

Emission Mechanism of Doubly *ortho*-Linked Quinoxaline/Diphenylfluorene or *cis*-Stilbene/Fluorene Hybrid Compounds Based on the Transient Absorption and Emission Measurements during the Pulse Radiolysis

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SUPPORTING INFORMATION

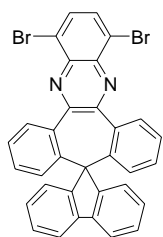
Experimental details, spectral data of compounds **1-4** and OLED device measurements for **1a-e**, **2a**, **3d**, **3f**, and **4f** (25 pages).

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General. ^1H NMR and ^{13}C NMR spectra were recorded on Jeol JNM-EX400 (400 MHz ^1H , 100 MHz ^{13}C) spectrometers in deuteriochloroform with chloroform as an internal reference unless otherwise stated. Chemical shifts are reported in ppm (δ). Coupling constants, J , are reported in Hz. Mass spectra were recorded on a Finnigan TCQ-700 GC/LC/MS spectrometer with an ionization voltage of 70 or 20 eV unless otherwise stated. High-resolution mass spectra were measured on a Finnigan MAT 95S spectrometer. Combustion analyses were performed on a Perkin-Elmer 2400-CHN analyzer by the Northern Instrument Center of Taiwan. Fast atom bombardment (FAB) mass spectra were recorded on a Finnigan MAT-95S spectrometer. Data are reported in the form m/e (intensity relative to base peak). Analytical TLC was performed on Merck silica gel plates with QF-254 indicator. Visualization was accomplished with UV light or with phosphomolybdic acid (PMA) and KMnO_4 staining agents. Column (flash) chromatography was performed using 32-63 μm silica gel. All reagents were purchased from ACROS, ALDRICH, and TCI with purification in advance before use. Solvents for extraction and chromatography were reagent grade. Dichloromethane and chlorobenzene were dried over CaH_2 before use. Diethyl ether, THF, 1,2-dimethoxyethane (DME) and toluene were dried over Na with benzophenone-ketyl intermediate as indicator. All reactions were run under argon.

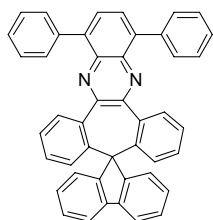
Spiro-fluorene-dibenzosuberene[d](1,4-dibromo-quinoxaline) (1)¹



To a 50-mL, two-necked, round-bottomed flask was placed **Spiro-fluorene-dibenzosuberene-10,11-dione** (745 mg, 2 mmol), 1,2-diamino-3,6-dibromobenzene (585 mg, 2.2 mmol) and catalytic *p*-TSA in CHCl_3 (20 mL). The reaction mixture was stirred under reflux for 12 hours. After having been quenched with saturated aqueous NaHCO_3 (20 mL), the mixture was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1**, which was further re-crystallized from CH_2Cl_2 to afford pure **1** (1084 mg, 90 %): m.p. 287 $^\circ\text{C}$ (DSC); M.W.: 602.32; ^1H NMR (400 MHz, CDCl_3) δ 8.52 (dd, $J = 7.6, 1.3$, 2H), 8.03 (s, 2H), 7.75 (d, $J = 7.6$, 2H), 7.47 (td, $J = 7.6, 1.6$, 2H), 7.34 (t, $J = 7.6$, 2H), 7.25-7.19 (m, 4H), 7.07 (t, $J = 7.6$, 2H), 6.76 (d, $J = 7.6$, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.31, 149.39, 145.86, 140.02, 140.00, 136.99,

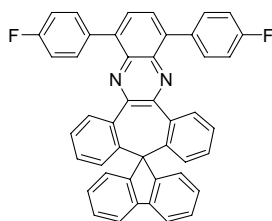
134.42, 133.36, 130.19, 128.55, 128.03, 128.01, 127.64, 127.23, 124.12, 120.48, 66.54; MS (ESI) 603.4 ($M+H^+$, 100); TLC R_f 0.30 (hexanes/ CH_2Cl_2 , 3/1).

Spiro-fluorene-dibenzosuberene[d](1,4-bis(4-methoxyphenyl)quinoxaline) (1a)²



To a 50-mL, two-necked, round-bottomed flask was placed **1** (602 mg, 1 mmol) and $Pd(PPh_3)_4$ (35 mg, 0.03 mmol) in DME (25 mL). A solution of phenylboronic acid (293 mg, 2.4 mmol) and Na_2CO_3 (318 mg, 3 mmol) in degassed water (12 mL) was added and the whole solution was refluxed for 24 hours. The reaction mixture was quenched with water (20 mL) and extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried ($MgSO_4$), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1a**, which was further re-crystallized from CH_2Cl_2 /hexanes to afford pure **1a** (555 mg, 93 %): m.p. 316 °C (DSC); T_d 361 °C (TGA); T_g 122 °C (DSC); M.W.: 596.72; 1H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, $J = 7.9, 1.3$, 2H), 8.04 (s, 2H), 7.94 (d, $J = 7.2$, 4H), 7.75 (d, $J = 7.6$, 2H), 7.54 (t, $J = 7.2$, 4H), 7.45 (t, $J = 7.2$, 4H), 7.37-7.32 (m, 4H), 7.20-7.13 (m, 4H), 7.08 (t, $J = 7.6$, 2H), 6.84 (d, $J = 7.6$, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.85, 149.71, 145.50, 140.09, 139.64, 138.43, 138.43, 138.25, 133.74, 131.01, 130.30, 129.33, 128.32, 128.01, 127.92, 127.85, 127.72, 127.62, 127.16, 120.39, 66.65; MS (ESI) 597.6 ($M+H^+$, 100); TLC R_f 0.35 (EtOAc/hexanes, 1/12); HR-MS calcd for $C_{45}H_{28}N_2$: 596.2252, found: 596.2256; Anal. Calcd for $C_{45}H_{28}N_2$: C, 90.58, H, 4.73, N, 4.69. Found: C, 90.19, H, 5.01, N, 4.52.

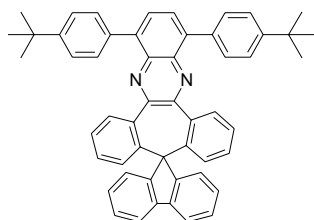
Spiro-fluorene-dibenzosuberene[d](1,4-bis(4-methoxyphenyl)quinoxaline) (1b)



To a 50-mL, two-necked, round-bottomed flask was placed **1** (602 mg, 1 mmol) and $Pd(PPh_3)_4$ (35 mg, 0.03 mmol) in DME (25 mL). A solution of 4-fluorophenylboronic acid (336 mg, 2.4 mmol) and Na_2CO_3 (318 mg, 3 mmol) in degassed water (12 mL) was added and the whole solution was refluxed for 24 hours. The reaction mixture was quenched with water (20 mL) and extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried ($MgSO_4$), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1b**, which was further re-crystallized from

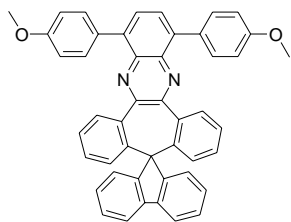
CH₂Cl₂/hexanes to afford pure **1b** (854 mg, 90 %): m.p. 298 °C (DSC); T_d 362 °C (TGA); T_g 161 °C (DSC); M.W.: 632.70; ¹H NMR (400 MHz, CDCl₃) δ 8.26 (d, *J* = 7.5, 2H), 7.97 (s, 2H), 7.88 (dd, *J* = 8.7, 5.5, 4H), 7.75 (d, *J* = 7.6, 2H), 7.37-7.32 (m, 4H), 7.24-7.13 (m, 8H), 7.07 (t, *J* = 7.6, 2H), 6.80 (d, *J* = 7.3, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 163.86, 161.41, 151.97, 145.30, 149.60, 145.44, 140.08, 139.48, 139.06, 138.04, 134.20, 133.57, 132.51, 130.01, 129.45, 128.36, 127.94, 127.72, 127.12, 120.42, 114.93, 66.58; MS (FAB) 633.07 (M⁺, 5); TLC R_f 0.32 (EtOAc/hexanes, 1/12); HR-MS calcd for C₄₅H₂₆N₂F₂: 632.2064, found: 632.2060; Anal. Calcd for C₄₅H₂₆N₂F₂: C, 85.42, H, 4.14, N, 4.43. Found: C, 85.15, H, 4.34, N, 4.53.

Spiro-fluorene-dibenzosuberene[d](1,4-bis(4-*t*-butylphenyl)Quinoxaline) (1c**)**



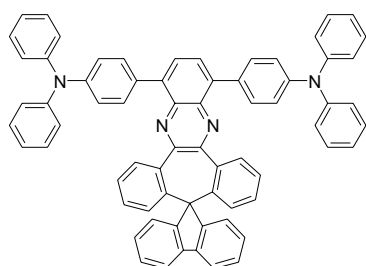
To a 50-mL, two-necked, round-bottomed flask was placed **1** (602 mg, 1 mmol) and Pd(PPh₃)₄ (35 mg, 0.03 mmol) in DME (25 mL). A solution of 4-*t*-butylphenylboronic acid (427 mg, 2.4 mmol) and Na₂CO₃ (318 mg, 3 mmol) in degassed water (12 mL) was added and the resulting mixture was refluxed for 24 hours. The reaction mixture was cooled to ambient temperature and quenched with water (20 mL). The whole mixture was extracted with dichloromethane (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1c**, which was further re-crystallized from CH₂Cl₂/hexanes to afford pure **1c** (631 mg, 89 %): m.p. 402 °C (DSC); T_d 395 °C (TGA); T_g 181 °C (DSC); M.W.: 708.93; ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, *J* = 7.6, 2H), 8.01 (s, 2H), 7.89 (d, *J* = 8.4, 4H), 7.71 (d, *J* = 7.6, 2H), 7.55 (d, *J* = 8.4, 4H), 7.36 (td, *J* = 7.6, 2.2, 2H), 7.30 (t, *J* = 7.6, 2H), 7.17-7.11 (m, 4H), 7.04 (bd, 2H), 6.80 (bd, 2H), 1.40 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 151.64, 150.45, 149.59, 145.35, 140.02, 139.72, 139.55, 138.31, 135.48, 133.69, 130.58, 130.24, 129.19, 128.27, 127.83, 127.69, 127.10, 124.98, 120.28, 66.56, 34.63, 31.40; MS (ESI) 709.7 (M+H⁺, 100); TLC R_f 0.30 (EtOAc/hexanes, 1/12).

Spiro-fluorene-dibenzosuberene[d](1,4-bis(4-methoxyphenyl)quinoxaline) (**1d**)



To a 50-mL, two-necked, round-bottomed flask was placed **1** (602 mg, 1 mmol) and Pd(PPh₃)₄ (35 mg, 0.03 mmol) in DME (25 mL). A solution of 4-methoxyphenylboronic acid (365 mg, 2.4 mmol) and Na₂CO₃ (318 mg, 3 mmol) in degassed water (12 mL) was added and the whole solution was refluxed for 24 hours. The reaction mixture was quenched with water (20 mL) and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1d**, which was further re-crystallized from CH₂Cl₂/hexanes to afford pure **1d** (624 mg, 95 %): m.p. 344 °C (DSC); T_d 372 °C (TGA); T_g 160 °C (DSC); M.W.: 656.77; ¹H NMR (400 MHz, CDCl₃) δ 8.32 (d, *J* = 7.6, 2H), 7.97 (s, 2H), 7.88 (d, *J* = 8.8, 4H), 7.74 (d, *J* = 7.6, 2H), 7.37-7.30 (m, 4H), 7.18-7.12 (m, 4H), 7.08 (bd, 2H), 7.06 (d, *J* = 8.8, 4H), 6.82 (bd, 2H), 3.89 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 159.27, 151.51, 149.66, 145.30, 140.05, 139.65, 139.04, 138.30, 133.66, 132.07, 130.90, 129.81, 129.21, 128.26, 127.86, 127.69, 127.11, 120.33, 113.50, 66.59, 55.33; MS (ESI) 657.7 (M+H⁺, 100); TLC R_f 0.32 (EtOAc/hexanes, 1/10).

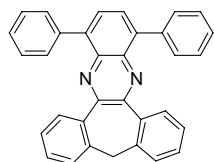
Spiro-fluorene-dibenzosuberene[d](1-(4-(*N,N*-diphenylamino)-phenyl)-quinoxaline) (**1e**)



To a 50-mL, two-necked, round-bottomed flask was placed **1** (602 mg, 1 mmol) and Pd(PPh₃)₄ (35 mg, 0.03 mmol) in DME (25 mL). A solution of 4-(*N,N*-diphenylamino)phenylboronic acid (694 mg, 2.4 mmol) and Na₂CO₃ (318 mg, 3 mmol) in degassed water (12 mL) was added and the whole solution was refluxed for 24 hours. The reaction mixture was quenched with water (20 mL) and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **1e**, which was further re-crystallized from CH₂Cl₂/hexanes to afford pure **1e** (857 mg, 92 %): m.p. 351 °C (DSC); T_d 412 °C (TGA); T_g 186 °C (DSC); M.W.: 931.13; ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 7.3, 2H), 7.98 (s, 2H), 7.81 (d, *J* = 8.7, 4H), 7.72 (d, *J* = 7.4, 2H), 7.34-7.26 (m, 12H), 7.22-7.13 (m, 16H), 7.04 (t,

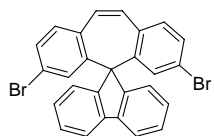
$J = 7.2$, 6H), 6.79 (d, $J = 7.1$, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 151.5, 149.7, 147.8, 147.4, 145.4, 140.1, 139.7, 139.1, 138.3, 133.7, 132.3, 131.7, 129.8, 129.3, 128.3, 127.9, 127.2, 124.7, 123.0, 122.7, 120.4, 66.6; MS (FAB) 931.4 ($\text{M}+\text{H}^+$, 100); TLC R_f 0.38 ($\text{EtOAc}/\text{CH}_2\text{Cl}_2$, 1/3).

5H-dibenzosuberene[d](1,4-bis(4-methoxyphenyl)quinoxaline) (2a)



To a 50-mL, two-necked, round-bottomed flask was placed **5H-dibenzo[a,d]cycloheptene-10,11-dione**³ (444 mg, 2 mmol), [1,1';4',1'']terphenyl-2',3'-diamine⁴ (573 mg, 2.2 mmol) and catalytic *p*-TSA in CHCl_3 (20 mL). The reaction mixture was stirred under reflux for 12 hours. After having been quenched with saturated aqueous NaHCO_3 (20 mL), the mixture was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **2a**, which was further re-crystallized from CH_2Cl_2 to afford pure **2a** (813 mg, 91 %): m.p. 298 °C (DSC); T_d 377 °C (TGA); T_g 98 °C (DSC); M.W.: 446.54; ^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, $J = 7.2$, 2H), 7.96 (s, 2H), 7.92 (d, $J = 7.4$, 4H), 7.54 (t, $J = 7.6$, 4H), 7.45 (t, $J = 7.4$, 2H), 7.40-7.32 (m, 6H), 4.00 (d, $J = 13.5$, 1H), 3.75 (d, $J = 13.5$, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.76, 142.24, 139.99, 139.42, 138.44, 136.55, 131.28, 130.94, 130.15, 129.81, 127.96, 127.54, 127.08, 126.90, 40.34; MS (ESI) 447.7 ($\text{M}+\text{H}^+$, 100); TLC R_f 0.4 ($\text{CH}_2\text{Cl}_2/\text{hexanes}$, 1/3); HR-MS calcd for $\text{C}_{33}\text{H}_{22}\text{N}_2$: 446.5412, found: 446.1788.

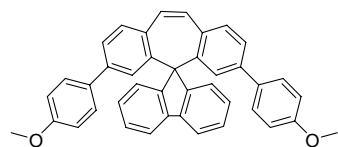
3,7-Dibromo-5,5-spirofluorenyl-5H-dibenzo[a,d]cycloheptene (3)⁵



To a 250-mL, three-necked, round-bottomed flask was placed a solution of 2-bromobiphenyl (3497 mg, 15 mmol) in THF (50 mL). The reaction flask was cooled to -78 °C and *n*-BuLi (2.5 M in hexanes, 6 mL, 15 mmol) was added dropwise. The whole solution was stirred at this temperature for 30 minutes followed by adding a solution of **3,7-Dibromo-dibenzo[a,d]cyclohepten-5-one** (3640 mg, 10 mmol) in THF (30 mL). The resulting mixture was gradually warmed to ambient temperature and then quenched with saturated, aqueous NaHCO_3 (30 mL). The mixture was extracted with CH_2Cl_2 (3×50 mL). The combined organic layers were dried (MgSO_4), filtered, and evaporated under reduced pressure. The crude residue dissolved in acetic acid

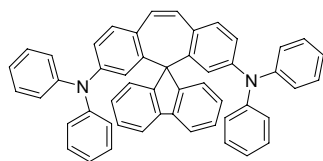
(15 mL) was placed in another 100-mL, two-necked, round-bottomed flask. Catalytic amount of aqueous HCl (12*N*, 5mol%) was then added and the whole mixture was refluxed for 30 minutes. After having been cooled to ambient temperature, the whole mixture was extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **3**, which was further re-crystallized from CH₂Cl₂/hexanes to afford 4852 mg of pure **3** (97 %): m.p. 283 °C (DSC); M.W.: 500.22; ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, *J* = 7.7, 2H), 7.76 (d, *J* = 7.6, 2H), 7.42 (t, *J* = 7.5, 2H), 7.32 (dd, *J* = 8.2, 2.0, 2H), 7.29 (d, *J* = 7.6, 2H), 7.20 (d, *J* = 8.2, 2H), 6.98 (dd, *J* = 1.9, 2H), 6.89 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 151.5, 143.4, 138.9, 135.2, 133.5, 132.7, 131.9, 130.5, 128.6, 127.9, 126.7, 122.8, 120.6, 65.2; MS(EI, 20eV) 500.0 (M⁺, 28); TLC R_f0.35 (CH₂Cl₂/hexanes, 1/5).

3,7-Bis(*N,N*-diphenylamino)-5,5-spirofluorenyl-5H-dibenzo[*a,d*]cycloheptene (**3d**)



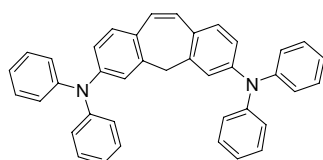
To a 25-mL, two-necked, round-bottomed flask was placed **3** (500 mg, 1 mmol) and Pd(PPh₃)₄ (35 mg, 0.03 mmol) in DME (25 mL). A solution of 4-methoxyphenylboronic acid (365 mg, 2.4 mmol) and Na₂CO₃ (318 mg, 3 mmol) in degassed water (12 mL) was added and the whole solution was refluxed for 24 hours. The reaction mixture was quenched with water (20 mL) and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **3d**, which was further re-crystallized from CH₂Cl₂/hexanes to afford pure **3d** (460 mg, 83 %): m.p. 242 °C (DSC); T_d 411 °C (TGA); T_g 118 °C (DSC); M.W.: 554.22; ¹H NMR (400 MHz, CDCl₃) δ 8.07 (d, *J* = 7.7, 2H), 7.73 (d, *J* = 7.6, 2H), 7.40-7.37 (m, 6H), 7.29 (t, *J* = 7.6, 2H), 7.19 (d, *J* = 8.7, 4H), 7.19 (d, *J* = 2.2, 2H), 6.99 (s, 2H), 6.83 (d, *J* = 8.8, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 159.1, 153.0, 142.0, 140.2, 139.0, 135.0, 133.0, 132.8, 132.6, 128.0, 127.6, 127.4, 127.4, 127.0, 125.1, 120.4, 114.1, 66.3, 55.3; MS (ESI) 554.2 (M⁺, 100); TLC R_f 0.35 (CH₂Cl₂/hexanes, 1/4); HR-MS calcd for C₆₉H₄₆N₄: 554.2246, found: 554.2248; Anal. Calcd for C₄₁H₃₀O₂: C, 88.78, H, 5.45. Found: C, 88.43, H, 5.46.

3,7-Bis(*N,N*-diphenylamino)-5,5-spirofluorenyl-5H-dibenzo[*a,d*]cycloheptene (3f)⁶



To a 25-mL, two-necked, round-bottomed flask was placed **3** (500 mg, 1 mmol), Pd₂(dba)₃ (18 mg, 0.02 mmol), sodium *tert*-butoxide (288 mg, 3 mmol), P(*t*-Bu)₃ (0.03 M in toluene, 2 mL, 0.06 mmol), and diphenylamine (372 mg, 2.2 mmol) in toluene (15 mL). The whole solution was refluxed for 12 hours. The reaction mixture was quenched with saturated aqueous NaHCO₃ (20 mL). The aqueous layer was separated and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel to give **3f**, which was further re-crystallized from CH₂Cl₂/hexanes to afford 643 mg of pure **3f** (95 %): m.p. 287 °C (DSC); T_d 443 °C (TGA); T_g 123 °C (DSC); M.W.: 676.84; ¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, *J* = 7.8, 2H), 7.49 (d, *J* = 7.6, 2H), 7.19-7.08 (m, 12H), 6.97 (t, *J* = 7.3, 4H), 6.89 (d, *J* = 8.2, 10H), 6.82 (s, 2H), 6.79 (t, *J* = 7.6, 2H), 6.54 (d, *J* = 2.2, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 152.0, 147.9, 147.1, 141.5, 138.6, 132.7, 130.7, 129.1, 128.8, 127.3, 127.0, 131.7, 124.8, 123.6, 123.1, 120.2, 119.7, 65.9; MS (ESI) 676.3 (M⁺, 53); TLC R_f 0.5 (CH₂Cl₂/hexane, 1/3).

N,N,N',N'-Tetraphenyl-5H-dibenzo[*a,d*]cycloheptene-3,7-diamine (4f)



To a 25-mL, two-necked, round-bottomed flask was placed **3,7-Dibromo-5H-dibenzo[*a,d*]cycloheptene** (350 mg, 1 mmol), Pd₂(dba)₃ (18 mg, 0.02 mmol), sodium *tert*-butoxide (288 mg, 3 mmol), P(*t*-Bu)₃ (0.03 M in toluene, 2 mL, 0.06 mmol), and diphenylamine (372 mg, 2.2 mmol) in anhydrous toluene (15 mL). The whole solution was stirred at reflux for 12 hours. The reaction mixture was quenched with saturated aqueous NaHCO₃ (20 mL). The aqueous layer was separated and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layers were dried (MgSO₄), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel (CH₂Cl₂/hexanes, 1/3) to give **4f**. The product was further re-crystallized from CH₂Cl₂/hexanes to afford 484 mg of analytically pure **4f** (485 mg, 92 %): m.p. 228 °C (DSC); T_d 397 °C (TGA); T_g 101 °C (DSC); M.W.: 526.67; ¹H NMR (400 MHz, CDCl₃) δ 7.24 (t, *J* = 7.7, 8H), 7.14 (d, *J* = 9.0, 2H), 7.09 (d, *J* = 7.7, 8H), 7.02 (t, *J* = 7.3, 4H), 6.92-6.90 (m, 4H), 6.86 (s,

2H), 3.53 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.1, 147.6, 138.6, 130.3, 129.6, 129.2, 129.0, 128.5, 122.9, 122.7, 121.2, 41.8; MS (ESI) 526.2 (M^+ , 100); TLC R_f 0.35 (CH_2Cl_2 /hexanes, 1/3).

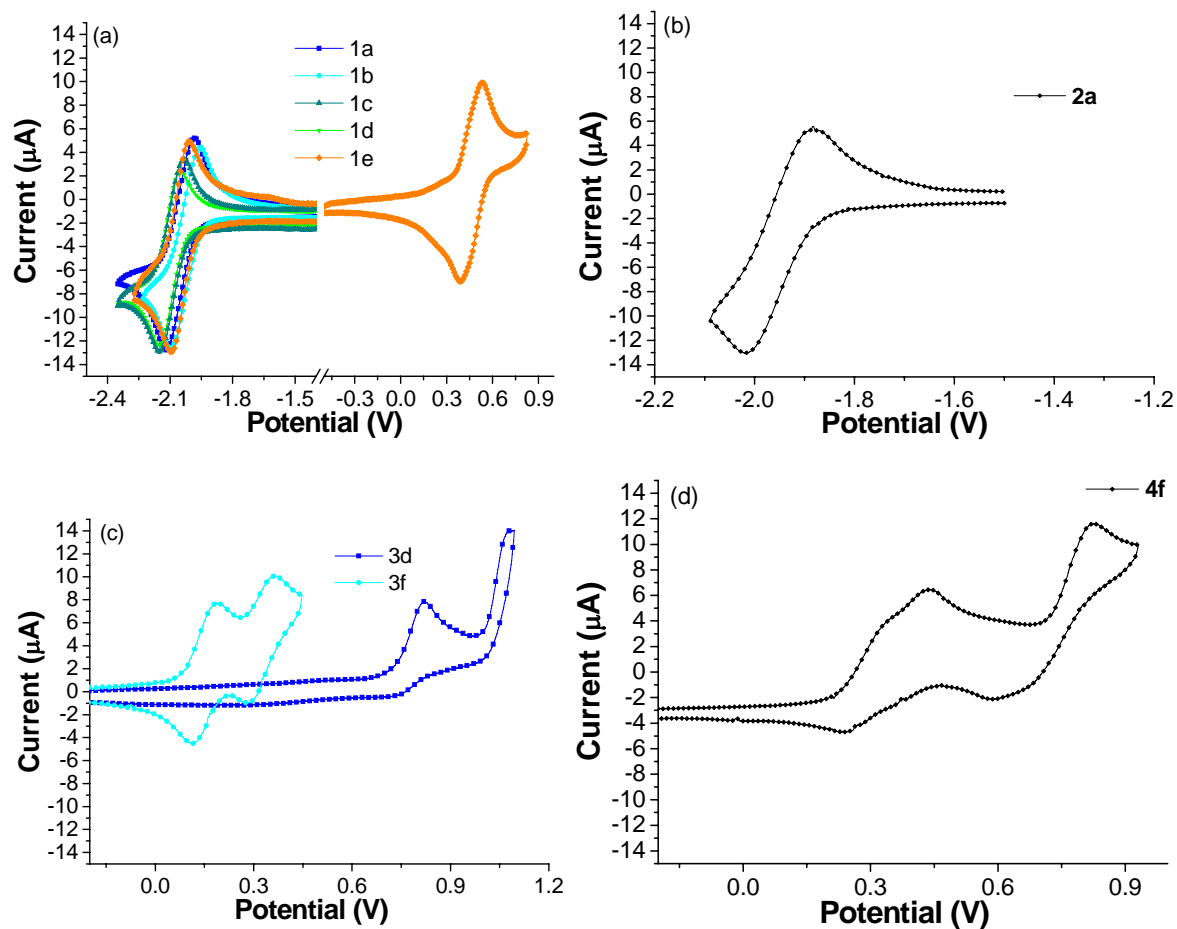


Figure S1. Stacked plots of cyclic voltammograms for (a) **1a-e**, (b) **2a**, (c) **3d** and **3f**, and (d) **4f**

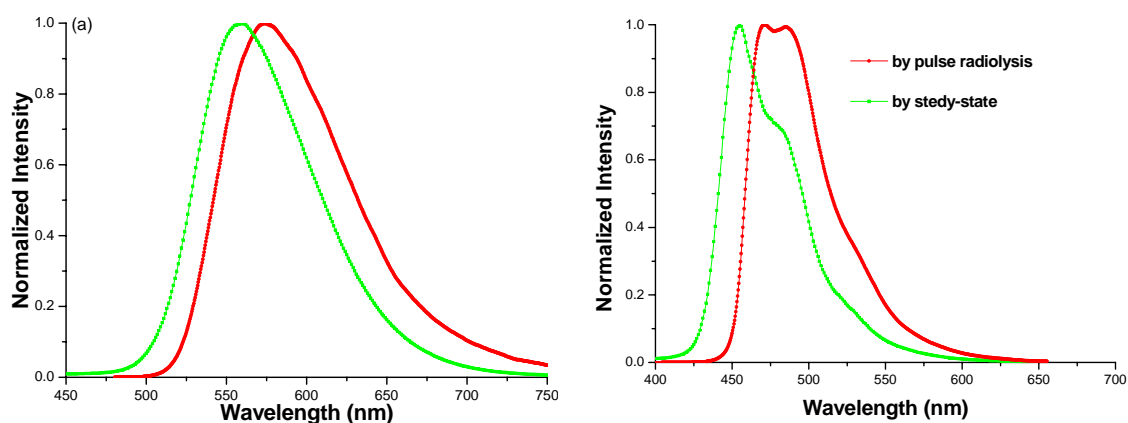


Figure S2. Stacked plots of emission spectra of **1e** (a) and **3f** (b) by steady-state at 10^{-5}M (green) and pulse radiolysis (red) measurements in Ar-saturated benzene.

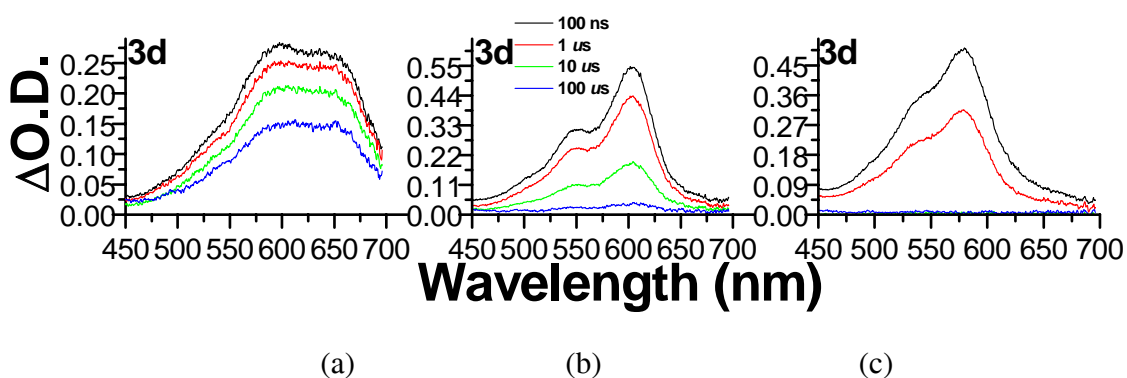


Figure S3. Time-resolved transient absorption spectrum stacked plots of **3d** observed at $t = 100$ ns (black), 1 (red), 10 (green), and 100 μ s (blue) after an electron pulse during pulse radiolysis measurements in Ar-saturated (a) DCE, (b) DMF, and (c) benzene solutions.

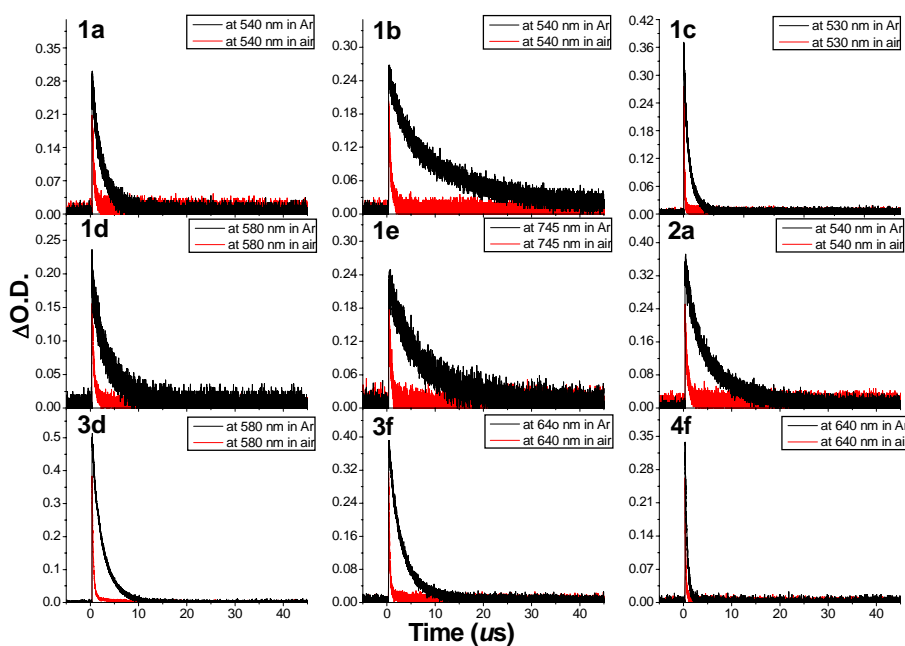


Figure S4. Decay profiles of the triplet excited state observed during the pulse radiolysis for **1a-e**, **2a**, **3d**, **3f**, and **4f** in Ar- and air-saturated benzene solution.

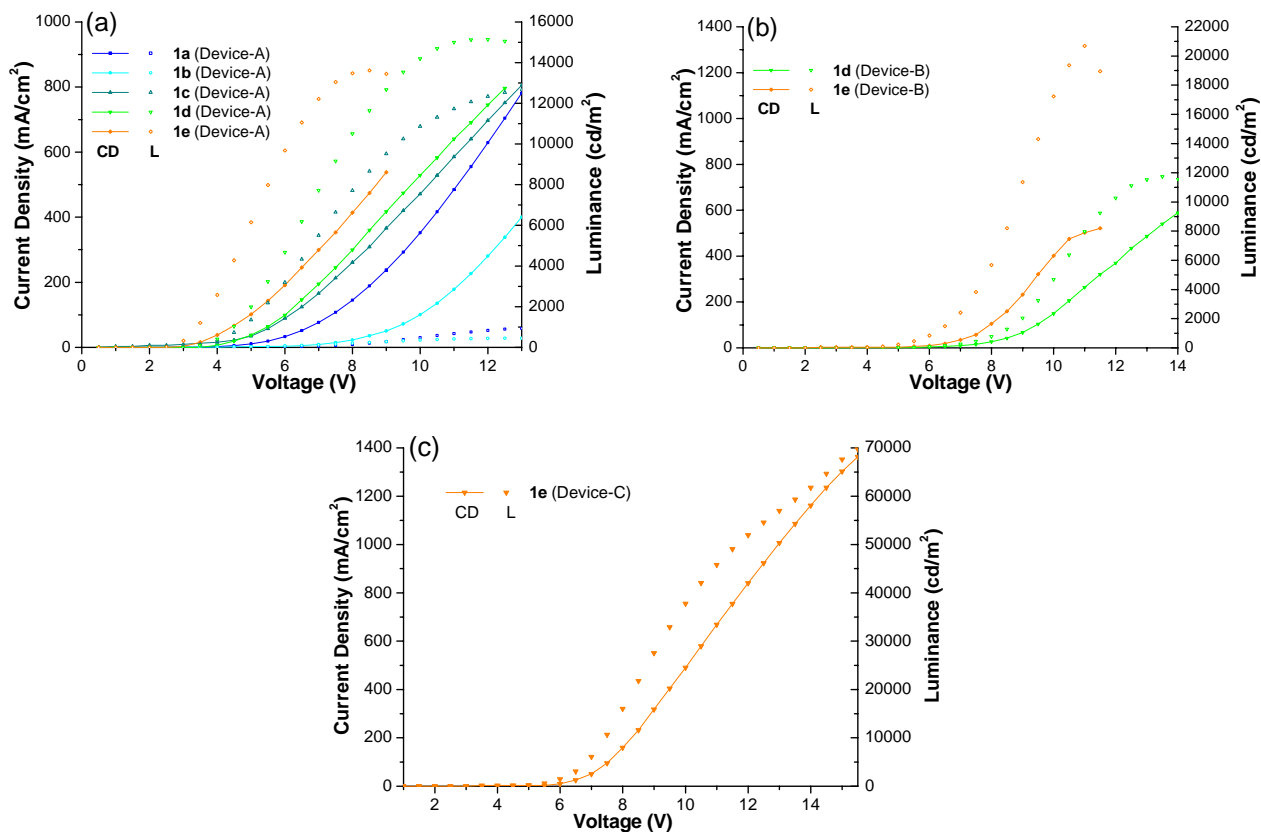


Figure S5. The stacked plots of the I-V-L characteristics [the plot of current density (mA/cm², I)/luminescence (cd/m², L) values vs. applied voltage (V, V) obtained for each device configuration] for (a) **1a-e** (Device-A), (b) **1d-e** (Device-B), and (c) **1e** (Device-C)

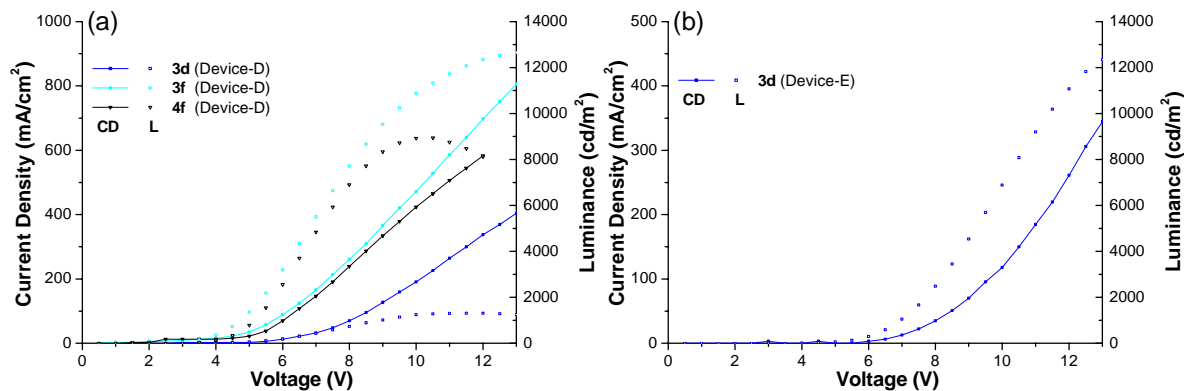


Figure S6. The stacked plots of the I-V-L characteristics for (a) **3d**, **3f**, and **4f** (Device-D) and (b) **3f** (Device-E)

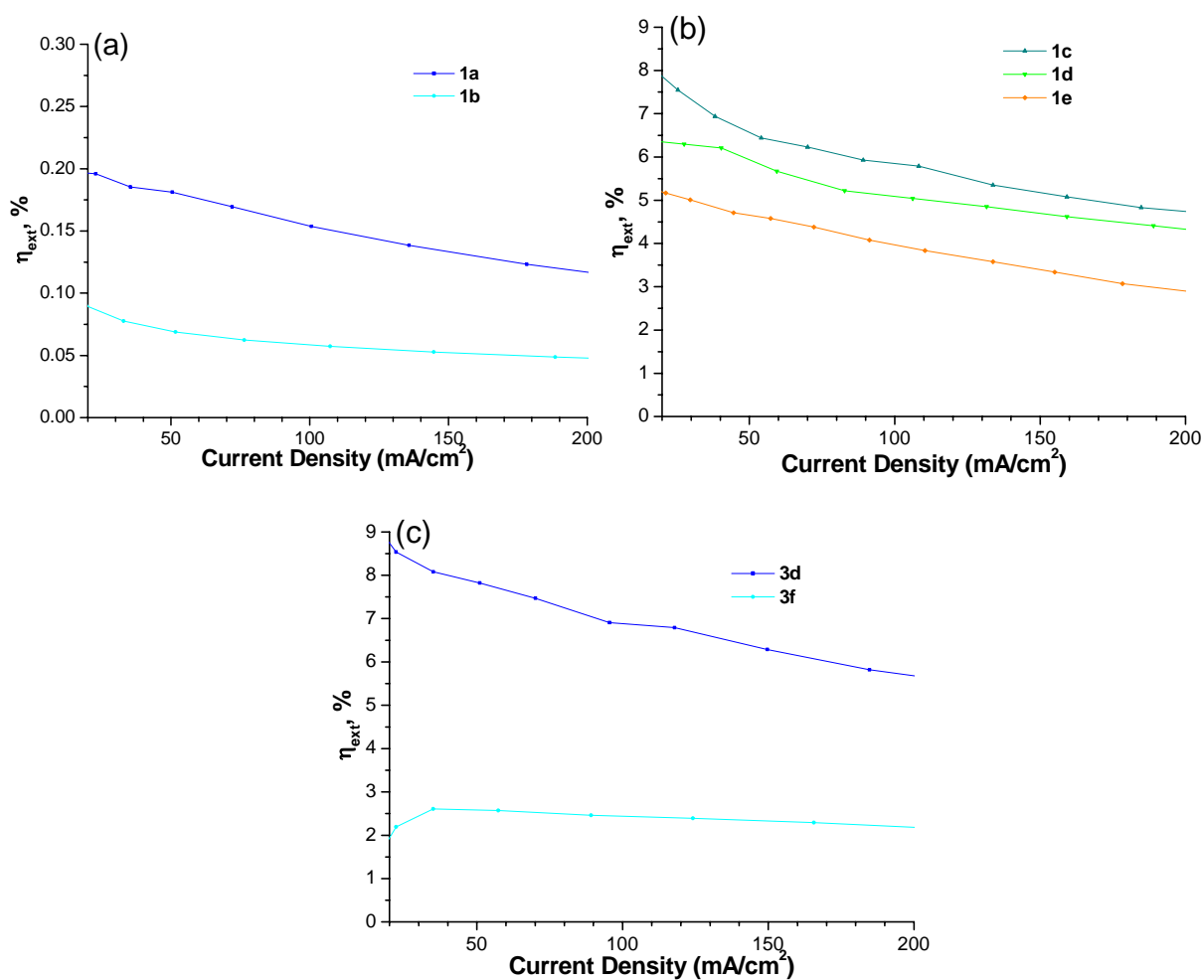


Figure S7. Current Density-External quantum efficiency stacked diagram for (a) **1a** and **1b**, (b) **1c-e**, and (c) **3d**, **3f**, and **4f**

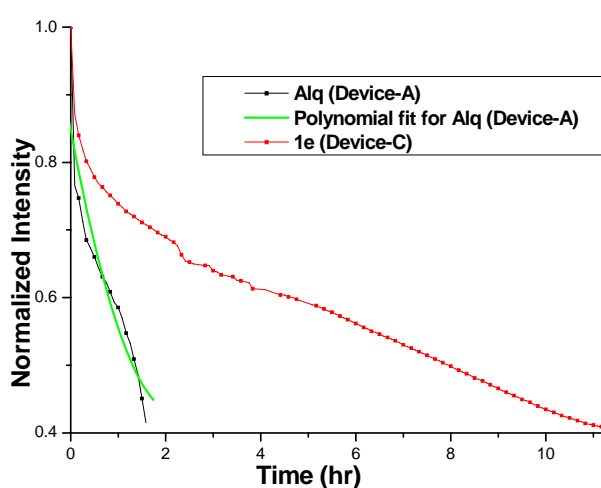
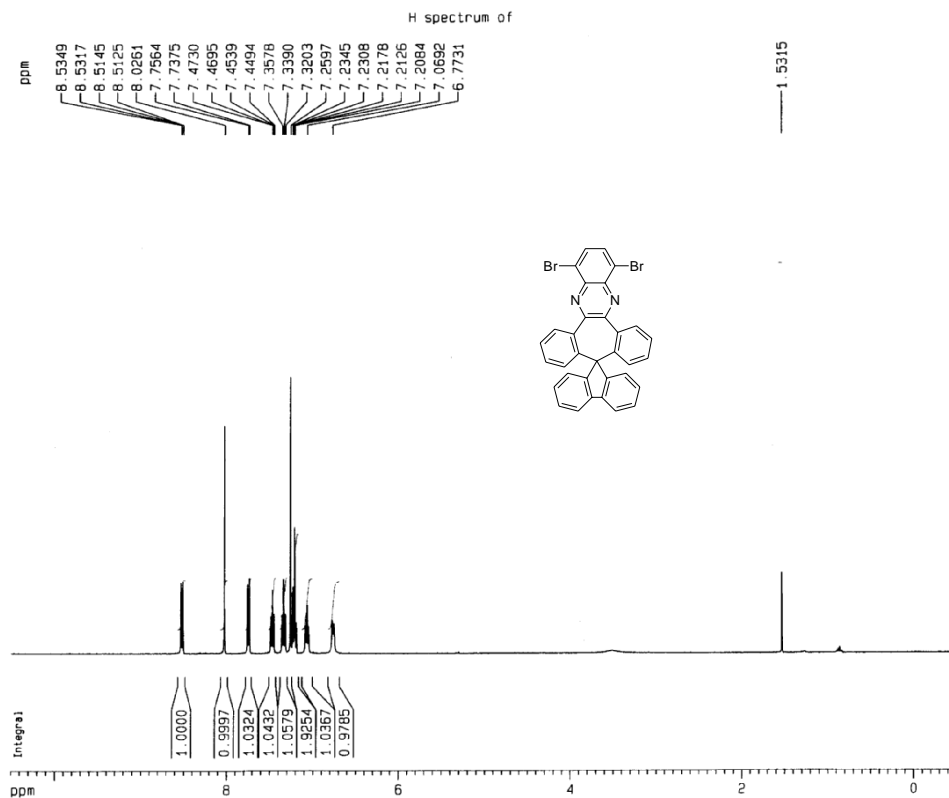


Figure S8. Stacked diagram of lifetime measurements for device-A of Alq and device-C of **1e**



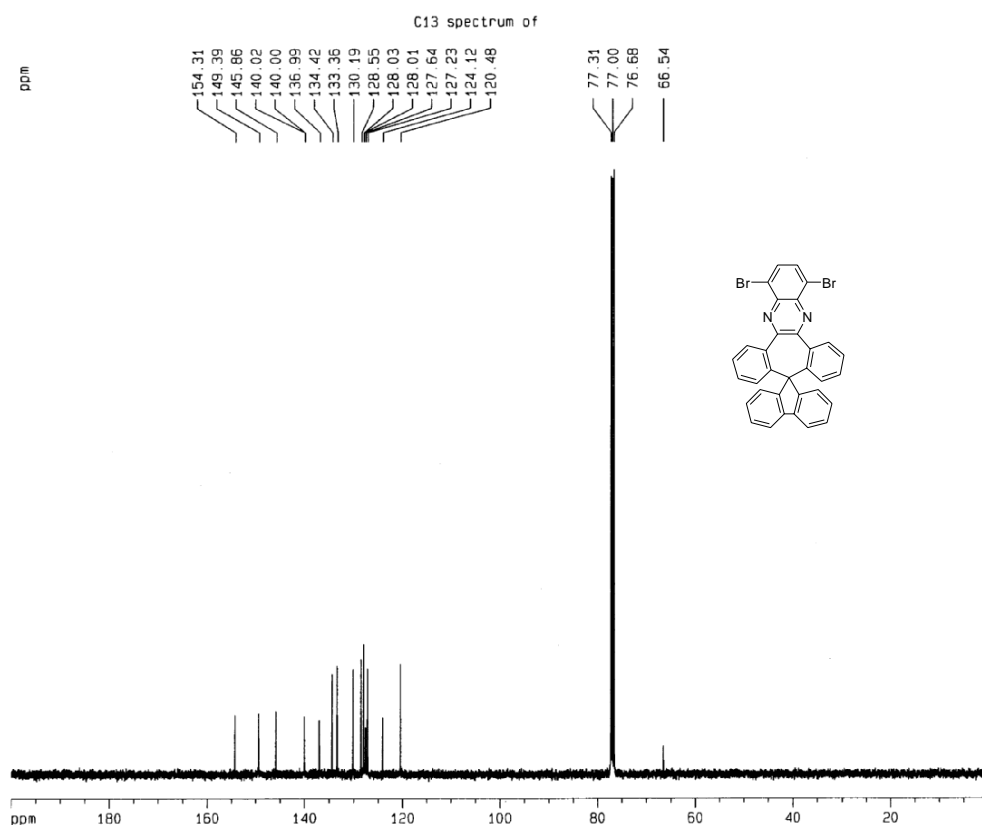
Current Data Parameters
NAME 2005-03-01
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050302
Time 8.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 15384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters
SI 15384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P 0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm



Current Data Parameters
NAME 2005-03-01
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050301
Time 8.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 837
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

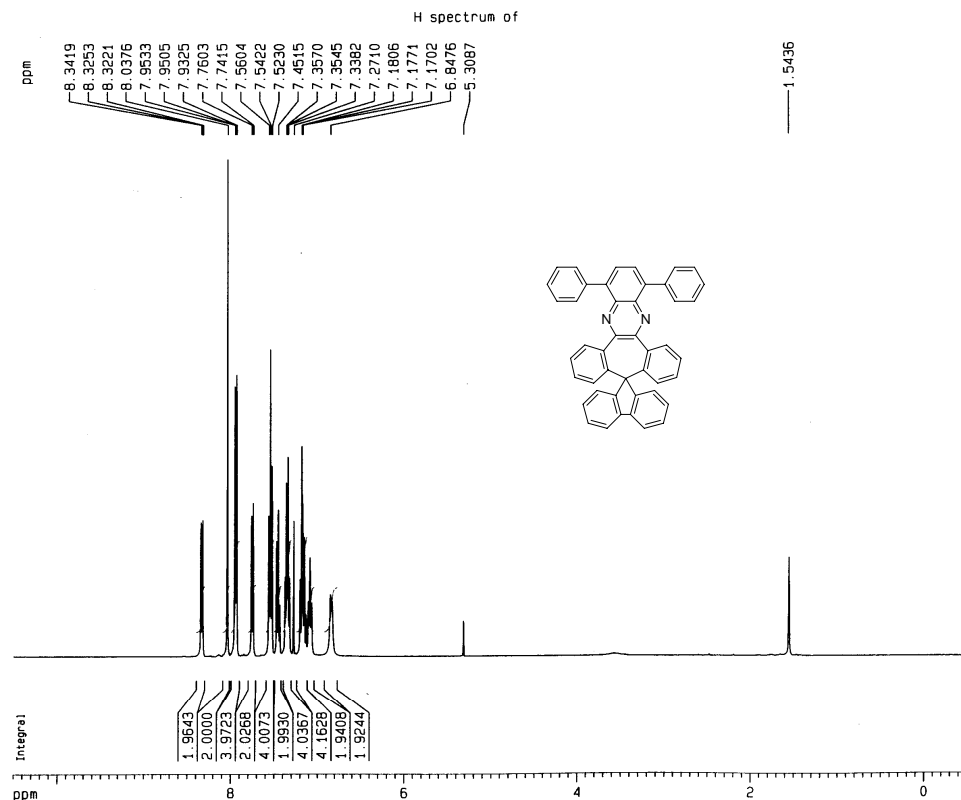
***** CHANNEL f1 *****
NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SF01 100.6242995 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SF02 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra for 1



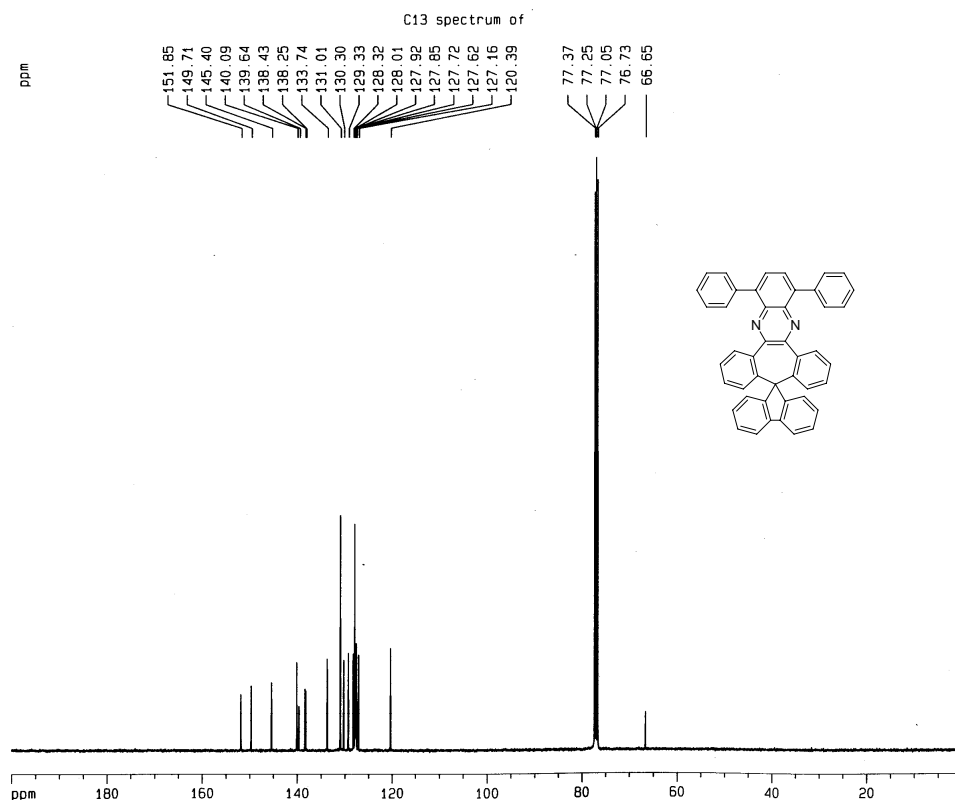
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NAME 05-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040610
Time 20.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 203.2
DM 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.05 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm



Current Data Parameters
NAME 05-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040612
Time 11.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4595
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8000
DM 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

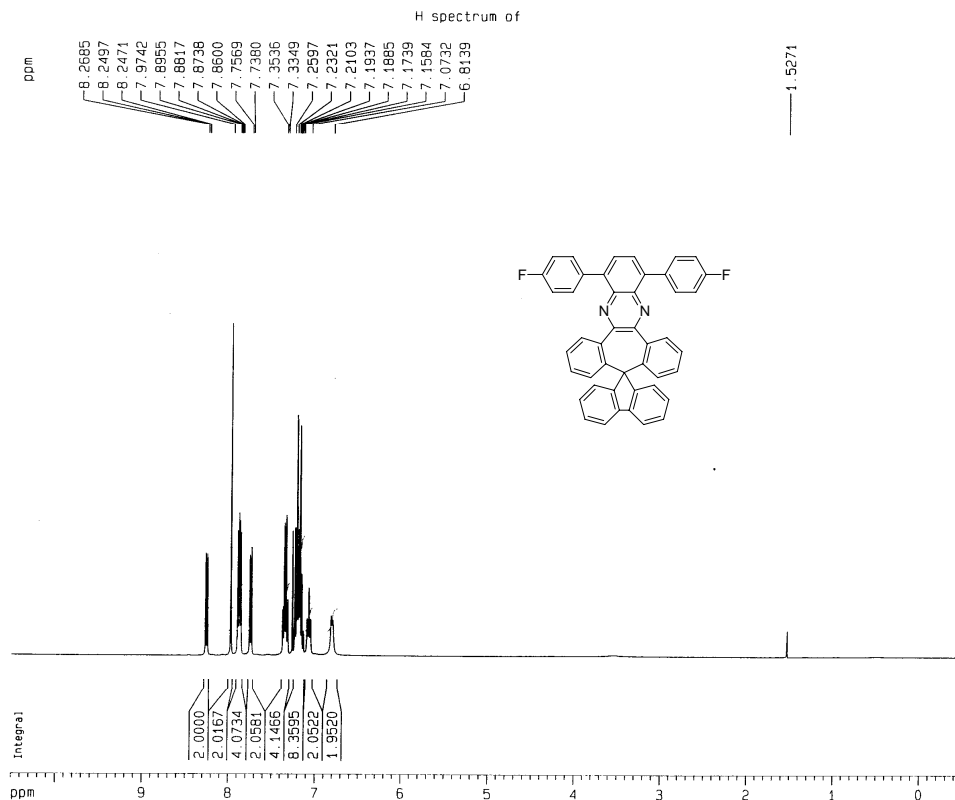
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NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SF01 100.6242995 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SF02 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127672 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra for 1a



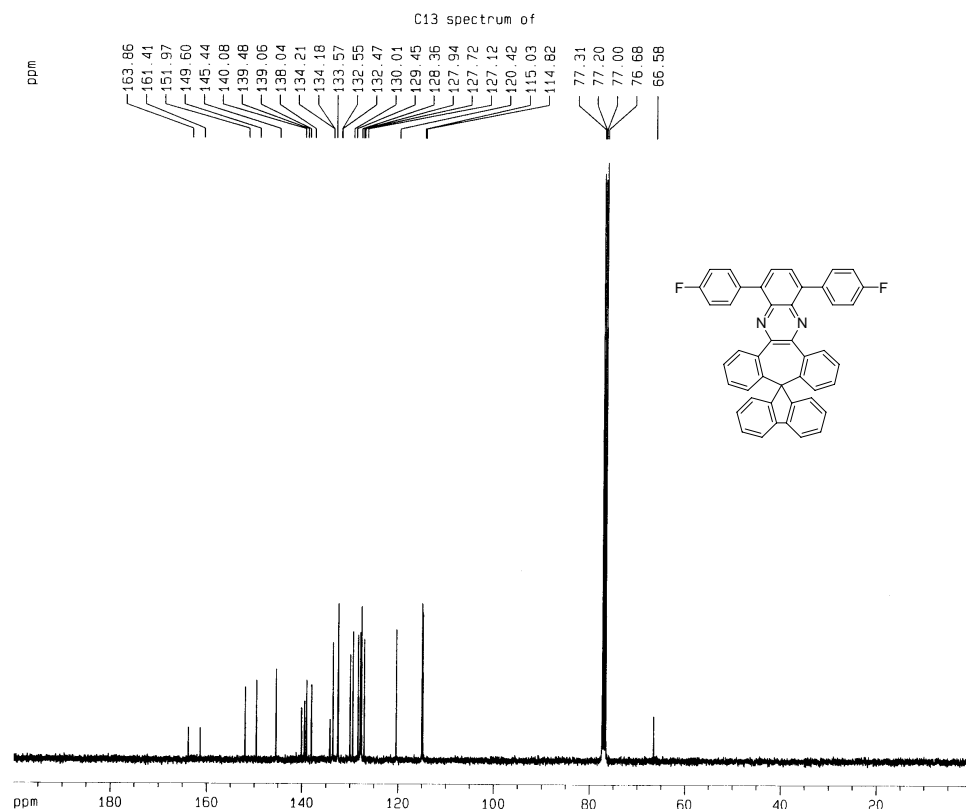
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NAME 2005-03-24
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 8.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07152 Hz/cm



Current Data Parameters
NAME 2005-03-24
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050324
Time 8.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1245
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

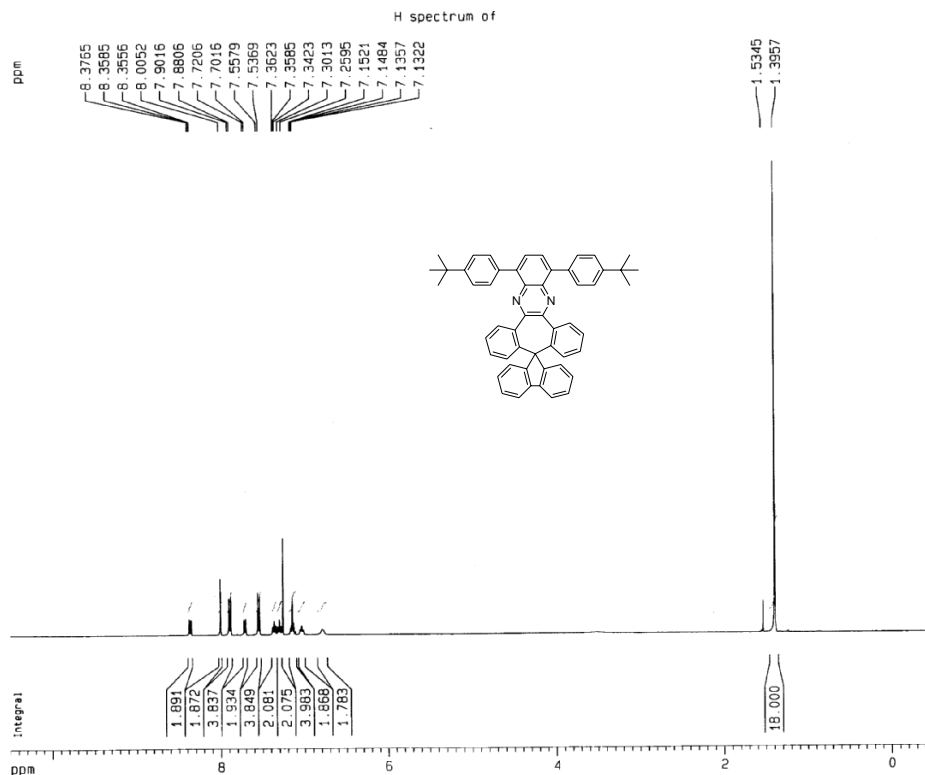
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NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SF01 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SF02 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra for **1b**



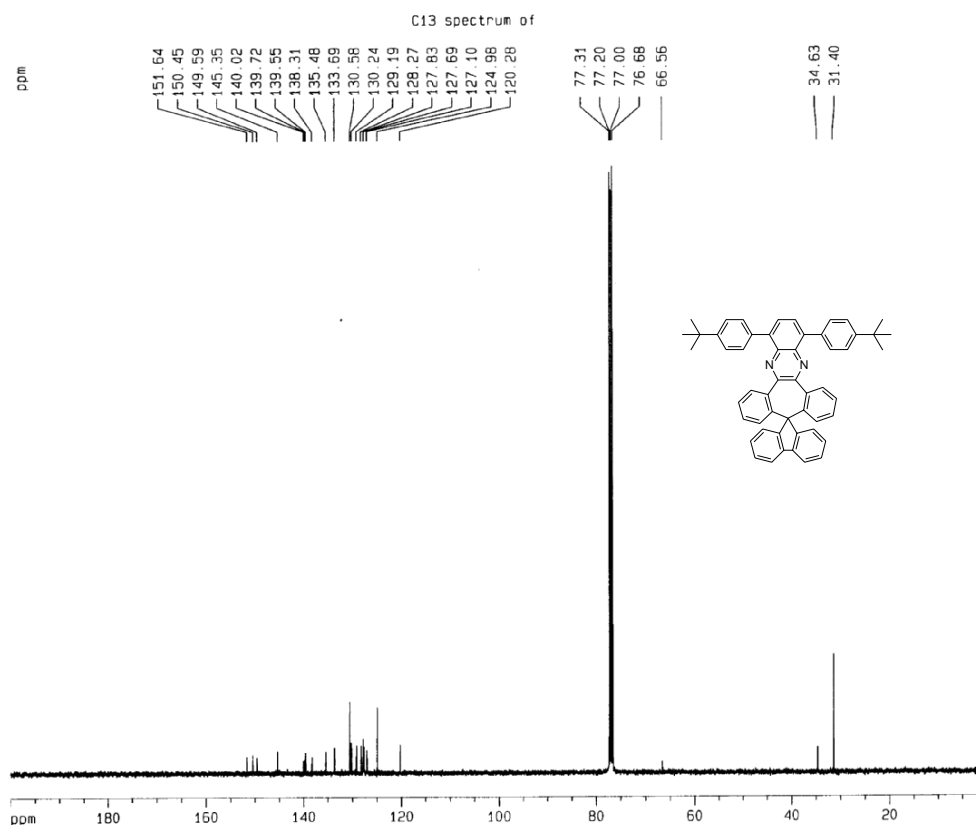
Current Data Parameters
NAME 2005-03-10
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050310
Time 9.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DM 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SFO1 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300959 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P ~200.06 Hz
F2 ~200.06 Hz
PPMCH 0.55000 ppm/cm
HZCM 220.07150 Hz/cm



Current Data Parameters
NAME 2005-03-10
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050310
Time 9.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1704
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DM 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

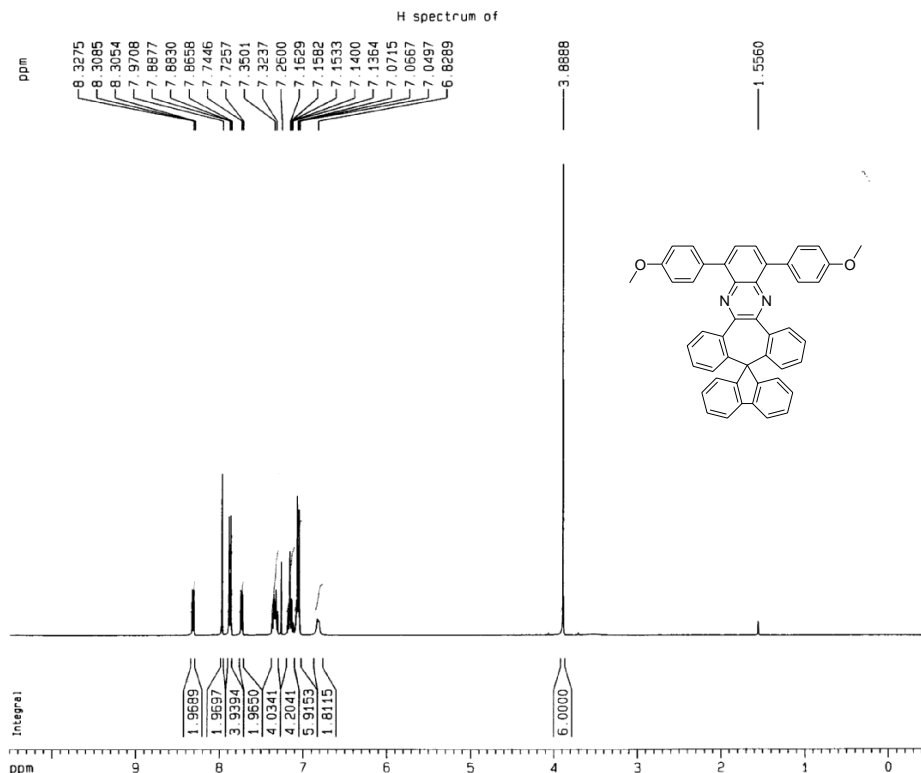
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NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SFO1 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SFO2 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCH 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra for **1c**



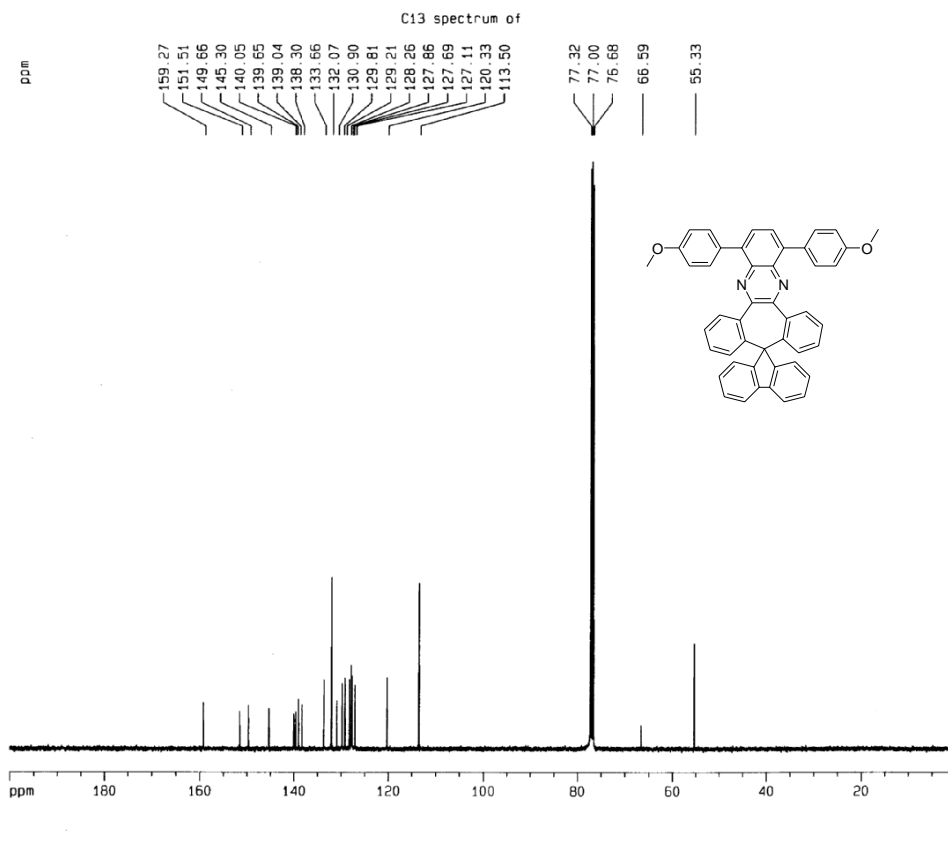
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050406
Time 6.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3654756 sec
RG 362
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SFO1 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07152 Hz/cm



Current Data Parameters
NAME 2005-04-06
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050406
Time 7.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2276
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

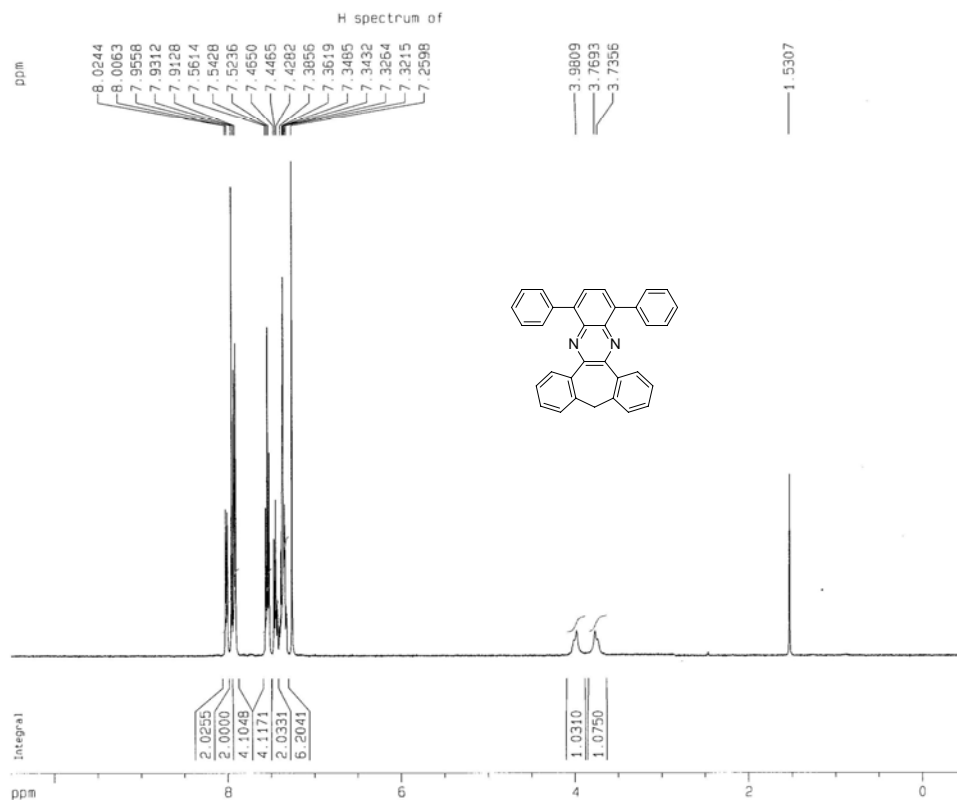
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NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SFO1 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SFO2 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra for **1d**



Current Data Parameters

NAME CH2-o-o-Ph
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20080430
Time 17.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22
DW 83.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.5000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

***** CHANNEL f1 *****

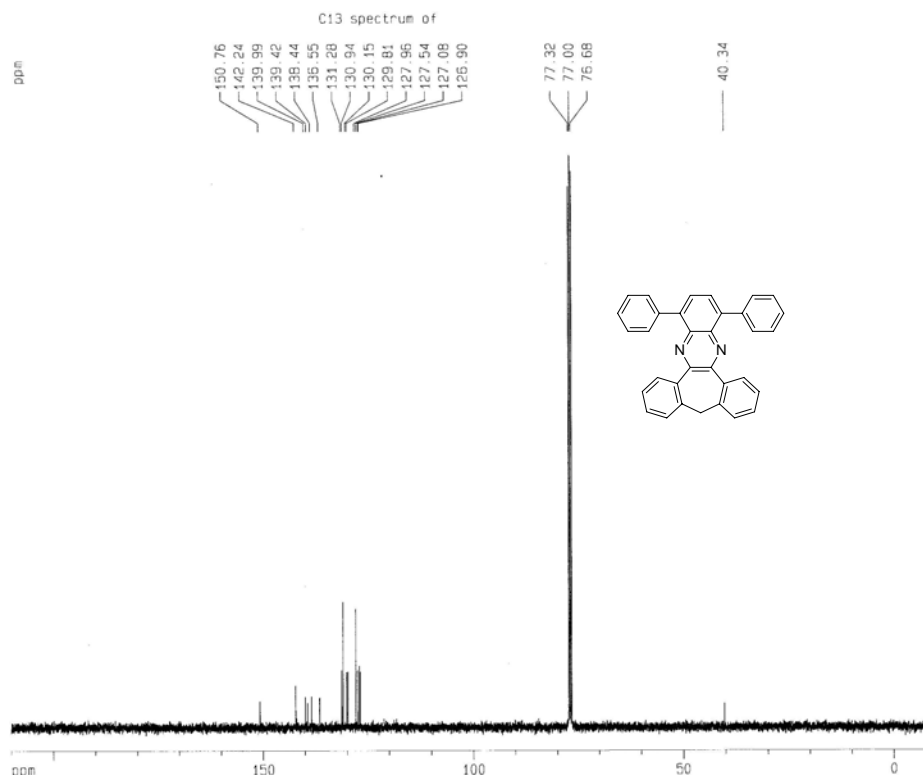
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters

SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm



Current Data Parameters

NAME CH2-o-o-Ph
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090501
Time 16.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 220
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8000
DW 19.900 usec
DE 6.50 usec
TE 298.6 K
D1 1.5000000 sec
d11 0.0300000 sec
DELTA 1.3999999 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

***** CHANNEL f1 *****

NUC1 13C
P1 9.80 usec
PL1 5.00 dB
SF01 100.6242999 MHz

***** CHANNEL f2 *****

CPDPRG2 waltz16
NUC2 1H
POPRG2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SF02 400.1319000 MHz

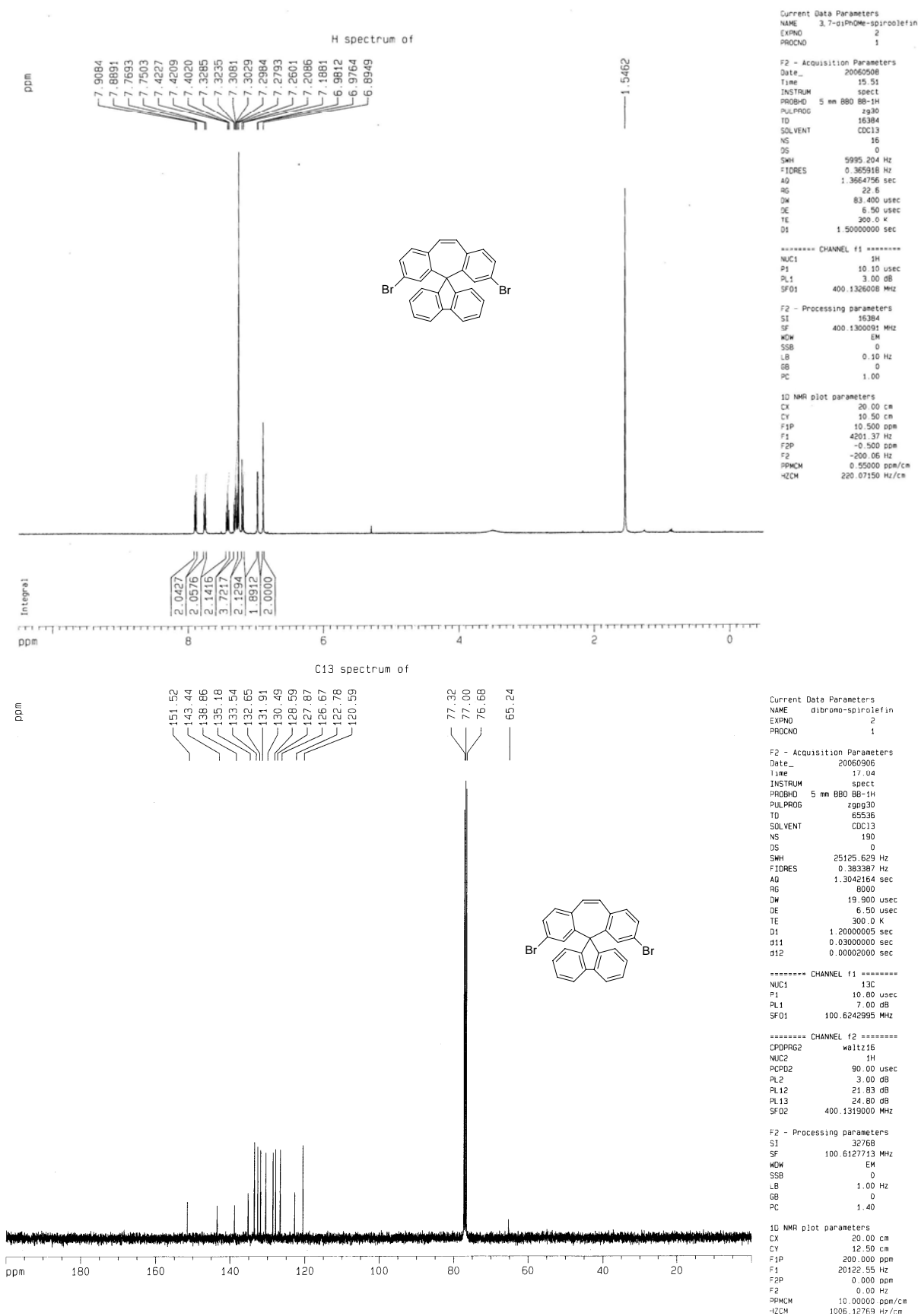
F2 - Processing parameters

SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

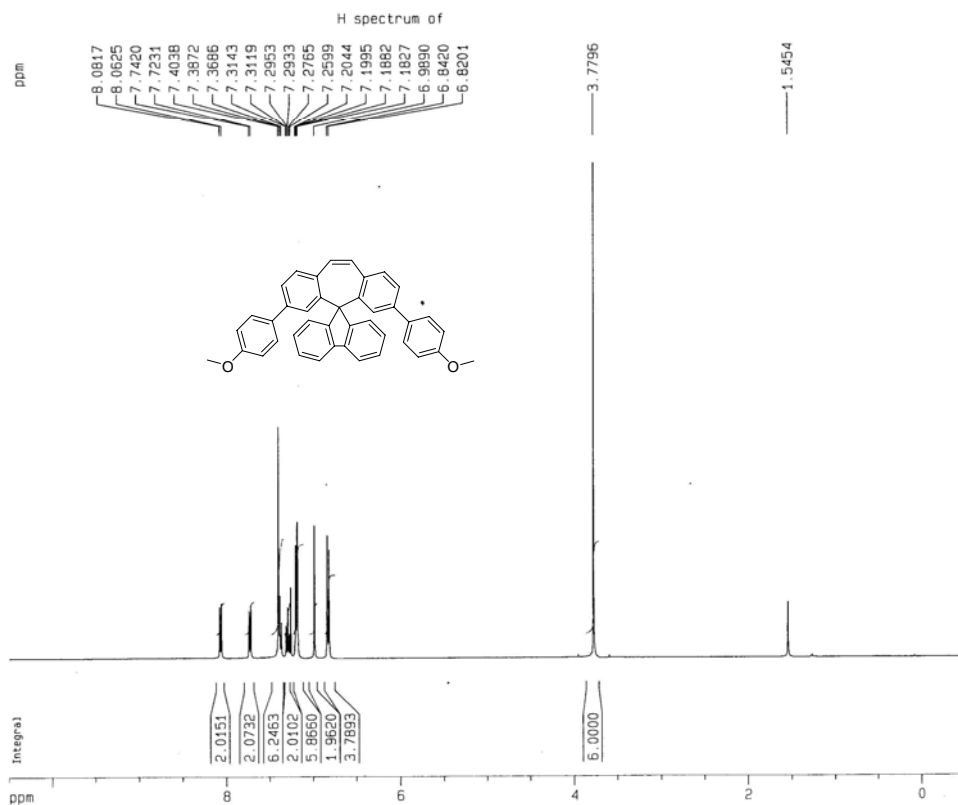
1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
F1P 210.000 ppm
F1 21129.68 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.74048 Hz/cm

^1H and ^{13}C NMR spectra for **2a**



^1H and ^{13}C NMR spectra of 3



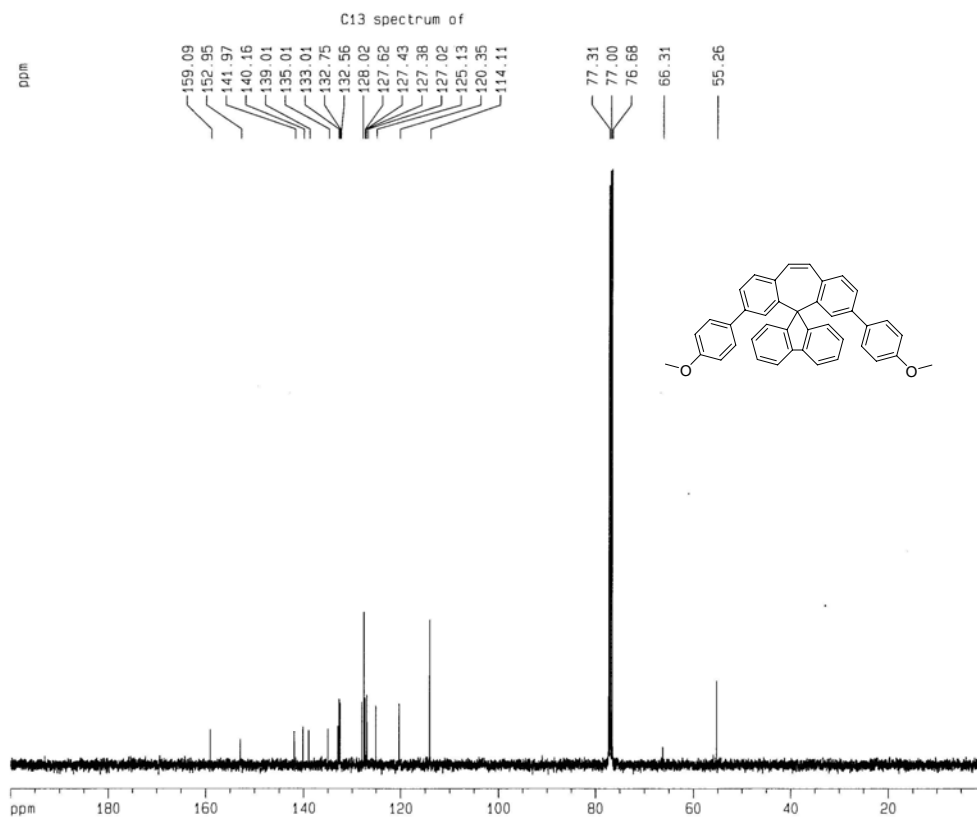
Current Data Parameters
NAME SSB-diPhOMe
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070928
Time 18.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22
DW 83.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm



Current Data Parameters
NAME SSB-diPhOMe
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070927
Time 18.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8000
DW 19.900 usec
DE 6.50 usec
TE 299.5 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999999 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

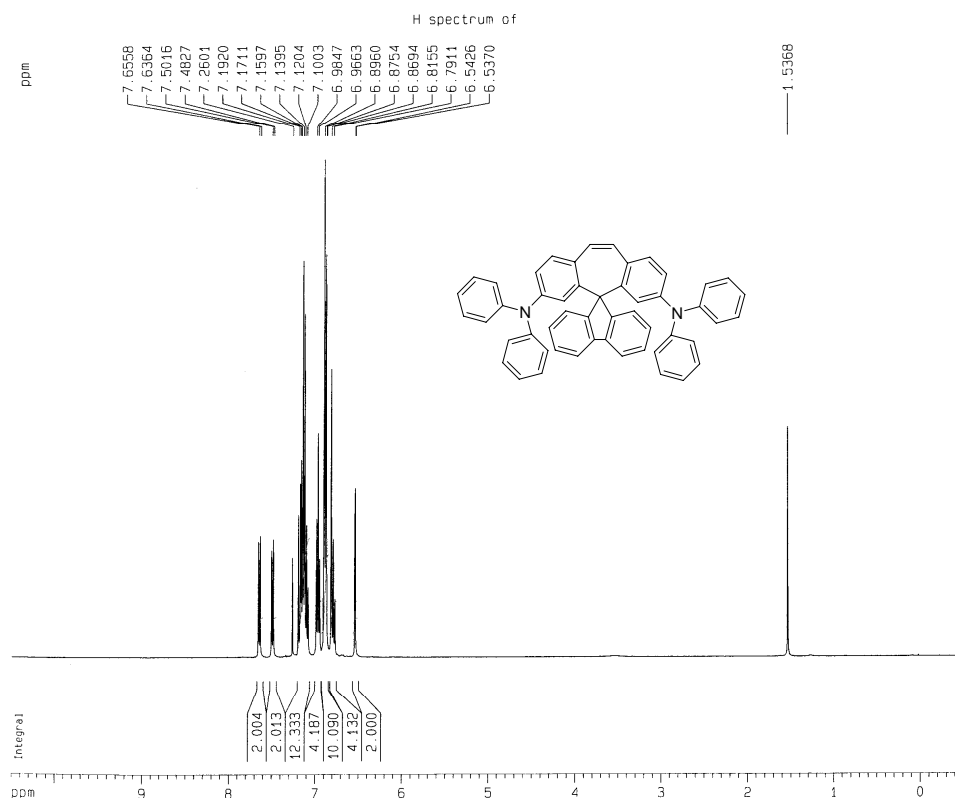
***** CHANNEL f1 *****
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SF01 100.6242995 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SF02 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra of **3d**



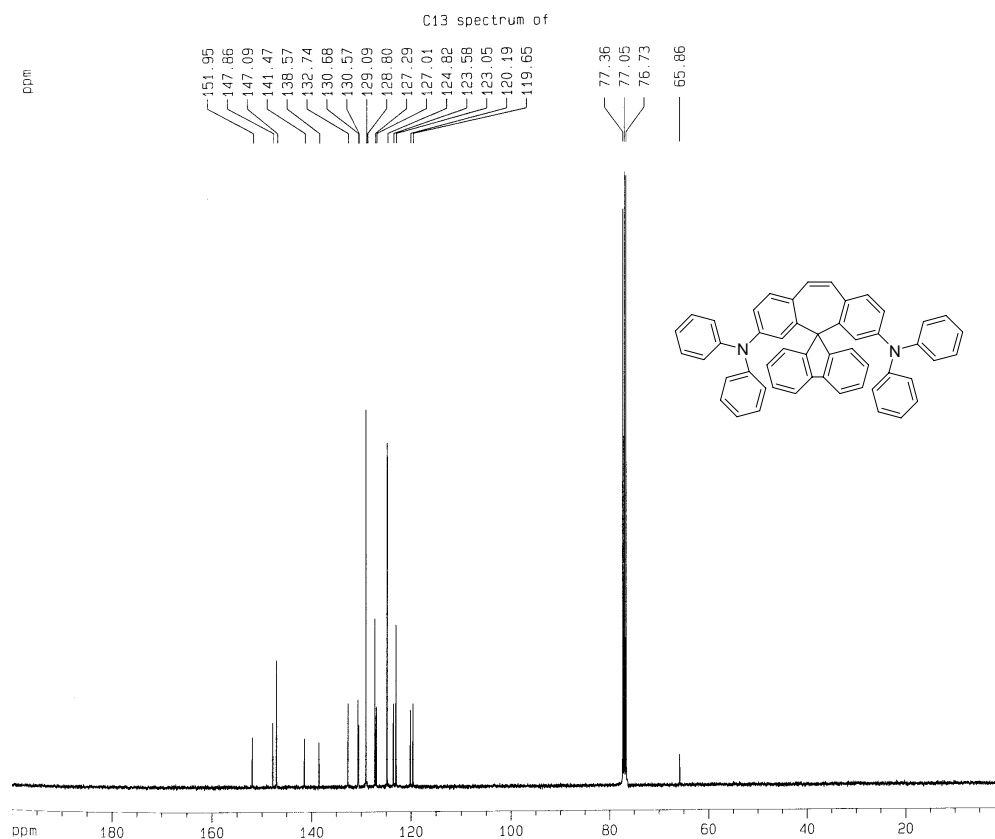
Current Data Parameters
NAME SSB-N-dPh
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060630
Time 20.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 3.00 dB
SF01 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07152 Hz/cm



Current Data Parameters
NAME sss-N-dPh
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060630
Time 20.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1913
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8000
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

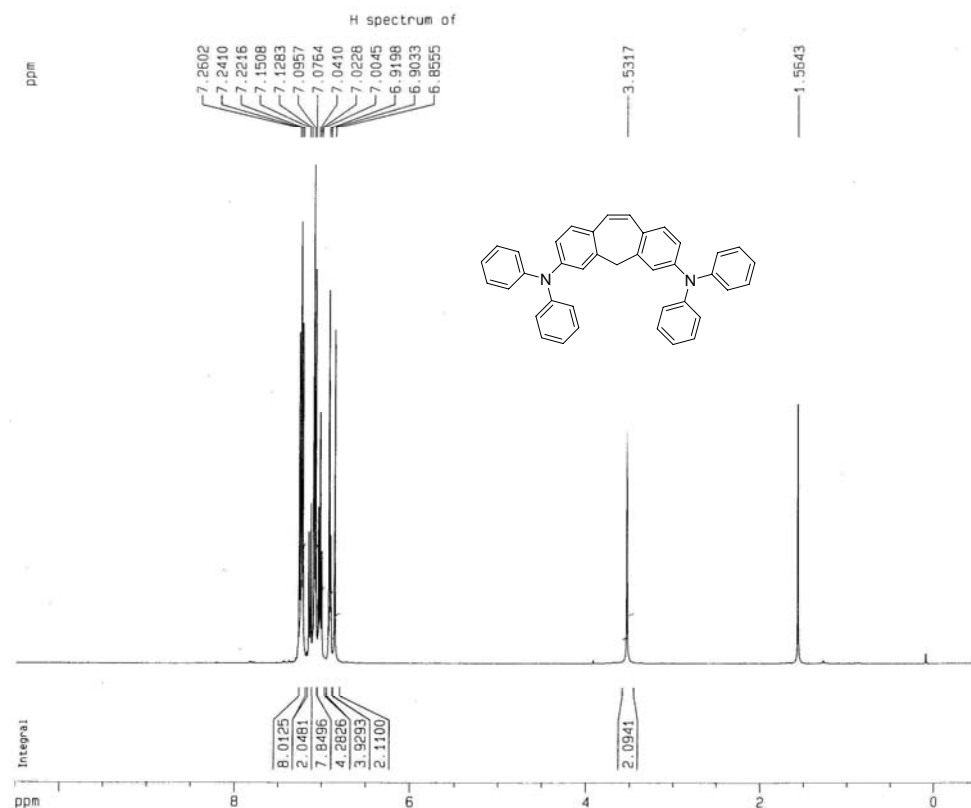
===== CHANNEL f1 =====
NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SF01 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SF02 400.1319000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127672 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1006.12768 Hz/cm

^1H and ^{13}C NMR spectra of **3f**



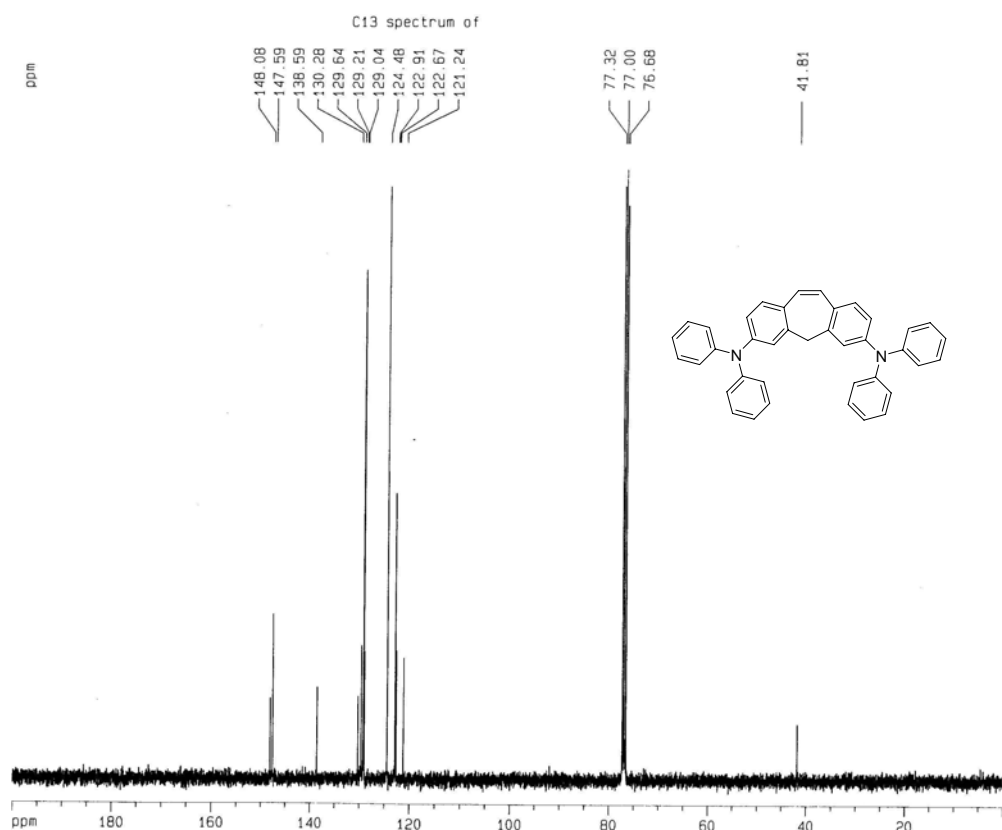
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070314
 Time 20.04
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 16384
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 181
 OW 83.400 usec
 DE 5.50 usec
 TE 296.7 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.70 usec
 PL1 2.00 dB
 SF01 400.1326008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.50 cm
 FIP 10.500 ppm
 F1 4201.37 Hz
 F2P -0.500 ppm
 F2 -200.06 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 220.07150 Hz/cm



Current Data Parameters
 NAME 20070313-01
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070314
 Time 20.08
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 156
 DS 0
 SWH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 8000
 OW 19.900 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.20000005 sec
 d11 0.03000000 sec
 DELTA 1.10000002 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 9.80 usec
 PL1 6.00 dB
 SF01 100.6242995 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 2.00 dB
 PL12 20.00 dB
 PL13 23.00 dB
 SF02 400.1319000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127729 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 200.000 ppm
 F1 20122.55 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1006.12769 Hz/cm

^1H and ^{13}C NMR spectra of **4f**

References and Notes

- (1) Chen, C.-T.; Wei, Y.; Lin, J.-S.; Moturu, M.V. R. K.; Chao, W.-S.; Tao, Y.-T.; Chien, C.-H. *J. Am. Chem. Soc.* **2006**, *128*, 10992.
- (2) Tsubata Y.; Suzuki T.; Miyashi T.; Yamashita Y. *J. Org. Chem.* **1992**, *57*, 6749.
- (3) Rigaudy, P. J.; Nédélec, L. *Bull. Soc. Chim. Fr.*; **1959**; 638, 642.
- (4) Mancilha, F. S.; Neto, B. A. D.; Lopes , A. S.; Moreira, P. F.; Quina, F. H.; Gonçalves, R. S.; Dupont, J. *Eur. J. Org. Chem.* **2006**, *21*, 4924.
- (5) Wei, Y.; Chen, C.-T. *J. Am. Chem. Soc.* **2007**, *129*, 7478.
- (6) Hartwig, J. F. *Acc. Chem. Res.* **1998**, *31*, 852.
- (7) Complete reference 5a in the manuscript: Anderson, J. D.; McDonald, E. M.; Lee, P. A.; Anderson, M. L.; Ritchie, E. L.; Hall, H. K.; Hopkins, T.; Padias, A.; Thayumanavan, S.; Barlow, S.; Marder, S. R.; Jabbour, G. E.; Shaheen, S.; Kippelen, B.; Peyghambarian, N.; Wightman, R. M.; Armstrong, N. R.; Mash, E. A.; Wang, J. *J. Am. Chem. Soc.* **1998**, *120*, 9646.