SUPPORTING INFROMATION FOR

Oxidative C-C Bond Formation (Scholl Reaction) Using DDQ as an Efficient and Easily Recyclable Oxidant

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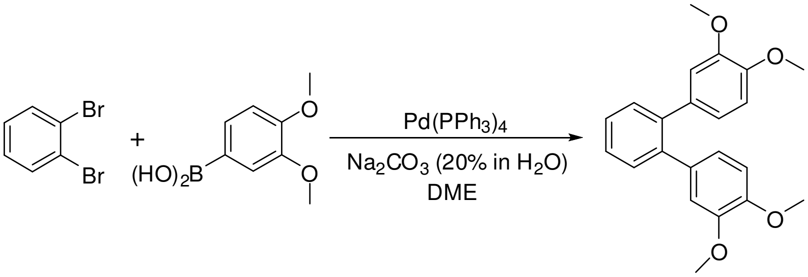
General Experimental Methods and Materials. All reactions were performed under argon atmosphere using conventional vacuum-line techniques unless otherwise noted. All commercial reagents were used without further purification unless otherwise noted. Anhydrous tetrahydrofuran (THF) was prepared by refluxing the commercial tetrahydrofuran (Aldrich) over lithium tetrahydroaluminate under an argon atmosphere for 24 hours followed by distillation. It was stored under an argon atmosphere in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. Dichloromethane (Aldrich) was repeatedly stirred with fresh aliquots of conc. Sulfuric acid (~10% by volume) until the acid layer remained colorless. After separation it was washed successively with water, aqueous sodium bicarbonate, water, and saturated aqueous sodium chloride and dried over anhydrous calcium chloride. The dichloromethane was distilled twice from P_2O_5 under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. The hexanes and toluene were distilled from P_2O_5 under an argon atmosphere and then refluxed over calcium hydride (~12 hrs). After distillation from CaH_2, the solvents were stored in Schlenk flasks under argon atmosphere.

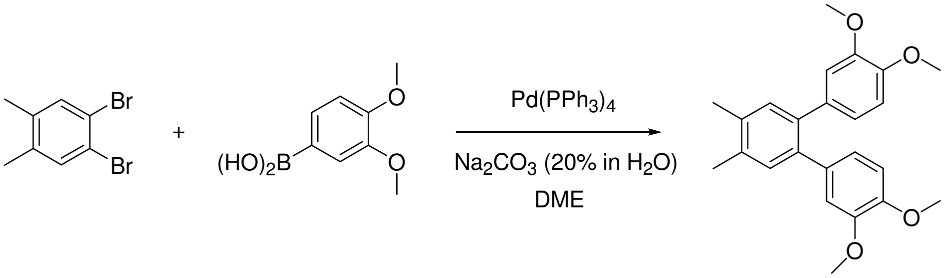
Syntheses of *o*-terphenyls, hexaarylbenzenes, and bichromophoric diarylpropanes as Scholl precursors. The Suzuki coupling[S1] provided a general route for the preparation of various substituted *o*-terphenyls (**1a-e** and **1k**). The hexaarylbenzene derivatives (**1l-1n**) were synthesized according to a previously known literature procedure.[S2] Bichromophoric 2,2-*bis*(3,4-dimethoxyphenyl)propane (**1f**),[S3] 9,9-*bis*(3,4-dimethoxyphenyl)fluorene (**1g**),[S4] and 1,3-*bis*(3,4-dimethoxyphenyl)propane (**1h**)[S4] were available from literature procedures. The details of the synthesis and spectral data for various Scholl precursors, utilized in this study, are summarized below:

General Method for Suzuki Reaction (Method A). Synthesis of 3,3",4,4"-tetramethoxy-*o*-terphenyl (1a).



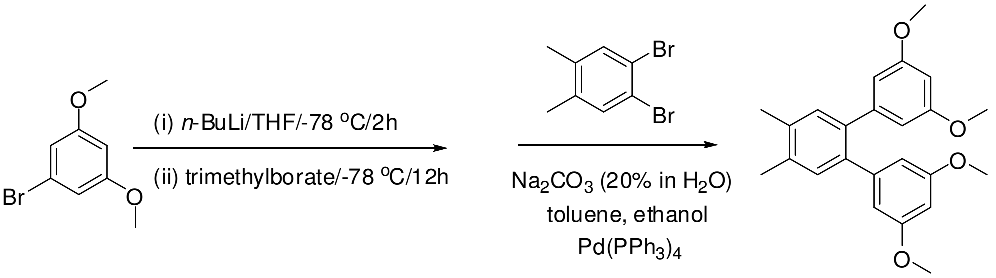
A solution of sodium carbonate (5 g) in water (20 mL) was prepared in a Schlenk flask and degassed (3x) and kept under argon atmosphere. In a separate Schlenk flask, 1,2-dibromobenzene (1.65 g, 7.0 mmol), 3,4-dimethoxyphenylboronic acid (3.82 g, 21 mmol), and DME (35 mL) were added under an argon atmosphere and the Schlenk flask was degassed (5x). Under an argon flow, a catalytic amount of $Pd(PPh_3)_4$ (35 mg) was added and the flask was covered by aluminum foil and degassed (3x). Into this mixture, the aqueous sodium carbonate solution was transferred with the aid of a syringe and the reaction was degassed again (3x). The resulting mixture was heated to reflux for ~24 hours, cooled to room temperature and poured onto 5% aqueous hydrochloric acid. The resulting mixture was extracted with dichloromethane (3 x 25 mL). The combined dichloromethane extracts were washed with water, brine, and dried over anhydrous $MgSO_4$. Removal of the solvent in *vacuo* afforded a crude solid which was purified by column chromatography on silica gel using a 95:5 mixture of hexanes: ethyl acetate as the eluent to afford pure 3,3",4,4"-tetramethoxy-*o*-terphenyl as white solid. Yield: 2.05 g, 84%; mp 138-139 °C; ^{1}H NMR ($CDCl_3$) δ: 3.61 (s, 6H), 3.86 (s, 6H), 6.61 (s, 2H), 6.78 (d, 4H), 7.41 (m, 4H); ^{13}C NMR ($CDCl_3$) δ: 55.83, 56.02, 110.94, 113.64, 122.01, 127.46, 130.52, 134.53, 140.37, 147.88, 148.39.

Synthesis of 3',4'-dimethyl-3,4,3",4"-tetramethoxy-*o*-terphenyl (1b)



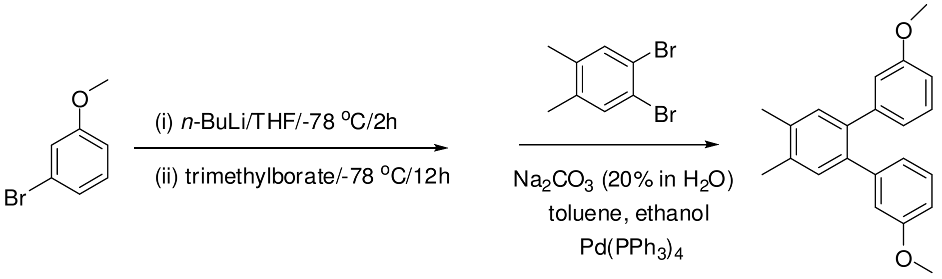
According to **Method A**, 1,2-dibromo-4,5-dimethylbenzene (1.1 g, 4.2 mmol) and 3,4-dimethoxyphenylboronic acid (2.3 g, 12.5 mmol) were mixed in 1,2-dimethoxyethane (25 mL) under argon atmosphere, followed by successive addition of a catalytic amount of $Pd(PPh_3)_4$ (35 mg) and aqueous sodium carbonate solution (20%, 20 mL). The resulting mixture was degassed and heated to reflux for 15h. Standard aqueous work up afforded the crude product which was purified by a column chromatography on silica gel using 10% ethyl acetate in hexanes as the eluent to furnish 3',4'-dimethyl-3,4,3",4"-tetramethoxyl-*o*-terphenyl (**1b**) as white solid. Yield: 1.5 g, 94%; mp 139-140 °C; ^{1}H NMR ($CDCl_3$) δ: 2.36 (s, 6H), 3.62 (s, 6H), 3.86 (s, 6H), 6.62 (s, 2H), 6.77 (s, 2H), 6.78 (s, 2H), 7.23 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 19.55, 55.79, 55.99, 110.91, 113.66, 121.92, 131.78, 134.50, 135.83, 137.81, 147.68, 148.32.

General *in situ* Suzuki Reaction (Method B): Synthesis of 3',4'-dimethyl-3,5,3",5"-tetramethoxy-*o*-terphenyl (1c).



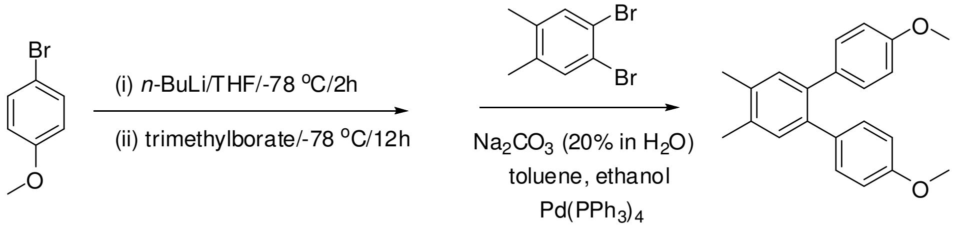
In a oven dried Schlenk flask, a solution of 1-bromo-3,5-dimethoxybenzene (3.25 g, 15 mmol) in anhydrous THF (30 mL) was cooled to -78 °C (dry ice-acetone bath) under argon atmosphere and *n*-butyllithium (2.5 M in hexane, 8 mL, 20 mmol) was added dropwise. After 2h of stirring at -78 °C, trimethylborate (1.5 equiv) was added dropwise with the aid of a syringe and the temperature was allowed to gradually rise to room temperature during an 8h period. To the resulting mixture were added 1,2-dibromo-4,5-dimethylbenzene (1.32 g, 5 mmol), anhydrous toluene (30 mL), dry ethanol (30 mL), aqueous Na_2CO_3 (7.5 g dissolved in 30 mL H_2O), and $Pd(PPh_3)_4$ (40 mg) successively. The flask containing the resulting mixture was repeatedly evacuated and filled with argon (3x), covered by aluminum foil and refluxed for 24 h. The reaction mixture was cooled to room temperature and then poured into 5% aqueous HCl solution. The organic layer was separated and the aqueous layer was extracted with dichloromethane (3 x 25 mL). The combined organic extracts were washed with water, brine and dried over anhydrous $MgSO_4$. Removal of the solvent in *vacuo* afforded the crude product which was purified by column chromatography on silica gel using 2% ethyl acetate in hexanes as the eluent to afford 3',4'-dimethyl-3,5,3'',5''-tetramethoxy-*o*-terphenyl (**1c**) as colorless oil. Yield: 0.75 g, 40%; ^{1}H NMR ($CDCl_3$) δ: 2.38 (s, 6H), 3.66 (s, 12H), 6.35 (t, J = 2.26 Hz, 2H), 6.39 (dd, J_1 = 2.26 Hz, J_2 = 0.86 Hz, 4H), 7.28 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 19.58, 55.41, 99.10, 107.99, 131.65, 136.21, 138.08, 143.66, 160.35.

Synthesis of 3,3''-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1d)



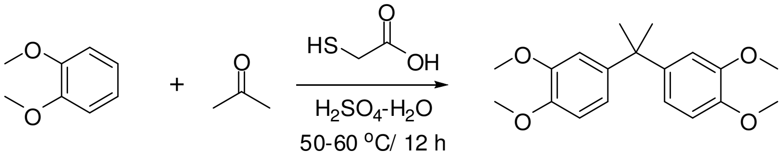
According to **Method B**, *n*-butyllithium (2.5M in hexane) (3.3 mL, 8.2 mmol) was added to a solution of *m*-bromoanisole (1.74 g, 9.3 mmol) in THF (20 mL) at -78 °C under argon atmosphere. After 2h, trimethylborate (1 mL, 9.4 mmol) was added and the mixture was allowed to warm to room temperature during a 12h period. 1,2-Dibromo-4,5-dimethylbenzene (0.42 g, 1.6 mmol), anhydrous toluene (20 mL), dry ethanol (20 mL), aqueous Na_2CO_3 (5 g dissolved in 20 mL H_2O), and $Pd(PPh_3)_4$ (40 mg) were added. The reaction mixture was refluxed for 16 h. Standard work up afforded a crude product which was purified by column chromatography on silica gel with hexanes as the eluent to afford 3,3"-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1d) as colorless oil. Yield: 0.4 g, 79%; ^{1}H NMR (CDCl$_3$) δ: 2.35 (s, 6H), 3.62 (s, 6H), 6.67 (dd, J_1 = 2.58 Hz, J_2 = 1.59 Hz, 2H), 7.74 (m, 4H), 7.13 (t, J = 7.77 Hz, 2H), 7.23 (s, 2H); ^{13}C NMR (CDCl$_3$) δ: 19.64, 50.31, 112.63, 115.31, 122.50, 129.02, 131.93, 136.18, 138.10, 143.08, 159.25.

Synthesis of 4,4"-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1e)



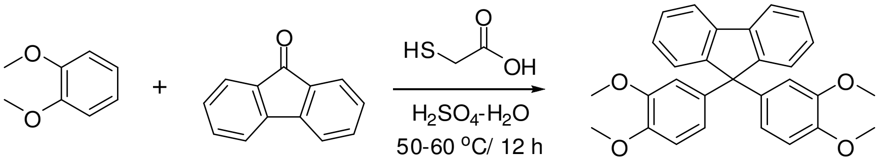
According to **Method B**, *n*-butyllithium (2.5M in hexane, 4.8 mL, 12 mmol) was added to a solution of *p*-bromoanisole (1.74 g, 9.3 mmol) in THF (25 mL) at -78 °C under an argon atmosphere. After 2 h, trimethylborate (1.56 mL, 14 mmol) was added and the resulting mixture was allowed to warm to room temperature during a 12h period. 1,2-Dibromo-4,5-dimethylbenzene (0.82 g, 3.1 mmol), anhydrous toluene (25 mL), dry ethanol (25 mL), aqueous Na_2CO_3 (5 g dissolved in 20 mL H_2O), and $Pd(PPh_3)_4$ (50 mg) were added. The reaction mixture was refluxed for 16 h. Standard work up afforded a crude product which was purified by column chromatography on silica gel using 2% ethyl acetate in hexanes as the eluent to afford 4,4"-dimethoxy-3',4'-dimethyl-*o*-terphenyl (**1e**) as white solid. Yield: 0.9 g, 91%; mp 78-79 °C; ^{1}H NMR (CDCl$_3$) δ: 2.37 (s, 6H), 3.81 (s, 6H), 6.79 (dt, J_1 = 8.74 Hz, J_2 = 2.25 Hz, 4H), 7.10 (dt, J_1 = 8.74 Hz, J_2 = 2.25 Hz, 4H), 7.21 (s, 2H); ^{13}C NMR (CDCl$_3$) δ: 19.58, 55.35, 113.52, 131.07, 132.09, 134.27, 135.66, 137.72, 158.27.

Synthesis of 2,2-Bis(3,4-dimethoxyphenyl)propane (1f)



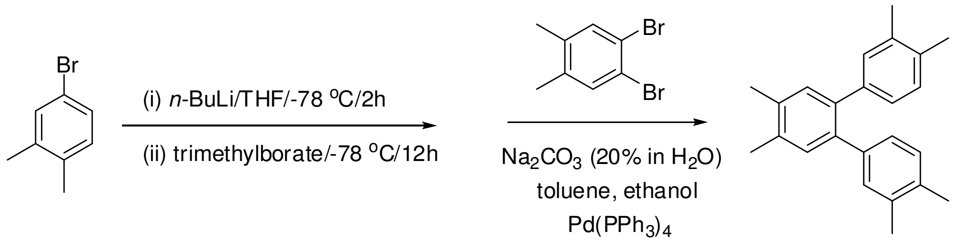
According to a literature procedure,[S4] 1,2-dimethoxybenzene (9.5 mL), acetone (2.0 mL), and mercaptoacetic acid (0.4 mL) were added to a solution prepared from conc. H_2SO_4 (*d* 1.84, 8.0 mL) and water (8.0 mL), and the resulting mixture was kept overnight at 50-60 °C. An standard aqueous workup and recrystallization from methanol afforded 2,2-bis(3,4-dimethoxyphenyl)propane (**1f**) as colorless crystalline solid. Yield: 3.1 g, mp 91-92 °C (lit.[S4] mp 92 °C); ^{1}H NMR ($CDCl_3$) δ: 1.65 (s, 6H), 3.77 (s, 6H), 3.86 (s, 6H), 6.69 (d, *J* = 2 Hz, 2H), 6.76-6.84 (m, 4H); ^{13}C NMR ($CDCl_3$) δ: 31.2, 42.4, 55.8, 55.9, 110.4, 110.8, 118.5, 143.5, 147.0, 148.4.

Synthesis of 9,9-Bis(3,4-dimethoxyphenyl)fluorene (1g)



Following a literature procedure[S4] similar to the one described above for (**1f**), 1,2-dimethoxybenzene (10 mL), fluorenone (1.8 g, 10 mmol), and mercaptoacetic acid (0.4 mL) were added to a solution prepared from conc. H_2SO_4 (*d* 1.84, 8.0 mL) and water (8.0 mL), and the resulting mixture was kept overnight at 80 °C. A standard aqueous workup and recrystallization from methanol afforded 9,9-bis(3,4-dimethoxyphenyl)fluorene (**1f**) as a colorless crystalline solid. Yield: 4.1 g, 94%; mp 216-218 °C; ^{1}H NMR ($CDCl_3$) δ: 3.69 (s, 6H), 3.81 (s, 6H), 6.69 (s, 4H), 6.77 (s, 2H), 7.24-7.29 (m, 2H), 7.33-7.42 (m, 4H), 7.76 (d, *J* = 7 Hz, 2H) ^{13}C NMR ($CDCl_3$) δ: 55.91, 55.96, 64.8, 110.7, 112.0, 120.3, 120.4, 126.0, 127.6, 127.7, 138.4, 140.0, 147.9, 148.5, 151.6.

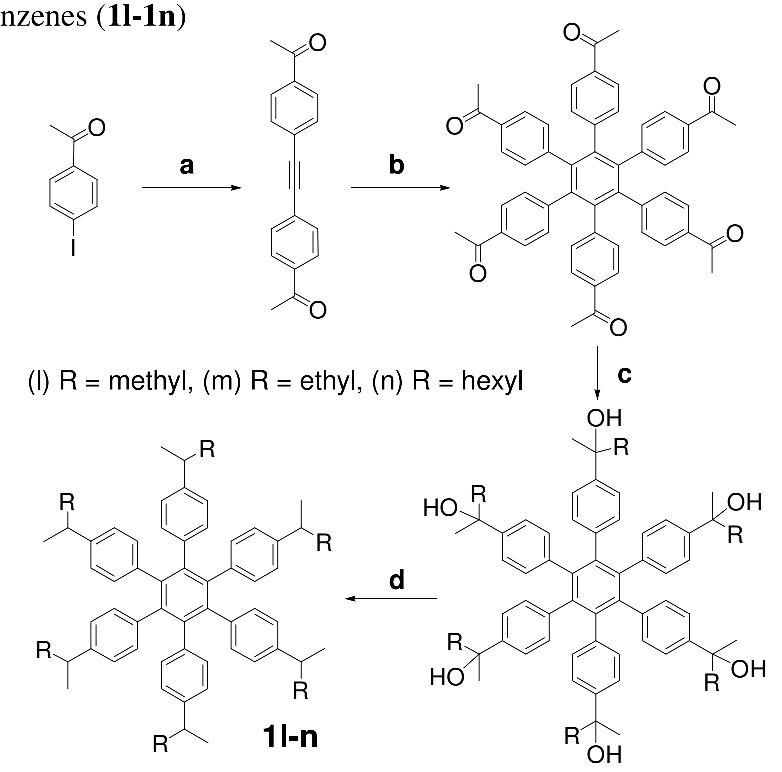
Synthesis of 3,4,3',4',3",4"-hexamethyl-*o*-terphenyl (1k)



According to **Method B**, *n*-butyllithium (2.5M in hexane, 8 mL, 20 mmol) was added to a solution of 4-bromo-*o*-xylene (2.78 g, 15 mmol) in 30 mL THF at -78 °C under argon atmosphere. After 2 h, trimethylborate (2.5 mL, 22.5 mmol) was added and the resulting mixture was allowed to warm to room temperature during a 12h period. 1,2-Dibromo-4,5-dimethylbenzene (1.32 g, 5 mmol), anhydrous toluene (30 mL), dry ethanol (30 mL), aqueous Na_2CO_3 (7.5 g dissolved in 30 mL H_2O), and $Pd(PPh_3)_4$ (40 mg) were added. The reaction mixture was refluxed for 16 h. Standard work up afforded a crude product which was purified by column chromatography on silica gel using hexanes as the eluent to afford 3,4,3',4',3",4"-hexamethyl-*o*-terphenyl (**1k**) as a colorless oil. Yield: 0.50 g, 32 %; ^{1}H NMR ($CDCl_3$) δ: 2.20 (s, 6H), 2.23 (s, 6H), 2.35 (s, 6H), 6.81 (dd, J_1 = 7.94 Hz, J_2 = 1.90 Hz, 2H), 6.94 (d, *J* = 7.94 Hz, 2H), 7.02 (d, *J* = 1.90 Hz, 2H), 7.20 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 19.58, 19.61, 19.67, 127.61, 129.15, 131.10, 132.17, 134.45, 135.57, 136.03, 138.16, 139.38.

Synthesis of Hexakis(4-isoalkylphenyl)benzenes (1l-1n). The hexaarylbenzenes **1l-1n** were obtained according to a published procedure[S2] from our laboratory according to the Scheme shown below:

Scheme . Synthesis of various soluble hexakis(4-isoalkylphenyl) benzenes (**1l-1n**)



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^{a} Benzene/DBU/H_2O/ $(PPh_3)PdCl_2$/CuI/ Me_3SiCCH, reflux. $^b Co_2(CO)_8$/Dioxane/reflux.
^{c} THF/RMgBr or RMgCl. ^{d} H^+/H_2 50 psi/ 10% Pd-C.

General Procedure for the Oxidative Cyclodehydrogenation with Acid and DDQ.

A solution of *o*-terphenyl **1a** (0.1 mmol) in dichloromethane (10 mL) containing protic acid (10% v/v) or Lewis acid (~10 equiv.) at ~0 ^oC was treated with DDQ (1 equivalent per C-C bond formation, i.e. 0.1 mmol), and the solution immediately took on a dark-green coloration. [Note that the solution colors varied depending on the Scholl precursors used (see Chart 1).] The progress of the reaction was monitored by TLC and ^1H NMR spectroscopy. After completion of the reaction, it was quenched with a saturated aqueous solution of $NaHCO_3$ (20 mL). The dichloromethane layer was separated and washed with water and brine solution and dried over anhydrous $MgSO_4$ and filtered. Removal of the solvent in *vacuo* afforded the crude product which by $^1H/^{13}C$ NMR analysis was shown to be 2,3,10,11-tetramethoxytriphenylene (**2a**). Various Scholl precursors were subjected to similar reaction conditions and the characterization data for the oxidative cyclodehydrogenation products are summarized below:

2,3,10,11-Tetramethoxytriphenylene (2a). Yield: quantitative; mp 215-216 °C; ^1H NMR ($CDCl_3$) δ: 4.11 (s, 12H), 7.59 (q, 2H), 7.71 (s, 2H), 7.94 (s, 2H), 8.46 (q, 2H); ^{13}C NMR ($CDCl_3$) δ: 56.08, 56.17, 104.11, 104.58, 122.99, 123.54, 123.94, 126.16, 128.93, 148.84, 149.39.

6,7-Dimethyl-2,3,10,11-tetramethoxytriphenylene (2b). White crystals, quantitative yield; mp 282-283 °C; ^1H NMR ($CDCl_3$) δ: 2.51 (s, 6H), 4.09 (s, 6H), 4.11 (s, 6H), 7.68 (s, 2H), 7.88 (s, 2H), 8.14 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 20.47, 56.14, 104.24, 104.46, 123.43, 123.54, 123.61, 127.15, 135.11, 148.79, 149.02.

6,7-Dimethyl-1,3,9,11-tetramethoxytriphenylene (2c). White solid, yield: 50%; mp 193-194 °C; ^1H NMR ($CDCl_3$) δ: 2.49 (s, 6H), 3.97 (s, 6H), 4.01 (s, 6H), 6.68 (s, 2H), 7.51 (s, 2H), 8.16 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 20.49, 55.78, 56.00, 96.96, 98.09, 112.94, 124.25, 128.74, 132.34, 136.41, 158.82, 158.91. Note that the triphenylene **2c** undergoes decomposition under the reaction conditions and thus the pure **2c** was isolated by column chromatography on silica gel using 5% ethyl acetate in hexanes as eluent.

3,10-Dimethoxy-6,7-dimethyltriphenylene (2d). Yield: 100%, mp 208-211 °C; ^1H NMR ($CDCl_3$) δ: 2.52 (s, 6H), 4.02 (s, 6H), 7.21 (dd, J_1 = 8.91 Hz, J_2 = 2.58 Hz, 2H), 7.99 (d, J = 2.58 Hz, 2H), 8.28 (s, 2H), 8.44 (d, J = 8.91 Hz, 2H); 20.53, 55.72, 105.76, 115.53, 123.93, 124.15, 124.51, 128.23, 130.30, 136.38, 158.34.

2,11-Dimethoxy-6,7-dimethyltriphenylene (2e). Yield: 60%; mp 214-215 °C; ^{1}H NMR ($CDCl_3$) δ: 2.49 (s, 6H), 4.02 (s, 6H), 7.25 (dd, J_1 = 8.83 Hz, J_2 = 2.56 Hz, 2H), 7.94 (d, J = 2.56 Hz, 2H), 8.26 (s, 2H), 8.53 (d, J = 8.83 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ: 20.48, 55.71, 106.32, 115.66, 123.54, 124.44, 124.95, 127.22, 130.79, 135.41, 158.56.

2,3,6,7-Tetramethoxy-9,9-dimethylfluorene (2f). White solid, yield: 100%; mp 178-180 °C; ^{1}H NMR ($CDCl_3$) δ: 1.65 (s, 6H), 3.77 (s, 6H), 3.86 (s, 6H), 6.69 (d, 2H, J = 2 Hz), 6.76-6.84 (m, 4H); ^{13}C NMR ($CDCl_3$) δ: 27.4, 46.7, 56.2, 56.3, 102.5, 106.1, 131.8, 146.1, 148.2, 148.7.

2,3,6,7-Tetramethoxy9,9-spirobifluorene (2g). White solid, yield: 100%; mp 242-244 °C; ^{1}H NMR ($CDCl_3$) δ: 3.61 (s, 6H), 4.03 (s, 6H), 6.18 (s, 2H), 6.75 (d, J = 7.6 Hz, 2H), 7.14 (t, J = 7 Hz, 2H), 7.26 (d, J = 5 Hz, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.85 (d, J = 7.6 Hz, 2H) ^{13}C NMR ($CDCl_3$) δ: 56.2, 56.3, 65.9, 102.3, 107.0, 120.0, 124.2, 127.8, 128.0, 134.7, 141.0, 141.7, 148.6, 149.1, 149.3.

6,7-Dihydro-2,3,9,10-tetramethoxydibenzo[1,c]cycloheptadiene (2h). White solid, yield: 100%; mp 152-153 °C (lit[S5] mp 158-159 °C); ^{1}H NMR ($CDCl_3$) δ: 2.11-2.20 (m, 2H), 2.43 (t, J = 7 Hz, 4H), 3.92 (s, 12H), 6.77 (s, 2H), 6.89 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 31.2, 34.0, 56.1, 56.3, 111.7, 112.0, 132.2, 133.1, 147.6, 147.9.

4,4’,5,5’-Tetramethoxy-2,2’-dimethylbiphenyl (2i). White solid, yield: 100%; mp 113-114 °C; ^{1}H NMR ($CDCl_3$) δ: 2.02 (s, 6H), 3.83 (s, 6H), 3.91 (s, 6H), 6.65 (s, 2H), 6.77 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 19.48, 56.04, 56.16, 112.91, 113.10, 128.36, 133.52, 146.66, 147.89.

2,2’,5,5’-Tetramethoxy-4,4’-dimethylbiphenyl (2j). White solid, yield: 100%; mp 129-130 °C; ^{1}H NMR ($CDCl_3$) δ: 2.29 (s, 6H), 3.75 (s, 6H), 3.81 (s, 6H), 6.79 (s, 2H), 6.83 (s, 2H); ^{13}C NMR ($CDCl_3$) δ: 16.60, 56.17, 56.82, 114.04, 115.08, 125.73, 126.71, 150.87, 151.87.

2,3,6,7,10,11-hexamethyltriphenylene (2k). Pale yellow crystals, quantitative yield, mp 303-306 °C; ^{1}H NMR ($CDCl_3$) δ: 2.51 (s, 18H), 8.33 (s, 6H); ^{13}C NMR ($CDCl_3$) δ: 20.50, 123.75, 127.80, 135.56.

Alkyl substituted hexa-*peri*-hexabenzocoronenes (2l-2o).

HBC 2l. Yellow/orange solid, Yield: qunatitative; mp >300 ºC; ^{1}H NMR ($CDCl_3$) δ: 1.73 (d, 36H), 3.58 (m, 6H), 8.9 (s, 12H); ^{13}C NMR ($CDCl_3$) δ: 24.97, 35.46, 120.04, 120.33, 124.15, 130.52, 146.56.

HBC 2m. Yellow/orange solid, Yield: quantitatve; mp >300 ºC; ^{1}H NMR ($CDCl_3$) δ: 1.11 (s, 18H), 1.69 (s, 18H), 2.07 (s, 12H), 3.29 (s, 6H), 9.03 (s, 12H); ^{13}C NMR ($CDCl_3$) δ: 12.12, 22.36, 31.25, 44.36, 120.11, 120.13, 124.89, 131.09, 146.78.

HBC 2n. Yellow/orange solid, Yield: quantitatve; mp 110-112 ºC; ^{1}H NMR ($CDCl_3$) δ: 0.84 (t, 18H), 1.06 (d, 18H), 1.33 (m, 60H), 2.38 (m, 6H), 6.59 (s, 12H), 6.67 (d, 12H); ^{13}C NMR ($CDCl_3$) δ: 14.32, 22.95, 28.33, 29.80, 32.02, 32.12, 39.24, 41.31, 120.70, 120.77, 124.94, 130.55, 146.26.

HBC 2o. Yellow/orange solid, Yield: quantitatve; mp >320 ºC (lit[S5] mp >300 °C) ; ^{1}H NMR ($CDCl_3$) δ: 1.83 (s, 54H), 9.32 (s, 12H); ^{13}C NMR ($CDCl_3$) δ: 32.25, 35.95, 119.13, 120.71, 124.22, 130.72, 149.22.

References:

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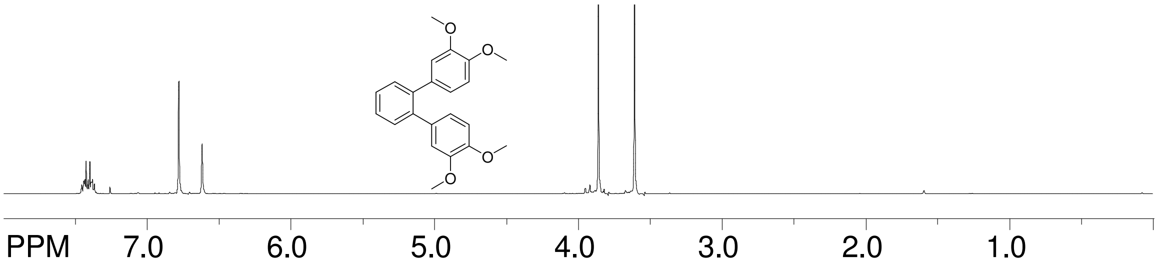
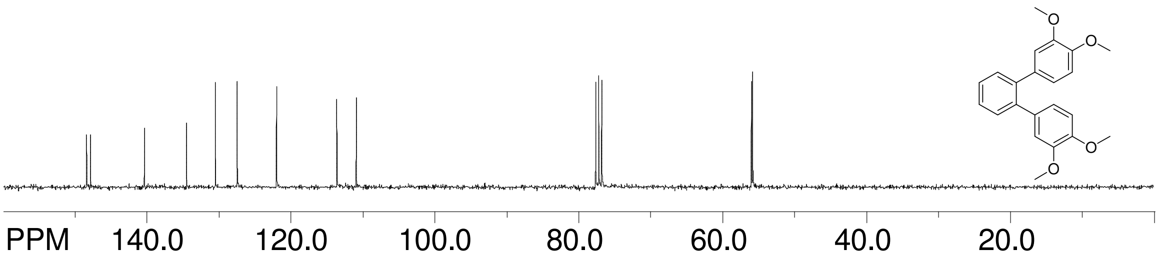
S6. Compare: Herwig, P. T.; Enkelmann, V.; Schmelz, O.; Muellen, K. *Chem. Eur. J.* **2000**, *6*, 1834.

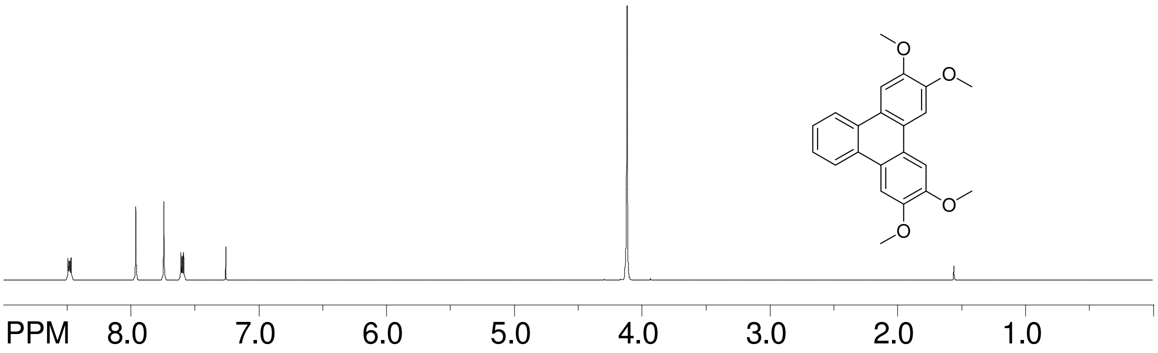
^{1}H NMR spectrum of 3,3',4,4'-tetramethoxy-*o*-terphenyl (1a).



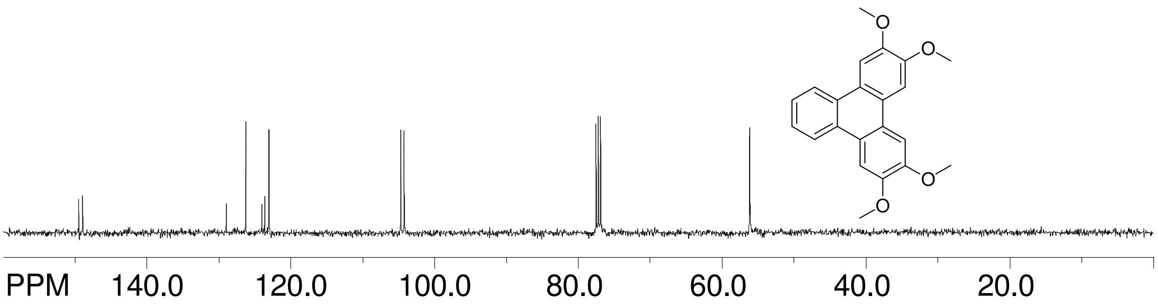
^{13}C NMR spectrum of 3,3',4,4'-tetramethoxy-*o*-terphenyl (1a).



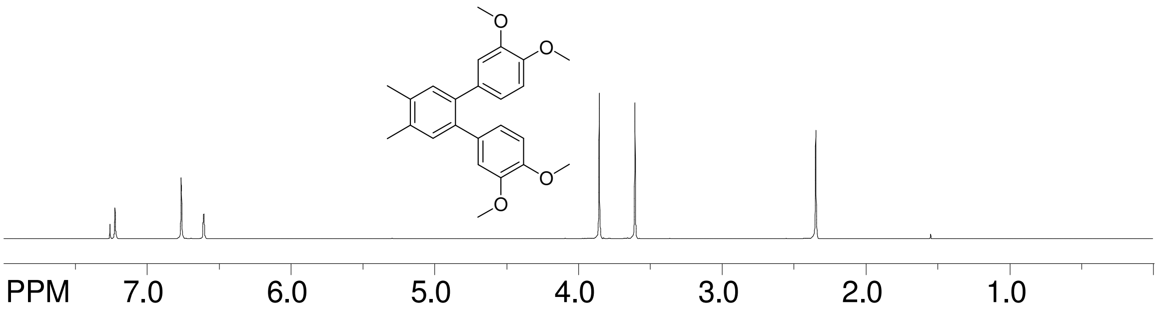
^{1}H NMR spectrum of 2,3,10,11-tetramethoxytriphenylene (2a).



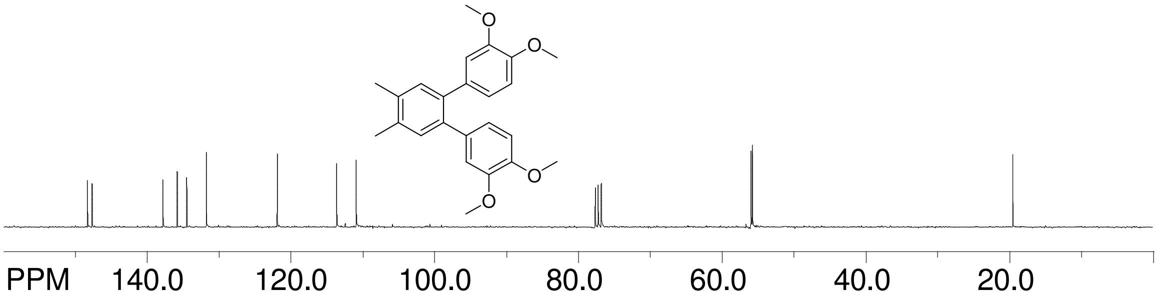
^{13}C NMR spectrum of 2,3,10,11-tetramethoxytriphenylene (2a).



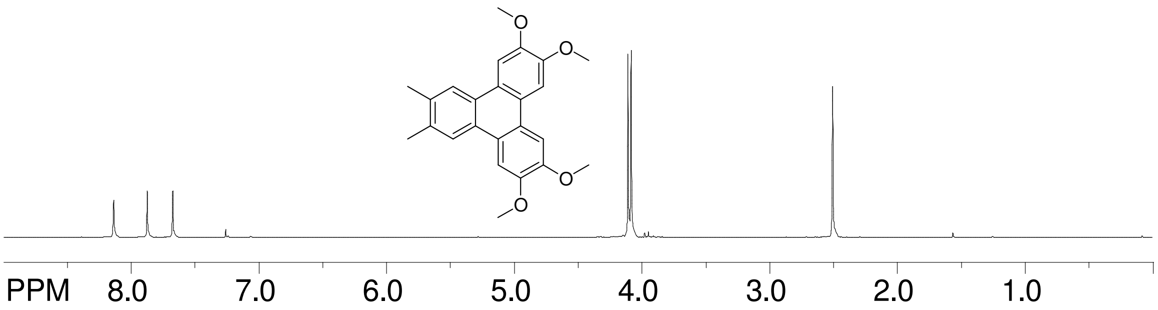
^{1}H NMR spectrum of 3',4'-dimethyl-3,4,3'',4''-tetramethoxyl-*o*-terphenyl (1b)



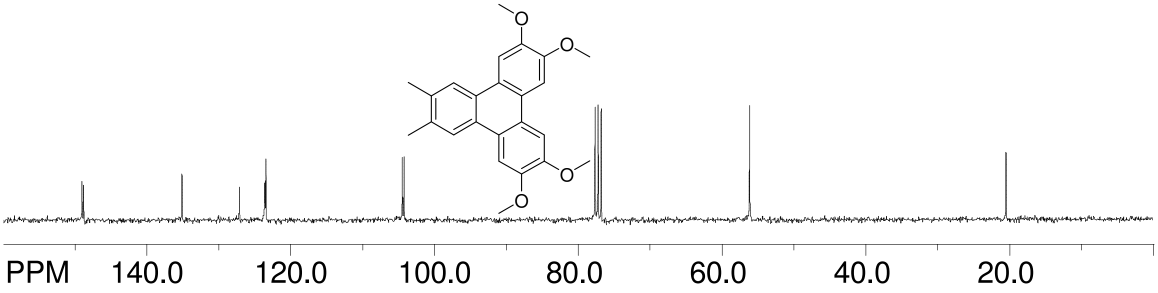
^{13}C NMR spectrum of 3',4'-dimethyl-3,4,3'',4''-tetramethoxyl-*o*-terphenyl (1b)



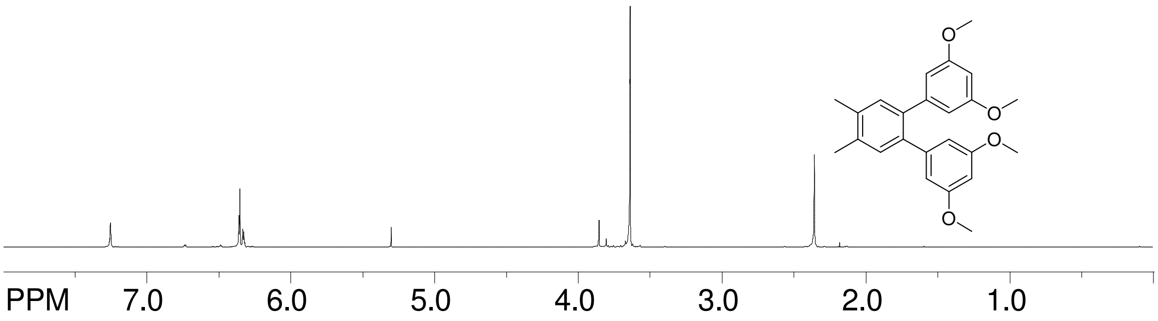
^{1}H NMR spectrum of 6,7-dimethyl-2,3,10,11-tetramethoxytriphenylene (2b).



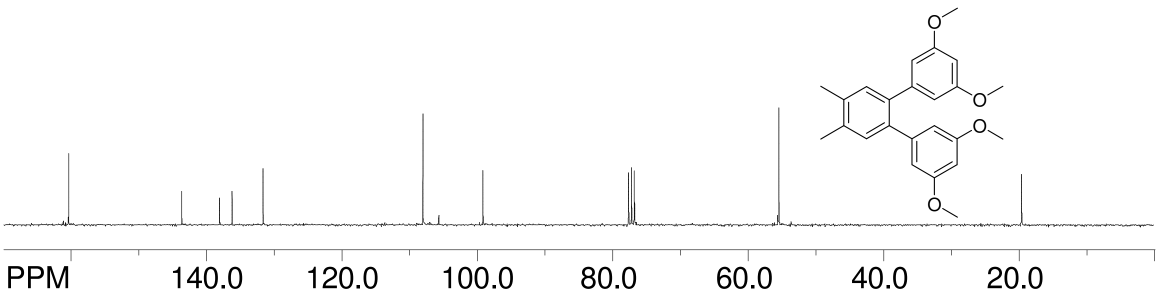
^{13}C NMR spectrum of 6,7-dimethyl-2,3,10,11-tetramethoxytriphenylene (2b).



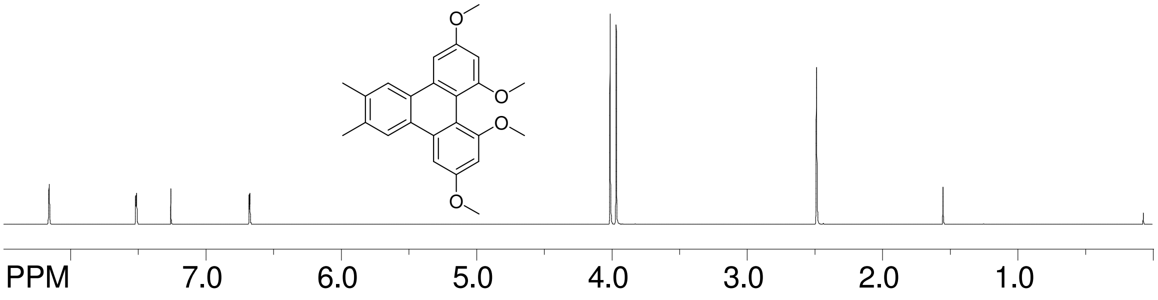
^{1}H NMR spectrum of 3',4'-dimethyl-3,5,3'',5''-tetramethoxy-*o*-terphenyl (1c)



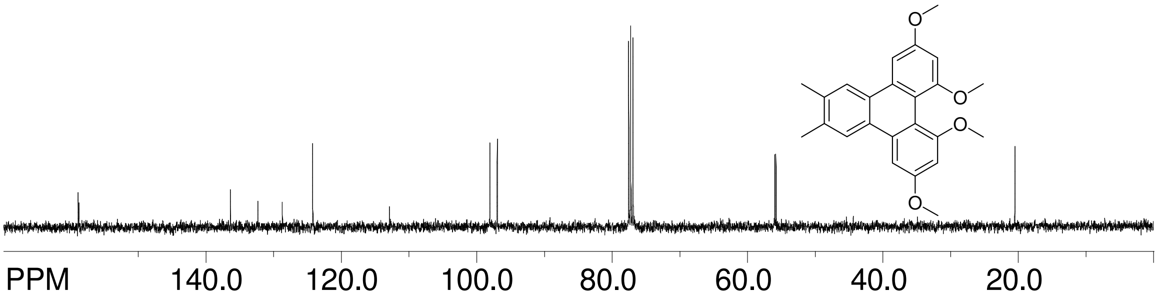
^{13}C NMR spectrum of 3',4'-dimethyl-3,5,3'',5''-tetramethoxy-*o*-terphenyl (1c)



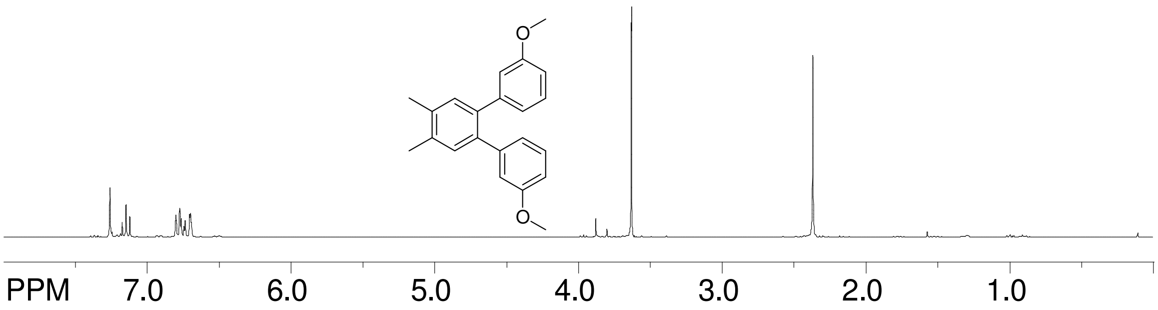
^{1}H NMR spectrum of 6,7-dimethyl-1,3,9,11-tetramethoxytriphenylene (2c)



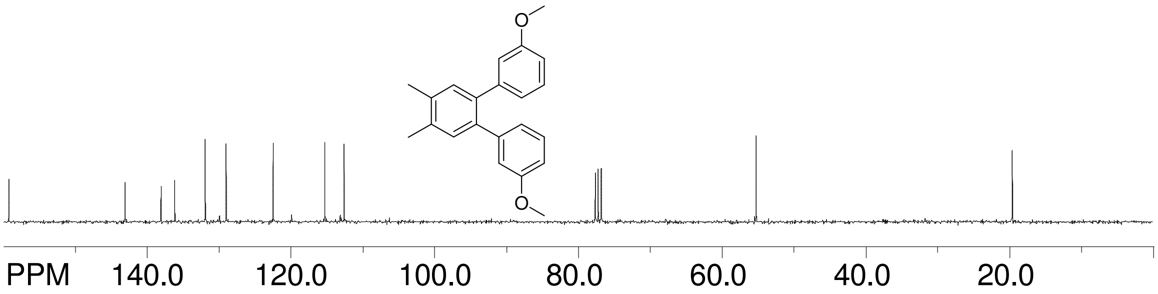
^{13}C NMR spectrum of 6,7-dimethyl-1,3,9,11-tetramethoxytriphenylene (2c)



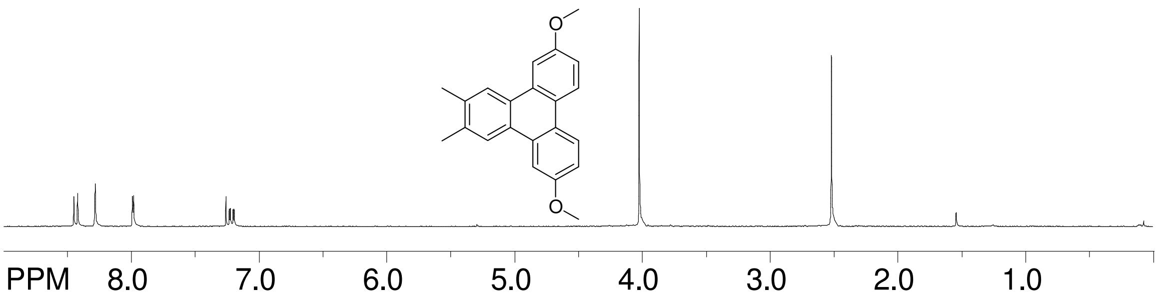
^{1}H NMR spectrum of 3,3''-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1d)



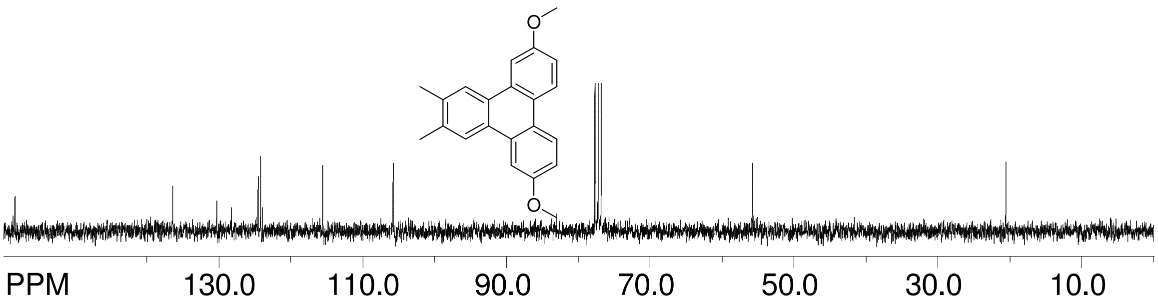
^{13}C NMR spectrum of 3,3''-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1d)



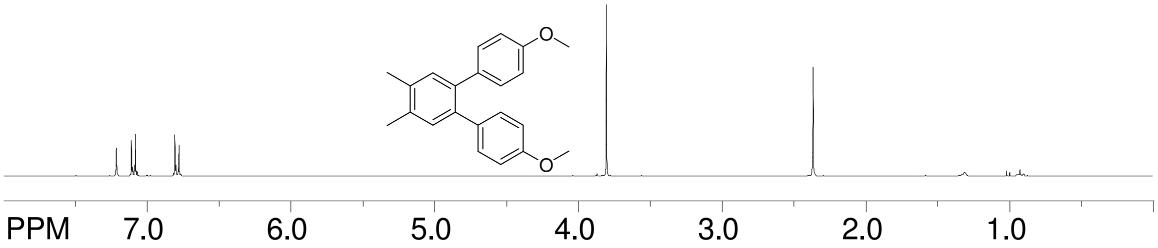
^{1}H NMR spectrum of 3,10-dimethoxy-6,7-dimethyltriphenylene (2d)



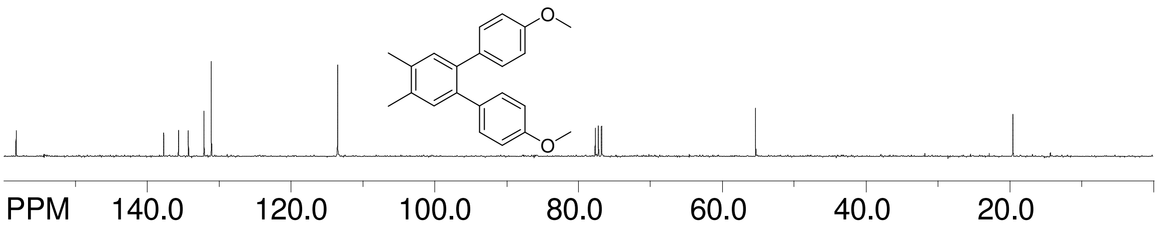
^{13}C NMR spectrum of 3,10-dimethoxy-6,7-dimethyltriphenylene (2d)



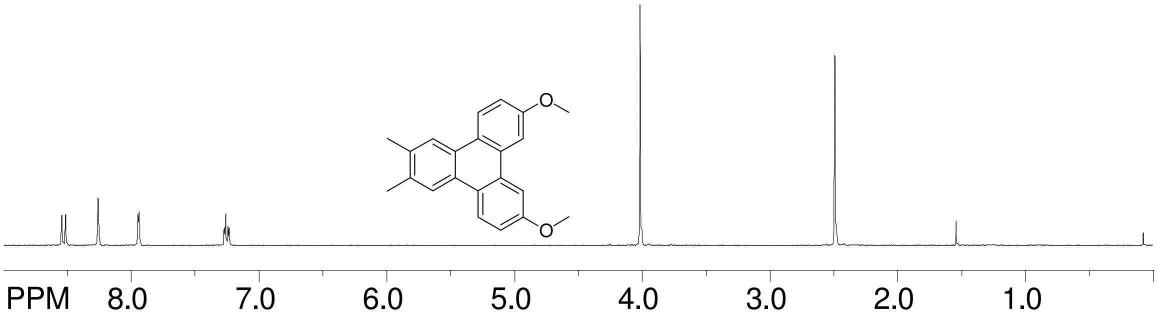
^{1}H NMR spectrum of 4,4''-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1e)



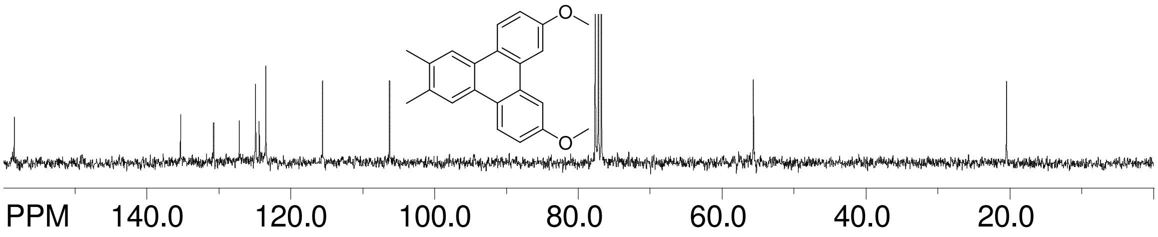
^{13}C NMR spectrum of 4,4''-dimethoxy-3',4'-dimethyl-*o*-terphenyl (1e)



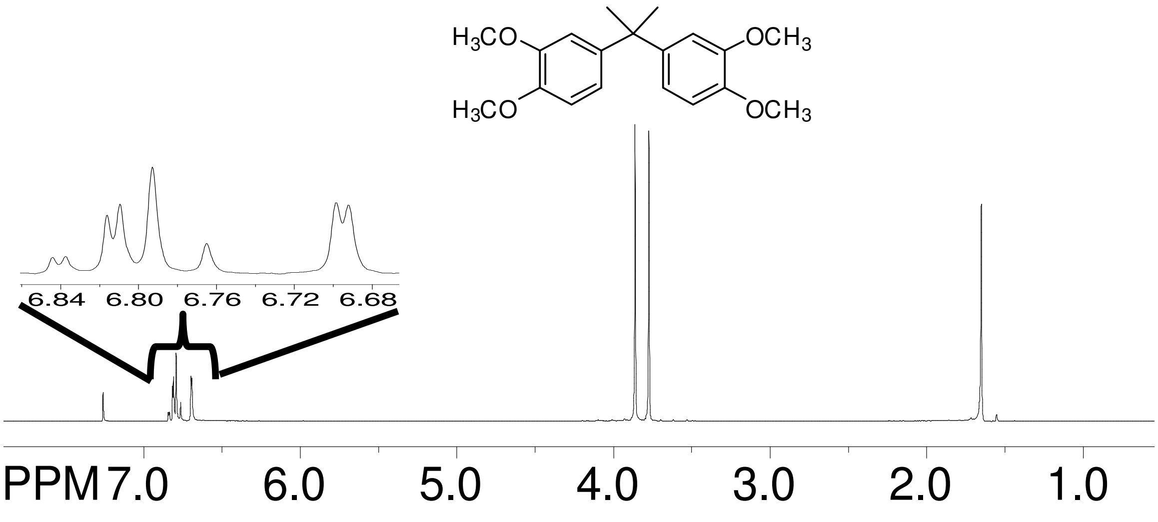
^{1}H NMR spectrum of 2,11-dimethoxy-6,7-dimethyltriphenylene (2e)



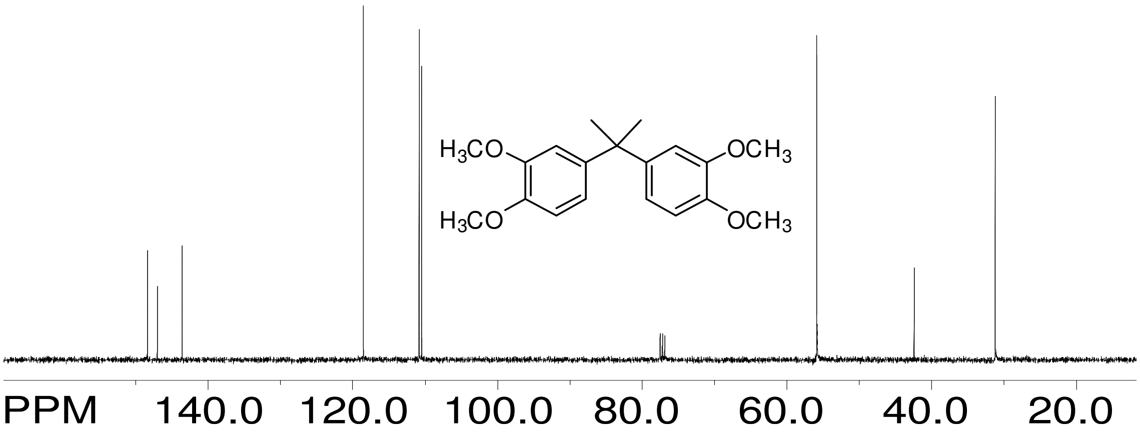
^{13}C NMR spectrum of 2,11-dimethoxy-6,7-dimethyltriphenylene (2e)



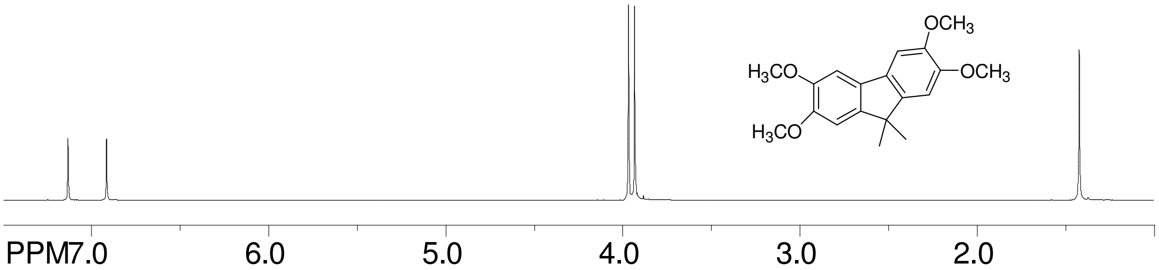
^{1}H NMR spectrum of 2,2-Bis(3,4-dimethoxyphenyl)propane (1f)



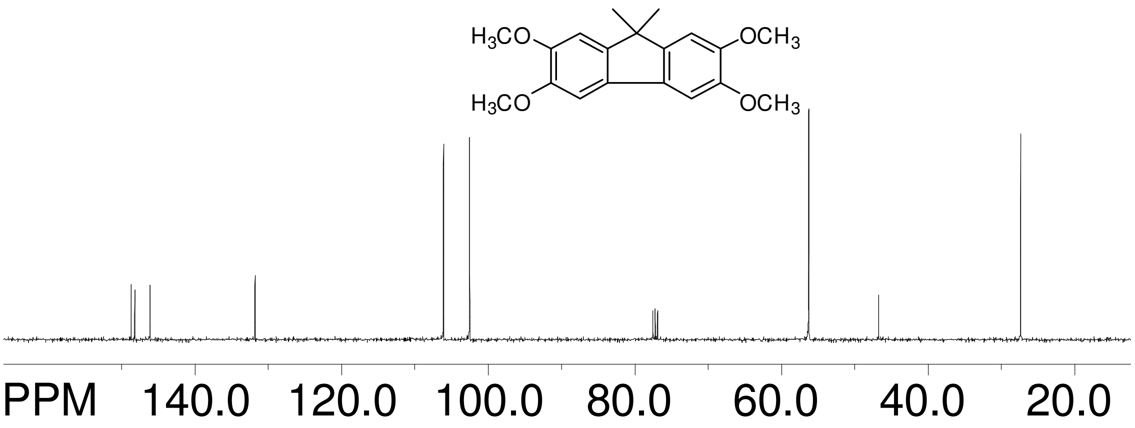
^{13}C NMR spectrum of 2,2-Bis(3,4-dimethoxyphenyl)propane (1f)



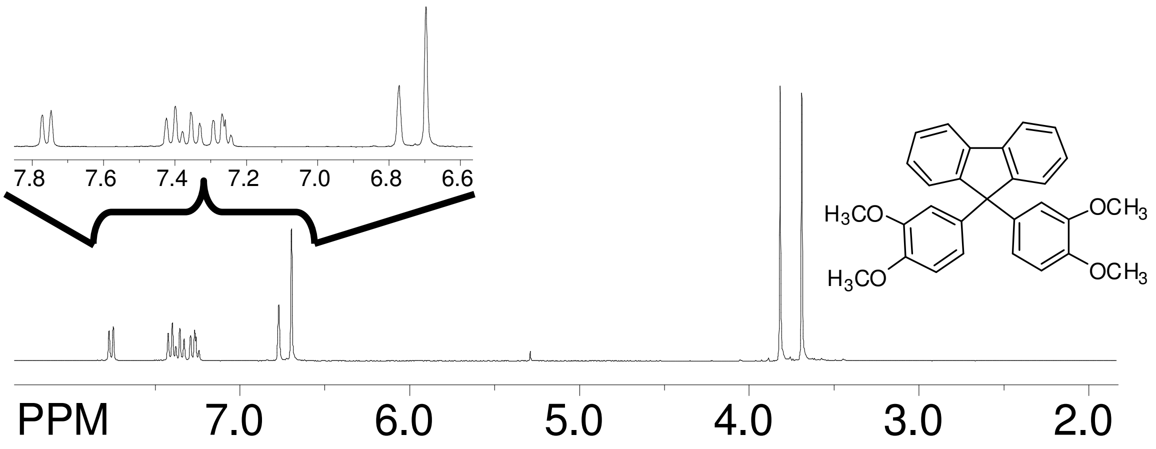
^{1}H NMR spectrum of 2,3,6,7-tetramethoxy-9,9-dimethylfluorene (2f)



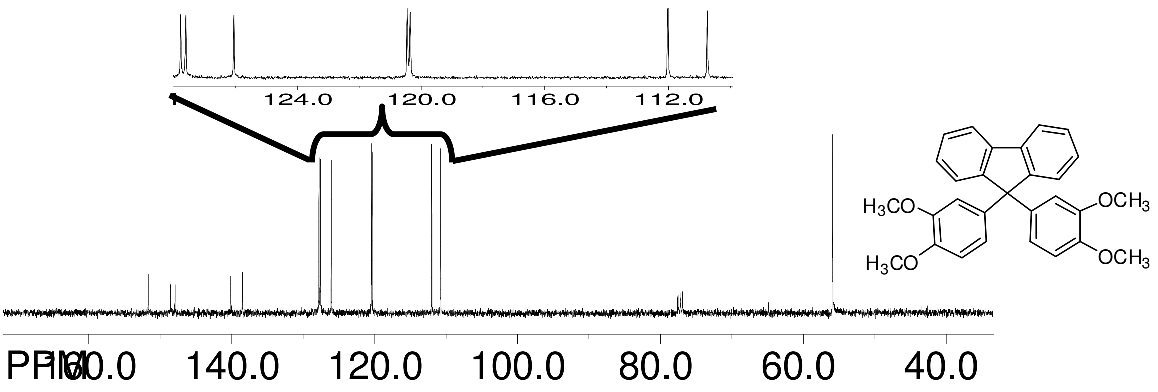
^{13}C NMR spectrum of 2,3,6,7-tetramethoxy-9,9-dimethylfluorene (2f)



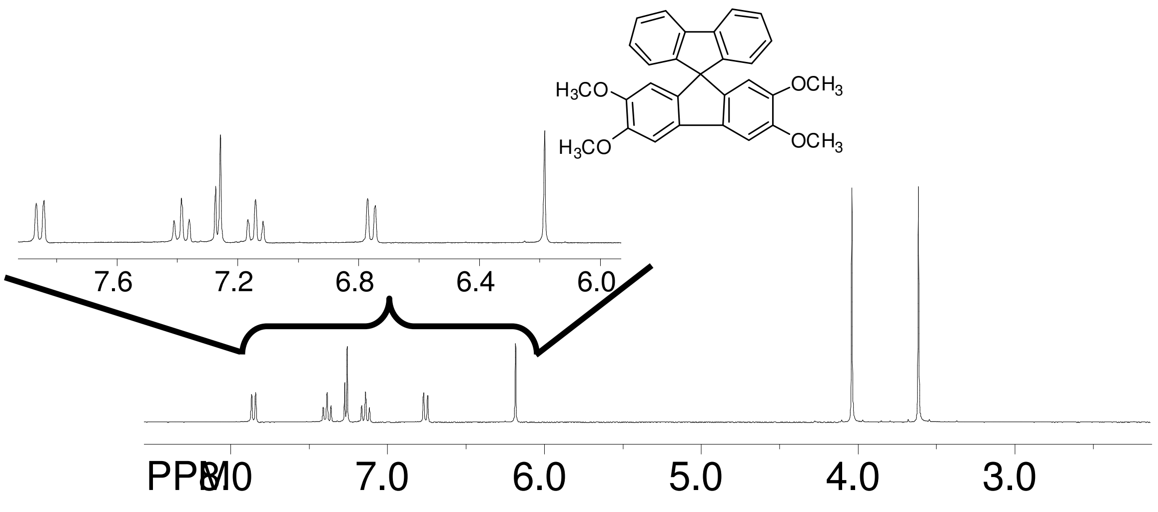
^{1}H NMR spectrum of 9,9-bis(3,4-dimethoxyphenyl)fluorene (1g)



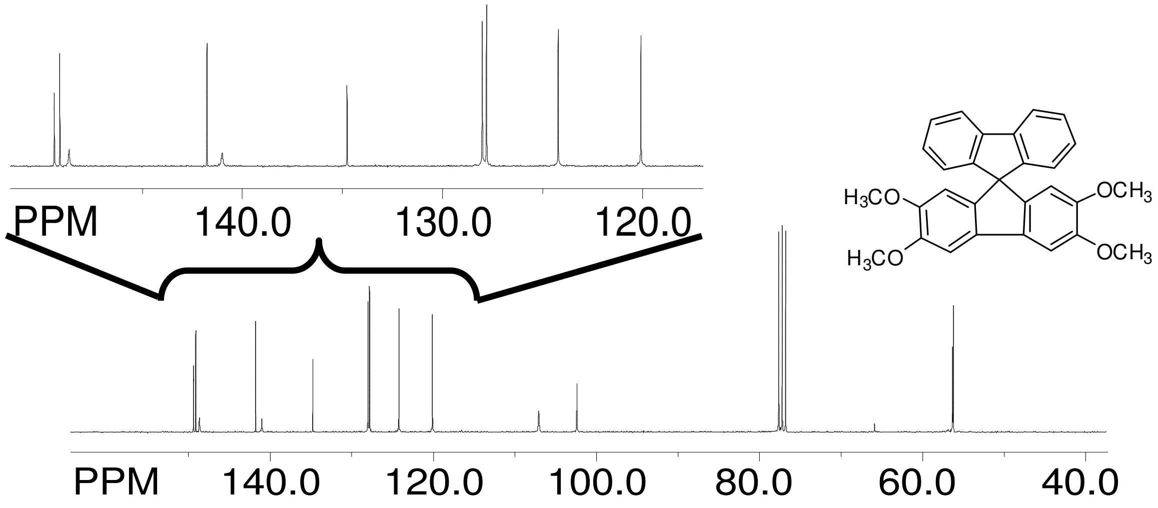
^{13}C NMR spectrum of 9,9-bis(3,4-dimethoxyphenyl)fluorene (1g)



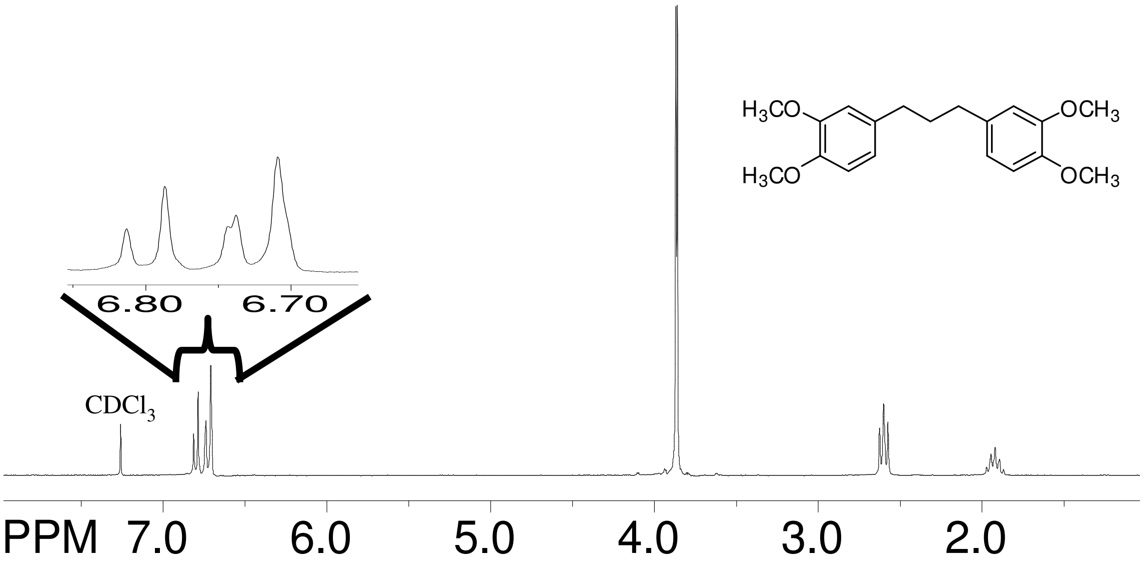
^{1}H NMR spectrum of 2,3,6,7-tetramethoxyspirobifluorene (2g)



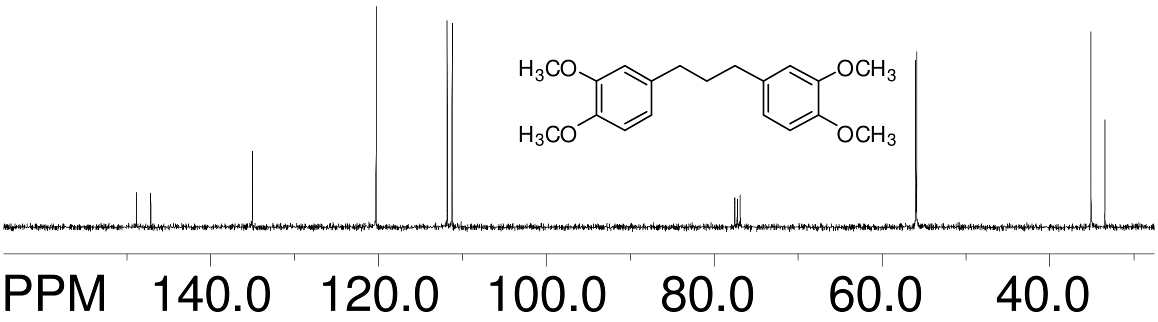
^{13}C NMR spectrum of 2,3,6,7-tetramethoxyspirobifluorene (2g)



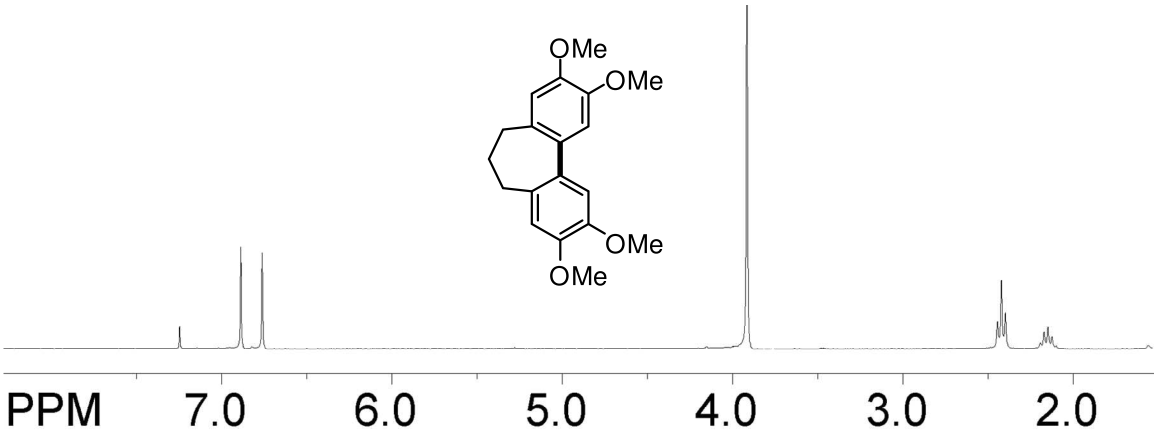
^{1}H NMR spectrum of 1,3-bis(3,4-dimethoxyphenyl)propane (1h)



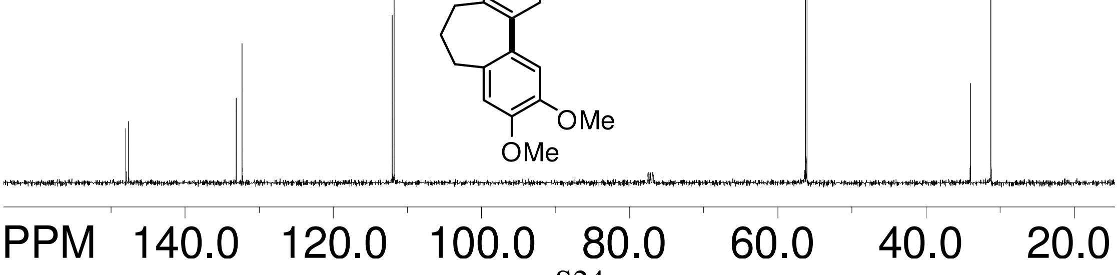
^{13}C NMR spectrum of 1,3-bis(3,4-dimethoxyphenyl)propane (1h)



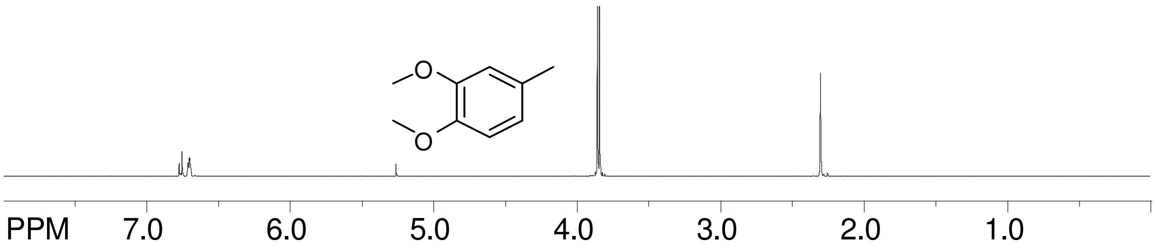
^{1}H NMR spectrum of 6,7-Dihydro-2,3,9,10-tetramethoxydibenzo-[1,c]cyclohepta-diene (2h)



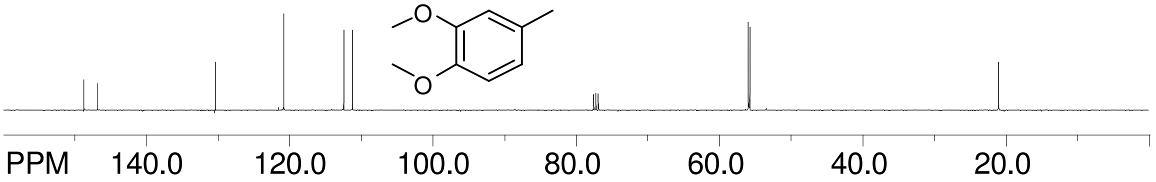
^{13}C NMR spectrum of 6,7-Dihydro-2,3,9,10-tetramethoxydibenzo-[1,c]cyclohepta-diene (2h)



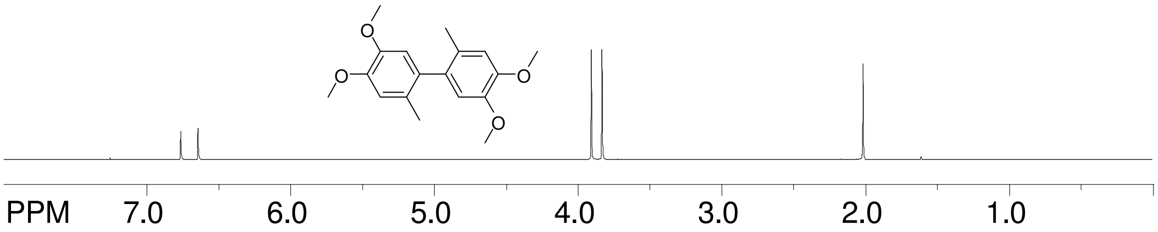
^{1}H NMR spectrum of 3,4-dimethoxytoluene (1i)



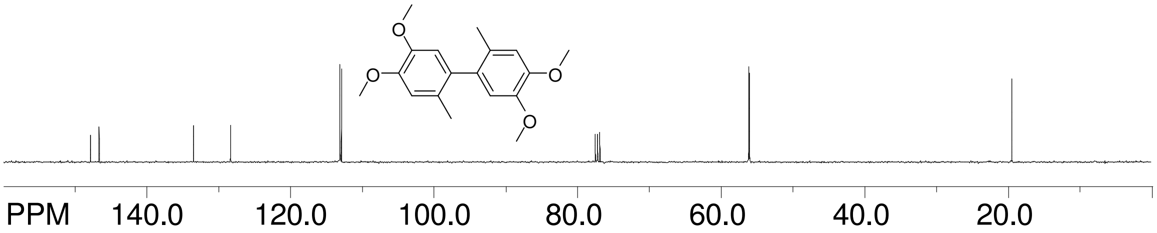
^{13}C NMR spectrum of 3,4-dimethoxytoluene (1i)



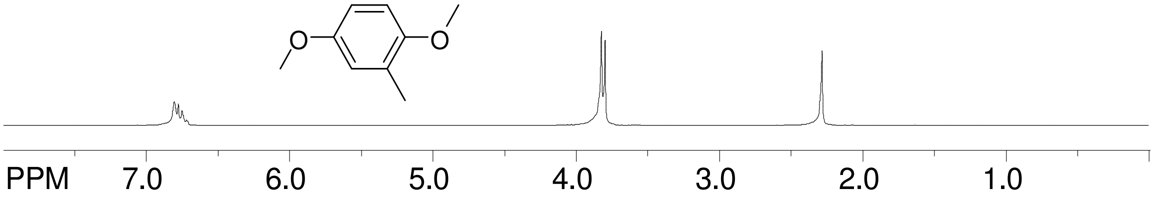
^{1}H NMR spectrum of 4,4’,5,5’-Tetramethoxy-2,2’-dimethylbiphenyl (2i)



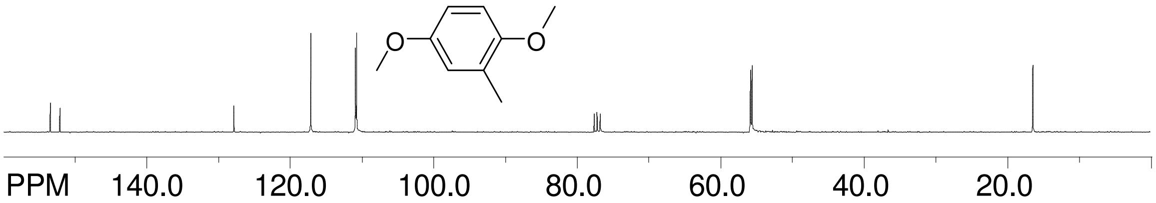
^{13}C NMR spectrum of 4,4’,5,5’-Tetramethoxy-2,2’-dimethylbiphenyl (2i)



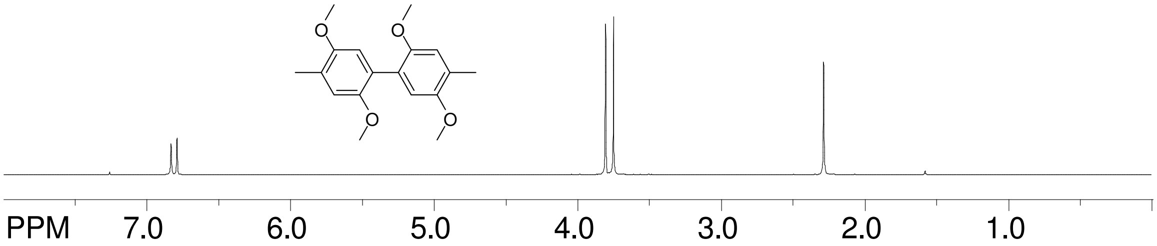
^1H NMR spectrum of 2,5-dimethoxytoluene (1j)



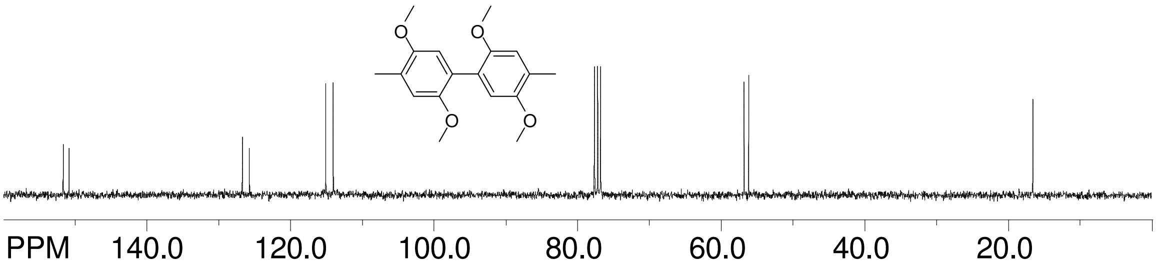
^{13}C NMR spectrum of 2,5-dimethoxytoluene (1j)



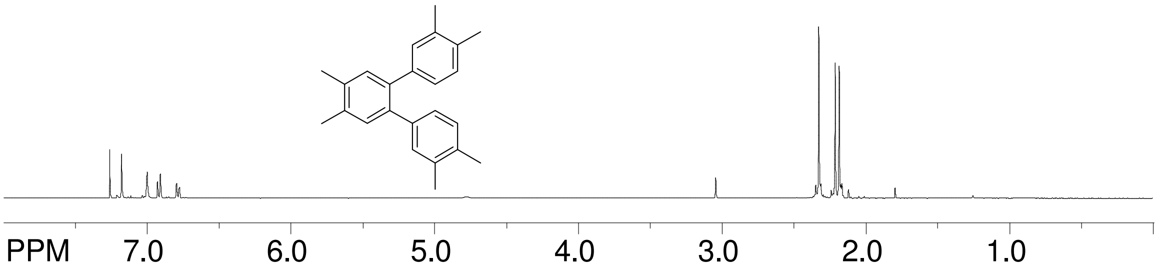
^1H NMR spectrum of 2,2’,5,5’-Tetramethoxy-4,4’-dimethylbiphenyl (2j)



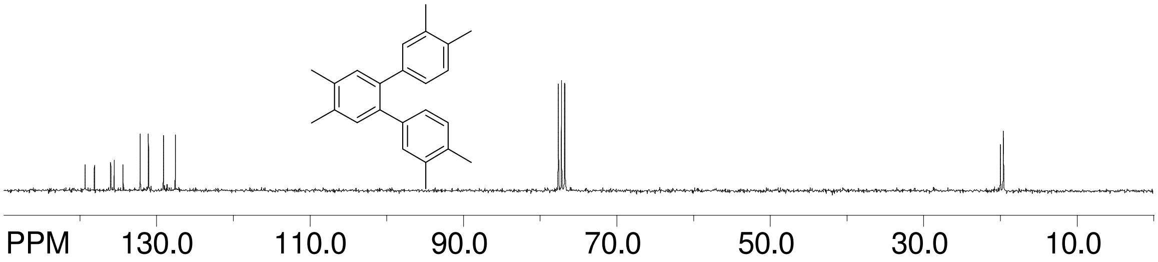
^{13}C NMR spectrum of 2,2’,5,5’-Tetramethoxy-4,4’-dimethylbiphenyl (2j)



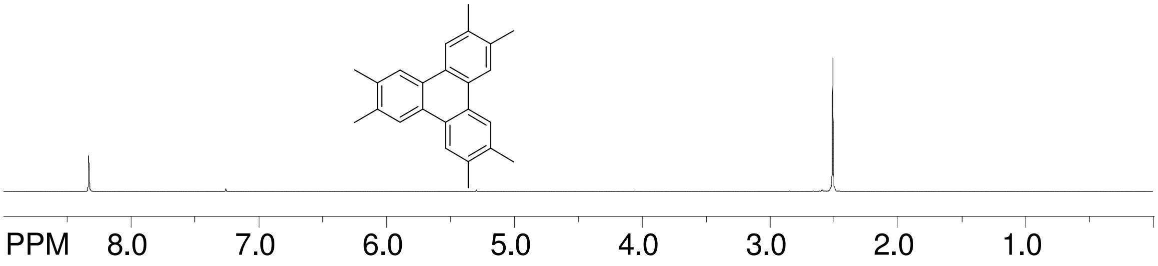
^{1}H NMR spectrum of (1k)



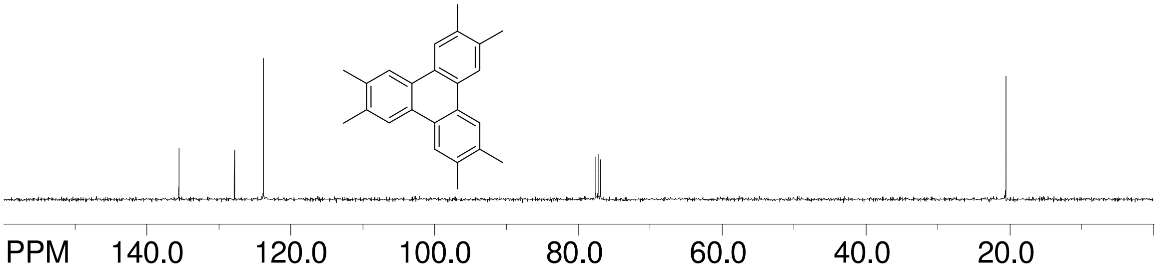
^{13}C NMR spectrum of (1k)



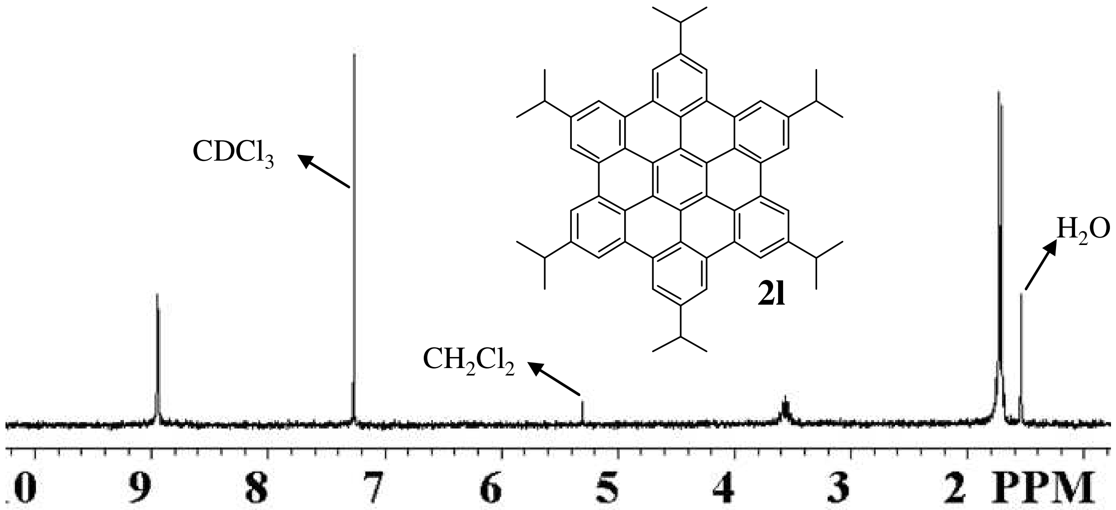
^{1}H NMR spectrum of (2k)



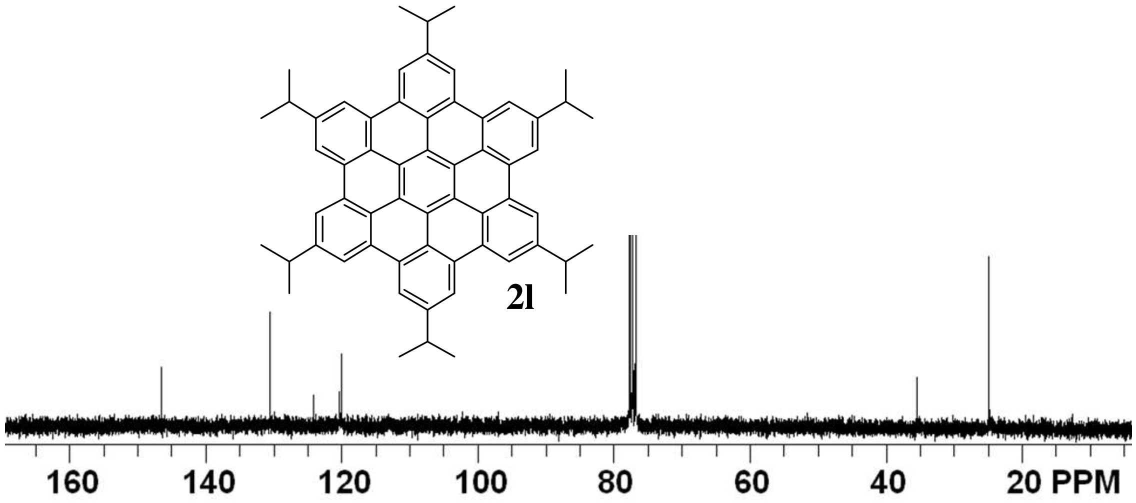
^{13}C NMR spectrum of (2k)



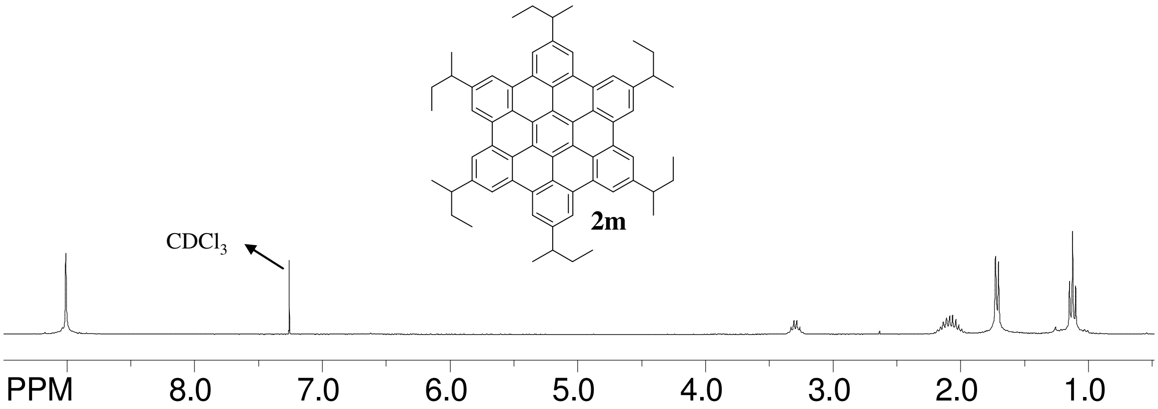
^{1}H NMR spectrum of HBC 2l



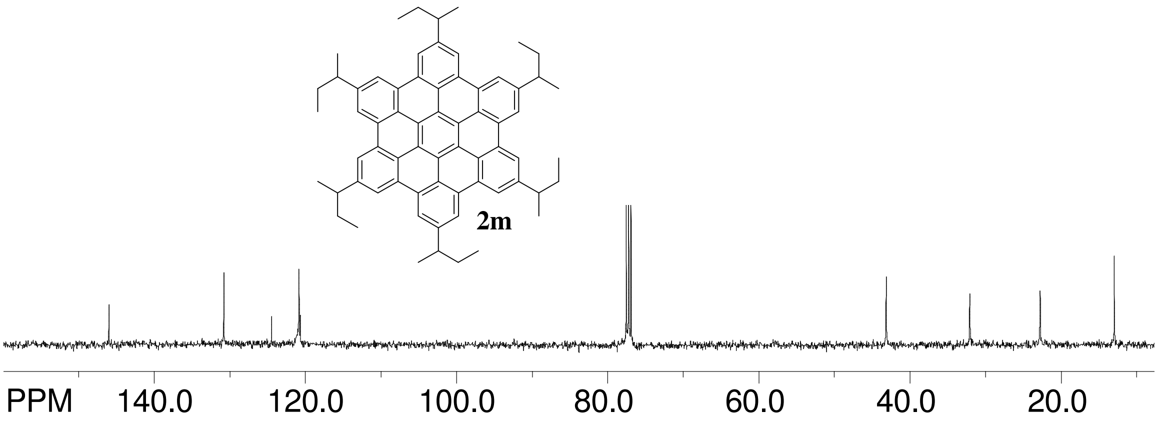
^{13}C NMR spectrum of HBC 2l



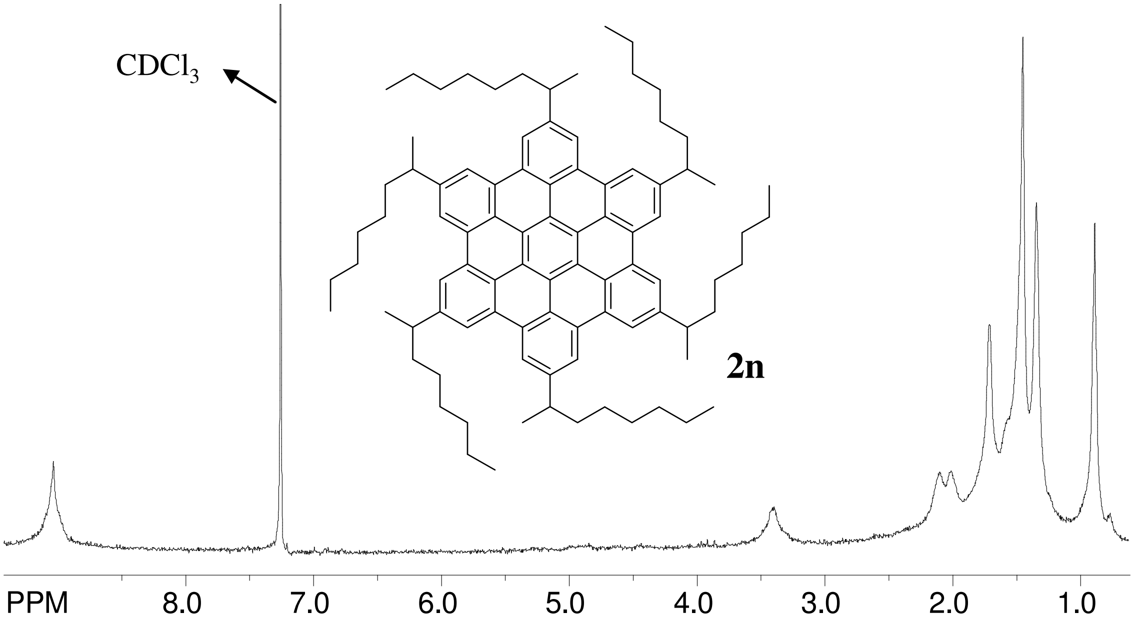
^{1}H NMR spectrum of HBC 2m



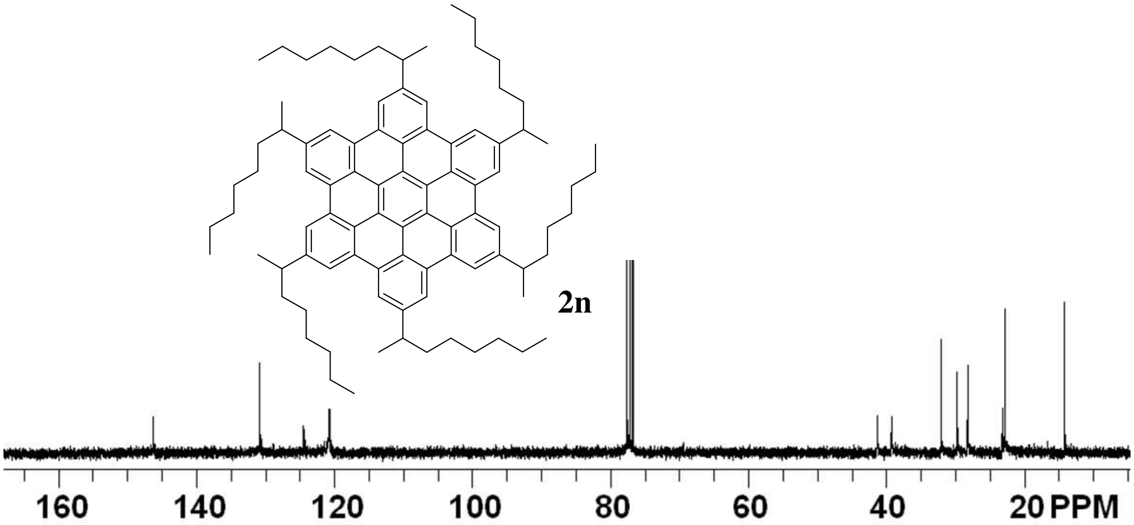
^{13}C NMR spectrum of HBC 2m



^{1}H NMR spectrum of HBC 2n



^{13}C NMR spectrum of HBC 2n



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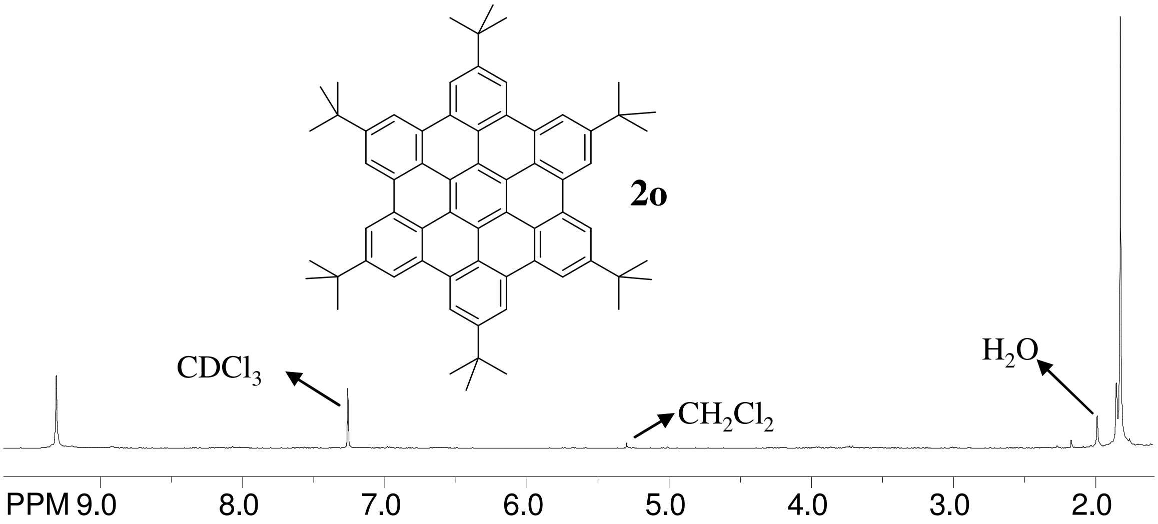
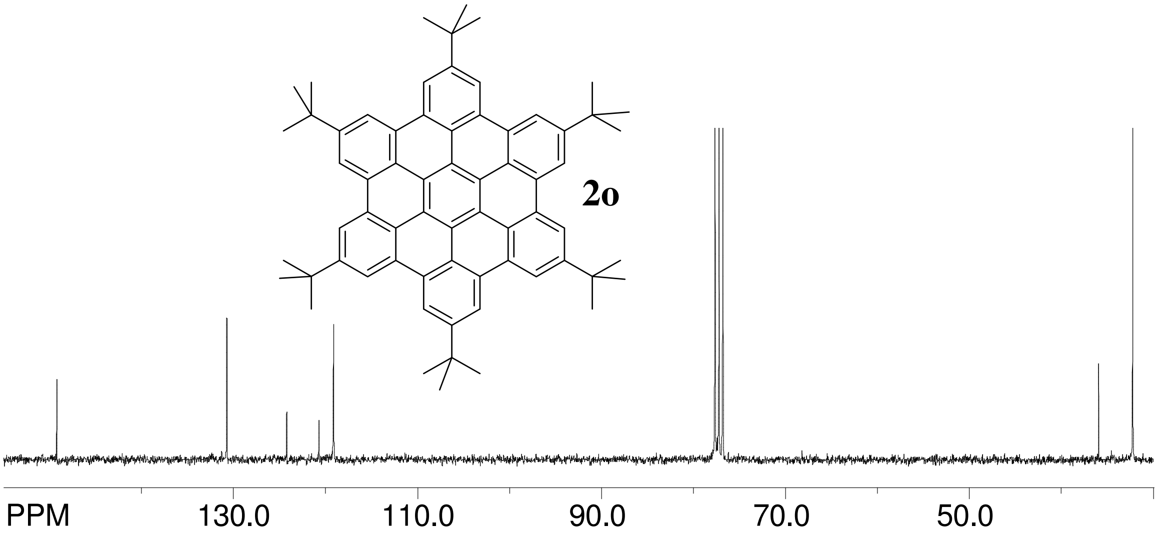
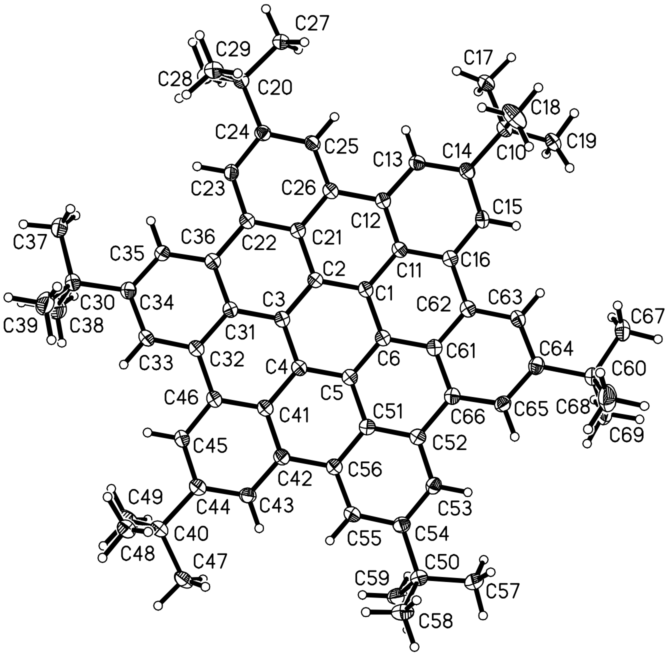


^{13}C NMR spectrum of HBC 2o



Crystal data and structure refinement for raj15n (HBC 2o).



Identification code	raj15n	
Empirical formula	C66 H66	
Formula weight	859.19	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.0858(4) Å	α= 90°.
	b = 17.9286(5) Å	β= 94.962(2)°.
	c = 17.9396(5) Å	γ = 90°.
Volume	4833.9(2) Å^3	
Z	4	
Density (calculated)	1.181 Mg/m^3	
Absorption coefficient	0.495 mm^{-1}	
F(000)	1848	
Crystal size	0.14 x 0.12 x 0.05 mm^3	
Theta range for data collection	2.94 to 67.80°.	
Index ranges	-17<=h<=17, 0<=k<=21, 0<=l<=21	
Reflections collected	39987	
Independent reflections	8596 [R(int) = 0.0306]	
Completeness to theta = 67.80°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9757 and 0.9340	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8596 / 0 / 613	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1157	
R indices (all data)	R1 = 0.0594, wR2 = 0.1253	
Largest diff. peak and hole	0.209 and -0.186 e.Å^{-3}	