120.32, 113.75, 113.15, 88.23, 85.00 (sp^3-*C* of C_{60}), 76.25 (sp^3-*C* of C_{60}), 55.03, 18.83. FT-IR ν/cm^{-1} (KBr) 2927, 1735, 1668, 1600, 1584, 1521, 1489, 1462, 1429, 1371, 1265, 1210, 1188, 1157, 1045, 942, 871, 839, 770, 698, 575, 554, 527. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 428, 696. MALDI-FT MS *m/z* calcd for $C_{70}H_{12}NO$ $[M+H]^+$ 882.0913, found 882.0924.



4da

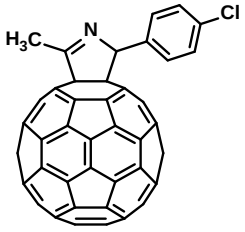
Spectral data of **4da**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.61 (d, *J* = 7.6 Hz, 1H), 7.56 (s, 1H), 7.43–7.40 (m, 2H), 7.31–7.27 (m, 1H), 3.03 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.57, 154.27, 151.89, 148.68, 147.86, 146.71, 146.66, 146.38 (2C), 146.11, 146.06, 145.85, 145.72, 145.65, 145.64, 145.61 (2C), 145.56, 145.34, 145.23, 145.17, 145.08, 145.04, 145.03 (2C), 145.01, 144.87, 144.81, 144.70, 144.16, 144.05, 143.78, 143.75, 142.88, 142.86, 142.46, 142.39, 142.35 (2C), 142.21, 142.05 (2C), 141.83, 141.77, 141.73, 141.71, 141.58, 141.56, 141.47, 141.39 (2C), 140.45, 140.13, 139.53, 139.24, 138.19, 135.96, 135.89, 134.19, 133.87, 133.63, 129.58, 129.21, 129.10, 127.11, 85.08, 83.70 (sp^3-*C* of C_{60}), 75.83 (sp^3-*C* of C_{60}), 18.78. FT-IR *v*/cm^{-1} (KBr) 2917, 1667, 1511, 1427, 1369, 1210, 1192, 1085, 1034, 932, 748, 733, 711, 642, 621, 595, 573, 554, 526. UV-vis ($CHCl_3$) λ_{max}/nm 257, 309, 428, 692. MALDI-FT MS *m/z* calcd for $C_{69}H_9ClN$ $[M+H]^+$ 886.0418, found 886.0437.



4ea

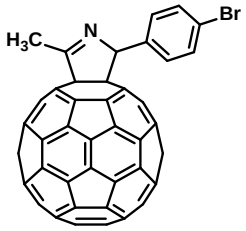
Spectral data of **4ea**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.62 (t, *J* = 2.0 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.30 (dq, *J* = 8.0, 2.0, 1.2 Hz, 1H), 6.95 (d, *J* = 2.0 Hz, 1H), 3.01 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.77, 154.43, 151.62, 148.47, 147.41, 146.74, 146.69, 146.40, 146.05, 146.02, 145.75, 145.68 (2C), 145.66 (2C), 145.60, 145.55, 145.28, 145.26, 145.22, 145.17, 145.14, 145.07, 145.05, 144.96,

144.90, 144.77 (2C), 144.67, 144.09, 143.98, 143.82, 143.77, 142.92, 142.90, 142.44, 142.41 (2C), 142.33, 142.20, 141.96, 141.92 (2C), 141.81 (2C), 141.70, 141.61, 141.58 (2C), 141.53, 141.49, 141.45, 140.44, 140.16 (2C), 139.54, 135.85 (2C), 134.91, 134.68, 133.71, 129.86, 128.23, 127.69, 126.01, 87.59, 84.98 (sp^3-C of C_{60}), 75.94 (sp^3-C of C_{60}), 18.80. FT-IR ν/cm^{-1} (KBr) 2919, 1666, 1595, 1571, 1511, 1427, 1371, 1251, 1213, 1194, 1079, 1044, 997, 943, 875, 840, 781, 763, 734, 720, 698, 646, 597, 574, 550, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 312, 429, 693. MALDI-FT MS *m/z* calcd for $C_{69}H_9ClN$ $[M+H]^+$ 886.0418, found 886.0422.



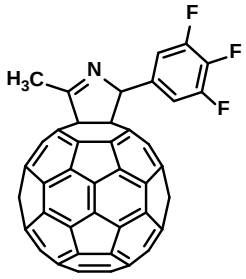
4fa

Spectral data of **4fa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 2.0 Hz, 1H), 3.01 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.35, 154.52, 151.77, 148.57, 147.43, 146.73, 146.70, 146.42, 146.05, 146.03, 145.74, 145.67 (4C), 145.61, 145.55, 145.29, 145.25 (2C), 145.15 (2C), 145.08, 145.04, 144.95, 144.89, 144.81, 144.77, 144.68, 144.09, 144.02, 143.81, 143.78, 142.93 (2C), 142.45, 142.42, 142.40, 142.34, 142.24, 141.96, 141.91 (2C), 141.80 (2C), 141.70, 141.61, 141.57, 141.52, 141.49, 141.44, 140.46, 140.16 (2C), 139.59, 138.14, 135.87, 135.81, 134.63, 134.21, 133.70, 129.02 (2C), 128.86 (2C), 87.62, 84.96 (sp^3-*C* of C_{60}), 76.07 (sp^3-*C* of C_{60}), 18.75. FT-IR ν/cm^{-1} (KBr) 2920, 1667, 1511, 1426, 1371, 1213, 1193, 1090, 1044, 1014, 932, 859, 822, 791, 733, 640, 595, 554, 525. UV-vis ($CHCl_3$) λ_{max}/nm 257, 309, 429, 693. MALDI-FT MS *m/z* calcd for $C_{69}H_9ClN$ $[M+H]^+$ 886.0418, found 886.0425.



4ga

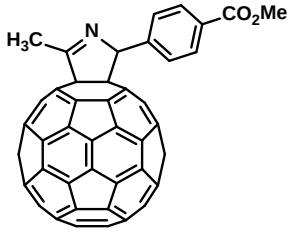
Spectral data of **4ga**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.58 (d, *J* = 8.8 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 2.0Hz, 1H), 3.02 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.61, 154.43, 151.70, 148.49, 147.36, 146.69, 146.64, 146.36, 146.00, 145.97, 145.71, 145.61 (4C), 145.55, 145.49, 145.23, 145.20, 145.16, 145.10, 145.08, 145.02, 144.99, 144.90, 144.84, 144.75, 144.72, 144.63, 144.03, 143.95, 143.76, 143.73, 142.86 (2C), 142.38, 142.35, 142.34, 142.28, 142.15, 141.90, 141.86 (2C), 141.75 (2C), 141.64, 141.51 (2C), 141.46, 141.43, 141.38, 140.39, 140.08 (2C), 139.54, 138.58, 135.82, 135.77, 134.58, 133.67, 131.78 (2C), 129.33 (2C), 122.41, 87.54, 84.91 (sp^3-*C* of C_{60}), 75.90 (sp^3-*C* of C_{60}), 18.80. FT-IR ν/cm^{-1} (KBr) 2919, 1666, 1511, 1486, 1426, 1371, 1212, 1188, 1070, 1044, 1011, 932, 858, 820, 790, 762, 732, 706, 638, 596, 553, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 428, 697. MALDI-FT MS *m/z* calcd for $C_{69}H_9BrN$ $[M+H]^+$ 929.9913, found 929.9918.



4ha

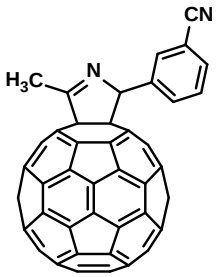
Spectral data of **4ha**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.28 (d, *J* = 6.8 Hz, 1H), 7.26 (d, *J* = 6.8 Hz, 1H), 6.88 (d, *J* = 2.0 Hz, 1H), 2.98 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 172.18, 154.04, 150.97, 148.29, 147.15, 146.93, 146.86, 146.40, 146.20, 146.17, 145.88, 145.85, 145.82 (3C), 145.77, 145.73 (2C), 145.42, 145.34, 145.28, 145.22 (4C), 145.13, 145.07, 145.03, 145.01, 144.95, 144.46 (2C), 144.19, 144.06, 143.96,

143.90, 143.05 (2C), 142.58 (2C), 142.55, 142.50, 142.23, 142.07, 142.03, 142.00, 141.94 (2C), 141.83, 141.70, 141.66 (3C), 141.62, 141.50, 140.59, 140.35 (2C), 139.78, 135.92, 135.78, 134.87, 133.93, 111.88 (2C), 86.82, 85.00 (sp^3-*C* of C_{60}), 75.67 (sp^3-*C* of C_{60}), 18.98. FT-IR ν/cm^{-1} (KBr) 2920, 1667, 1612, 1528, 1447, 1354, 1236, 1211, 1082, 1042, 960, 857, 836, 807, 763, 706, 693, 619, 574, 554, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 428, 692. MALDI-FT MS *m/z* calcd for $C_{69}H_7F_3N$ $[M+H]^+$ 906.0525, found 906.0525.



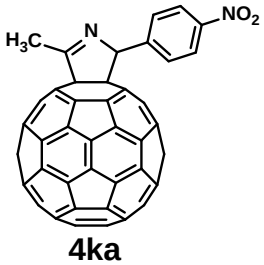
4ia

Spectral data of **4ia**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.16 (d, *J* = 8.4 Hz, 2H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 2.0 Hz, 1H), 3.93 (s, 3H), 3.05 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 171.28, 166.33, 154.55, 151.71, 148.62, 147.58, 146.94, 146.88, 146.57, 146.24, 146.20, 145.94, 145.86 (4C), 145.78, 145.73, 145.45 (2C), 145.35, 145.31 (2C), 145.25 (2C), 145.14, 145.07, 144.95, 144.93, 144.84, 144.68, 144.27, 144.14, 143.98, 143.96, 143.09, 143.08, 142.61, 142.58 (2C), 142.51, 142.36, 142.12, 142.09, 142.03, 141.98 (2C), 141.84, 141.74 (2C), 141.69, 141.66, 141.59, 140.61, 140.34, 140.31, 139.65, 136.03, 135.97, 134.82, 133.93, 130.15 (2C), 129.94, 127.89 (2C), 87.99, 85.16 (sp^3-*C* of C_{60}), 76.10 (sp^3-*C* of C_{60}), 51.99, 19.02. FT-IR ν/cm^{-1} (KBr) 2943, 1722, 1667, 1610, 1571, 1520, 1430, 1381, 1276, 1236, 1192, 1106, 1044, 1019, 963, 934, 837, 768, 729, 705, 681, 595, 571, 527. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 428, 693. MALDI-FT MS *m/z* calcd for $C_{71}H_{12}NO_2$ $[M+H]^+$ 910.0863, found 910.0870.



4ja

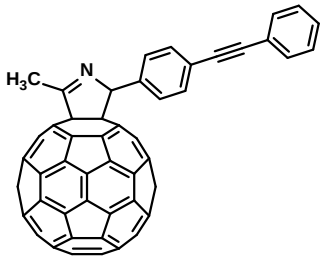
Spectral data of **4ja**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.92 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.63 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 6.99 (s, 1H), 3.02 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 171.95, 154.15, 151.18, 148.35, 147.23, 146.92, 146.84, 146.43, 146.19, 146.16, 145.84 (4C), 145.77 (2C), 145.71, 145.44, 145.35, 145.30, 145.21 (3C), 145.13, 145.07, 144.94 (3C), 144.52, 144.19, 144.03, 143.97, 143.91, 143.06 (2C), 142.57 (3C), 142.50, 142.27, 142.03 (2C), 141.96 (3C), 141.79, 141.70 (3C), 141.64, 141.51, 141.43, 140.60, 140.38, 140.35, 139.74, 135.95, 135.76, 134.84, 133.95, 132.21, 131.77, 131.15, 129.55, 118.18, 113.14, 87.33, 85.11 (sp^3-*C* of C_{60}), 75.76 (sp^3-*C* of C_{60}), 18.99. FT-IR *v*/cm^{-1} (KBr) 2923, 2227, 1732, 1666, 1427, 1371, 1207, 1084, 1045, 944, 790, 766, 733, 693, 664, 595, 575, 562, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 311, 428, 690. MALDI-FT MS *m/z* calcd for $C_{70}H_9N_2$ $[M+H]^+$ 877.0760, found 877.0752.



4ka

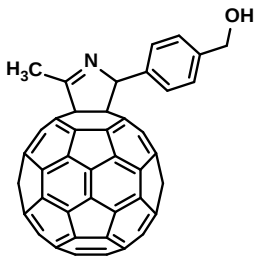
Spectral data of **4ka**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.35 (d, *J* = 8.0 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.12 (s, 1H), 3.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 172.51, 154.15, 151.08, 148.38, 147.74, 147.32, 147.08, 147.00, 146.96, 146.52, 146.34, 146.30, 146.00 (2C), 145.97, 145.96, 145.90 (2C), 145.86, 145.56, 145.50, 145.42, 145.35 (2C), 145.33, 145.28, 145.20, 145.13, 145.09 (2C), 144.64, 144.32, 144.14, 144.09, 144.05, 143.20,

143.19, 142.71 (3C), 142.64, 142.36, 142.17, 142.15, 142.10, 142.06 (2C), 141.92, 141.80 (4C), 141.61, 140.73, 140.51, 140.43, 139.83, 136.09, 135.86, 135.00, 134.14, 128.86 (2C), 124.15 (2C), 87.43, 85.25 (sp^3-*C* of C_{60}), 75.84 (sp^3-*C* of C_{60}), 19.22. FT-IR ν/cm^{-1} (KBr) 2920, 1665, 1597, 1518, 1425, 1371, 1344, 1259, 1214, 1188, 1108, 1080, 1044, 934, 856, 836, 778, 733, 696, 639, 596, 575, 554, 526. UV-vis ($CHCl_3$) λ_{max}/nm 257, 309, 428, 688. MALDI-FT MS *m/z* calcd for $C_{69}H_9N_2O_2$ $[M+H]^+$ 897.0659, found 897.0653.



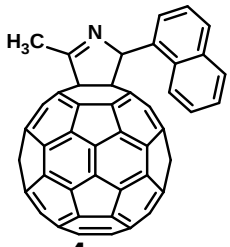
4la

Spectral data of **4la**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.67 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.51−7.48 (m, 2H), 7.33−7.31 (m, 3H), 7.02 (d, *J* = 2.0 Hz, 1H), 3.04 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.66, 154.61, 151.91, 148.63, 147.55, 146.77, 146.74, 146.47, 146.08, 146.06, 145.82, 145.69 (4C), 145.63, 145.56, 145.35, 145.30 (2C), 145.21, 145.16, 145.11, 145.07, 144.97, 144.90, 144.80 (3C), 144.13, 144.06, 143.83, 143.81, 142.93 (2C), 142.46, 142.42 (2C), 142.35, 142.26, 142.00, 141.94 (2C), 141.83 (2C), 141.73, 141.61, 141.58, 141.53, 141.50, 141.48, 140.44, 140.15 (2C), 139.69, 139.55, 135.90 (2C), 134.64, 133.72, 131.95 (2C), 131.40 (2C), 128.12 (2C), 128.09, 127.75 (2C), 123.11, 122.94, 90.20, 89.13, 88.01, 84.98 (sp^3-*C* of C_{60}), 76.21 (sp^3-*C* of C_{60}), 18.83. FT-IR ν/cm^{-1} (KBr) 2921, 1733, 1667, 1508, 1426, 1371, 1213, 1188, 1080, 1044, 961, 933, 827, 806, 753, 688, 596, 572, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 310, 428, 693. MALDI-FT MS *m/z* calcd for $C_{77}H_{14}N$ $[M+H]^+$ 952.1121, found 952.1113.



4ma

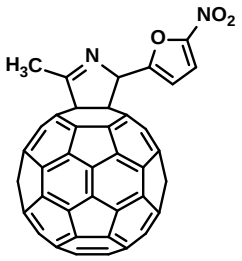
Spectral data of **4ma**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 2.0 Hz, 1H), 4.68 (d, *J* = 5.6 Hz, 2H), 3.00 (d, *J* = 2.0 Hz, 3H), 1.72 (t, *J* = 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.07, 154.71, 152.15, 148.68, 147.58, 146.69, 146.65, 146.43, 146.01, 145.97, 145.79, 145.61 (4C), 145.55, 145.49, 145.41, 145.25 (2C), 145.13, 145.09, 145.02 (2C), 144.90, 144.79 (2C), 144.70, 144.66, 144.06, 143.96, 143.77, 143.74, 142.87 (2C), 142.75, 142.39, 142.34 (2C), 142.28, 142.23, 141.89 (3C), 141.76 (2C), 141.60, 141.55, 141.52, 141.47, 141.44, 141.40, 140.38, 140.07 (2C), 139.43, 138.71, 135.88, 135.83, 134.57, 133.59, 127.91 (2C), 127.10 (2C), 88.02, 84.92 (sp^3-*C* of C_{60}), 76.18 (sp^3-*C* of C_{60}), 65.01, 18.71. FT-IR *v*/cm^{-1} (KBr) 2921, 1734, 1667, 1571, 1519, 1381, 1277, 1191, 1017, 932, 821, 772, 679, 659, 610, 594, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 694. MALDI-FT MS *m/z* calcd for $C_{70}H_{12}NO$ $[M+H]^+$ 882.0913, found 882.0912.



4na

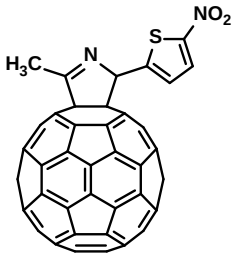
Spectral data of **4na**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.55 (d, *J* = 8.4 Hz, 1H), 7.89−7.79 (m, 4H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.50−7.46 (m, 2H), 3.10 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 169.61, 153.95, 151.73, 148.57, 148.05, 146.49, 146.42, 146.20, 145.90, 145.86, 145.70, 145.62, 145.50, 145.41 (2C), 145.38, 145.36, 145.30, 145.10, 145.03, 144.93, 144.91, 144.85, 144.84, 144.75 (2C), 144.66, 144.61, 144.35, 143.86,

143.77, 143.66, 143.59, 142.70, 142.64, 142.21, 142.18, 142.14, 142.09, 142.05, 141.71 (2C), 141.60 (2C), 141.58, 141.40, 141.34, 141.26 (2C), 141.22, 141.19, 140.30, 139.93, 139.18, 138.95, 136.35, 135.89, 135.62, 134.02 (2C), 133.57, 130.93, 128.68, 128.43, 126.08, 125.50, 125.40, 125.30, 123.90, 85.19, 83.12 (sp^3-*C* of C_{60}), 76.29 (sp^3-*C* of C_{60}), 18.64. FT-IR ν/cm^{-1} (KBr) 2920, 1668, 1510, 1426, 1371, 1206, 1165, 1094, 1046, 960, 931, 840, 790, 773, 734, 705, 667, 648, 635, 624, 573, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 693. MALDI-FT MS *m/z* calcd for $C_{73}H_{12}N$ $[M+H]^+$ 902.0694, found 902.0693.



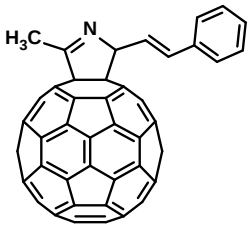
4oa

Spectral data of **4oa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.38 (d, *J* = 3.6 Hz, 1H), 7.09 (d, *J* = 2.0 Hz, 1H), 6.92 (d, *J* = 3.6 Hz, 1H), 3.02 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 173.87, 155.94, 152.99, 149.77, 147.77, 147.07, 147.00, 146.92, 146.26, 146.22 (2C), 145.98, 145.95, 145.87 (2C), 145.83 (4C), 145.44, 145.37 (2C), 145.31, 145.26, 145.24 (2C), 145.20, 145.18 (2C), 145.07, 144.80, 144.24, 144.11, 143.97, 143.94, 143.06, 143.03, 142.63, 142.61, 142.58, 142.55, 142.14, 142.12, 142.10, 141.98, 141.96, 141.87 (2C), 141.83, 141.70, 141.64, 141.60 (2C), 140.60, 140.46, 140.27, 139.77, 136.00, 135.84, 135.18, 134.24, 112.33, 111.86, 84.91 (sp^3-*C* of C_{60}), 81.91, 74.64 (sp^3-*C* of C_{60}), 19.25. FT-IR ν/cm^{-1} (KBr) 2922, 1665, 1587, 1529, 1496, 1425, 1350, 1295, 1237, 1211, 1014, 952, 806, 775, 736, 706, 631, 574, 553, 526. UV-vis ($CHCl_3$) λ_{max}/nm 257, 317, 428, 690. MALDI-FT MS *m/z* calcd for $C_{67}H_7N_2O_3$ $[M+H]^+$ 887.0451, found 887.0447.



4pa

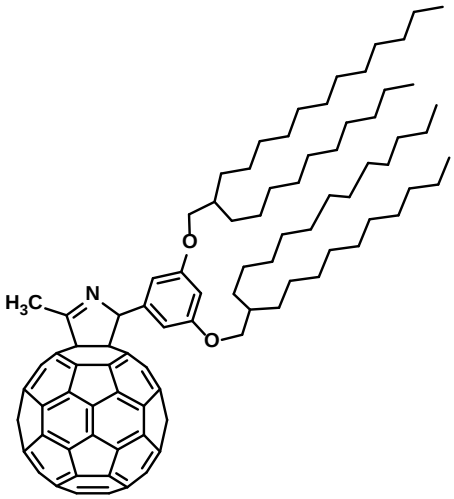
Spectral data of **4pa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.90 (d, *J* = 4.0 Hz, 1H), 7.34 (dd, *J* = 4.0, 0.4 Hz, 1H), 7.21 (d, *J* = 2.0 Hz, 1H), 3.03 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 172.96, 153.11, 151.39，149.73, 147.89, 146.76, 146.65 (2C), 146.06, 145.98 (2C), 145.73, 145.68, 145.64 (2C), 145.57, 145.52, 145.42, 145.25, 145.14, 145.04 (3C), 145.03 (3C), 144.98, 144.92, 144.91, 144.79, 144.14, 143.94, 143.85, 143.76, 143.68, 142.85 (2C), 142.42 (2C), 142.38, 142.32, 141.95, 141.88, 141.83, 141.75 (2C), 141.73, 141.68, 141.53 (2C), 141.42 (2C), 141.35, 140.44, 140.22, 140.14, 139.51, 135.66 (2C), 134.99, 133.94, 128.19, 125.03, 84.77 (sp^3-*C* of C_{60}), 83.71, 75.42 (sp^3-*C* of C_{60}), 18.76. FT-IR *v*/cm^{-1} (KBr) 2921, 1662, 1537, 1500, 1432, 1370, 1333, 1220, 1178, 1030, 960, 813, 775, 731, 640, 596, 574, 553, 526. UV-vis ($CHCl_3$) λ_{max}/nm 257, 322, 428, 692. MALDI-FT MS *m/z* calcd for $C_{67}H_7N_2O_2S$ $[M+H]^+$ 903.0223, found 903.0222.



4qa

Spectral data of **4qa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.43 (d, *J* = 1.2 Hz, 1H), 7.41 (s, 1H), 7.29−7.26 (m, 2H), 7.23−7.19 (m, 1H), 7.04 (d, *J* = 15.6 Hz, 1H), 6.74 (dd, *J* = 15.6, 8.4 Hz, 1H), 6.47 (dd, *J* = 8.4, 2.0 Hz, 1H), 2.90 (d, *J* = 2.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 169.36, 154.61, 151.66, 148.68, 147.80, 146.82, 146.79, 146.53, 146.13, 146.10, 146.06, 145.84, 145.82, 145.79, 145.76 (2C), 145.69 (2C), 145.40, 145.36

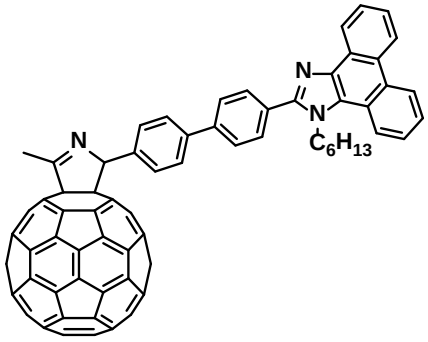
(2C), 145.24, 145.16 (3C), 145.05, 145.02, 144.97, 144.88, 144.23, 144.16, 143.93, 143.86, 143.03, 143.00, 142.54, 142.52, 142.46, 142.42, 142.32, 142.22, 142.07, 142.02, 141.90, 141.88, 141.81, 141.73, 141.71, 141.64, 141.60 (2C), 140.44, 140.27, 140.19, 140.02, 136.14, 135.95, 135.93, 134.99, 133.71 (2C), 128.50 (2C), 128.03, 127.90, 126.80 (2C), 86.98, 85.03 (sp^3-*C* of C_{60}), 75.49 (sp^3-*C* of C_{60}), 18.90. FT-IR ν/cm^{-1} (KBr) 2921, 1665, 1509, 1425, 1370, 1206, 958, 942, 763, 745, 689, 640, 595, 571, 561, 525. UV-vis ($CHCl_3$) λ_{max}/nm 257, 309, 429, 697. MALDI-FT MS *m/z* calcd for $C_{71}H_{12}N$ $[M+H]^+$ 878.0964, found 878.0970.



4ra

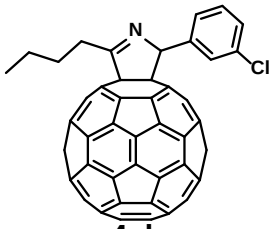
Spectral data of **4ra**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 6.92 (d, *J* = 1.6 Hz, 1H), 6.80 (s, 2H), 6.41 (s, 1H), 3.84 (d, *J* = 4.8 Hz, 4H), 3.03 (d, *J* = 1.6 Hz, 3H), 1.76 (s, 2H), 1.24 (s, 80H), 0.87 (t, *J* = 1.6 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.19, 160.66 (2C), 154.98, 152.36, 148.94, 147.86, 146.83, 146.81, 146.63, 146.17, 146.12, 145.98, 145.87, 145.75 (4C), 145.69, 145.63, 145.42, 145.37 (2C), 145.20 (2C), 145.14, 145.03 (2C), 144.93, 144.84 (2C), 144.22, 144.16, 143.90 (2C), 143.01, 142.96, 142.55, 142.48, 142.45, 142.42, 142.39, 142.09, 142.07, 142.05, 141.91 (2C), 141.78, 141.67 (2C), 141.56 (2C), 141.52, 141.35, 140.49, 140.16 (2C), 139.39, 136.11, 135.97, 134.68, 133.72, 106.47 (2C), 100.96, 88.44, 85.04 (sp^3-*C* of C_{60}), 76.34 (sp^3-*C* of C_{60}), 70.71 (2C), 37.86 (2C), 31.96 (4C), 31.33 (4C), 30.14 (4C), 29.76 (8C), 29.72 (8C), 29.42 (4C), 26.90 (4C), 22.81 (4C), 18.92, 14.19 (4C). FT-IR ν/cm^{-1} (KBr) 2922, 2851, 1670, 1595, 1463, 1374, 1350, 1209, 1164, 1056, 831, 766, 722, 575, 554, 527.

UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 695. ESI FT-ICR MS *m/z* calcd for $C_{117}H_{106}NO_2$ $[M+H]^+$ 1556.8218, found 1556.8225.



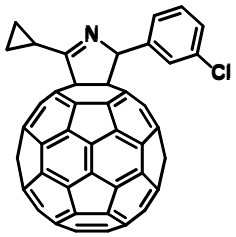
4sa

Spectral data of **4sa**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.81 (d, *J* = 7.6 Hz, 1H), 8.74 (d, *J* = 6.8 Hz, 1H), 8.66 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.81−7.79 (m, 7H), 7.66−7.60 (m, 5H), 7.08 (d, *J* = 2.0 Hz, 1H), 4.65 (t, *J* = 7.6 Hz, 2H), 3.06 (d, *J* = 2.0 Hz, 3H), 1.96 (t, *J* = 6.8 Hz, 2H), 1.25−1.20 (m, 6H), 0.81 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.85, 154.86, 152.33, 152.21, 148.89, 147.77, 146.90, 146.85, 146.64, 146.20, 146.15, 146.02, 145.82, 145.80 (4C), 145.74, 145.69, 145.60, 145.47, 145.39, 145.34, 145.27, 145.21, 145.20, 145.09, 145.01, 144.98, 144.90 (2C), 144.25, 144.12, 143.96, 143.94, 143.03 (3C), 142.56, 142.51 (2C), 142.45, 142.38, 142.12, 142.10, 142.07, 141.95 (2C), 141.80, 141.71, 141.68, 141.66, 141.60 (2C), 141.33, 140.53, 140.23 (2C), 139.89, 139.69, 139.32, 138.00, 136.08, 136.02, 134.83, 133.83, 130.35 (2C), 129.96, 129.02, 128.59, 127.98, 127.54, 127.25 (3C), 127.14, 126.65, 126.09, 125.39, 124.64, 124.37, 123.35, 122.93, 122.50, 120.58, 88.05, 85.16 (sp^3-*C* of C_{60}), 76.36 (sp^3-*C* of C_{60}), 46.92, 30.99, 30.23, 25.91, 22.33, 19.09, 13.81. FT-IR *v*/cm^{-1} (KBr) 2923, 2852, 1727, 1668, 1609, 1574, 1518, 1450, 1427, 1384, 1261, 1187, 1086, 1038, 1005, 943, 822, 806, 753, 723, 677, 615, 553, 527. UV-vis ($CHCl_3$) λ_{max}/nm 256, 313, 428, 690. MALDI-FT MS *m/z* calcd for $C_{96}H_{34}N_3$ $[M+H]^+$ 1228.2747, found 1228.2761.



4eb

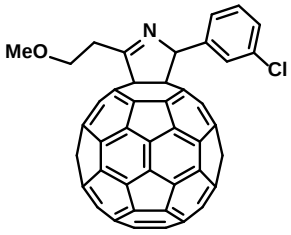
Spectral data of **4eb**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.62 (s, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.31 (dt, *J* = 8.0, 2.0 Hz, 1H), 6.98 (t, *J* = 2.0 Hz, 1H), 3.41−3.25 (m, 2H), 2.26−2.17 (m, 2H), 1.72−1.63 (m, 2H), 1.10 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 174.42, 154.69, 151.94, 148.82, 147.81, 146.87, 146.81, 146.61, 146.16, 146.12, 145.98, 145.79 (4C), 145.72, 145.66, 145.41, 145.34 (2C), 145.32, 145.17 (3C), 145.08, 144.98, 144.90, 144.86, 144.81, 144.21, 144.09, 143.93, 143.89, 143.02 (2C), 142.54, 142.51 (2C), 142.46, 142.29, 142.07, 142.04 (2C), 141.94 (2C), 141.90, 141.82, 141.74, 141.66 (2C), 141.61 (2C), 140.46, 140.27, 140.18, 139.65, 135.82, 135.78, 134.90, 134.79, 133.82, 129.99, 128.33, 127.83, 126.17, 87.72, 85.24 (sp^3-*C* of C_{60}), 76.18 (sp^3-*C* of C_{60}), 32.36, 29.19, 22.93, 14.05. FT-IR ν/cm^{-1} (KBr) 2922, 2853, 1661, 1594, 1571, 1510, 1461, 1427, 1376, 1266, 1151, 1077, 1030, 991, 943, 876, 780, 763, 725, 698, 574, 562, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 310, 429, 695. MALDI-FT MS *m/z* calcd for $C_{72}H_{15}ClN$ $[M+H]^+$ 928.0888, found 928.0882.



4ec

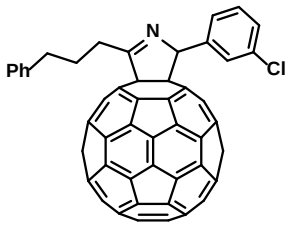
Spectral data of **4ec**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.53 (t, *J* = 1.6 Hz, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 7.26 (dt, *J* = 8.0, 1.6 Hz, 1H), 6.85 (s, 1H), 2.69−2.65 (m, 1H), 1.68−1.57 (m, 2H), 1.35−1.26 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 176.38, 154.57, 151.88, 148.91, 147.99, 146.89, 146.82, 146.80, 146.21, 146.16, 146.13, 145.80 (2C), 145.77, 145.76, 145.72, 145.65, 145.45, 145.34 (2C), 145.30, 145.20,

145.17, 145.14, 145.09, 144.99, 144.91, 144.86, 144.80, 144.22, 144.11, 143.95, 143.92, 143.02, 143.01, 142.53, 142.50 (2C), 142.44, 142.31, 142.25, 142.08, 142.05 (2C), 141.93 (2C), 141.81 (2C), 141.69, 141.65 (2C), 141.57, 140.51, 140.24, 140.22, 139.63, 135.90, 135.79, 134.86, 134.83, 133.87, 129.95, 128.28, 127.74, 126.09, 86.77, 85.09 (sp^3-*C* of C_{60}), 76.56 (sp^3-*C* of C_{60}), 12.92, 12.02, 11.97. FT-IR ν/cm^{-1} (KBr) 2921, 2851, 1655, 1595, 1508, 1428, 1390, 1188, 1085, 1020, 991, 941, 885, 781, 763, 723, 699, 598, 574, 561, 525. UV-vis ($CHCl_3$) λ_{max}/nm ($CHCl_3$) 258, 309, 429, 696. MALDI-FT MS *m/z* calcd for $C_{71}H_{11}ClN$ $[M+H]^+$ 912.0575, found 912.0577.



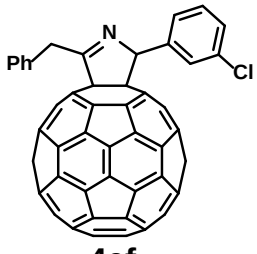
4ed

Spectral data of **4ed**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.60 (t, *J* = 1.6 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.27 (dt, *J* = 7.6, 1.6 Hz, 1H), 6.97 (t, *J* = 2.0 Hz, 1H), 4.24−4.14 (m, 2H), 3.68−3.60 (m, 1H), 3.54−3.42 (m, 1H), 3.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 171.70, 154.44, 151.78, 148.35, 147.38, 146.80, 146.73, 146.40, 146.08, 146.05, 145.85, 145.72 (4C), 145.68, 145.64, 145.57, 145.30 (2C), 145.21, 145.19, 145.14, 145.11, 145.08, 144.99, 144.93, 144.83, 144.77, 144.70, 144.10, 144.02, 143.86, 143.82, 142.92 (2C), 142.47, 142.43 (2C), 142.37, 142.22, 141.99, 141.96 (2C), 141.85 (3C), 141.73, 141.60, 141.57 (2C), 141.50, 140.41, 140.20, 140.10, 139.56, 135.96, 135.82, 134.94, 134.76, 133.78, 129.87, 128.25, 127.74, 126.08, 87.64, 85.15 (sp^3-*C* of C_{60}), 75.92 (sp^3-*C* of C_{60}), 69.47, 58.73, 32.66. FT-IR ν/cm^{-1} (KBr) 2920, 1732, 1663, 1594, 1570, 1530, 1474, 1427, 1393, 1186, 1115, 1031, 993, 964, 943, 876, 781, 763, 727, 699, 574, 562, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 695. MALDI-FT MS *m/z* calcd for $C_{71}H_{13}ClNO$ $[M+H]^+$ 930.0680, found 930.0677.



4ee

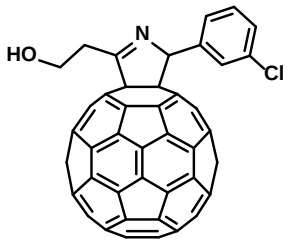
Spectral data of **4ee**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.58 (t, *J* = 1.6 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.24−7.22 (m, 4H), 7.15−7.11 (m, 1H), 6.94 (t, *J* = 2.0 Hz, 1H), 3.39−3.24 (m, 2H), 2.94 (td, *J* = 6.8, 2.0 Hz, 2H), 2.55−2.48 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 173.70, 154.58, 151.76, 148.59, 147.57, 146.77, 146.71, 146.45, 146.07, 146.04, 145.80, 145.70 (3C), 145.63, 145.57, 145.30, 145.26 (2C), 145.22, 145.09 (2C), 145.06, 144.99, 144.92, 144.81, 144.79, 144.69, 144.11, 144.01, 143.84, 143.79, 142.94, 142.92, 142.46, 142.43 (2C), 142.38, 142.22, 141.99, 141.95 (2C), 141.84 (2C), 141.82, 141.75, 141.64, 141.57 (2C), 141.49 (2C), 141.00, 140.38, 140.21, 140.10, 139.59, 135.72, 135.70, 134.95, 134.71, 133.72, 129.88, 128.35 (2C), 128.32 (2C), 128.28, 128.24, 127.76, 126.01, 125.94, 87.73, 85.14 (sp^3-*C* of C_{60}), 76.11 (sp^3-C of C_{60}), 35.60, 31.74, 28.56. FT-IR *v*/cm^{-1} (KBr) 2923, 2853, 1661, 1594, 1508, 1452, 1427, 1095, 943, 875, 781, 763, 745, 697, 574, 562, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 309, 429, 697. MALDI-FT MS *m/z* calcd for $C_{77}H_{17}ClN$ $[M+H]^+$ 990.1044, found 990.1053.



4ef

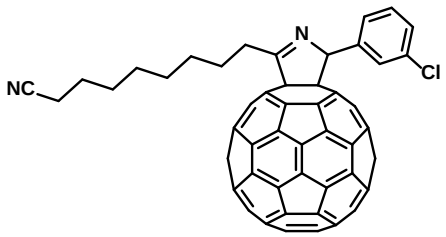
Spectral data of **4ef**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.59 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.39−7.35 (m, 3H), 7.31−7.28 (m, 2H), 7.00 (s, 1H), 4.71 (d, *J* = 15.2 Hz, 1H), 4.65 (d, *J* = 15.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 172.94, 154.55, 151.83, 148.35, 147.39, 146.85, 146.81, 146.51, 146.15, 146.11, 145.92,

145.78 (3C), 145.75, 145.72, 145.65, 145.38, 145.30, 145.27 (2C), 145.18, 145.15 (2C), 145.08, 144.96, 144.89, 144.84, 144.72, 144.18, 144.06, 143.89, 143.86, 142.99, 142.97, 142.53, 142.51 (2C), 142.46, 142.22, 142.06, 142.02, 141.97, 141.94 (2C), 141.83, 141.80, 141.66 (3C), 141.58 (2C), 140.29, 140.26, 140.01, 139.64, 135.85, 135.77, 135.40, 134.85, 134.81, 133.82, 130.00, 129.76 (2C), 128.71 (2C), 128.34, 127.93, 127.19, 126.21, 87.63, 84.87 (sp^3-*C* of C_{60}), 76.38 (sp^3-*C* of C_{60}), 38.80. FT-IR ν/cm^{-1} (KBr) 2920, 1654, 1594, 1509, 1427, 1183, 1076, 1030, 993, 942, 874, 780, 762, 693, 574, 550, 526. UV-vis ($CHCl_3$) λ_{max}/nm 258, 310, 429, 693. MALDI-FT MS *m/z* calcd for $C_{75}H_{13}ClN$ $[M+H]^+$ 962.0731, found 962.0732.



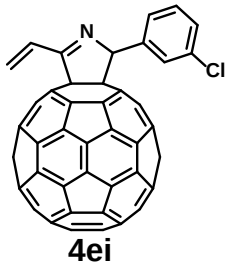
4eg

Spectral data of **4eg**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.61 (t, *J* = 1.6 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.32 (dt, *J* = 8.0, 2.0 Hz, 1H), 6.99 (t, *J* = 2.4 Hz, 1H), 4.39−4.33 (m, 2H), 3.77 (t, *J* = 6.4 Hz, 1H), 3.64−3.57 (m, 1H), 3.53−3.46 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 174.68, 154.35, 151.59, 148.23, 147.23, 147.06, 147.00, 146.51, 146.36, 146.32, 145.97 (3C), 145.90 (2C), 145.85, 145.60, 145.49, 145.45, 145.40, 145.37 (2C), 145.34, 145.24, 145.21, 145.07 (2C), 144.87, 144.35, 144.25, 144.07, 144.03, 143.19, 143.17, 142.73, 142.70, 142.69, 142.63, 142.42, 142.23, 142.19, 142.15, 142.08 (2C), 141.98, 141.84, 141.83, 141.79, 141.75, 141.68, 141.59 (2C), 140.70, 140.49, 140.43, 139.88, 136.22, 136.19, 135.28, 134.96, 134.00, 130.23, 128.66, 127.91, 126.07, 87.73, 85.16 (sp^3-*C* of C_{60}), 75.54 (sp^3-*C* of C_{60}), 59.85, 34.93. FT-IR ν/cm^{-1} (KBr) 3451, 2922, 1713, 1660, 1595, 1572, 1477, 1428, 1366, 1274, 1164, 1106, 1069, 878, 783, 711, 686, 568, 526. UV-vis ($CHCl_3$) λ_{max}/nm 256, 312, 428, 690. MALDI-FT MS *m/z* calcd for $C_{70}H_{11}ClNO$ $[M+H]^+$ 916.0524, found 916.0517.



4eh

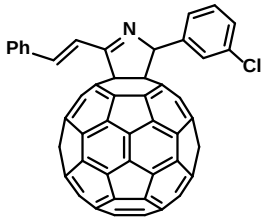
Spectral data of **4eh**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.59 (s, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.30 (dt, *J* = 8.0, 1.6 Hz, 1H), 6.96 (t, *J* = 2.0 Hz, 1H), 3.40−3.26 (m, 2H), 2.33 (t, *J* = 6.8 Hz, 2H), 2.27−2.17 (m, 2H), 1.70−1.63 (m, 4H), 1.55−1.44 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 173.82, 154.39, 151.60, 148.46, 147.45, 146.59, 146.54, 146.29, 145.90, 145.86, 145.66, 145.52 (4C), 145.45, 145.40, 145.12, 145.06 (2C), 145.03, 144.91 (2C), 144.89, 144.82, 144.73, 144.63, 144.61, 144.51, 143.94, 143.84, 143.66, 143.61, 142.77, 142.75, 142.29, 142.26 (2C), 142.21, 142.03, 141.81, 141.77 (2C), 141.66 (2C), 141.63, 141.56, 141.47, 141.40 (2C), 141.33 (2C), 140.21, 140.04, 139.92, 139.42, 135.56, 135.53, 134.74, 134.51, 133.53, 129.74, 128.10, 127.51, 125.92, 118.77, 87.49, 84.94 (sp^3-*C* of C_{60}), 75.91 (sp^3-*C* of C_{60}), 32.34, 29.36, 29.06, 28.59, 28.47, 26.70, 25.31, 16.88. FT-IR ν/cm^{-1} (KBr) 2923, 2851, 1662, 1594, 1570, 1459, 1426, 1185, 1077, 1037, 991, 943, 875, 781, 763, 746, 726, 698, 599, 574, 562, 526. UV-vis ($CHCl_3$) λ_{max}/nm 259, 311, 428, 693. MALDI-FT MS *m/z* calcd for $C_{77}H_{22}ClN_2$ $[M+H]^+$ 1009.1466, found 1009.1475.



4ei

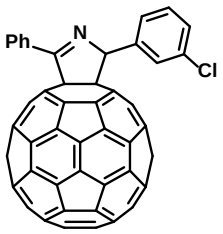
Spectral data of **4ei**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.60 (s, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.39 (dd, *J* = 17.2, 10.8 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.02 (s, 1H), 6.93 (d, *J* = 17.2 Hz, 1H), 5.98 (d, *J* = 10.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 167.69, 154.42, 151.60, 148.28, 147.36, 146.84, 146.80, 146.48, 146.15, 146.11,

145.85, 145.79 (2C), 145.76, 145.74, 145.71, 145.64, 145.36 (2C), 145.29, 145.22 (2C), 145.17, 145.15, 145.05, 144.97, 144.86, 144.84, 144.67, 144.19, 144.08, 143.88, 143.84, 142.99, 142.98, 142.52, 142.49, 142.47, 142.41, 142.26, 142.04, 142.00 (2C), 141.99, 141.89 (2C), 141.76 (2C), 141.61 (3C), 141.53, 140.40, 140.23, 140.10, 139.64, 136.18, 136.10, 134.99, 134.81, 133.84, 129.96, 128.34, 128.11, 127.93, 127.30, 126.21, 87.37, 83.76 (sp^3-*C* of C_{60}), 76.40 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2920, 1638, 1595, 1571, 1475, 1429, 1406, 1250, 1162, 1103, 1086, 993, 973, 949, 877, 782, 764, 747, 734, 699, 683, 574, 563, 527. UV-vis ($CHCl_3$) λ_{max}/nm 257, 310, 429, 695. MALDI-FT MS *m/z* calcd for $C_{70}H_9ClN$ $[M+H]^+$ 898.0418, found 898.0425.



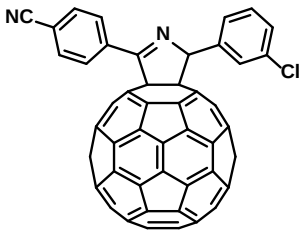
4ej

Spectral data of **4ej**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.32 (d, *J* = 15.6 Hz, 1H), 7.69−7.64 (m, 4H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.41−7.36 (m, 4H), 7.33−7.29 (m, 1H), 7.10 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 167.58, 154.69, 151.84, 148.73, 147.79, 146.98, 146.93, 146.66, 146.28, 146.25, 146.01, 145.91 (2C), 145.88 (2C), 145.83, 145.77, 145.50 (2C), 145.44, 145.41, 145.36, 145.03, 145.27, 145.19, 145.12, 145.01, 145.98, 144.87, 144.34, 144.24, 144.03, 143.98, 143.14, 143.13, 142.66, 142.63 (2C), 142.56, 142.43 (2C), 142.19, 142.18, 142.16, 142.03 (2C), 141.98, 141.91, 141.83, 141.79, 141.76, 141.72 (2C), 140.67, 140.38 (2C), 139.80, 136.28, 136.19, 135.33, 135.20, 135.00, 134.01, 130.05, 130.02, 128.96 (2C), 128.42, 128.24, 128.12, 128.05 (2C), 118.16, 87.65, 84.00 (sp^3-*C* of C_{60}), 76.57 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2921, 1638, 1596, 1574, 1494, 1448, 1429, 1336, 1261, 1162, 1130, 1042, 995, 969, 879, 783, 765, 747, 690, 616, 574, 551, 527. UV-vis ($CHCl_3$) λ_{max}/nm 256, 312, 428, 691. MALDI-FT MS *m/z* calcd for $C_{76}H_{13}ClN$ $[M+H]^+$ 974.0731, found 974.0734.



4ek

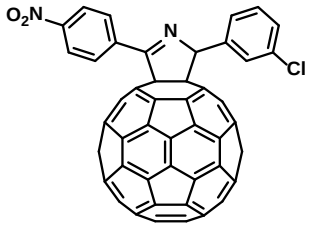
Spectral data of **4ek**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.25−8.22 (m, 2H), 7.73 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.57−7.56 (m, 3H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.17 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 171.62, 154.57, 151.77, 148.17, 147.20, 146.87, 146.78 (2C), 146.25, 146.17, 146.13, 145.80 (3C), 145.72 (2C), 145.61, 145.44, 145.36, 145.32, 145.16 (3C), 145.12, 145.04, 144.93, 144.85, 144.83, 144.52, 144.20, 144.09, 143.85, 143.81, 142.97, 142.96, 142.56, 142.53, 142.51, 142.45, 142.20, 142.08, 142.04, 141.98 (2C), 141.95, 141.88, 141.79, 141.72, 141.70, 141.56, 141.53, 141.44, 140.36, 139.96, 139.75, 139.66, 136.01, 135.99, 135.01, 134.78, 134.10, 133.73, 130.60, 130.01, 129.06 (2C), 128.59 (2C), 128.42, 127.98, 126.27, 87.33, 84.46 (sp^3-*C* of C_{60}), 76.85 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2921, 1653, 1559, 1428, 1275, 1183, 1077, 1044, 985, 903, 879, 765, 730, 692, 574, 526. UV-vis ($CHCl_3$) λ_{max}/nm 256, 310, 429, 690. MALDI-FT MS *m/z* calcd for $C_{74}H_{11}ClN$ $[M+H]^+$ 948.0575, found 948.0569.



4el

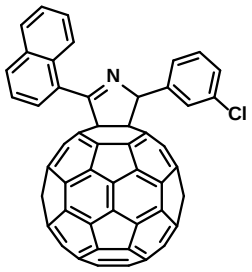
Spectral data of **4el**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.38 (d, *J* = 8.4 Hz, 2H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.68 (s, 1H), 7.62 (s, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.13 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.02, 154.02, 151.18, 147.14, 146.76, 146.73, 146.24, 146.18, 146.15, 146.10, 145.75 (2C), 145.69 (2C), 145.59 (2C), 145.34, 145.23, 145.17 (3C), 145.13, 144.98, 144.89, 144.83, 144.79

(2C), 144.23, 144.13, 144.03, 143.70, 143.65, 142.95, 142.92, 142.55, 142.52, 142.48, 142.42, 142.06, 142.01, 141.97, 141.84 (2C), 141.82 (2C), 141.80, 141.64, 141.54, 141.48, 141.39, 141.37, 141.20, 140.38, 140.00, 139.77, 139.72, 138.01, 136.25 (2C), 135.13, 134.57, 133.53, 132.10 (2C), 130.00, 129.68 (2C), 128.53, 127.82, 126.08, 117.23, 114.67, 87.37, 83.96 (sp^3-*C* of C_{60}), 76.92 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2927, 2227, 1726, 1628, 1594, 1464, 1428, 1276, 1187, 1123, 1074, 1042, 985, 876, 825, 780, 763, 688, 574, 562, 524. UV-vis ($CHCl_3$) λ_{max}/nm 256, 311, 428, 690. MALDI-FT MS *m/z* calcd for $C_{75}H_{10}ClN_2$ $[M+H]^+$ 973.0527, found 973.0528.



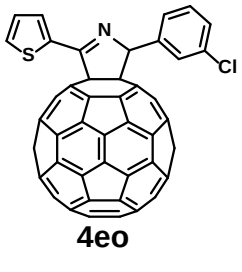
4em

Spectral data of **4em**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.44 (d, *J* = 8.8 Hz, 2H), 8.37 (d, *J* = 8.8 Hz, 2H), 7.64 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.44 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.15 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.11, 153.98, 151.16, 148.84, 147.06, 146.81, 146.22, 146.20, 146.10, 145.80 (2C), 145.73, 145.63, 145.57, 145.40, 145.27, 145.24, 145.21 (2C), 145.18, 145.02, 144.94, 144.86, 144.84, 144.26, 144.17, 144.07, 143.74, 143.71, 143.69, 142.98, 142.97, 142.59, 142.57, 142.52, 142.46, 142.10, 142.05, 142.01, 141.96, 141.88, 141.85 (4C), 141.68, 141.56, 141.53, 141.44, 141.39, 141.16, 140.41, 140.08, 139.84, 139.81, 139.79, 136.32, 136.30, 135.14, 133.58, 132.54, 130.27, 130.08 (2C), 128.61, 127.86, 127.39, 126.14, 123.70, 123.60 (2C), 87.49, 84.08 (sp^3-*C* of C_{60}), 76.70 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2926, 1733, 1596, 1518, 1428, 1341, 1276, 1187, 1107, 1077, 1042, 986, 846, 802, 763, 750, 692, 574, 524. UV-vis ($CHCl_3$) λ_{max}/nm 258, 312, 428, 689. MALDI-FT MS *m/z* calcd for $C_{74}H_{10}ClN_2O_2$ $[M+H]^+$ 993.0425, found 993.0426.



4en

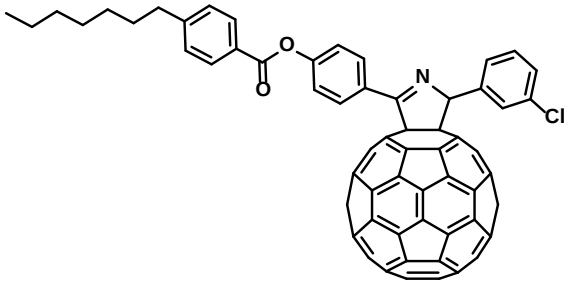
Spectral data of **4en**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.92−7.87 (m, 2H), 7.64 (s, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.65−7.61 (m, 1H), 7.58−7.52 (m, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.58−7.52 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 171.58, 154.74, 151.73, 148.23, 147.00, 146.91, 146.75, 146.28, 146.23, 146.14, 146.01, 145.99, 145.92, 145.90, 145.86, 145.80, 145.51, 145.47 (2C), 145.46 (2C), 145.30 (4C), 145.21, 145.13, 145.01, 144.72, 144.30, 144.20, 144.03, 143.95, 143.11 (2C), 142.70 (2C), 142.60, 142.55, 142.46, 142.25, 142.24, 142.20, 142.05, 142.04, 142.02, 141.86 (2C), 141.81, 141.68, 141.64, 141.60, 140.43 (2C), 140.10, 139.86, 135.71, 135.68, 135.26, 135.13, 133.95, 133.86, 131.36, 131.34, 130.26, 130.20, 128.70, 128.58, 128.26, 127.34, 126.80, 126.65, 126.42, 125.54, 124.54, 88.80, 86.74 (sp^3-*C* of C_{60}), 76.37 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2919, 1652, 1594, 1572, 1506, 1473, 1428, 1280, 1246, 1182, 1110, 1030, 970, 881, 787, 726, 700, 668, 575, 526. UV-vis ($CHCl_3$) λ_{max}/nm 255, 311, 428, 688. MALDI-FT MS *m/z* calcd for $C_{78}H_{13}ClN$ $[M+H]^+$ 998.0731, found 998.0723.



4eo

Spectral data of **4eo**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.37 (d, *J* = 3.2 Hz, 1H), 7.63 (s, 1H), 7.60 (d, *J* = 4.8 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 4.4 Hz, 1H), 7.05 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 163.75,

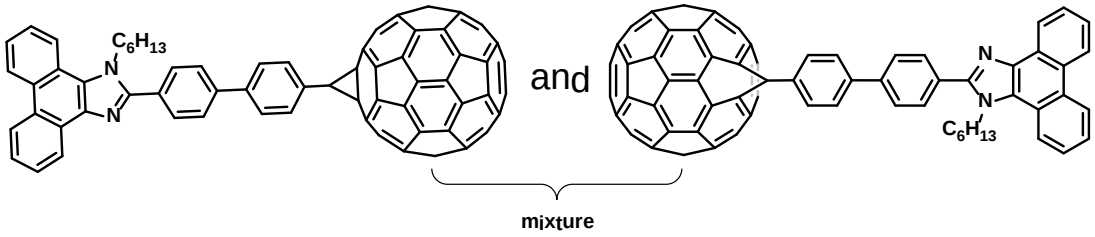
154.47, 151.67, 148.08, 147.24, 146.88, 146.80, 146.73, 146.40, 146.13, 146.12, 145.77 (2C), 145.74, 145.67 (2C), 145.56, 145.40, 145.38, 145.32, 145.23, 145.11 (2C), 145.09, 145.00, 144.85, 144.80, 144.72, 144.47, 144.21, 144.11, 143.80, 143.75, 142.95, 142.93, 142.55, 142.53, 142.51, 142.46, 142.10, 142.06, 142.01 (3C), 141.81 (2C), 141.74, 141.64, 141.61, 141.58, 141.43, 141.35, 140.44, 139.77 (2C), 139.37, 137.43, 136.32, 136.26, 134.95, 134.72, 133.66, 131.38, 130.98, 129.93, 128.38, 128.01, 127.98, 126.29, 86.41, 82.75 (sp^3-*C* of C_{60}), 77.71 (sp^3-*C* of C_{60}). FT-IR ν/cm^{-1} (KBr) 2920, 1610, 1510, 1424, 1355, 1265, 1188, 1060, 969, 877, 837, 796, 781, 764, 708, 574, 525. UV-vis ($CHCl_3$) λ_{max}/nm 256, 310, 429, 690. MALDI-FT MS *m/z* calcd for $C_{72}H_9ClNS$ $[M+H]^+$ 954.0139, found 954.0142.



4ep

Spectral data of **4ep**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 8.39 (d, *J* = 8.8 Hz, 2H), 8.13 (d, *J* = 8.0 Hz, 2H), 7.75 (t, *J* = 1.6 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.44 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.18 (s, 1H), 2.70 (t, *J* = 7.6 Hz, 2H), 1.69−1.62 (m, 2H), 1.33−1.27 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 170.48, 163.92, 154.46, 152.76, 151.65, 149.12, 147.97, 147.04, 146.71 (3C), 146.09 (2C), 146.05, 145.73 (3C), 145.65, 145.63, 145.52, 145.30 (2C), 145.15, 145.10, 145.09, 145.01, 144.96, 144.83, 144.76, 144.73, 144.40, 144.12, 144.01, 143.78, 143.73, 142.89 (2C), 142.48, 142.45, 142.43, 142.37, 142.11, 142.00, 141.96, 141.93 (2C), 141.85, 141.79, 141.66, 141.64, 141.61, 141.48 (2C), 141.39, 140.30, 139.94, 139.69, 139.63, 136.05, 134.96, 134.71, 133.65, 131.34, 130.46, 130.10 (4C), 129.96, 128.44 (4C), 128.37, 127.93, 126.34, 126.19, 121.91, 87.10, 84.14 (sp^3-*C* of C_{60}), 77.48 (sp^3-*C* of C_{60}), 36.08, 31.77, 31.08, 29.24, 29.15, 22.75, 14.11. FT-IR ν/cm^{-1} (KBr) 2922, 2852, 1738, 1603, 1506, 1463, 1430, 1261,

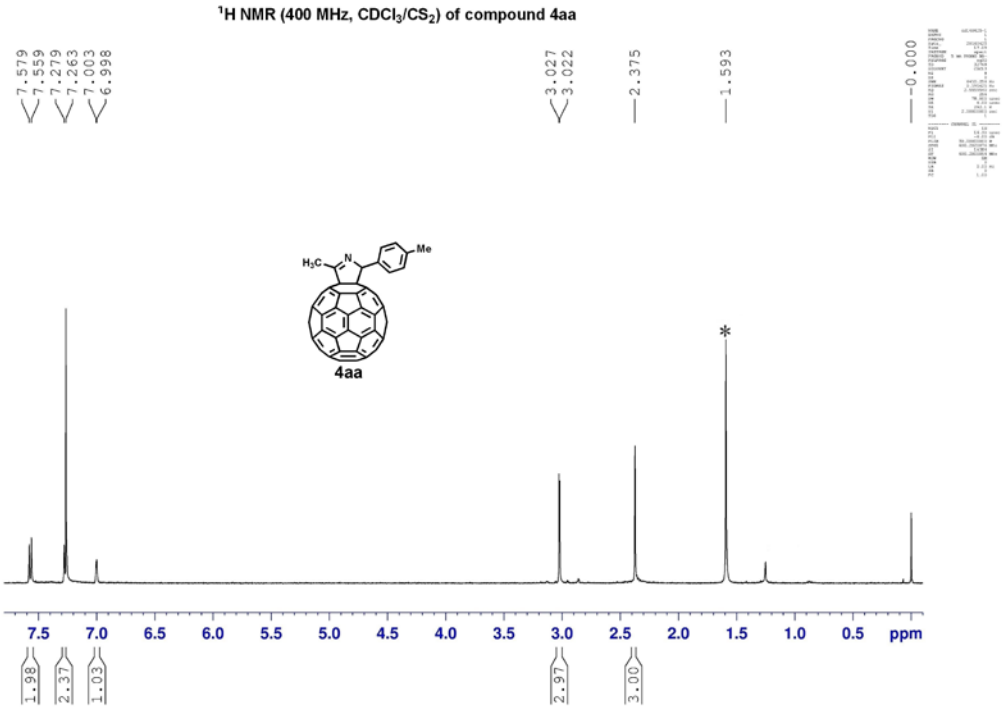
1207, 1168, 1064, 1017, 987, 879, 784, 723, 693, 660, 645, 598, 581, 552, 5262. UV-vis ($CHCl_3$) λ_{max}/nm 256, 312, 429, 688. ESI FT-ICR MS *m/z* calcd for $C_{88}H_{29}ClNO_2$ $[M+H]^+$ 1166.1881, found 1166.1872.

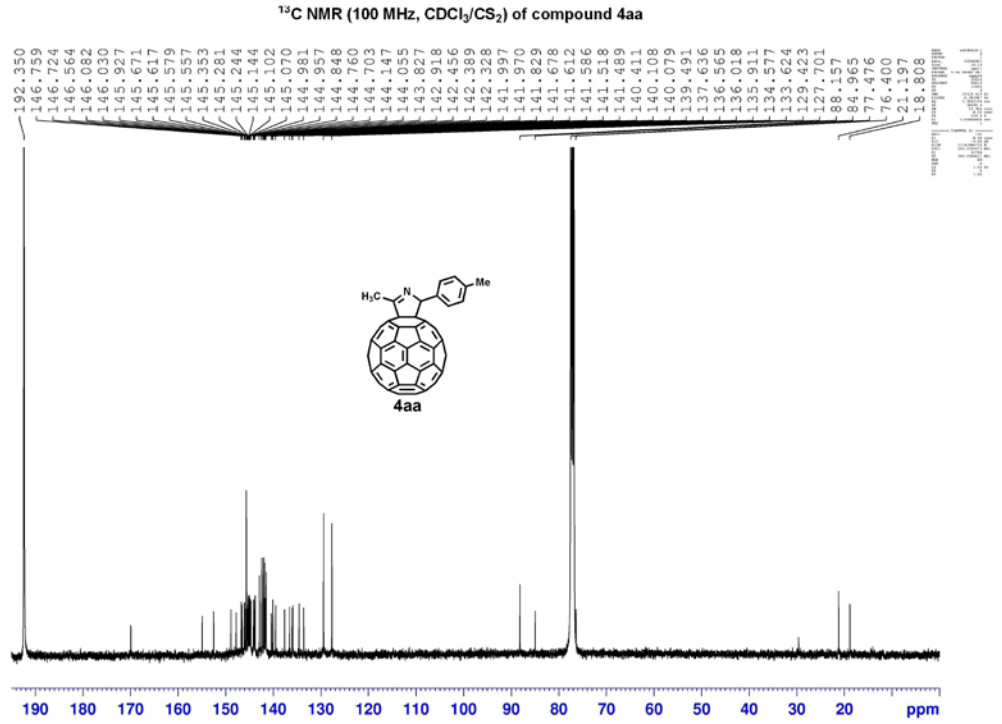


5s

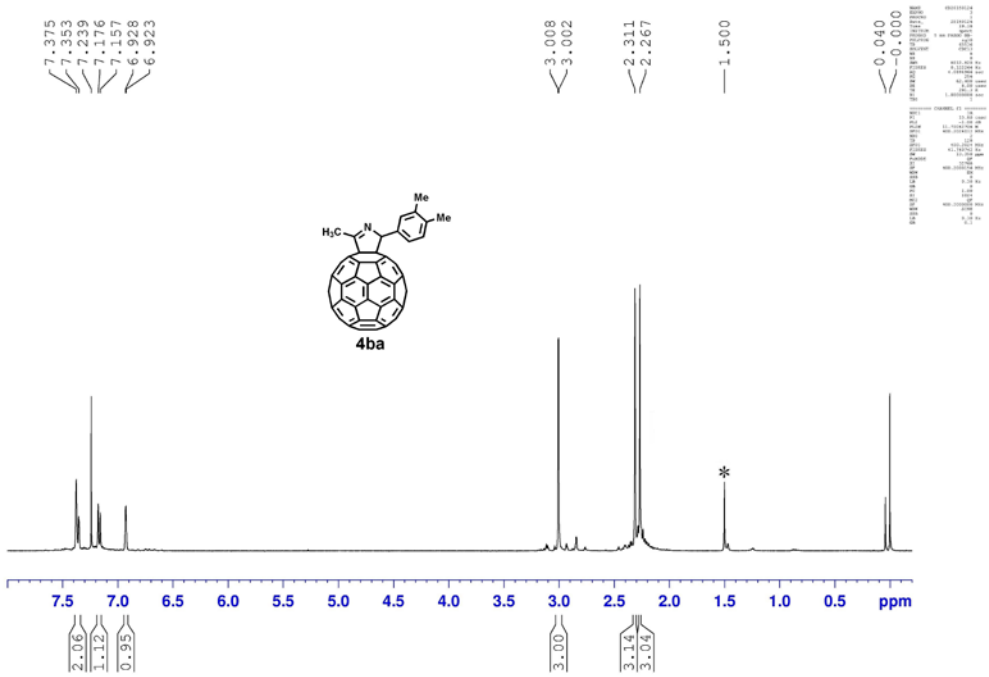
The mixture of methanofullerene and fulleroid **5s**: ESI FT-ICR MS *m/z* calcd for $C_{94}H_{31}N_2$ $[M+H]^+$ 1187.2482, found 1187.2480.

6. ^{1}H NMR and ^{13}C NMR Spectra of Compounds 4aa−4sa and 4eb−4en

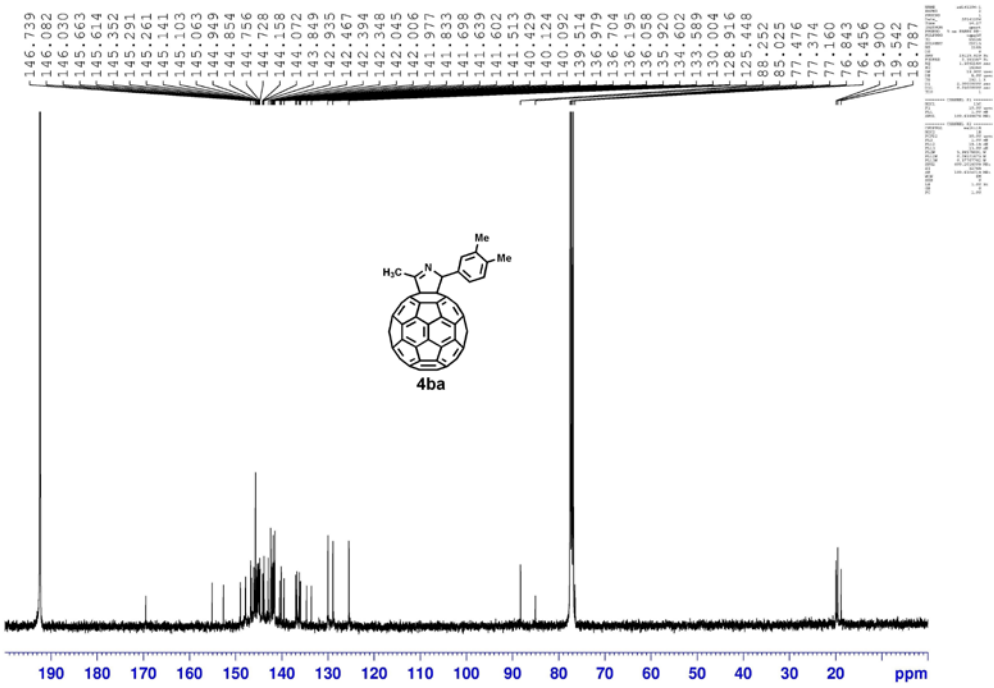




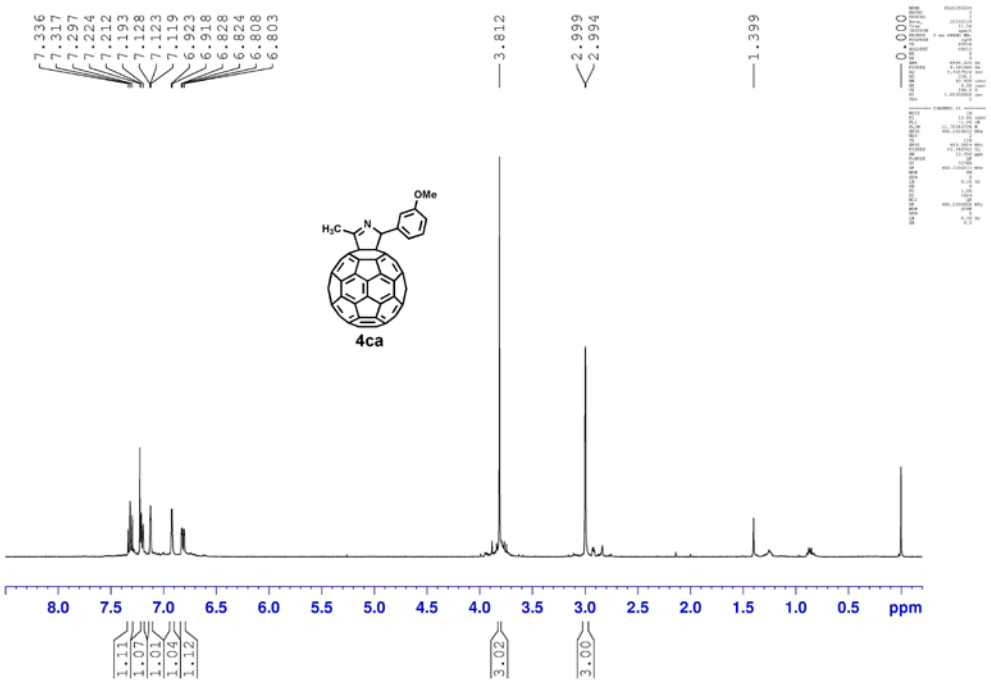
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ba



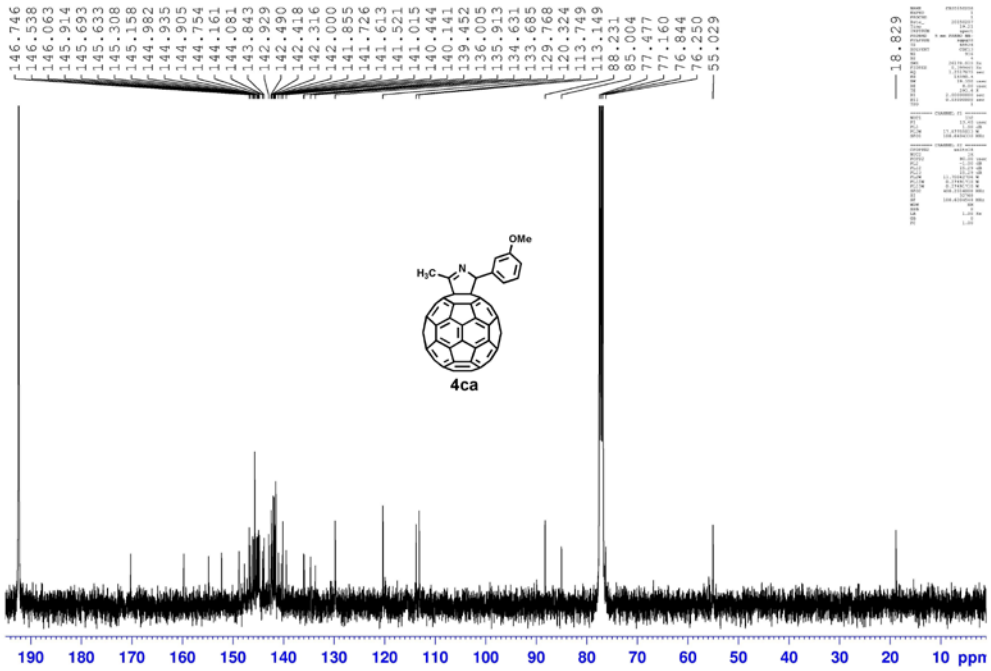
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ba



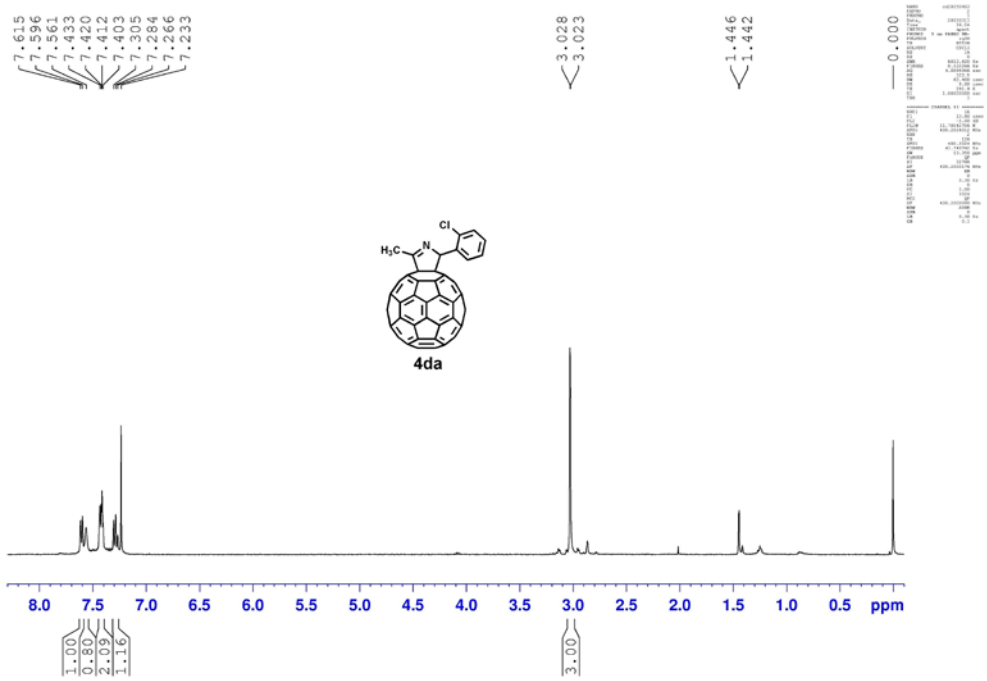
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ca



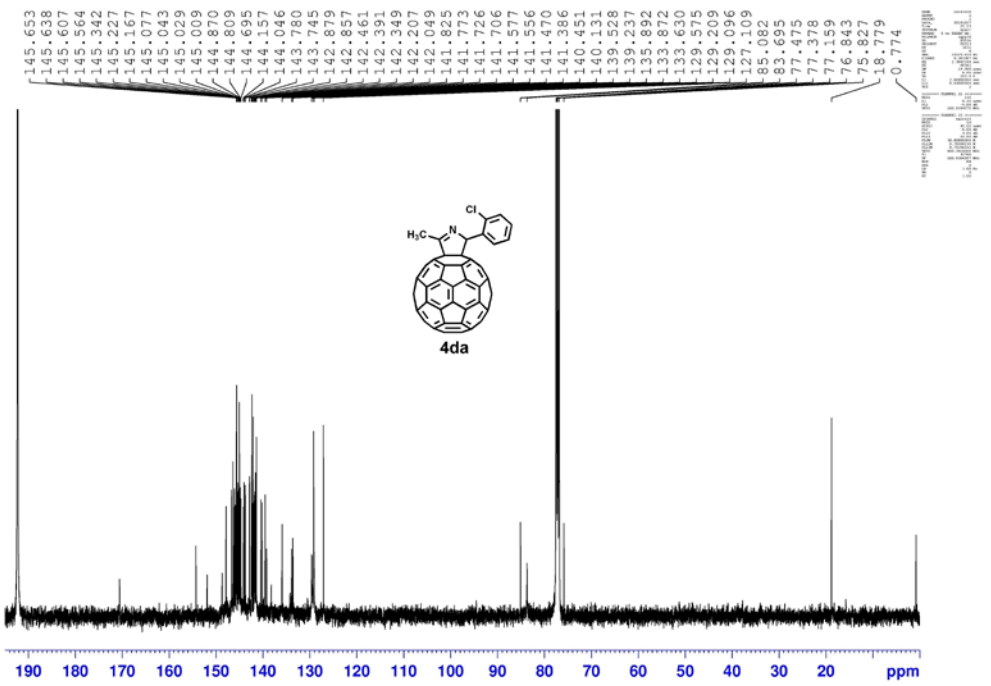
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ca



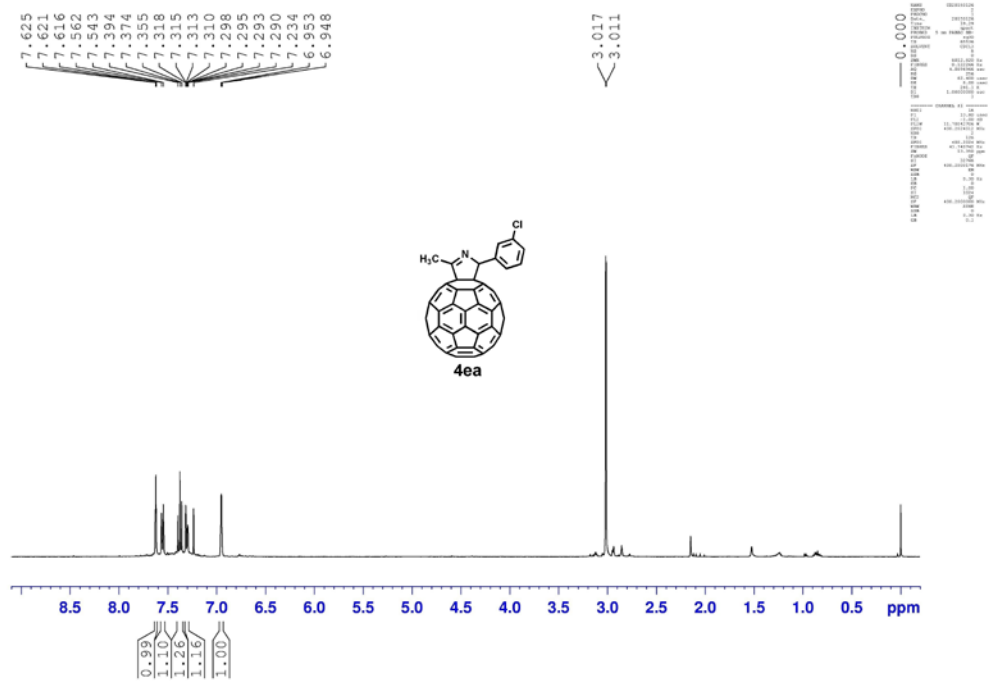
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4da



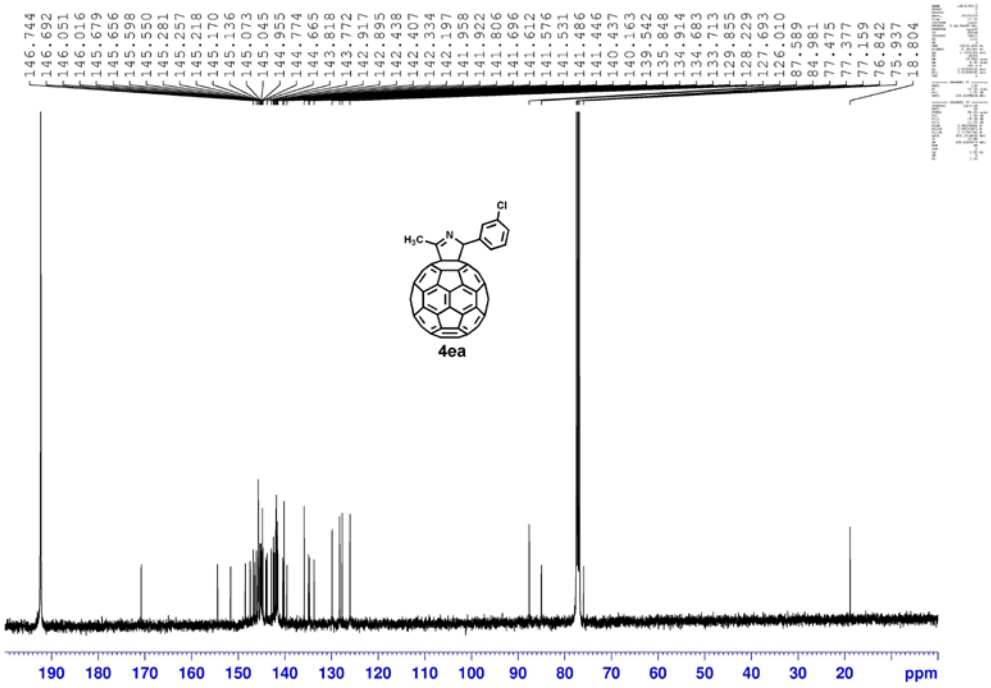
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4da



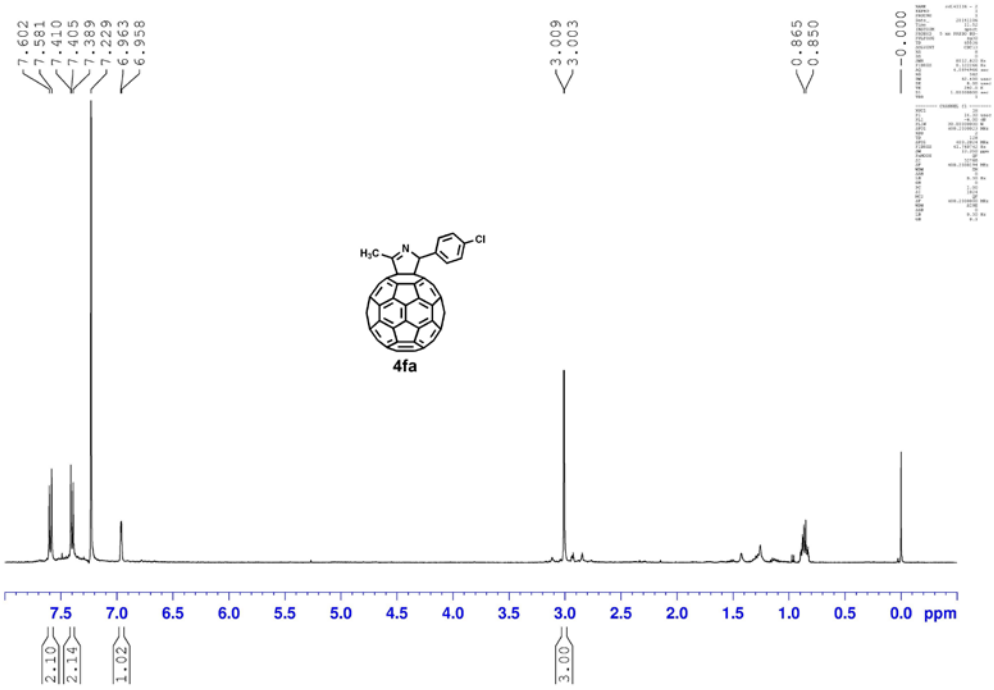
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ea



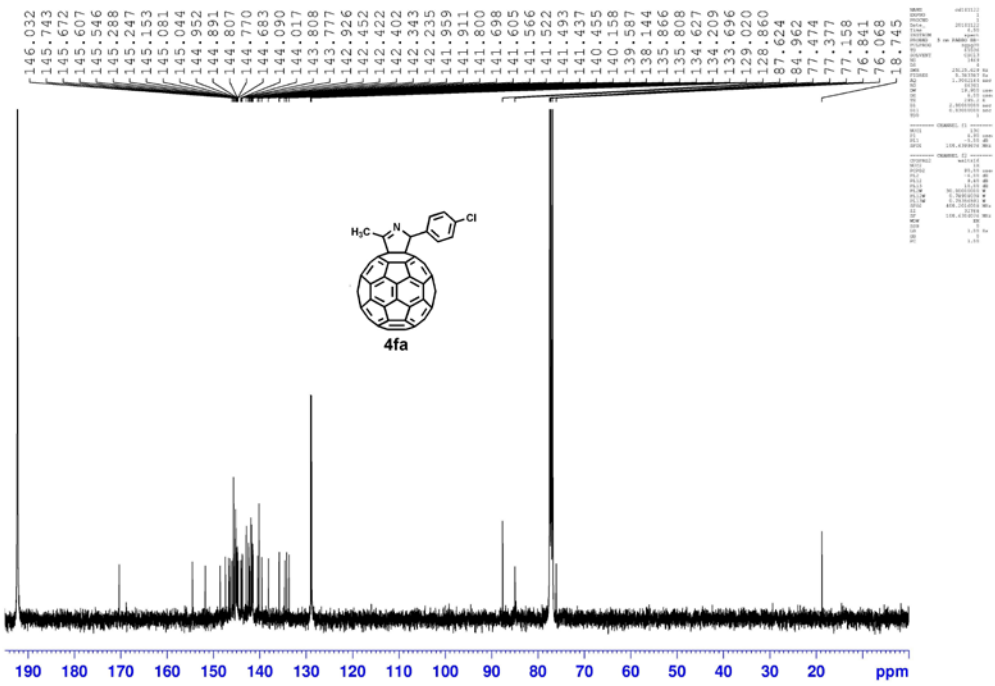
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ea



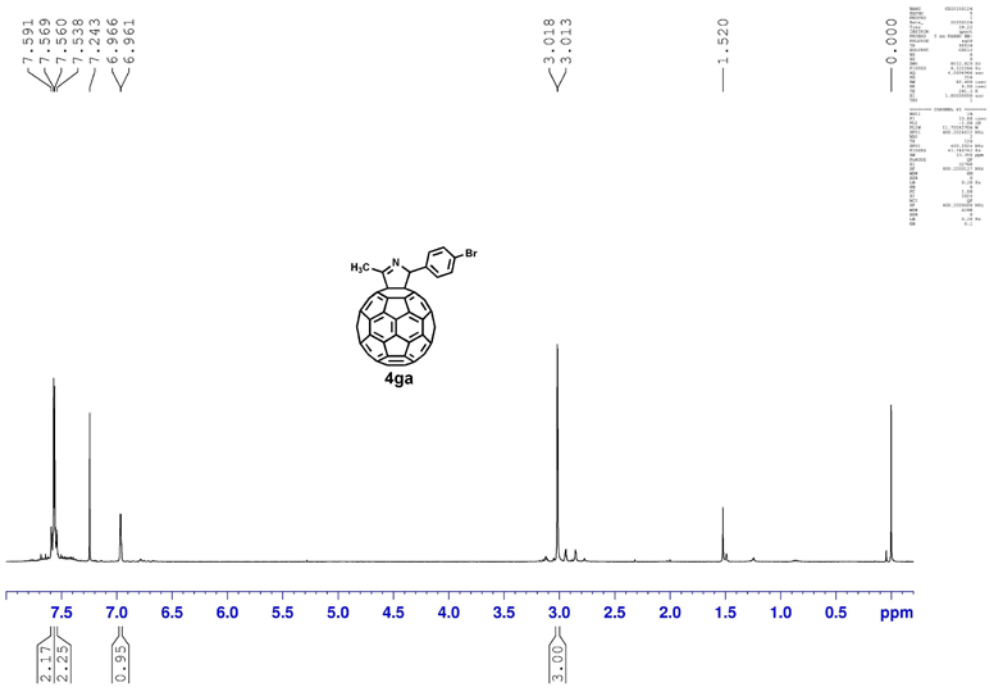
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4fa



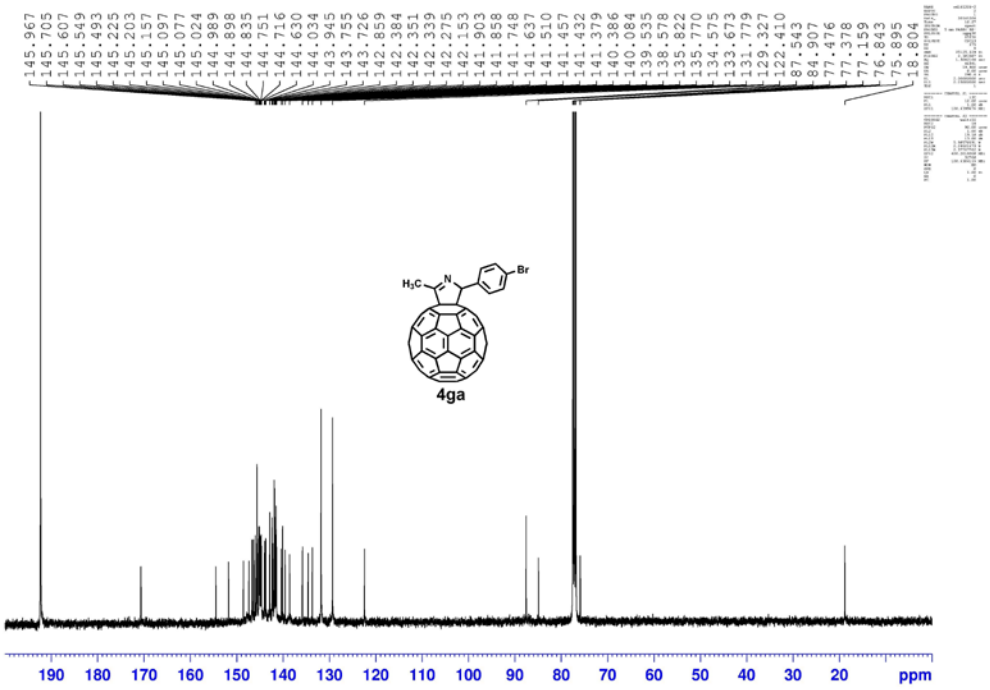
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4fa



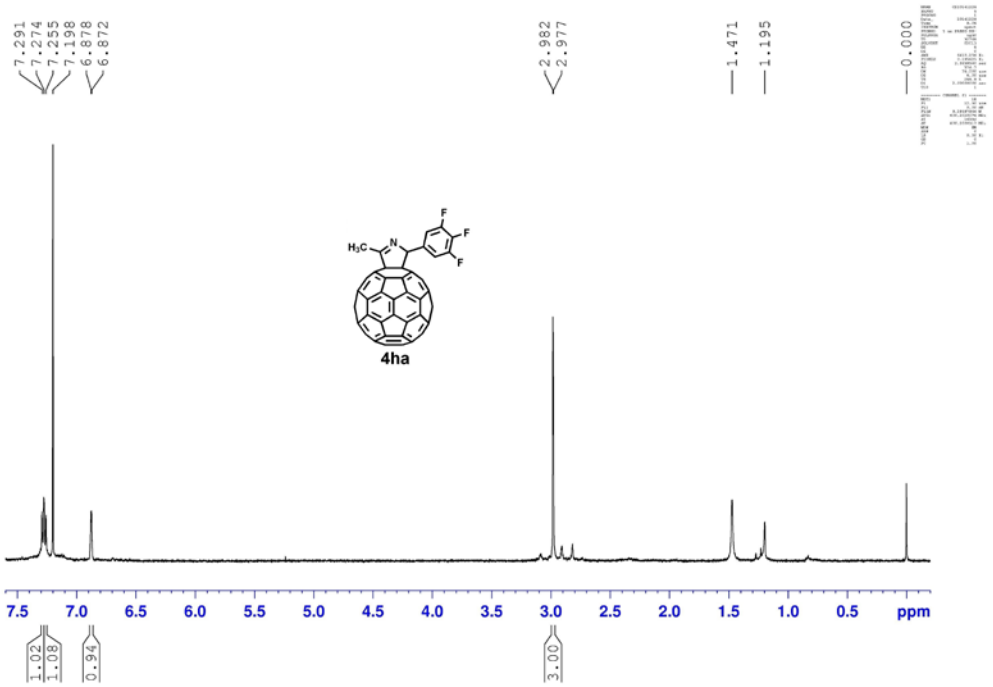
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ga



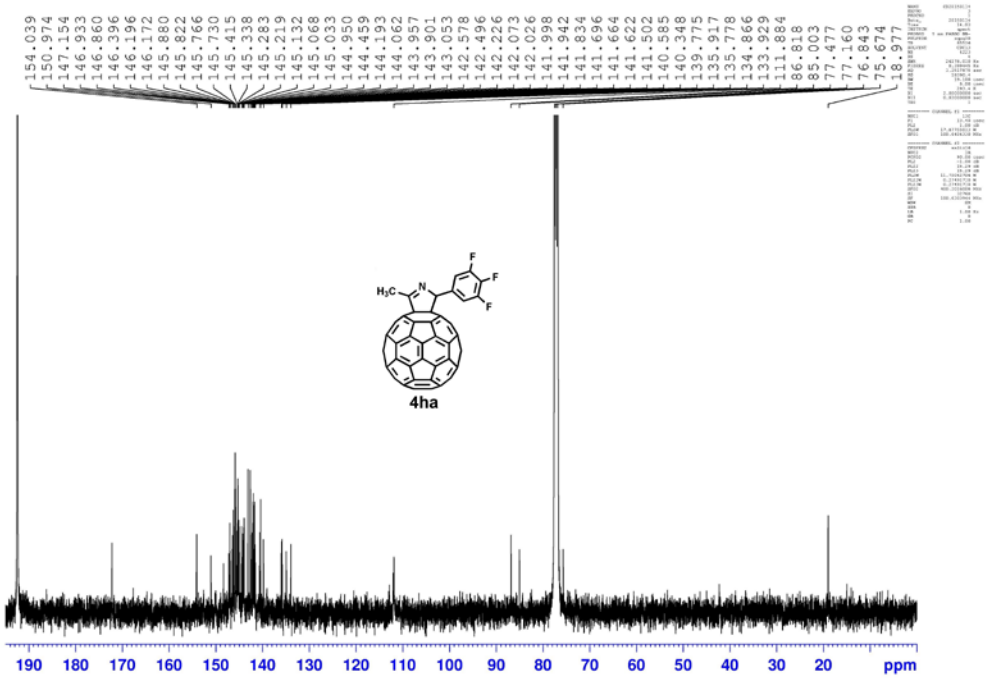
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ga



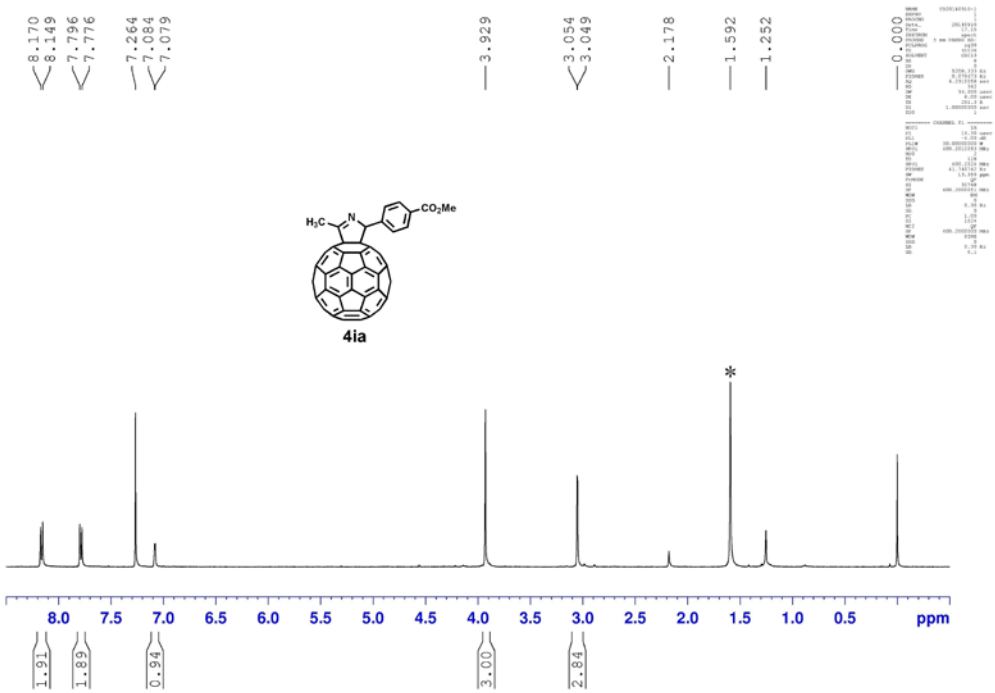
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ha



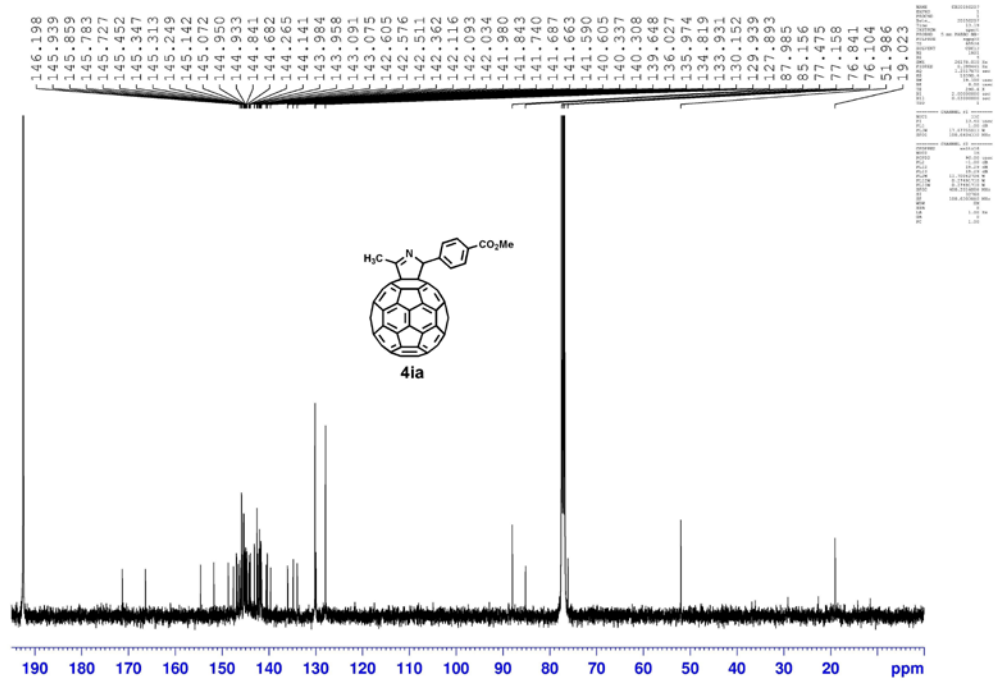
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ha



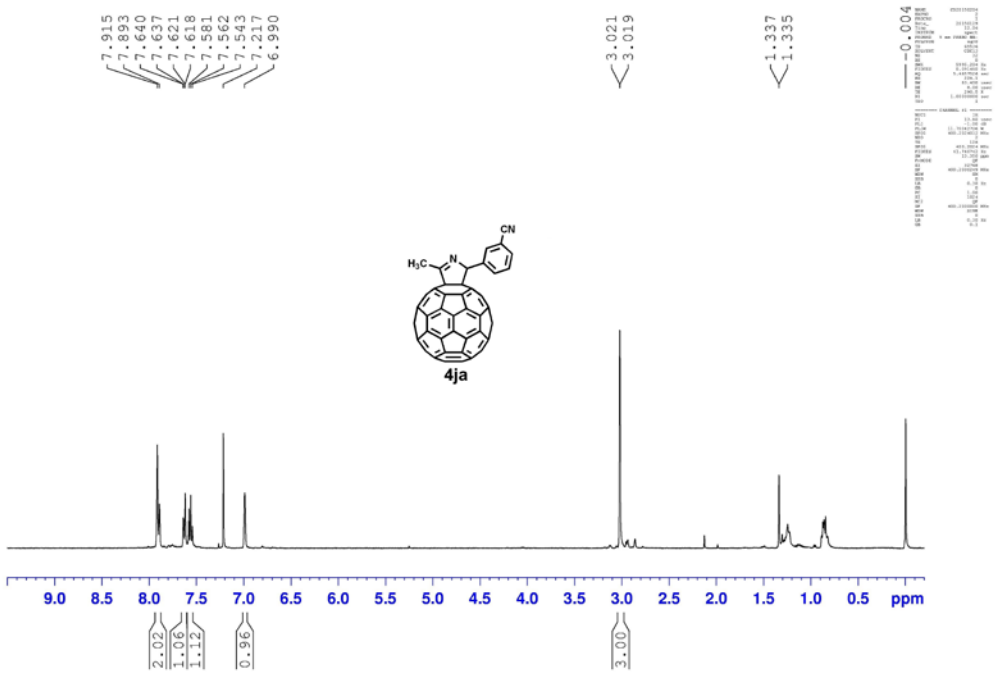
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ia



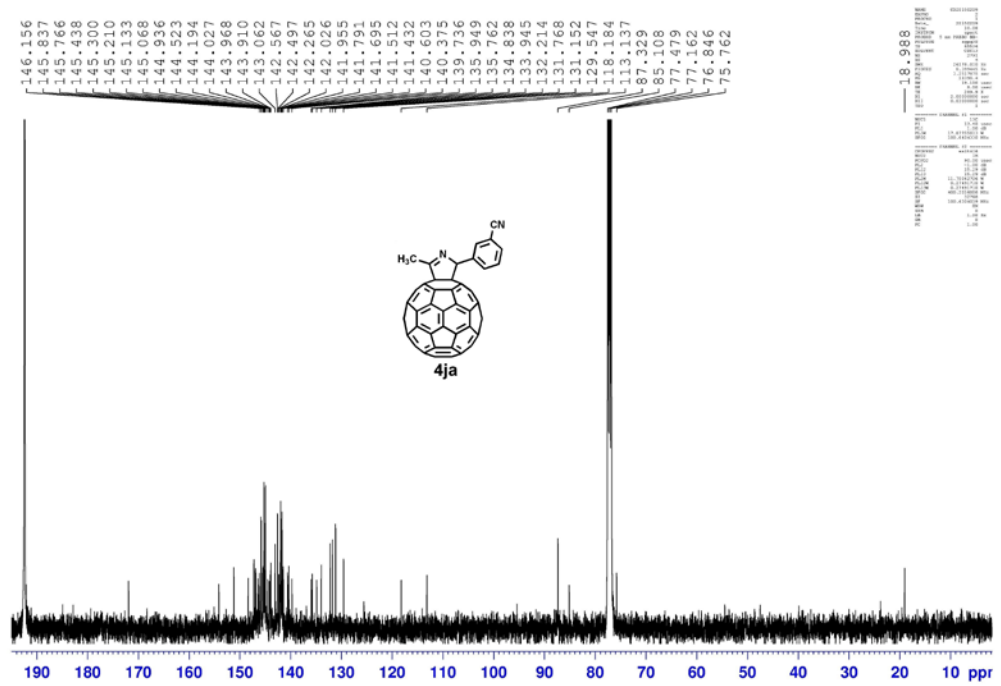
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ia



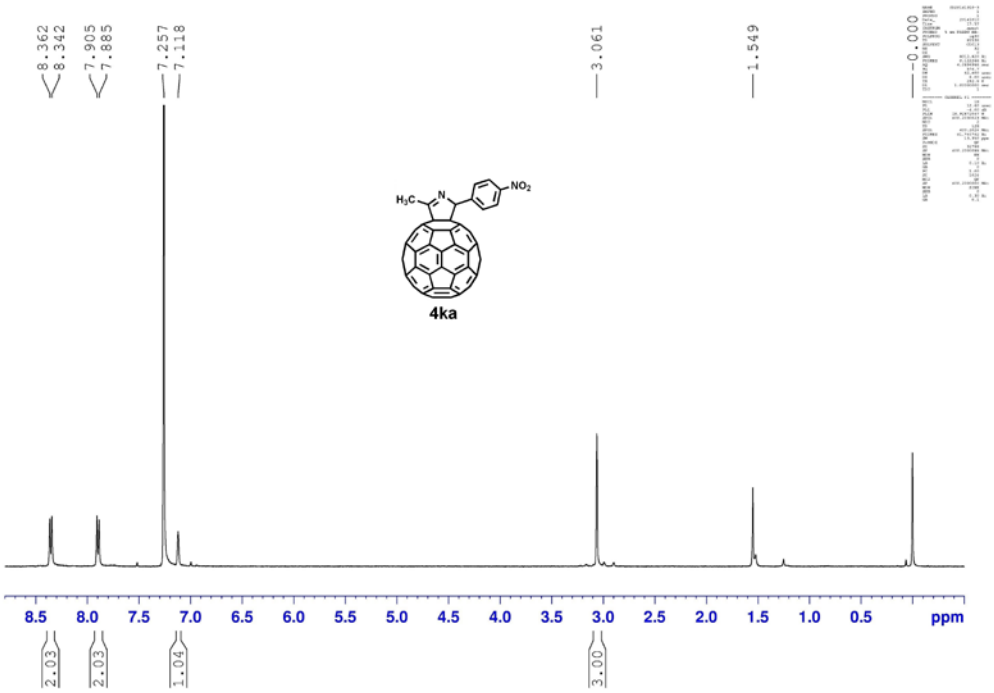
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ja



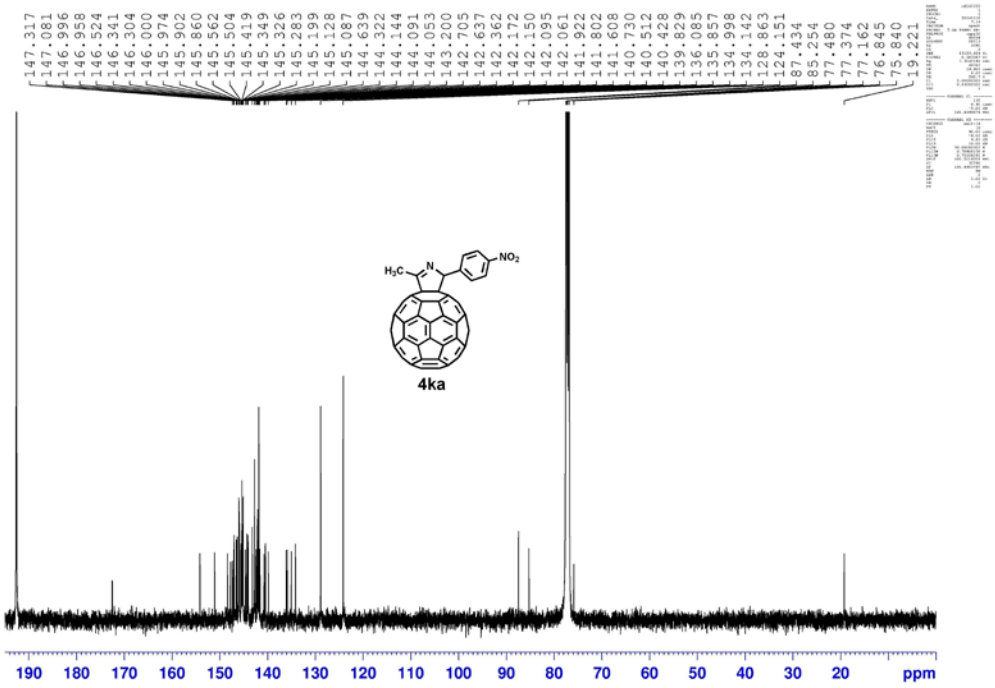
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ja



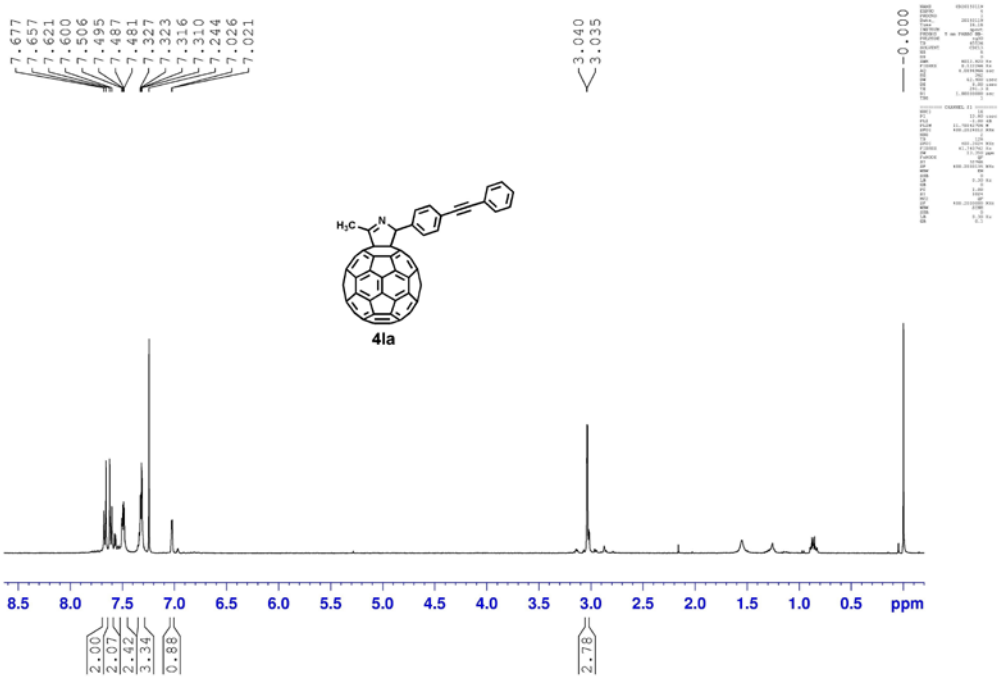
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ka



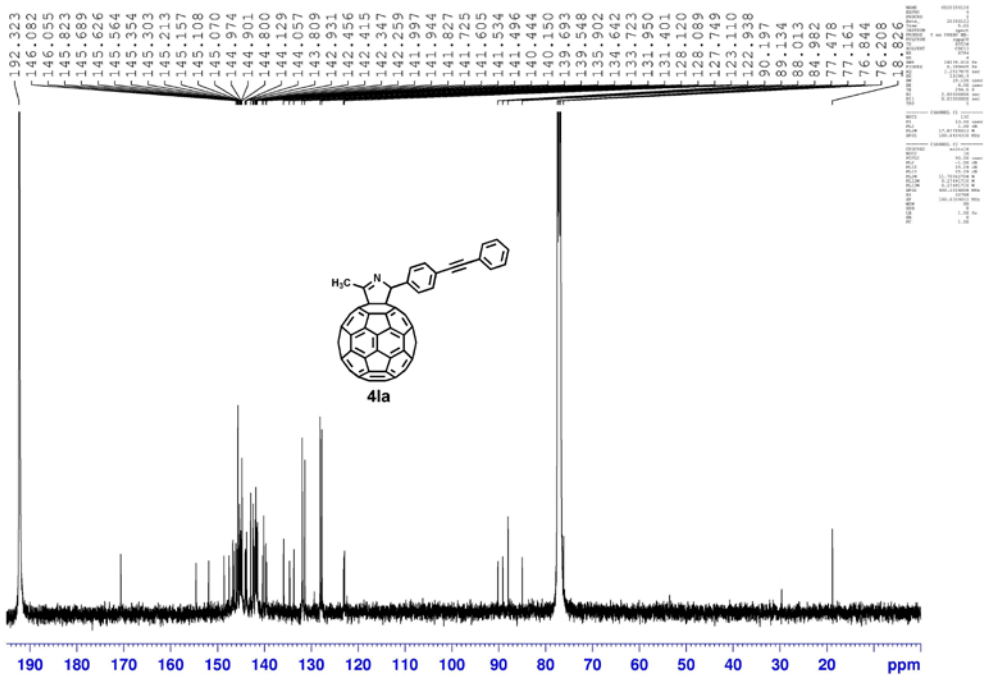
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ka



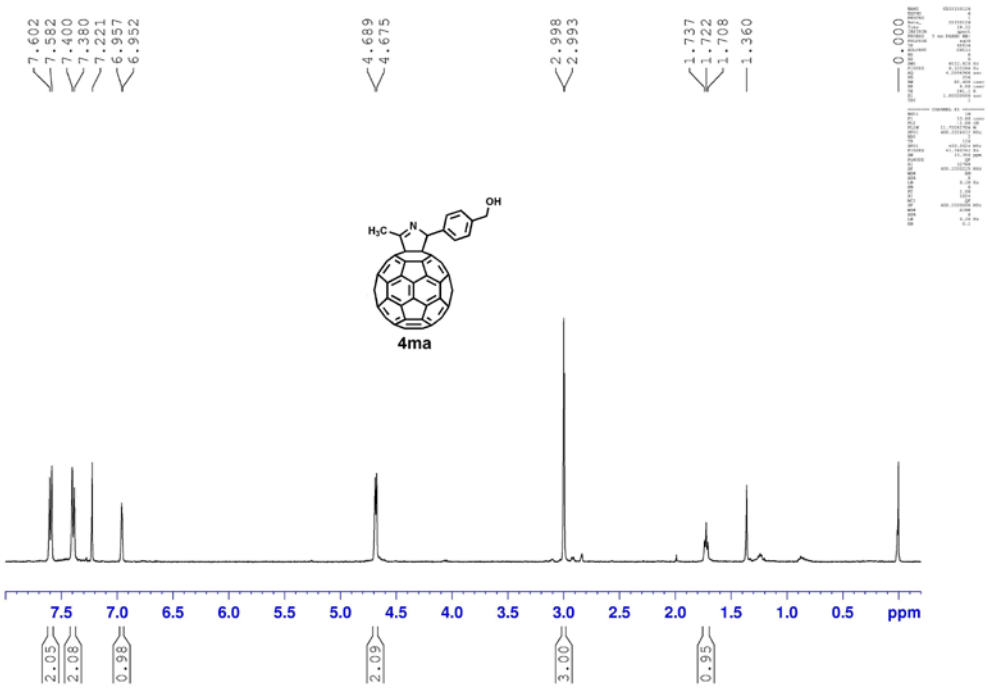
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4la



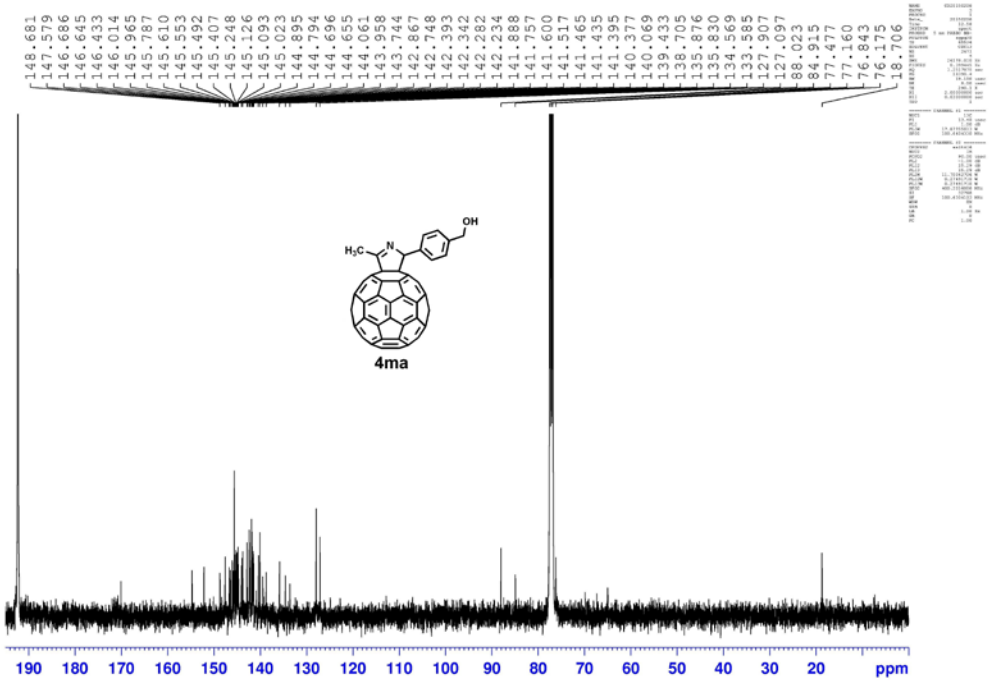
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4la



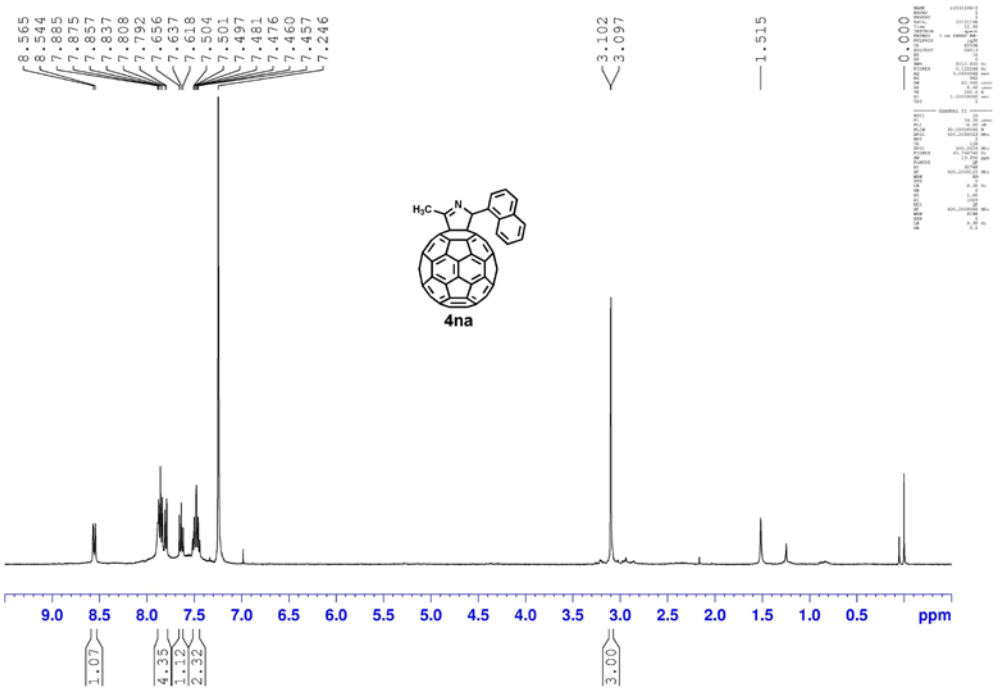
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ma



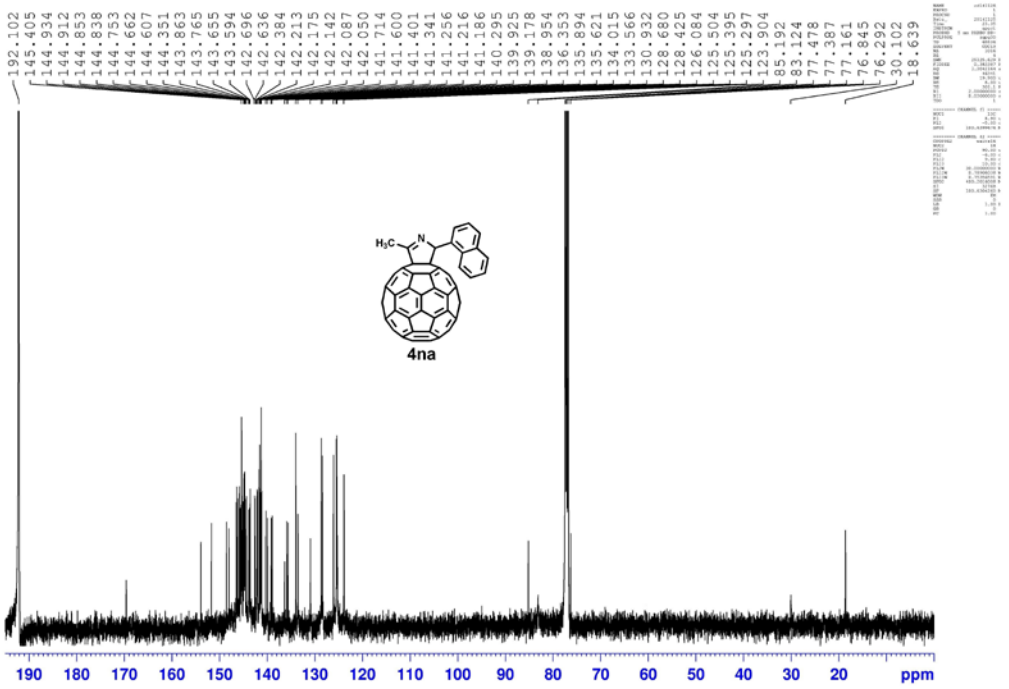
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ma



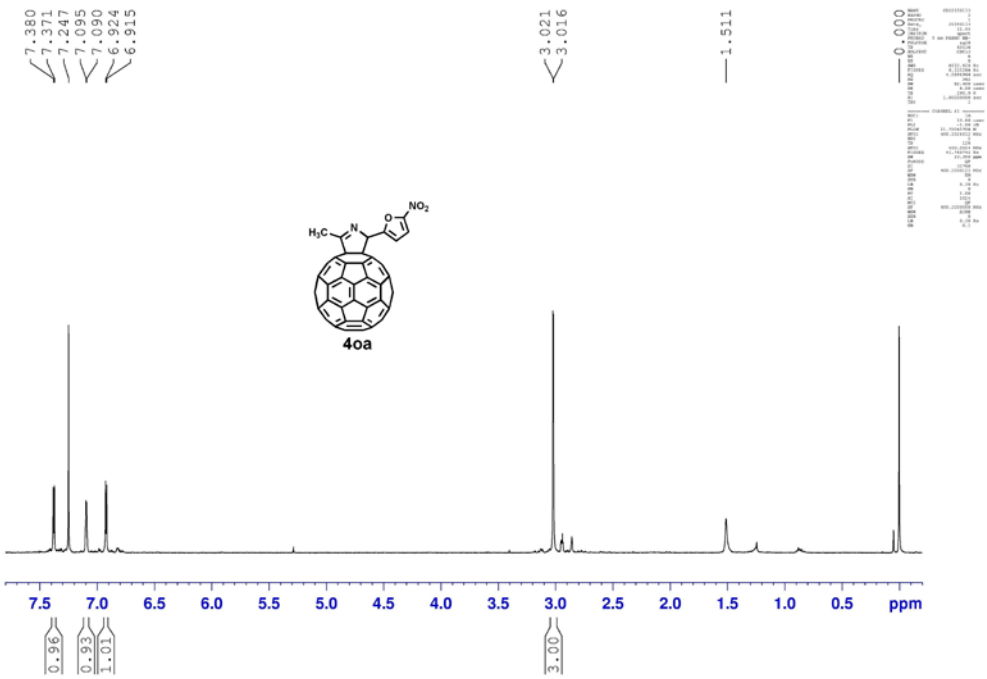
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4na



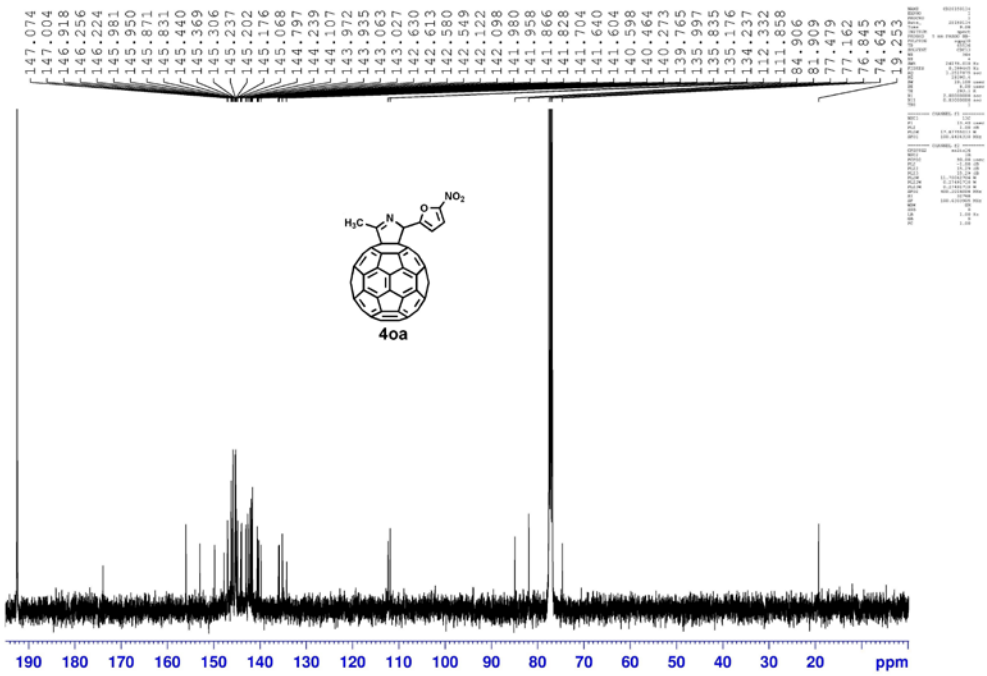
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4na



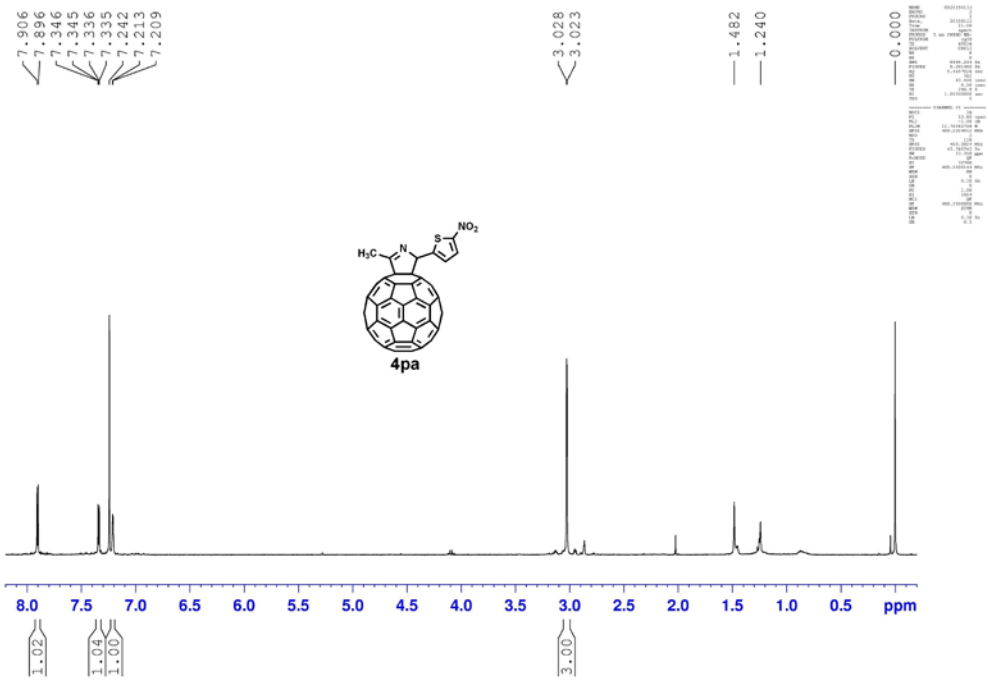
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4oa



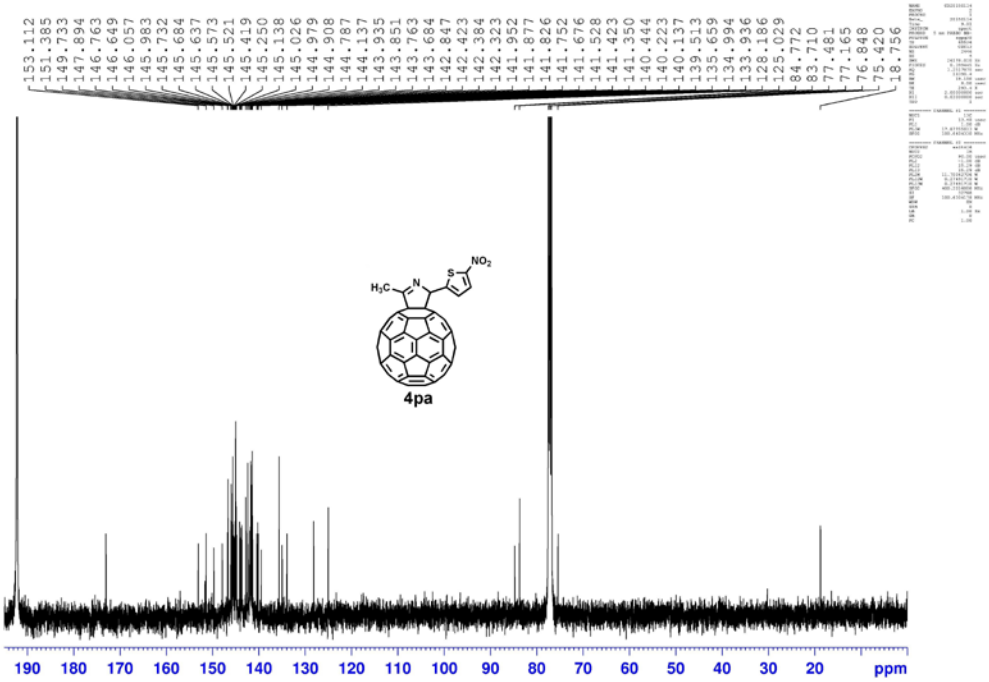
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4oa



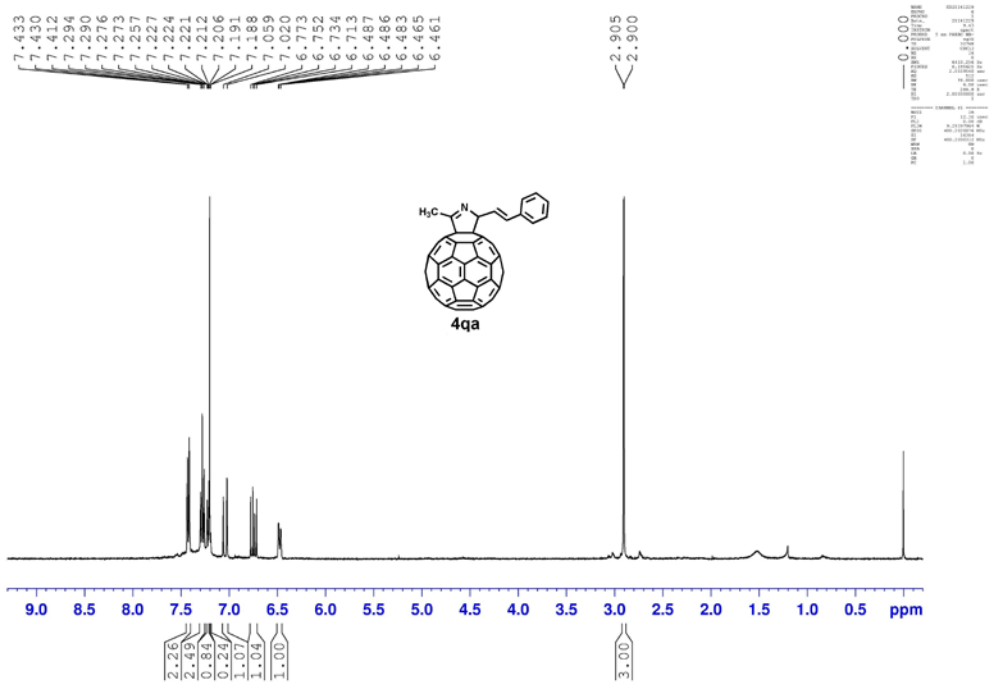
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4pa



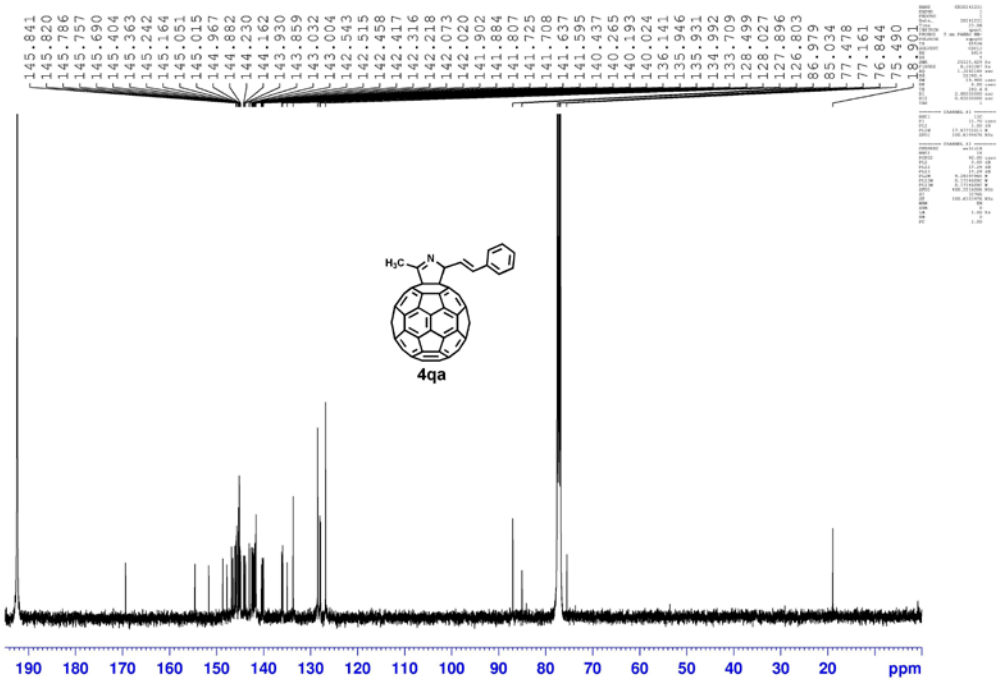
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4pa



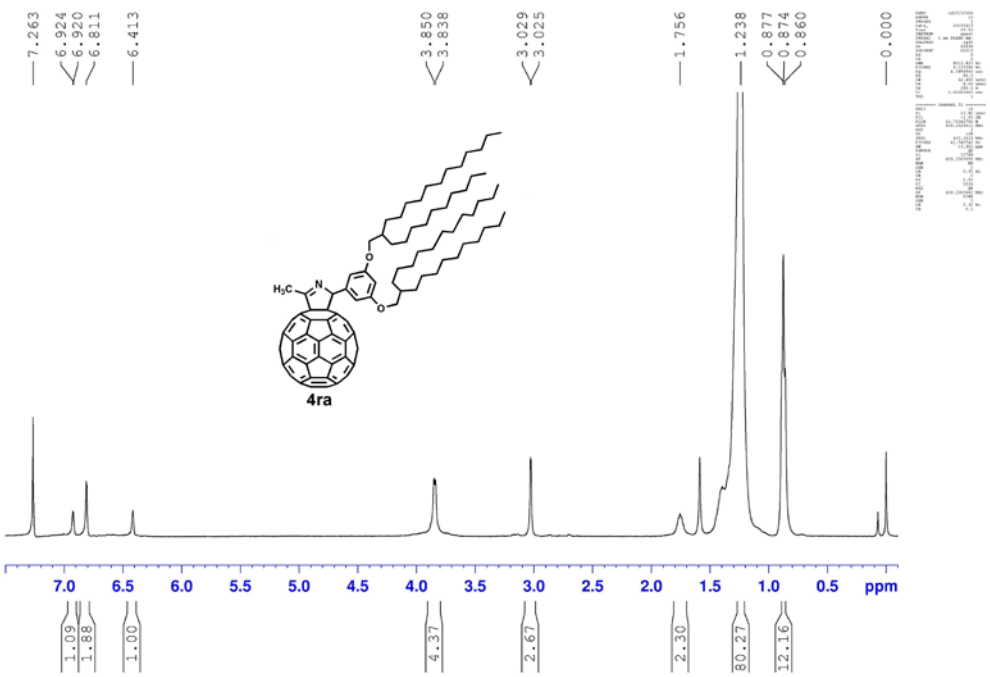
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4qa



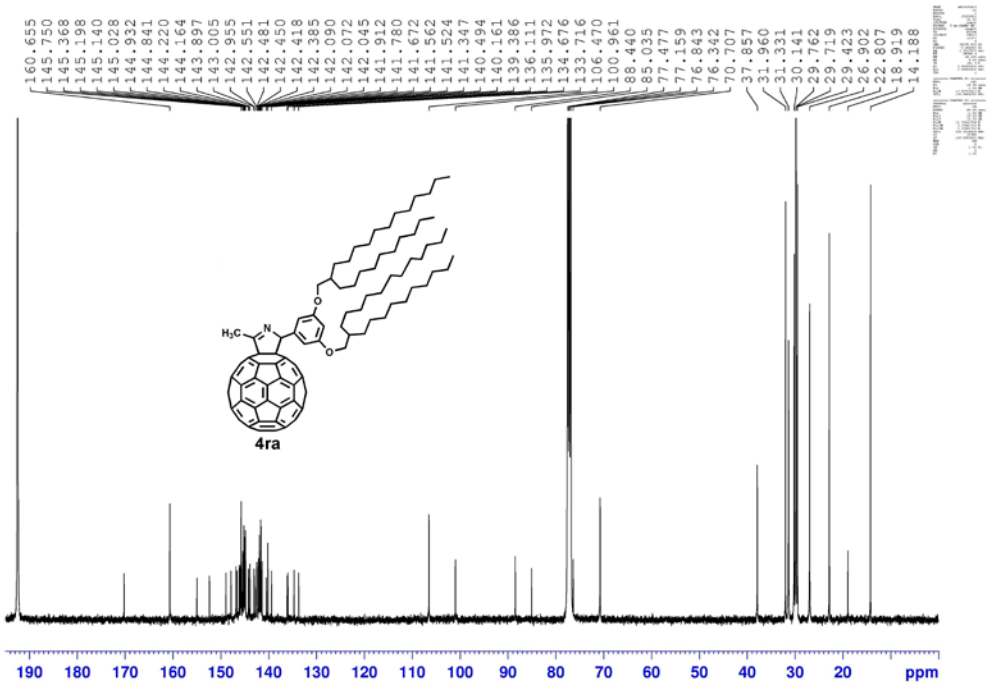
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4qa



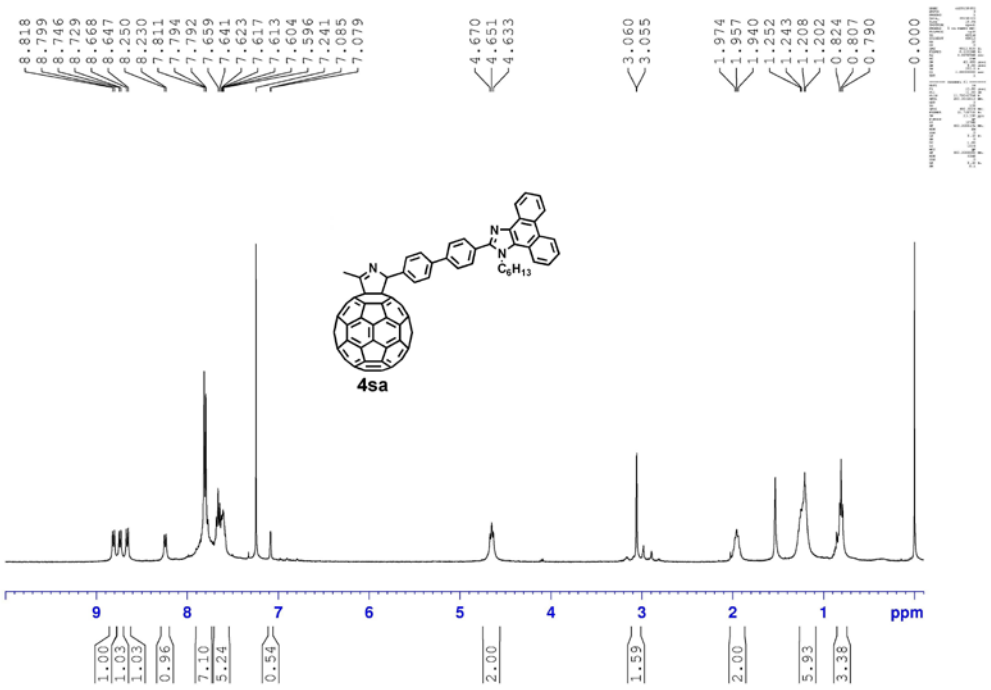
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ra



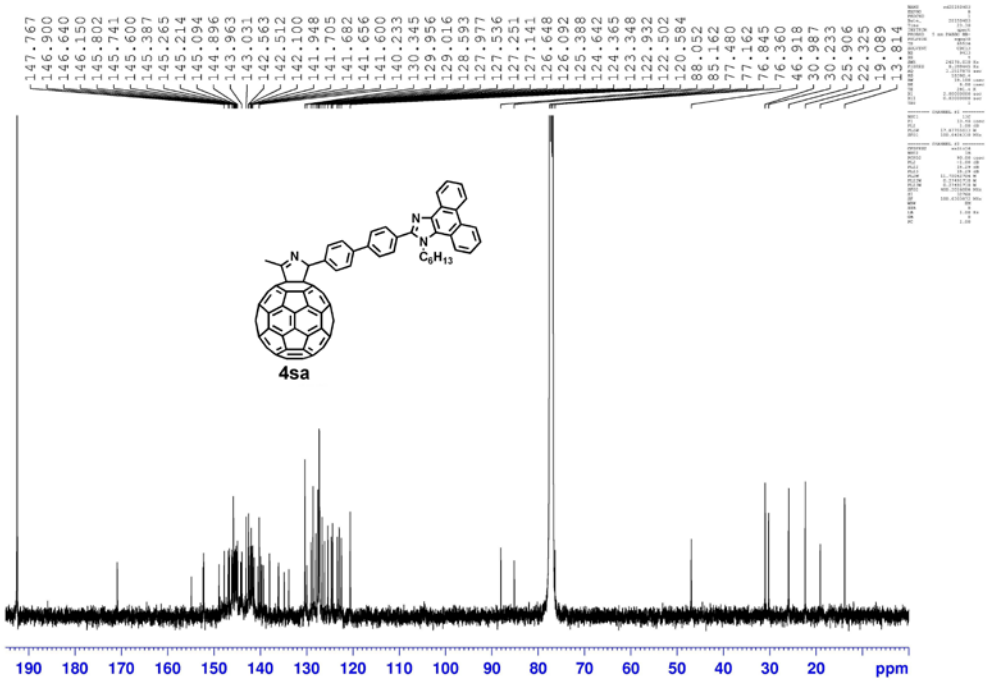
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ra



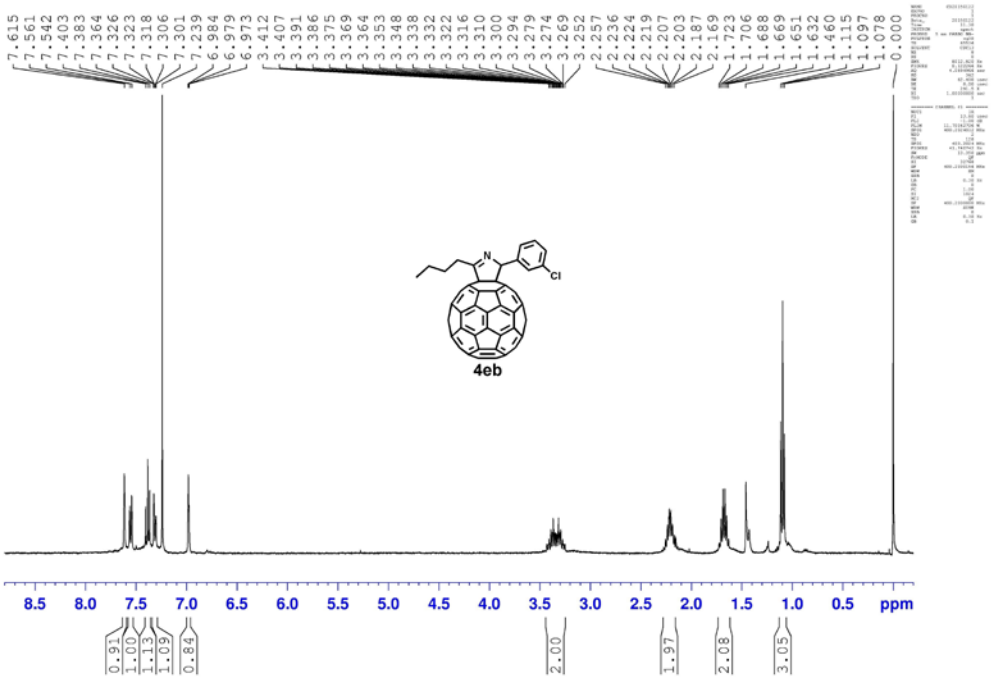
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4sa



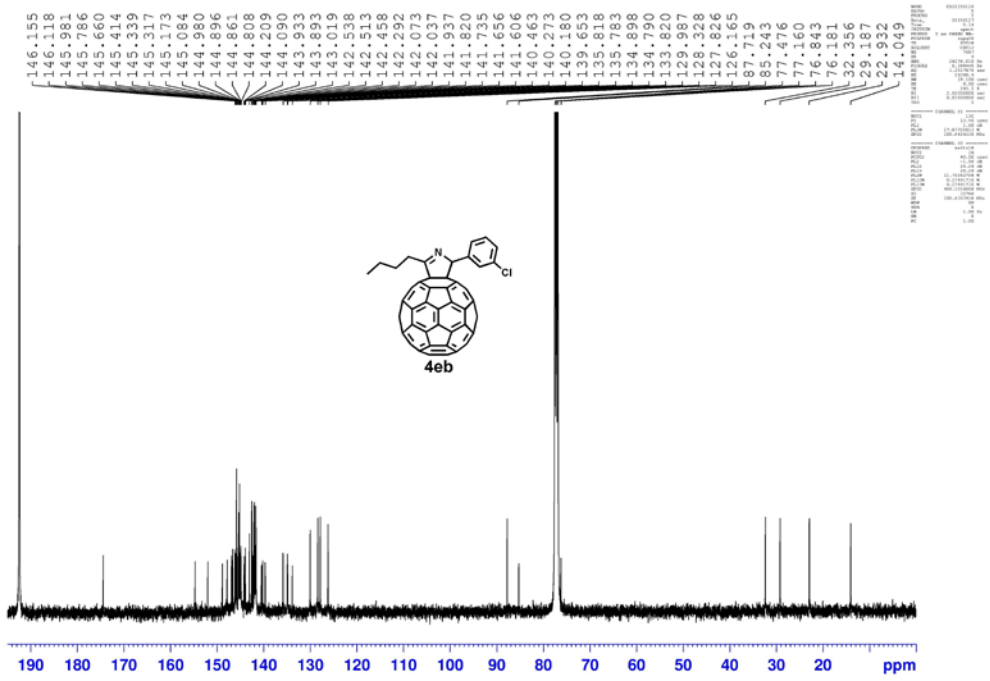
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4sa



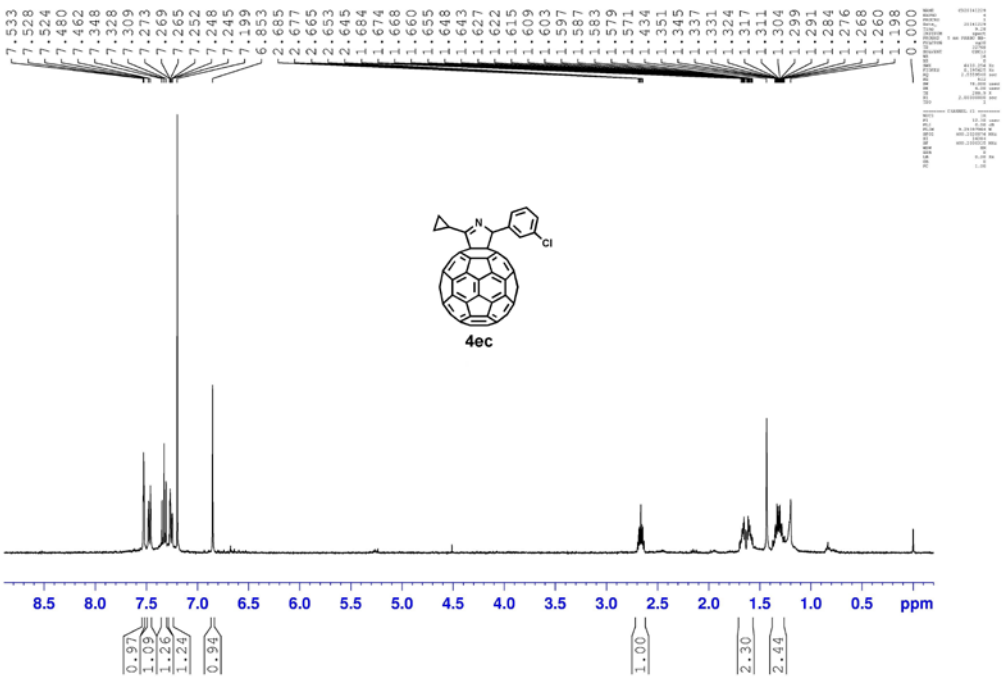
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4eb



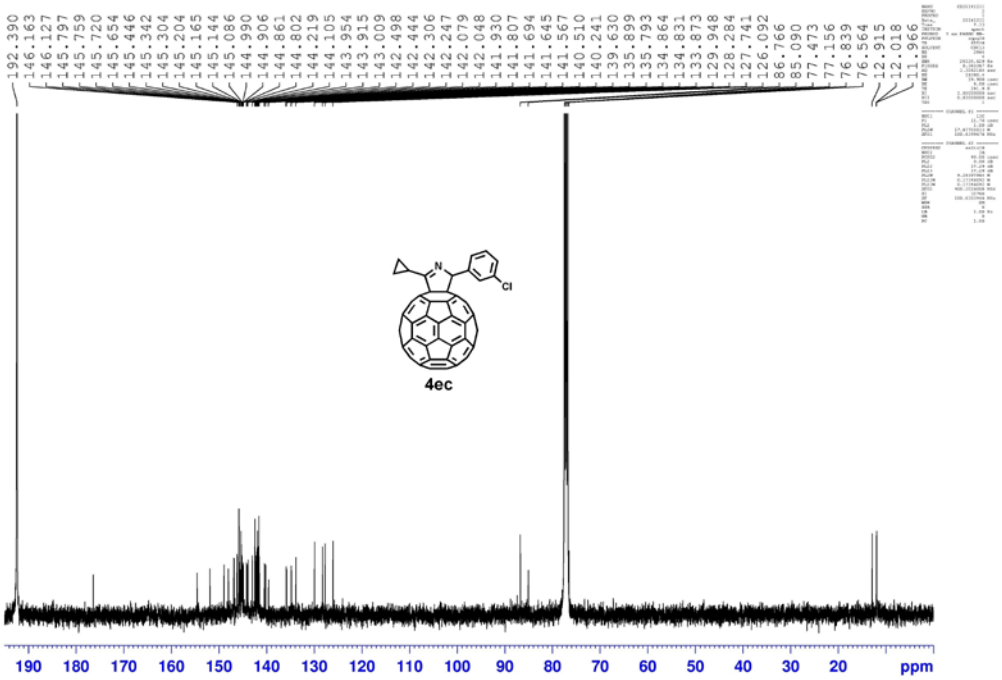
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4eb



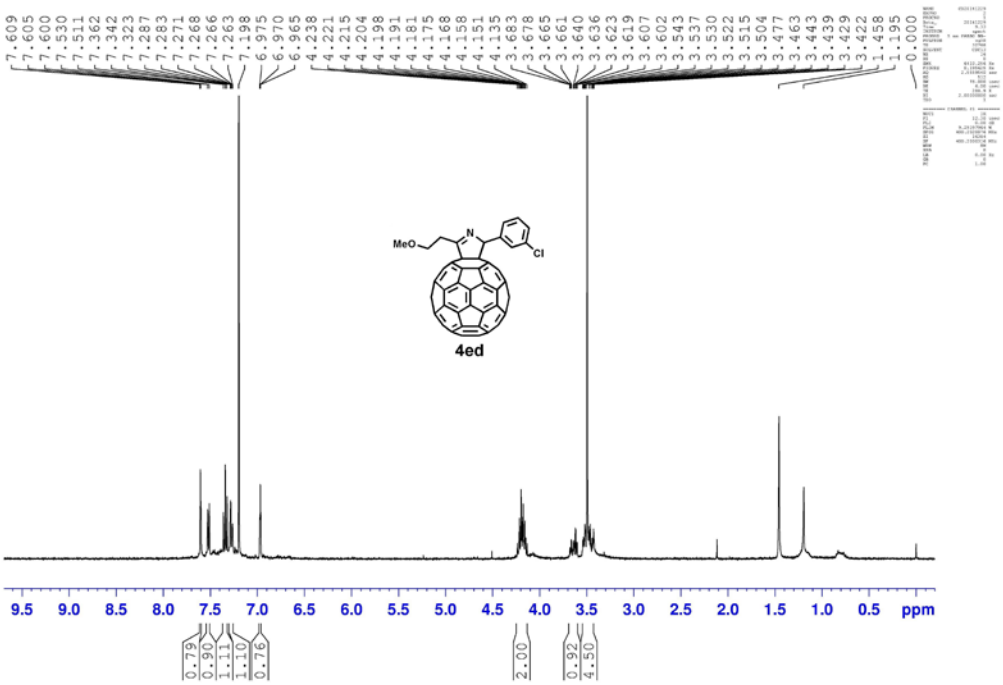
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ec



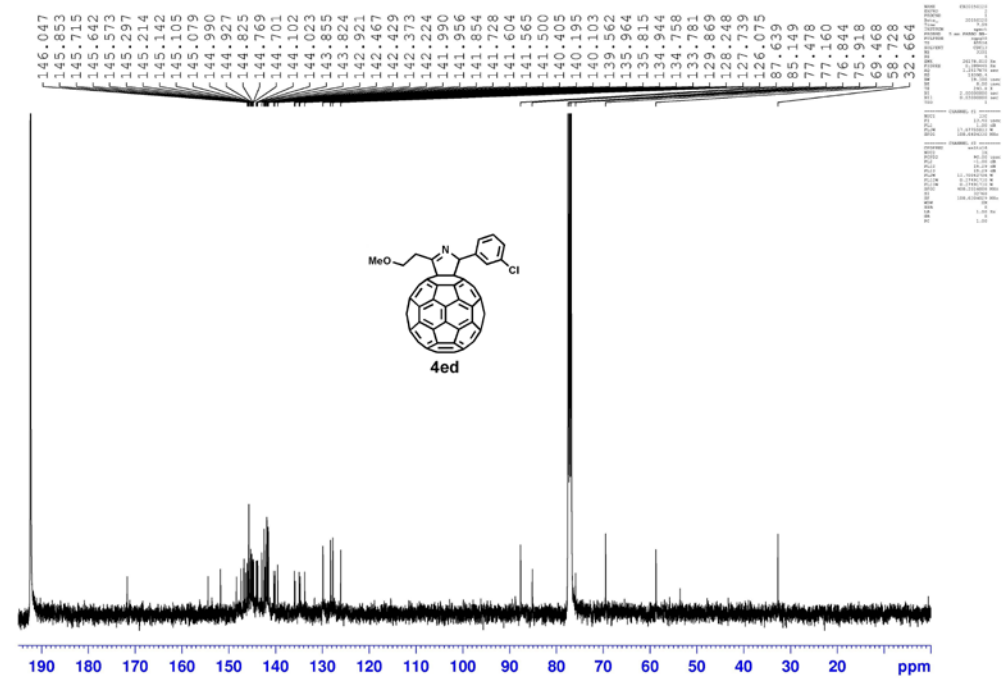
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ec



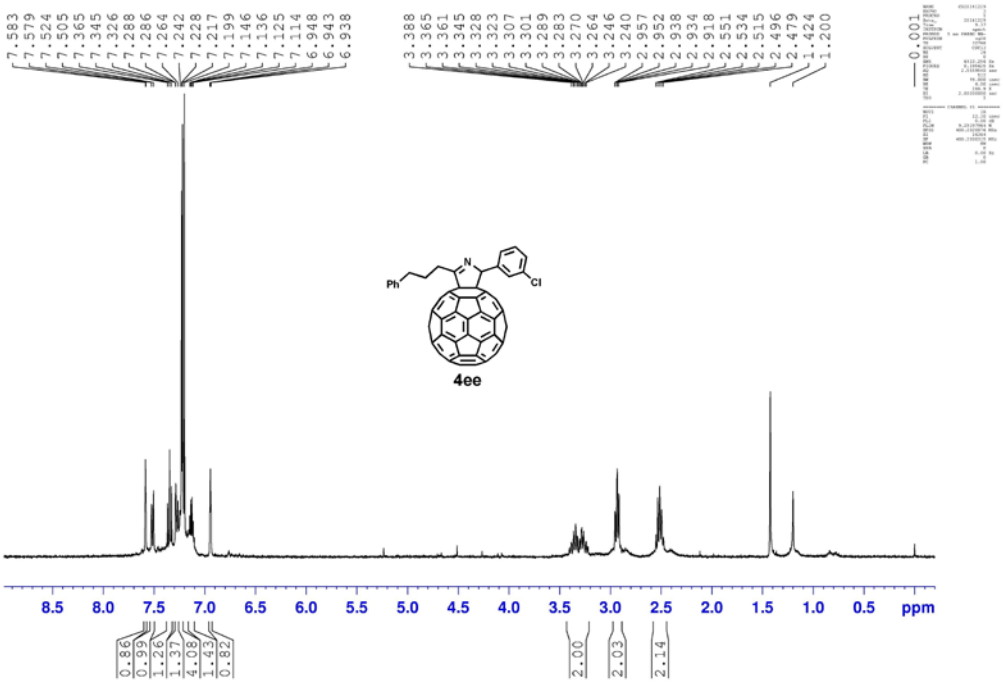
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ed



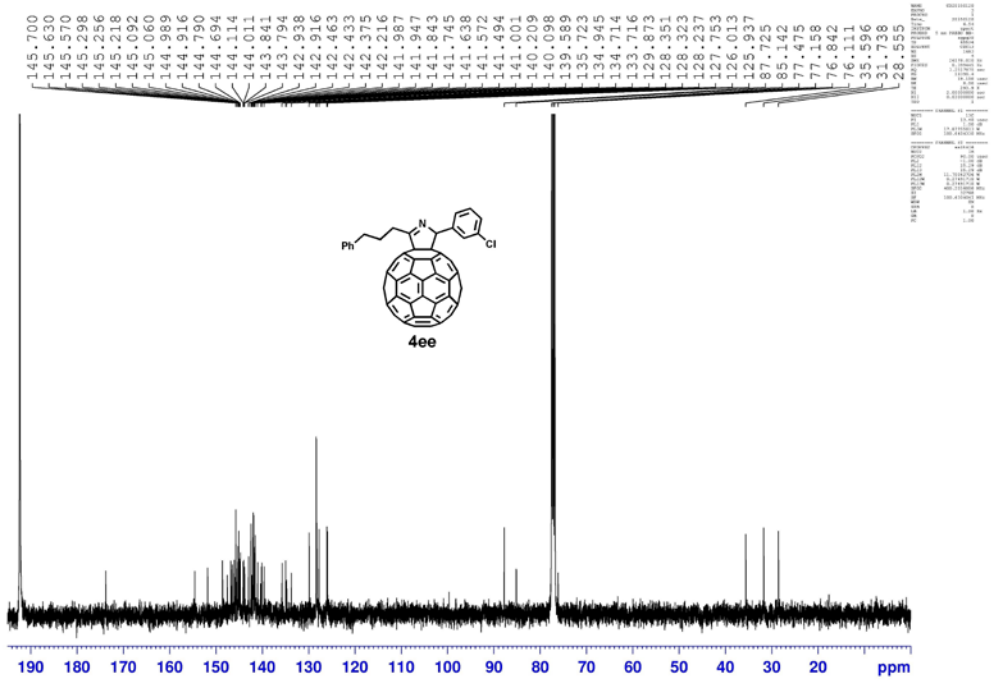
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ed



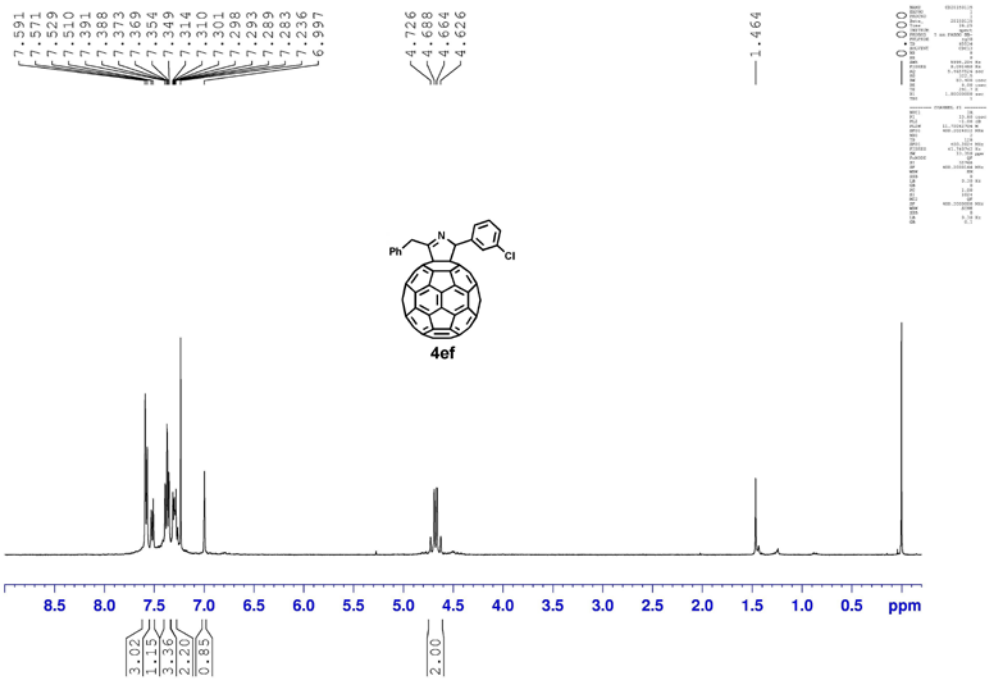
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ee



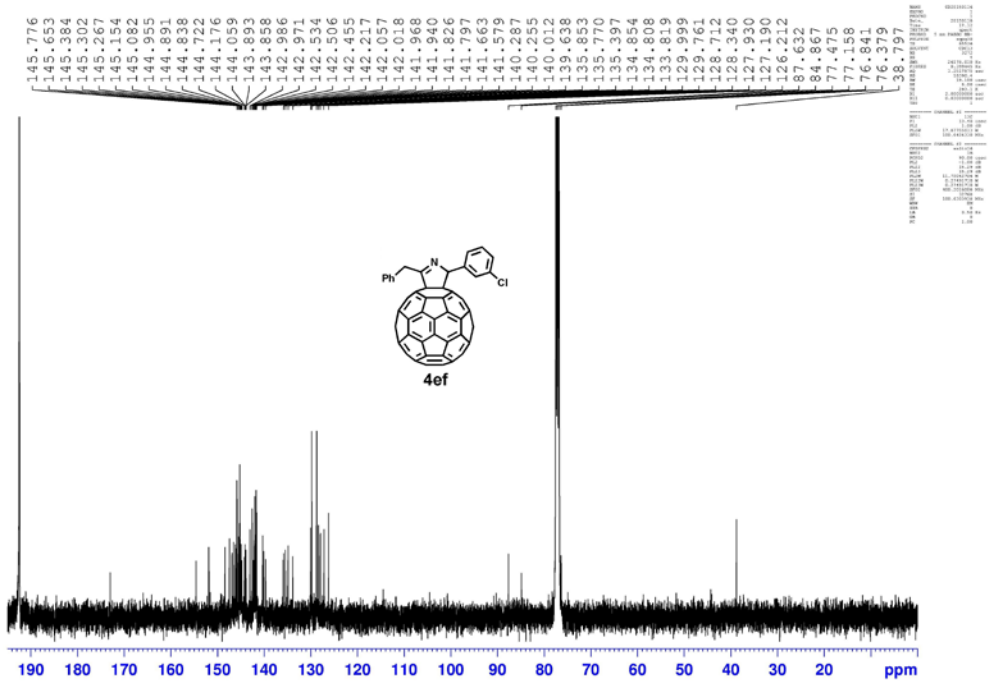
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ee



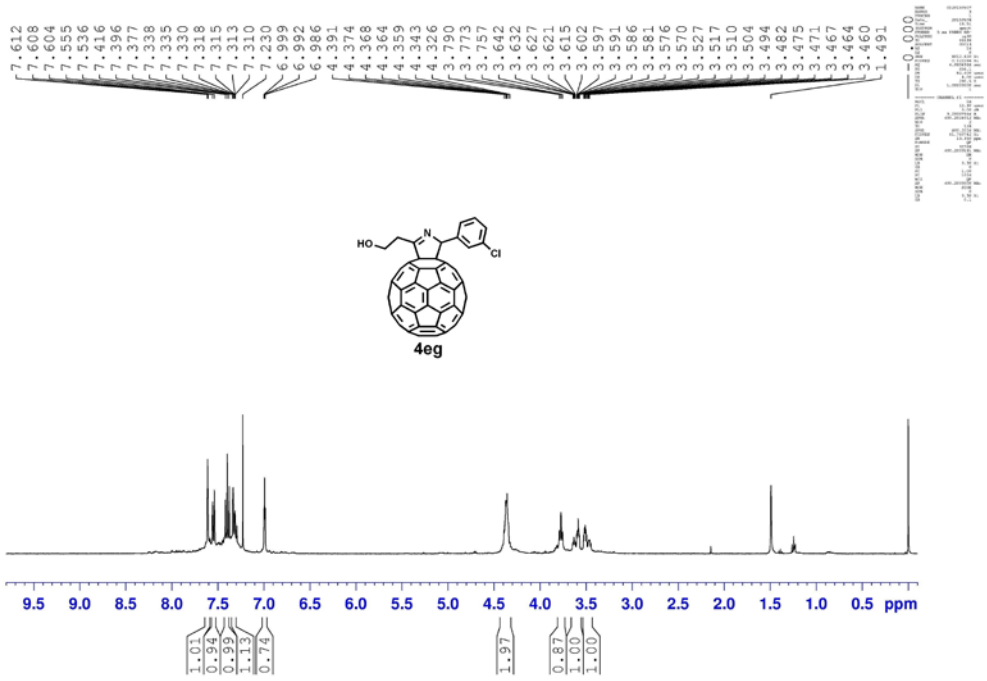
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ef



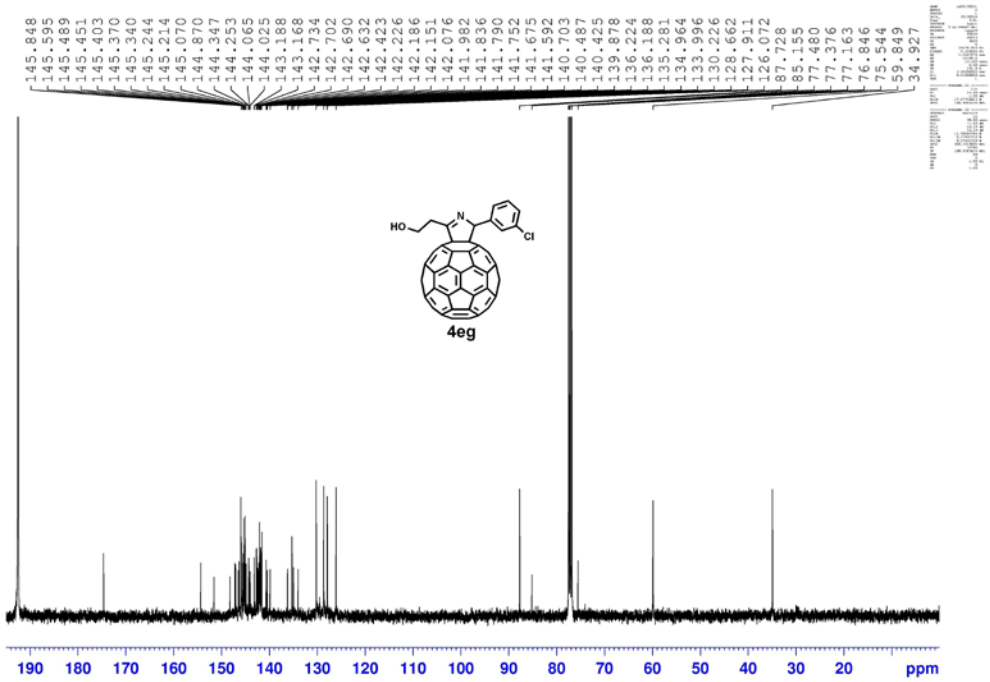
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ef



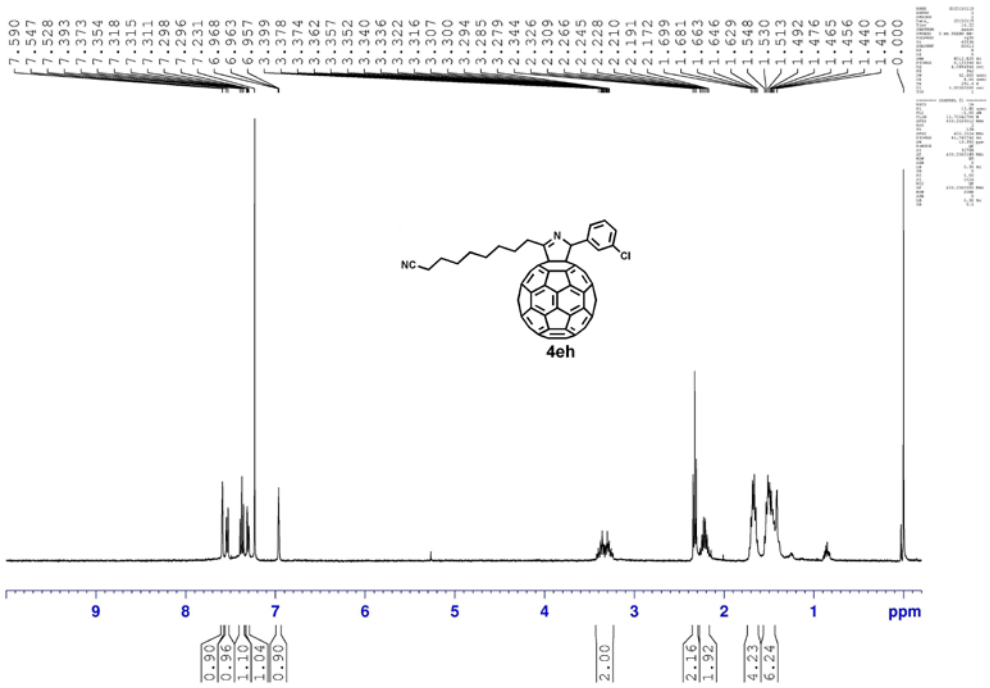
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4eg



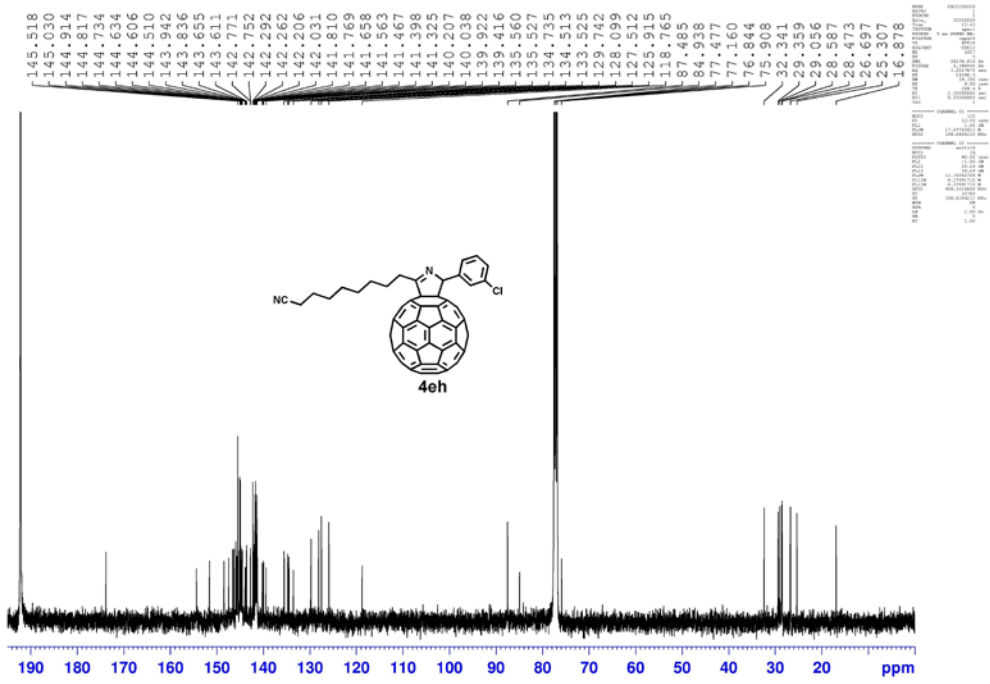
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4eg



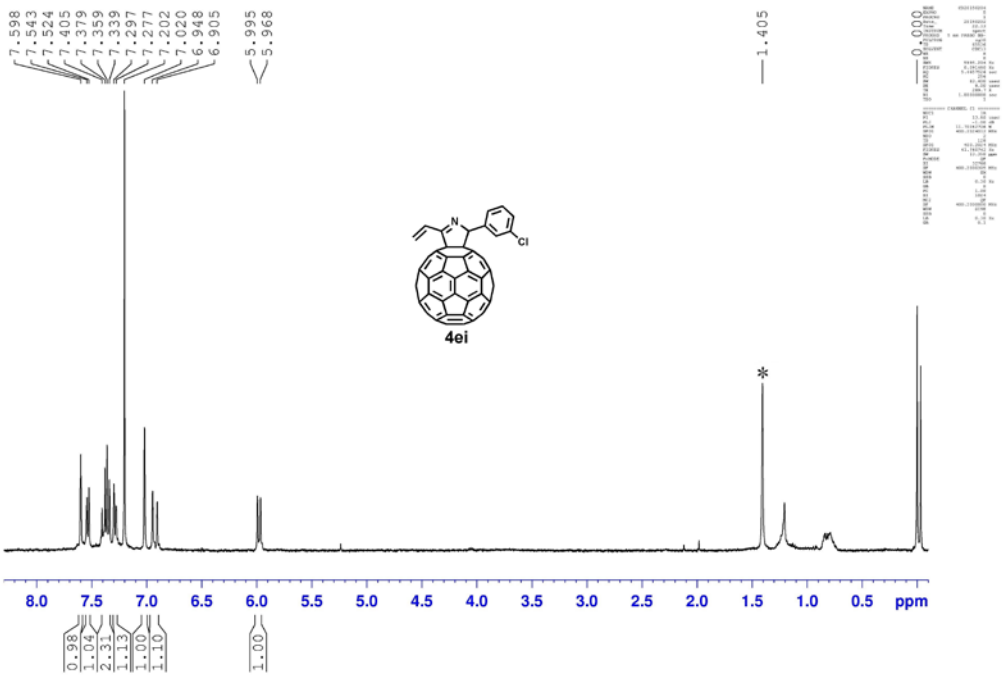
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4eh



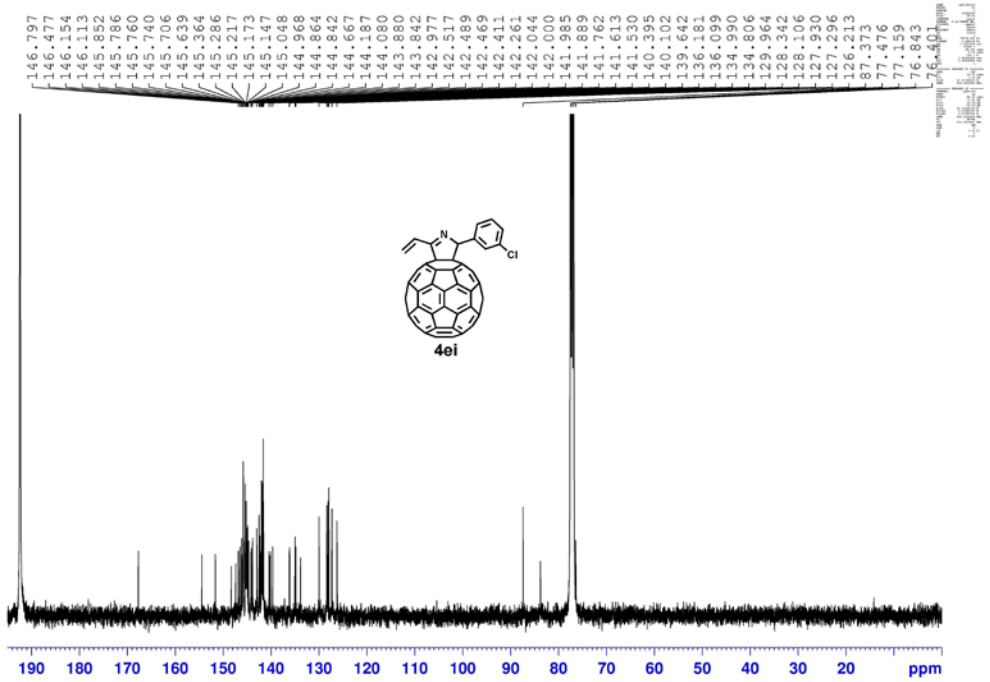
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4eh



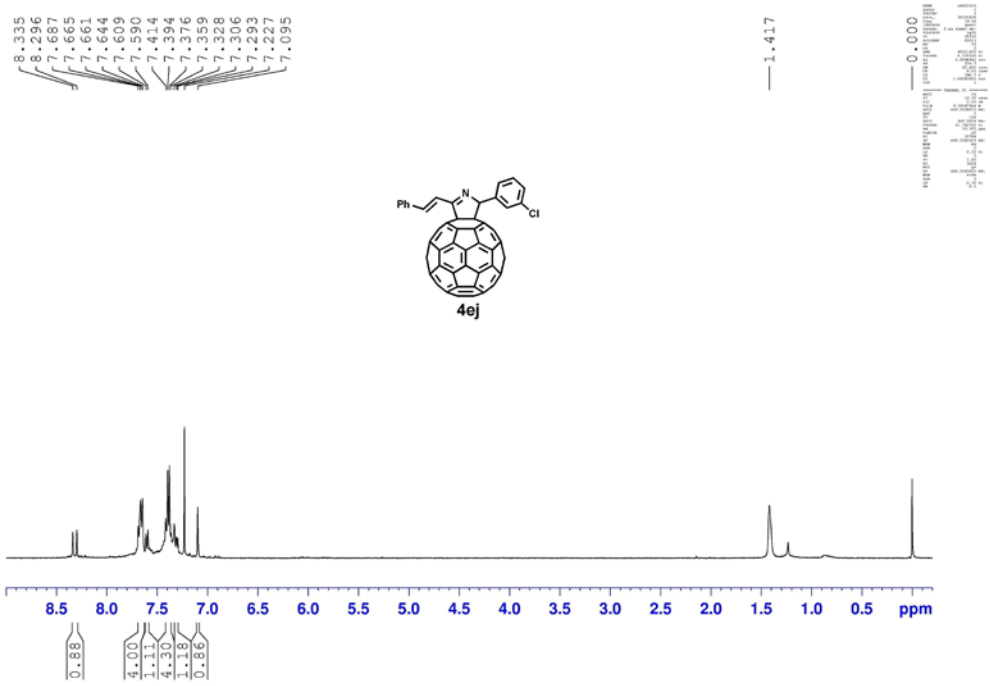
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ei



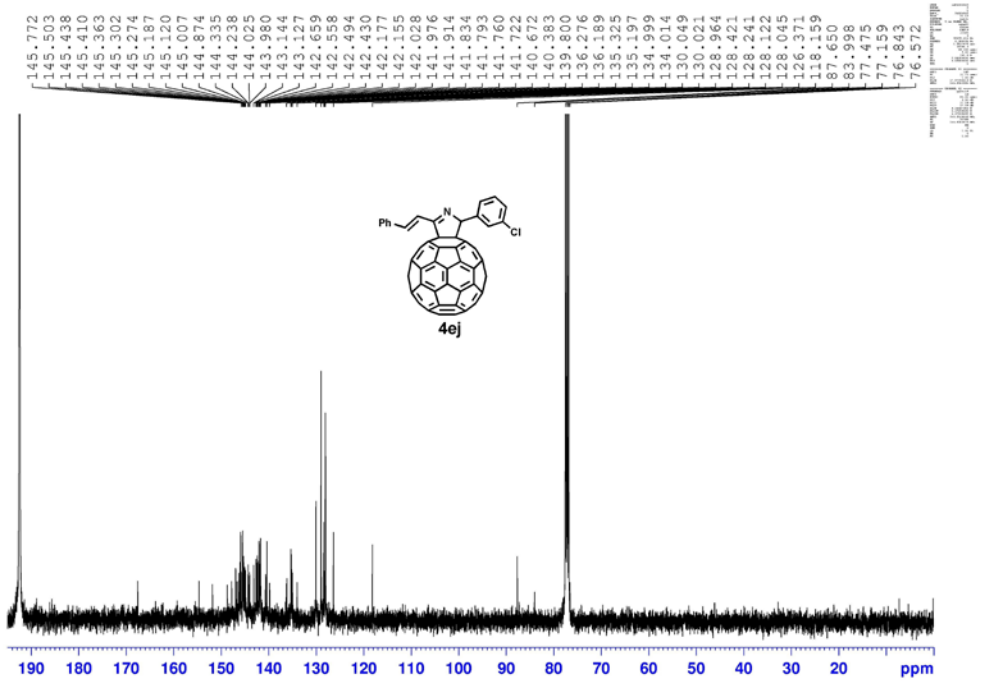
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ei



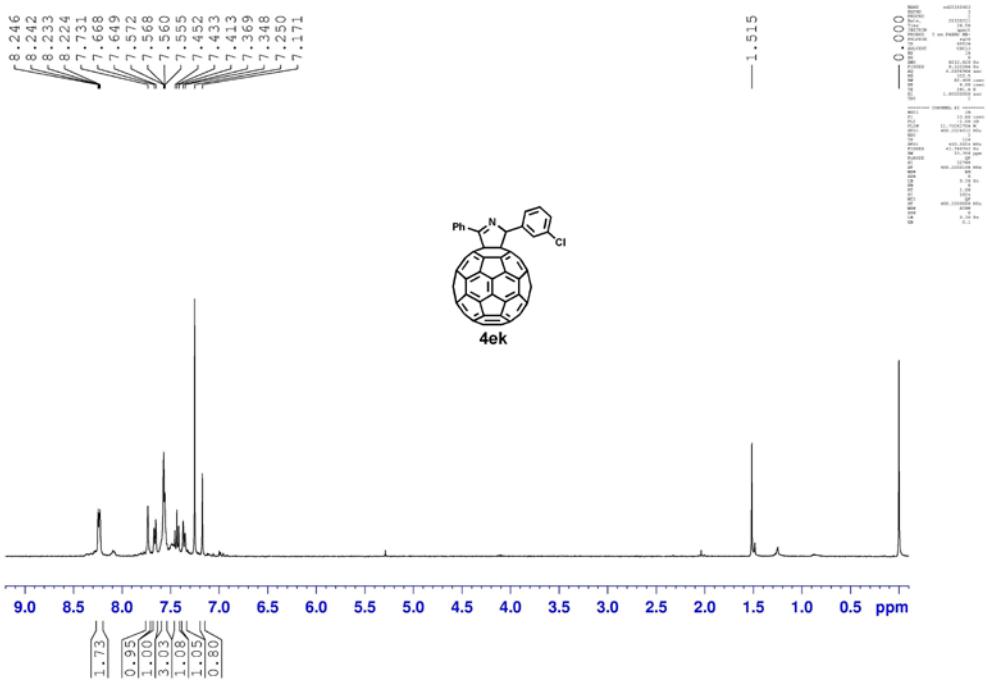
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ej



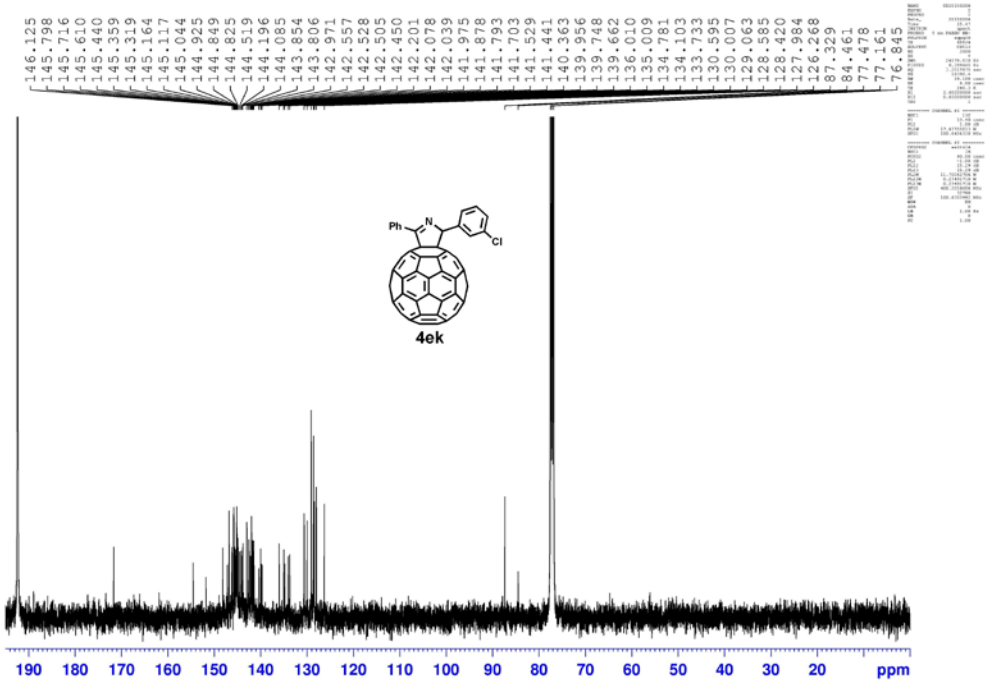
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ej



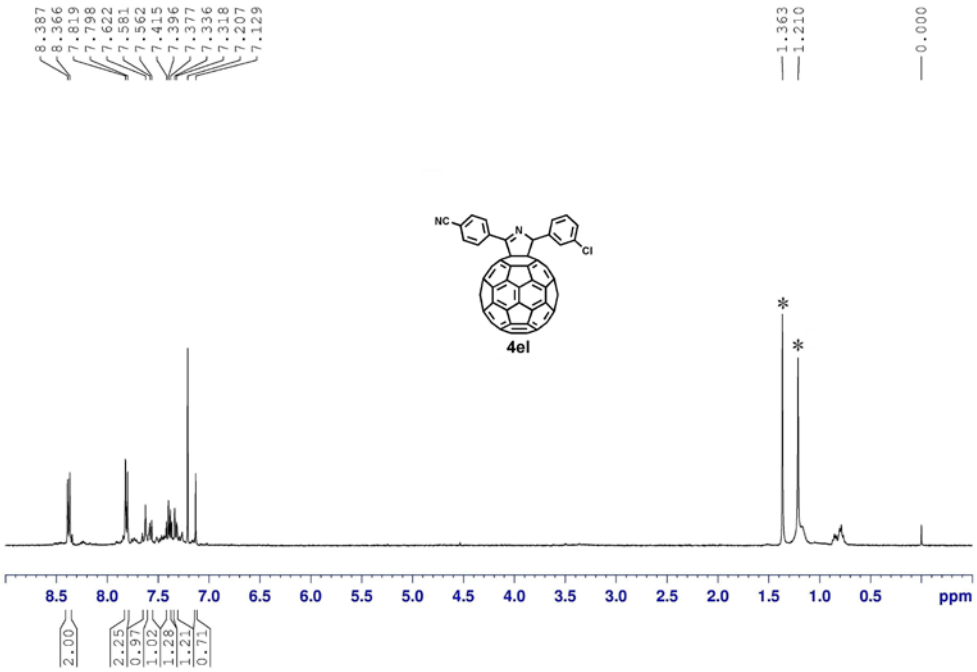
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ek



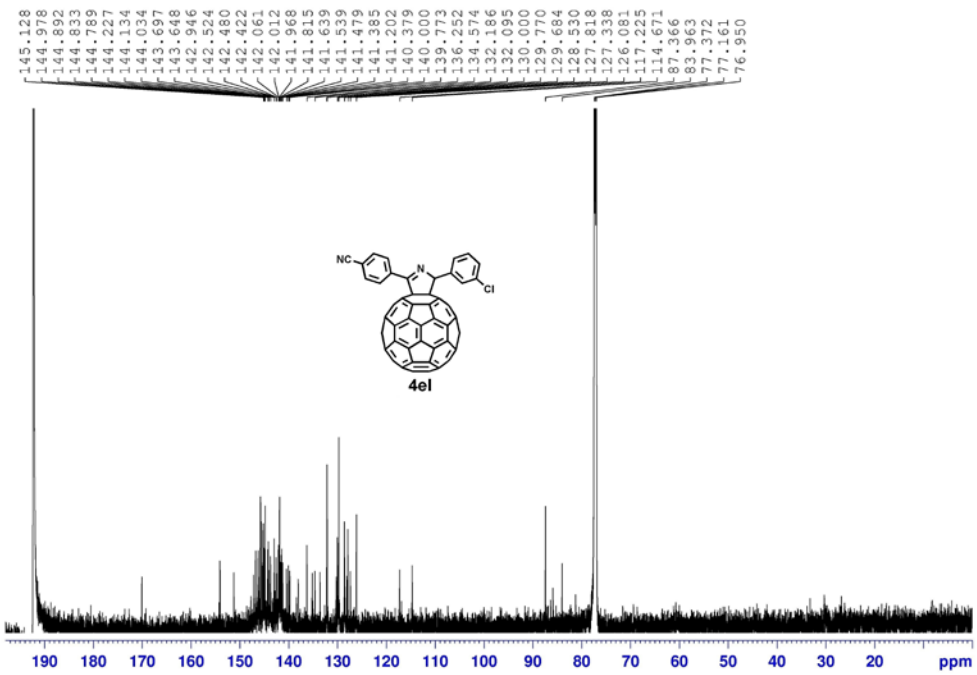
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ek



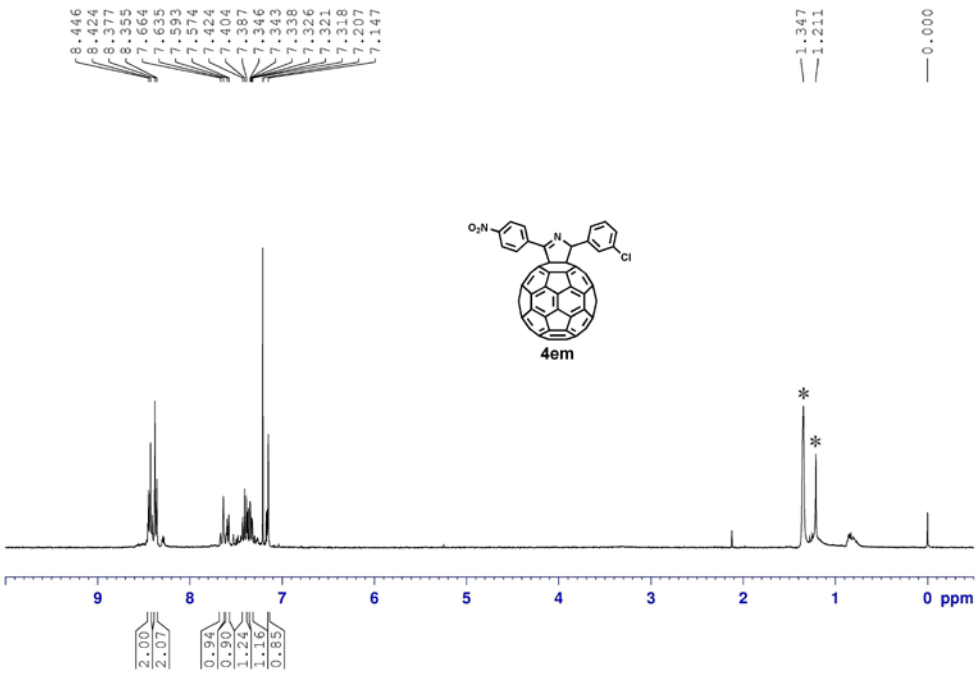
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4el



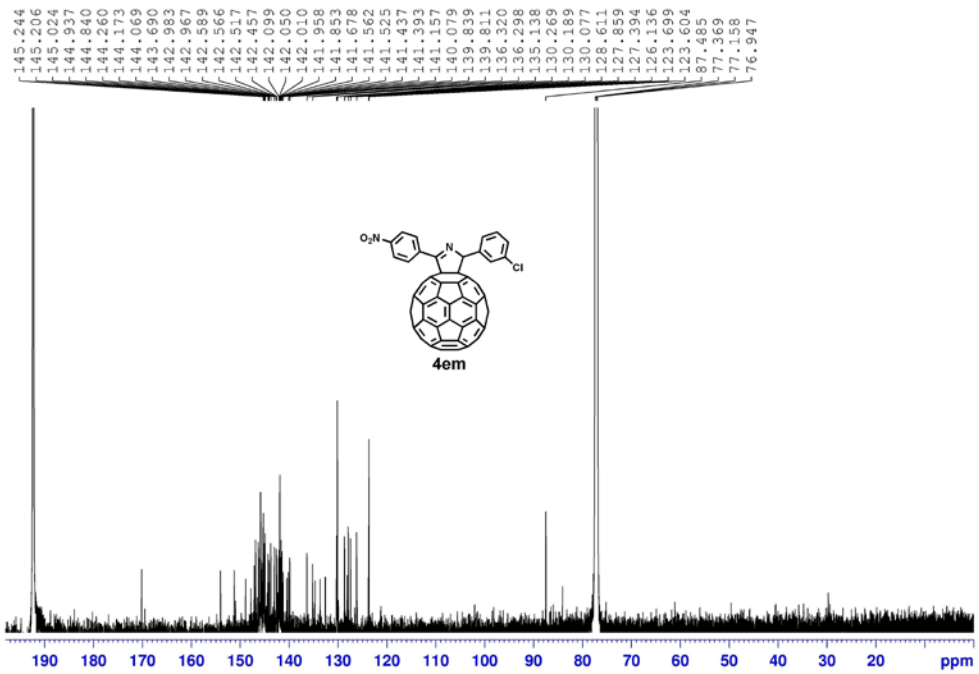
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 4el



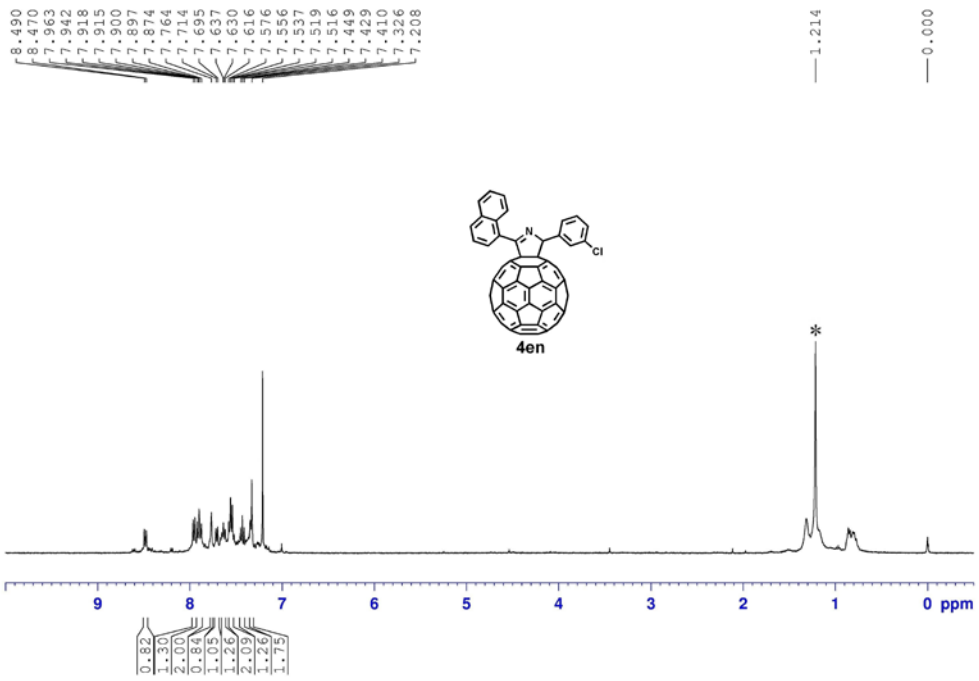
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4em



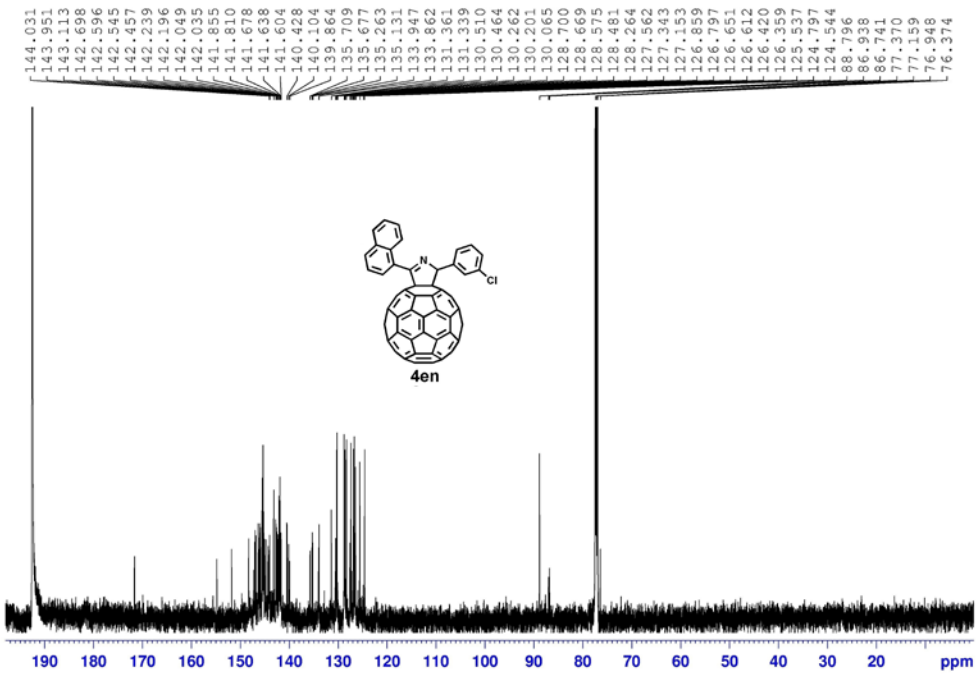
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 4em



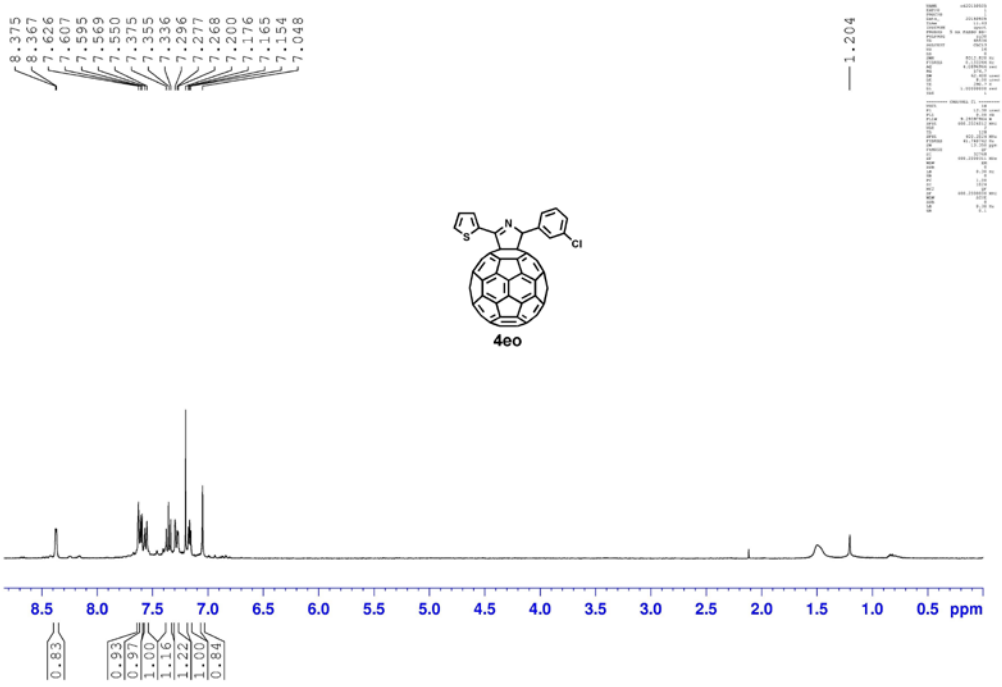
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4en



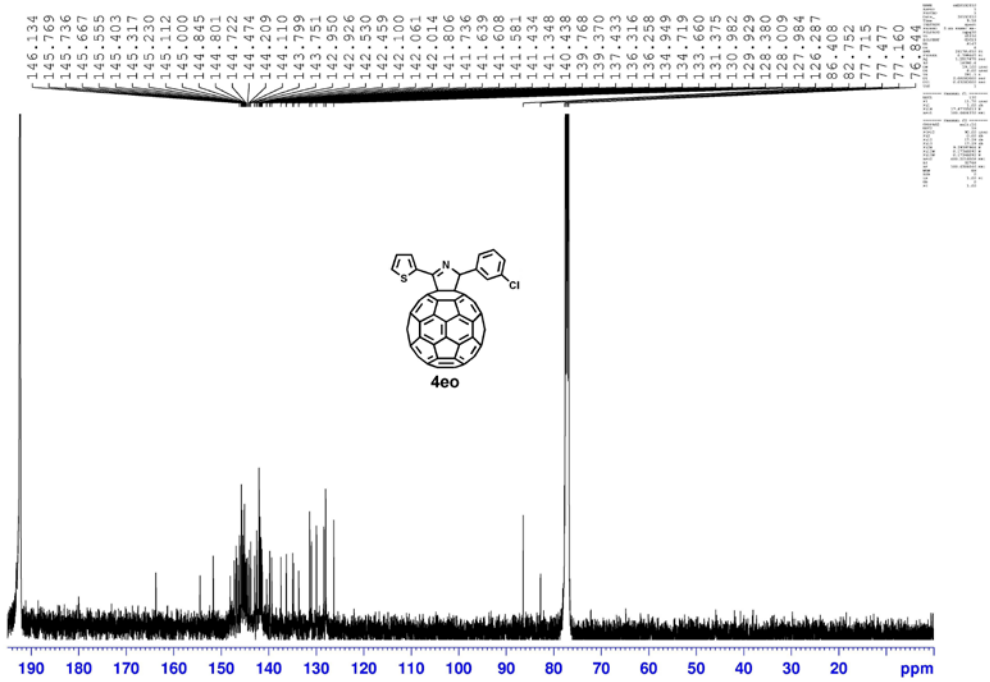
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 4en



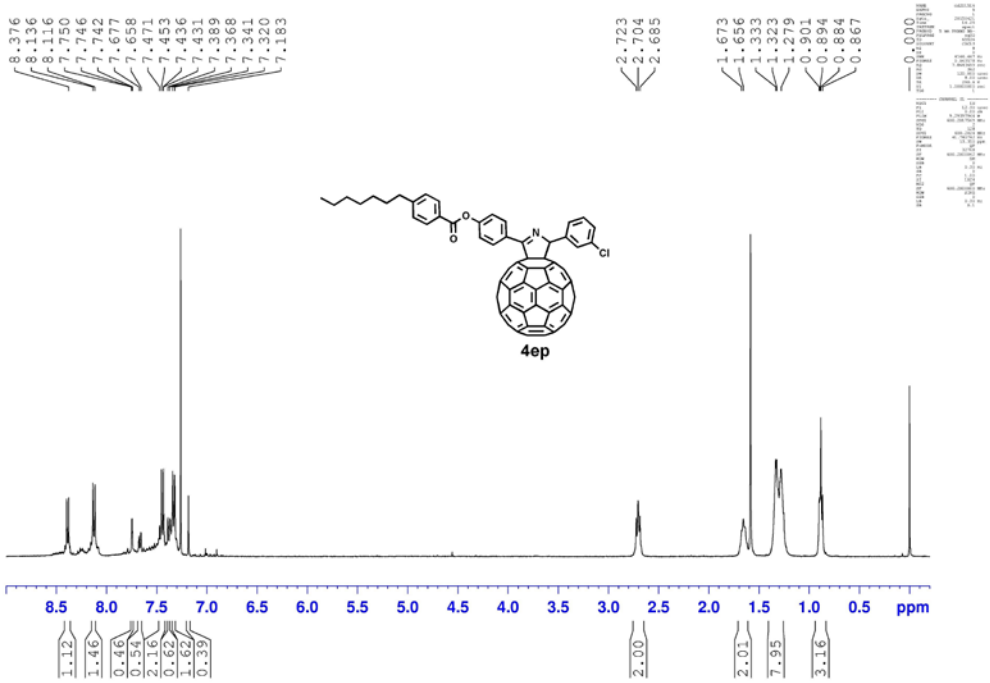
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4eo



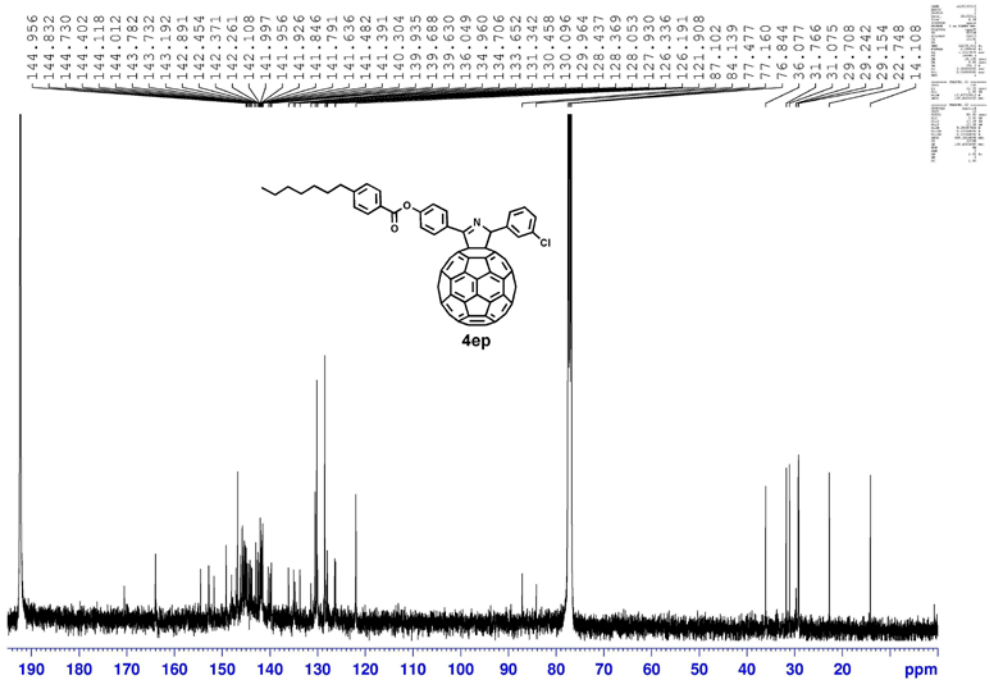
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4eo



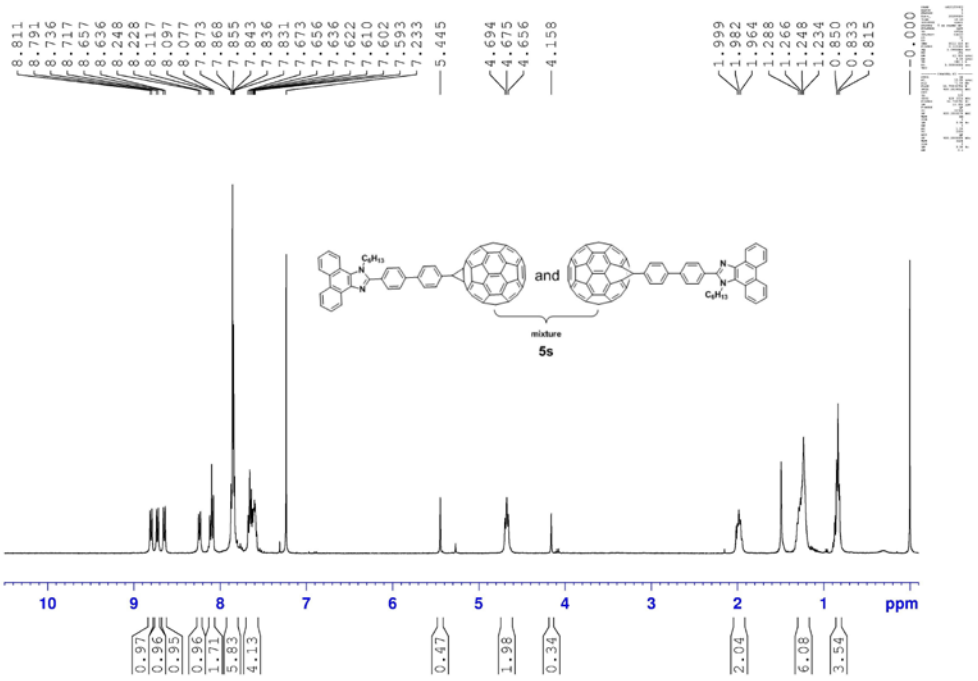
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 4ep



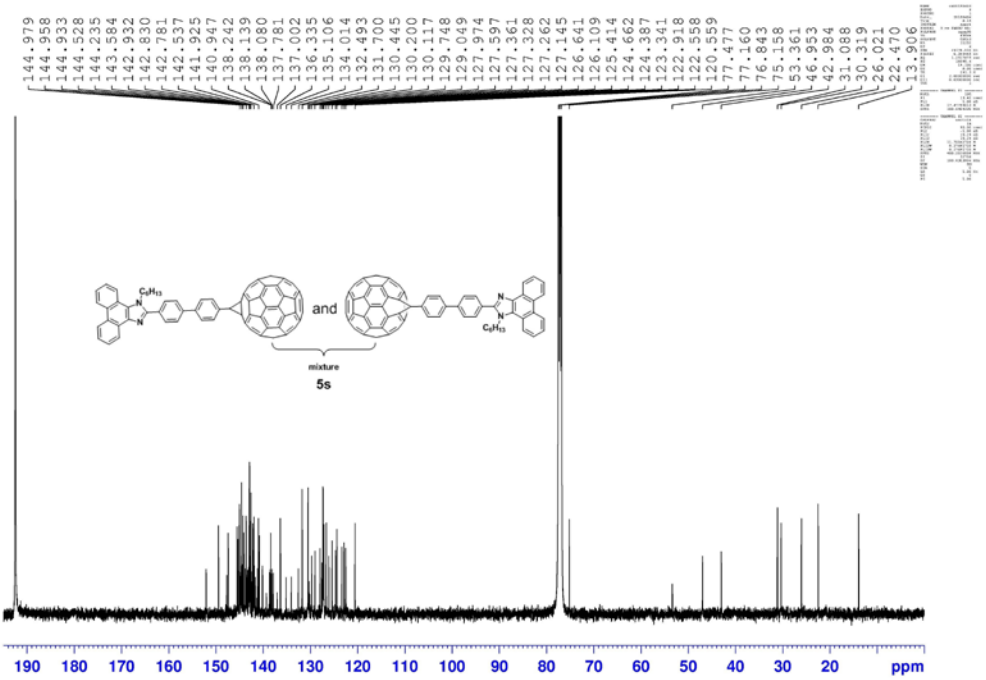
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 4ep



^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 5s



^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 5s



7. Optimized cartesian coordinates

4aa

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6	-0.234569	3.278793	0.190585
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6	0.293745	2.390896	-2.010242
6	-1.106132	2.491575	-2.363511
6	-3.337871	2.379057	-1.309554
6	-3.695365	2.401478	0.099942
6	-2.611194	3.040734	0.825239
6	-2.244111	2.574818	2.086852
6	0.147037	2.794794	1.504136
6	1.933945	2.181238	-0.042158
6	2.508757	0.847587	-0.707333
6	1.744170	0.382890	-1.946791
6	0.821230	1.151857	-2.622804
6	-0.268680	0.520368	-3.336429
6	-1.454989	1.342833	-3.179824
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6	-2.831387	-0.700807	-3.067071
6	-1.692510	-1.494421	-3.218186

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6	1.312475	-1.485511	2.098918
6	0.361300	-0.962287	3.062653
6	-0.884331	-1.569853	3.223141
6	-1.237207	-2.724165	2.412635
6	-0.780817	-3.644219	0.168848
6	0.240193	-3.271733	-0.794720
6	1.323416	-2.628689	-0.067750
6	1.984840	-1.530822	-0.627094
6	2.370824	-0.398024	0.172722
6	2.022942	-0.372212	1.505838
6	0.474734	0.484683	3.071645
6	-0.669984	1.271039	3.242406
6	-1.969279	0.641898	3.395088
6	-2.075275	-0.750225	3.384566
6	-3.158390	-1.391233	2.663977
6	-2.639975	-2.611374	2.062782
6	-3.079525	-3.007577	0.797779
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6	-3.698478	-2.221443	-1.330145
6	-4.048853	-2.196889	0.080042
6	-4.545975	-1.026990	0.656443

6	-4.094328	-0.616746	1.975261
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6	-2.944706	1.449089	2.679874
6	1.494894	0.866687	2.118881
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6	-0.323494	-3.230965	1.486067
6	4.026576	1.261149	-1.070252
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6	5.503462	-0.768212	-1.373454
6	5.667291	0.442530	0.695949
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1	5.075707	-0.893998	-2.365898
6	6.622464	-0.465811	1.146901
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1	8.014992	-3.475370	0.330823
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1	8.016492	-2.678367	1.913628
7	4.231267	2.615400	-0.579665
6	3.177617	3.101243	-0.061546
6	3.121197	4.493130	0.492713
1	2.361845	5.087754	-0.029190
1	2.844301	4.479996	1.553507
1	4.094326	4.974677	0.379647

5aa

	X	Y	Z
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6	0.411923	-0.187522	2.900355
6	0.903532	1.014678	2.286488
6	0.085439	2.114458	2.208043
6	-1.254738	2.069926	2.749567
6	-3.082948	0.456020	3.132924
6	-3.061343	-0.996377	3.066753
6	-1.690373	-1.431916	3.268619
6	-1.191525	-2.520310	2.555032
6	0.931924	-1.320591	2.160074
6	2.024722	0.676795	1.292144
6	2.005291	1.560074	-0.060064
6	0.819547	2.550638	-0.113595
6	0.038208	2.906345	0.960926
6	-1.329656	3.331766	0.765865
6	-2.128344	2.819172	1.864795
6	-3.436357	2.390307	1.639558
6	-3.921807	1.179196	2.281693
6	-3.878304	-1.666424	2.154386
6	-4.750014	-0.912115	1.271246
6	-4.770413	0.482808	1.334998
6	-4.817325	1.266478	0.108763
6	-3.996394	2.445939	0.298015
6	-3.231818	2.943266	-0.759459
6	-1.875721	3.400207	-0.519718
6	-1.065191	3.013500	-1.647231

6	0.247100	2.577146	-1.431871
6	1.748467	-0.821396	1.087926
6	-0.016402	-0.646253	-3.180478
6	0.823359	-1.353809	-2.314373
6	0.344202	-2.566326	-1.674898
6	-0.949355	-3.025204	-1.918610
6	-1.827336	-2.278429	-2.806240
6	-2.235219	0.050486	-3.511030
6	-1.413989	1.232735	-3.316541
6	-0.043265	0.793173	-3.109282
6	0.772666	1.452167	-2.180895
6	1.675980	0.724724	-1.330600
6	1.676543	-0.652057	-1.382586
6	0.897623	-2.621269	-0.334265
6	0.131051	-3.136702	0.716760
6	-1.220517	-3.601347	0.468594
6	-1.751547	-3.546475	-0.822351
6	-3.119172	-3.112996	-1.026809
6	-3.166277	-2.329574	-2.253581
6	-3.999161	-1.211472	-2.335543
6	-3.524214	0.001942	-2.976422
6	-1.913798	2.319115	-2.601708
6	-3.257181	2.274389	-2.050224
6	-4.045643	1.136514	-2.231018
6	-4.841587	0.622712	-1.130550
6	-4.813895	-0.828404	-1.194827
6	-4.769130	-1.579627	-0.019226
6	-3.907576	-2.746685	0.066346
6	-3.357919	-2.801876	1.409336

6	-2.040787	-3.220953	1.607406
6	1.719741	-1.451065	-0.135918
6	0.149770	-2.469567	1.995496
6	-1.368734	-1.113662	-3.425553
7	3.305471	0.736855	2.208729
7	4.447737	0.596201	1.778510
6	4.685280	0.477843	0.286548
1	3.949238	-0.224408	-0.116105
6	6.070745	-0.065347	0.041621
6	6.249868	-1.426295	-0.212927
6	7.197186	0.763193	0.109212
6	7.529629	-1.952945	-0.396389
1	5.385134	-2.084426	-0.270177
6	8.470698	0.233693	-0.073800
1	7.062124	1.824318	0.292031
6	8.661110	-1.133753	-0.328165
1	7.648369	-3.014971	-0.598240
1	9.335639	0.891685	-0.020047
6	10.050432	-1.696755	-0.517787
1	10.646262	-1.604414	0.399207
1	10.019375	-2.756975	-0.787947
1	10.594287	-1.165003	-1.308064
6	3.353331	2.326422	-0.329846
7	4.520309	1.825176	-0.228316
6	3.270149	3.759745	-0.796614
1	2.699678	3.852078	-1.727501
1	2.768717	4.387703	-0.050871
1	4.284279	4.128492	-0.958931

6aa (i) Coordinate

6	1.761973	2.805361	1.950037
6	1.635660	3.353006	0.620989
6	0.401016	3.283740	-0.033108
6	-0.752611	2.722406	0.614588
6	-0.628391	2.180835	1.871680
6	0.646381	2.217385	2.555769
6	3.063975	2.173401	2.055811
6	3.746600	2.336926	0.782247
6	2.862382	3.069151	-0.107388
6	2.810334	2.745091	-1.462047
6	0.347337	2.942004	-1.442586
6	-1.774493	2.247504	-0.447824
6	-2.486183	0.826674	-0.084864
6	-2.012947	0.220122	1.251685
6	-1.276217	0.891468	2.201509
6	-0.384849	0.169697	3.079948
6	0.798262	0.981822	3.301418
6	2.051145	0.380135	3.418322
6	3.206852	0.984445	2.774680
6	4.543251	1.306012	0.279975
6	4.691561	0.071862	1.030459
6	4.036939	-0.084231	2.254497
6	3.398122	-1.351252	2.581507
6	2.174684	-1.064727	3.304243
6	1.038179	-1.848914	3.094563
6	-0.266140	-1.221149	2.987517
6	-1.022524	-1.924964	1.983002

6	-1.856826	-1.202244	1.122053
6	-0.834627	2.161310	-1.673205
6	-0.459931	-2.425661	-2.051977
6	-0.610247	-1.225276	-2.754699
6	0.540229	-0.620619	-3.402648
6	1.792141	-1.231481	-3.325414
6	1.948468	-2.470554	-2.580256
6	0.976051	-3.613652	-0.621220
6	-0.247765	-3.324185	0.105562
6	-1.129669	-2.586892	-0.785467
6	-1.911087	-1.539259	-0.286823
6	-2.106188	-0.327018	-1.034005
6	-1.448795	-0.168445	-2.233313
6	0.422603	0.820640	-3.284698
6	1.568467	1.599856	-3.092654
6	2.869879	0.965972	-2.996122
6	2.980650	-0.421605	-3.109430
6	3.864464	-1.154239	-2.224494
6	3.226108	-2.421284	-1.897304
6	3.353658	-2.955951	-0.613372
6	2.206352	-3.564109	0.037155
6	-0.195559	-3.000911	1.460186
6	1.082717	-2.951872	2.148177
6	2.260743	-3.226135	1.450459
6	3.441151	-2.409920	1.671525
6	4.117744	-2.243455	0.396391
6	4.729991	-1.028761	0.082594
6	4.604743	-0.474289	-1.254610
6	4.489826	0.968603	-1.133303

6	3.640528	1.675069	-1.987176
6	-0.796039	1.118884	-2.564542
6	1.528873	2.689042	-2.147302
6	0.843827	-3.056410	-1.958108
7	-2.663223	3.390816	-0.749077
7	-4.346917	1.838932	1.147112
6	-4.059112	1.042855	-0.074930
7	-4.173666	3.071459	1.121137
6	-3.695115	3.717237	-0.075584
6	-4.474025	4.957464	-0.410902
1	-4.051767	5.429339	-1.299478
1	-5.528836	4.713713	-0.588057
1	-4.444516	5.655960	0.433008
1	-4.296863	1.610772	-0.981975
6	-4.905156	-0.213623	-0.055858
6	-5.379166	-0.740720	-1.263741
6	-5.244651	-0.867236	1.135018
6	-6.155300	-1.897366	-1.283755
1	-5.132704	-0.246086	-2.200720
6	-6.026173	-2.022166	1.108771
1	-4.908817	-0.461361	2.082682
6	-6.494738	-2.559477	-0.096443
1	-6.506588	-2.288773	-2.235865
1	-6.277149	-2.514287	2.045752
6	-7.364260	-3.794777	-0.115642
1	-8.430274	-3.530664	-0.107724
1	-7.186653	-4.396387	-1.013572
1	-7.179677	-4.427581	0.758594

6aa (ii) Coordinate

6	-1.411495	3.387689	0.821063
6	-0.823584	2.801746	2.001494
6	0.446170	2.218604	1.918597
6	1.191648	2.235466	0.690455
6	0.623825	2.774994	-0.438313
6	-0.698573	3.359126	-0.382144
6	-2.832508	3.092649	0.830333
6	-3.122992	2.323227	2.029460
6	-1.878389	2.143271	2.756072
6	-1.621053	0.941078	3.412797
6	0.712109	0.964413	2.598653
6	2.237623	1.090920	0.687746
6	2.380943	0.329500	-0.736109
6	1.437991	0.896454	-1.828110
6	0.750430	2.083372	-1.739313
6	-0.491768	2.264155	-2.453905
6	-1.386902	3.047773	-1.621735
6	-2.755345	2.779424	-1.618153
6	-3.491996	2.794237	-0.364392
6	-4.060840	1.289450	1.985997
6	-4.746550	0.983217	0.743035
6	-4.466792	1.722266	-0.408516
6	-4.338432	1.047752	-1.692515
6	-3.284527	1.702990	-2.441309
6	-2.425971	0.950767	-3.245825
6	-1.004177	1.240730	-3.257999
6	-0.290782	-0.008872	-3.343949

6	0.897550	-0.171866	-2.621077
6	1.619778	0.197700	1.792449
6	-0.046362	-3.234075	-0.816464
6	0.617632	-2.915659	0.373038
6	-0.112869	-2.903500	1.628114
6	-1.474035	-3.205437	1.651436
6	-2.167031	-3.518739	0.411302
6	-2.062722	-2.949866	-1.987352
6	-1.007430	-2.289078	-2.735963
6	0.236983	-2.468095	-2.004433
6	1.170648	-1.425302	-1.942725
6	1.891153	-1.136063	-0.732138
6	1.595382	-1.853038	0.404735
6	0.409795	-1.826341	2.447607
6	-0.453487	-1.089782	3.264396
6	-1.872258	-1.391640	3.279593
6	-2.373811	-2.428265	2.488861
6	-3.616080	-2.251759	1.762839
6	-3.488258	-2.926269	0.478732
6	-4.061566	-2.365143	-0.664460
6	-3.334551	-2.376939	-1.921575
6	-1.265160	-1.086961	-3.392285
6	-2.588872	-0.491705	-3.329595
6	-3.602862	-1.122484	-2.606397
6	-4.495329	-0.337685	-1.772148
6	-4.780180	-1.105606	-0.571978
6	-4.903122	-0.459001	0.659333
6	-4.312239	-1.044332	1.850921
6	-3.792631	0.035493	2.671600

6	-2.596772	-0.134149	3.372302
6	1.462369	-1.164132	1.708708
6	-0.297598	0.342969	3.341277
6	-1.466659	-3.534437	-0.797060
7	3.477345	1.627125	1.278832
7	4.088867	1.861417	-1.669214
6	3.831825	0.403436	-1.340430
1	3.728532	-0.040093	-2.335588
7	4.333006	2.656331	-0.747754
6	4.383917	2.246705	0.633211
6	5.596543	2.785520	1.336707
1	5.560624	2.510631	2.391984
1	6.506808	2.375888	0.882282
1	5.640487	3.875264	1.233116
6	5.023464	-0.295150	-0.695306
6	6.209094	-0.316844	-1.451959
6	5.030290	-0.943407	0.543823
6	7.355909	-0.946611	-0.979926
1	6.230956	0.170802	-2.423957
6	6.180104	-1.586812	1.006536
1	4.149332	-0.945920	1.172970
6	7.362331	-1.600822	0.260652
1	8.257708	-0.938276	-1.588255
1	6.152314	-2.082244	1.974225
6	8.598934	-2.310651	0.758755
1	8.767113	-3.247568	0.211680
1	9.496189	-1.695390	0.624950
1	8.516120	-2.560655	1.821120

7aa (i) Coordinate

6	1.814560	1.949685	-2.900858
6	0.975112	0.869669	-3.358308
6	-0.318608	0.739904	-2.839393
6	-0.837200	1.684226	-1.889782
6	-0.033199	2.706529	-1.448336
6	1.315150	2.846160	-1.949847
6	3.171991	1.450006	-2.784380
6	3.169260	0.050473	-3.178758
6	1.807651	-0.309845	-3.535752
6	1.311421	-1.571090	-3.210591
6	-0.836850	-0.573188	-2.504919
6	-1.968991	1.042499	-1.070225
6	-1.980479	1.452767	0.490996
6	-0.808232	2.388983	0.874563
6	-0.018571	3.072288	-0.015776
6	1.339417	3.426744	0.330793
6	2.163157	3.288130	-0.856843
6	3.472481	2.819684	-0.750913
6	3.985203	1.875292	-1.731146
6	3.979247	-0.866023	-2.505190
6	4.825025	-0.421032	-1.411879
6	4.827065	0.923471	-1.033912
6	4.840759	1.281997	0.377331
6	4.008133	2.455629	0.551227
6	3.217700	2.589798	1.695207
6	1.860711	3.091015	1.584475
6	1.034586	2.362820	2.516341

6	-0.269114	2.008629	2.148707
6	-1.681061	-0.444004	-1.348614
6	0.011142	-1.604385	2.797627
6	-0.803377	-2.013163	1.736798
6	-0.296066	-2.957332	0.757683
6	0.999294	-3.459474	0.872119
6	1.850856	-3.022423	1.967630
6	2.213416	-1.029172	3.376936
6	1.379820	0.148143	3.548246
6	0.019148	-0.214048	3.184051
6	-0.788309	0.697357	2.492653
6	-1.660113	0.262979	1.436188
6	-1.648056	-1.058920	1.054252
6	-0.825820	-2.591712	-0.543823
6	-0.034340	-2.744195	-1.687432
6	1.319485	-3.253037	-1.569279
6	1.827233	-3.602906	-0.315755
6	3.185015	-3.245486	0.043627
6	3.199777	-2.886784	1.455043
6	4.015199	-1.844461	1.901695
6	3.511884	-0.897509	2.880632
6	1.876226	1.408474	3.220084
6	3.229269	1.548541	2.710095
6	4.030216	0.417589	2.540534
6	4.853080	0.281916	1.351833
6	4.844895	-1.116213	0.956767
6	4.830778	-1.460158	-0.396126
6	3.986816	-2.547322	-0.862209
6	3.461325	-2.181342	-2.165372

6	2.153716	-2.526948	-2.512805
6	-1.659939	-1.424307	-0.381960
6	-0.040535	-1.709236	-2.692531
6	1.364954	-2.114283	2.911623
7	-3.239264	1.387236	-1.914728
7	-3.189572	2.145672	0.996523
7	-4.384183	1.128707	-1.545772
6	-4.654094	0.556487	-0.190925
6	-4.371851	1.732574	0.755810
6	-5.530449	2.482782	1.352305
1	-6.135623	1.824427	1.985915
1	-5.153891	3.319402	1.943301
1	-6.194940	2.857592	0.564450
1	-3.924130	-0.229602	0.021775
6	-6.041816	-0.044066	-0.137078
6	-6.305454	-1.071959	0.776546
6	-7.081605	0.400659	-0.961850
6	-7.577624	-1.633195	0.871055
1	-5.508860	-1.437102	1.421941
6	-8.350746	-0.169219	-0.866001
1	-6.888214	1.181515	-1.689714
6	-8.623643	-1.194269	0.048652
1	-7.758801	-2.429245	1.589748
1	-9.144465	0.189195	-1.517805
6	-9.992664	-1.828792	0.123581
1	-10.069646	-2.688320	-0.555727
1	-10.211976	-2.192901	1.132938
1	-10.778517	-1.120672	-0.159799

7aa (ii) Coordinate

6	1.806241	-2.003984	2.840514
6	0.883517	-1.015142	3.341850
6	-0.428406	-0.991609	2.854859
6	-0.879177	-1.956285	1.892002
6	-0.000030	-2.894366	1.412755
6	1.367202	-2.921253	1.879736
6	3.109143	-1.379785	2.704904
6	2.988618	0.004843	3.132702
6	1.609669	0.231130	3.530094
6	0.991889	1.448388	3.247730
6	-1.074580	0.274538	2.567168
6	-2.097219	-1.405942	1.121820
6	-2.111641	-1.776588	-0.445028
6	-0.861314	-2.595957	-0.879039
6	0.010082	-3.226044	-0.027432
6	1.385319	-3.447001	-0.414160
6	2.222994	-3.259831	0.756790
6	3.481788	-2.671659	0.632291
6	3.930622	-1.705866	1.623033
6	3.695020	1.006224	2.463701
6	4.549752	0.664595	1.340128
6	4.664448	-0.665514	0.929490
6	4.674826	-0.990217	-0.489864
6	3.948145	-2.230932	-0.672743
6	3.144145	-2.411638	-1.800836
6	1.841739	-3.037965	-1.671236
6	0.928525	-2.367578	-2.564789

6	-0.391694	-2.141119	-2.156786
6	-1.935480	0.094975	1.430013
6	-0.458123	1.493839	-2.726427
6	-1.278810	1.802077	-1.636335
6	-0.835206	2.767018	-0.646816
6	0.405926	3.387796	-0.779175
6	1.265247	3.055081	-1.904611
6	1.772269	1.135911	-3.370364
6	1.045030	-0.108649	-3.550727
6	-0.333388	0.119547	-3.147118
6	-1.035792	-0.875745	-2.456832
6	-1.915968	-0.545490	-1.371290
6	-2.014574	0.760789	-0.956278
6	-1.297541	2.325616	0.657240
6	-0.493872	2.526031	1.785351
6	0.804849	3.159595	1.648300
6	1.247232	3.580228	0.391746
6	2.622099	3.357447	-0.007594
6	2.633496	3.032815	-1.427357
6	3.529033	2.080022	-1.917986
6	3.089596	1.112896	-2.908018
6	1.662233	-1.325295	-3.265427
6	3.034784	-1.351800	-2.790367
6	3.734060	-0.156295	-2.612657
6	4.570836	0.027883	-1.440079
6	4.445417	1.410116	-1.010756
6	4.435089	1.721850	0.350193
6	3.506736	2.716110	0.862078
6	3.050284	2.275561	2.167976

6	1.725802	2.492502	2.554367
6	-2.027869	1.091823	0.485920
6	-0.380287	1.474177	2.765514
6	0.840361	2.128192	-2.859645
7	-3.251321	-1.841852	2.076970
7	-3.237319	-2.546511	-0.988812
7	-4.450902	-1.928971	1.831820
6	-5.095059	-1.702200	0.496688
1	-6.084136	-2.147567	0.657761
6	-5.334246	-0.214250	0.234001
6	-5.675678	0.629598	1.302107
6	-5.331500	0.315969	-1.058882
6	-5.983294	1.967683	1.077011
1	-5.698952	0.235705	2.313859
6	-5.649902	1.658190	-1.276899
1	-5.072004	-0.310095	-1.907339
6	-5.974586	2.509877	-0.216750
1	-6.238753	2.602993	1.922232
1	-5.638418	2.047077	-2.292394
6	-6.288501	3.969038	-0.448251
1	-7.154039	4.291404	0.141724
1	-5.444255	4.607526	-0.156821
1	-6.503832	4.170134	-1.502399
6	-4.458538	-2.498582	-0.635408
6	-5.433205	-3.359930	-1.408194
1	-6.272883	-2.757381	-1.779229
1	-4.926519	-3.837836	-2.248185
1	-5.860901	-4.133371	-0.756569

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6	-1.988424	3.216322	-1.078355
6	-1.570946	3.445521	0.283987
6	-0.230014	3.246711	0.631202
6	0.745427	2.864643	-0.352374
6	0.342258	2.624342	-1.646431
6	-1.043864	2.799531	-2.022765
6	-3.304887	2.606250	-1.050634
6	-3.701985	2.460195	0.340518
6	-2.628238	2.981207	1.168523
6	-2.306583	2.352848	2.370877
6	0.104779	2.592765	1.884154
6	1.927511	2.148008	0.324216
6	2.497709	0.882017	-0.498337
6	1.754374	0.590258	-1.804774
6	0.863358	1.458657	-2.397397
6	-0.216045	0.946577	-3.212950
6	-1.390408	1.769380	-2.984878
6	-2.660169	1.192522	-2.969897
6	-3.634506	1.613899	-1.976316
6	-4.412061	1.329105	0.748165
6	-4.755496	0.300188	-0.217338
6	-4.375020	0.441596	-1.553446
6	-3.863140	-0.705395	-2.290021
6	-2.807527	-0.240743	-3.168300
6	-1.680334	-1.034816	-3.389750
6	-0.360873	-0.429812	-3.420220
6	0.563495	-1.338969	-2.787618

6	1.585795	-0.825953	-1.980981
6	1.286667	1.803183	1.678259
6	0.836604	-2.765858	1.052288
6	1.168337	-1.755257	1.960581
6	0.201308	-1.335697	2.958675
6	-1.058676	-1.931673	3.010242
6	-1.409397	-2.967647	2.051787
6	-0.906419	-3.612068	-0.276695
6	0.148422	-3.144504	-1.159389
6	1.222238	-2.621100	-0.329734
6	1.923978	-1.478143	-0.729508
6	2.309116	-0.464016	0.215982
6	1.915020	-0.593572	1.530106
6	0.342107	0.095213	3.154002
6	-0.791299	0.879727	3.393729
6	-2.105654	0.264841	3.430961
6	-2.237732	-1.112752	3.242810
6	-3.311328	-1.634519	2.420005
6	-2.799064	-2.781001	1.683337
6	-3.209532	-3.005438	0.367447
6	-2.244323	-3.428417	-0.631785
6	-0.174064	-2.517750	-2.362373
6	-1.565240	-2.328171	-2.734752
6	-2.580623	-2.773742	-1.886116
6	-3.752688	-1.946845	-1.659889
6	-4.142787	-2.090320	-0.267341
6	-4.633610	-0.990877	0.438679
6	-4.212489	-0.759084	1.809902
6	-4.076336	0.673830	2.002036

6	-3.044935	1.176706	2.797608
6	1.394108	0.572008	2.282637
6	-0.913495	2.161193	2.741462
6	-0.479371	-3.377052	1.093519
7	3.054209	3.079487	0.516748
6	4.004805	1.305990	-0.771174
6	4.113312	2.638095	-0.039560
6	5.395850	3.416995	-0.024396
1	5.258482	4.353353	0.519995
1	6.200353	2.837373	0.441269
1	5.718163	3.641126	-1.049593
1	4.106736	1.514507	-1.844275
6	5.073570	0.291204	-0.411150
6	5.736189	-0.423055	-1.413945
6	5.426600	0.036498	0.923519
6	6.715452	-1.366421	-1.097557
1	5.482865	-0.244693	-2.456759
6	6.406506	-0.901131	1.235615
1	4.928066	0.575441	1.725652
6	7.069611	-1.622275	0.230764
1	7.212085	-1.909391	-1.898343
1	6.660981	-1.078901	2.278280
6	8.137069	-2.632557	0.580122
1	8.469810	-3.184591	-0.304361
1	9.017972	-2.147346	1.019651
1	7.773066	-3.361680	1.313834