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SUPPORTING INFORMATION

STRUCTURE-PROPERTY RELATIONSHIPS FOR TWO-PHOTON ABSORBING CHROMOPHORES: *BIS*-DONOR DIPHENYLPOLYENE AND *BIS*(STYRYL)BENZENE DERIVATIVES

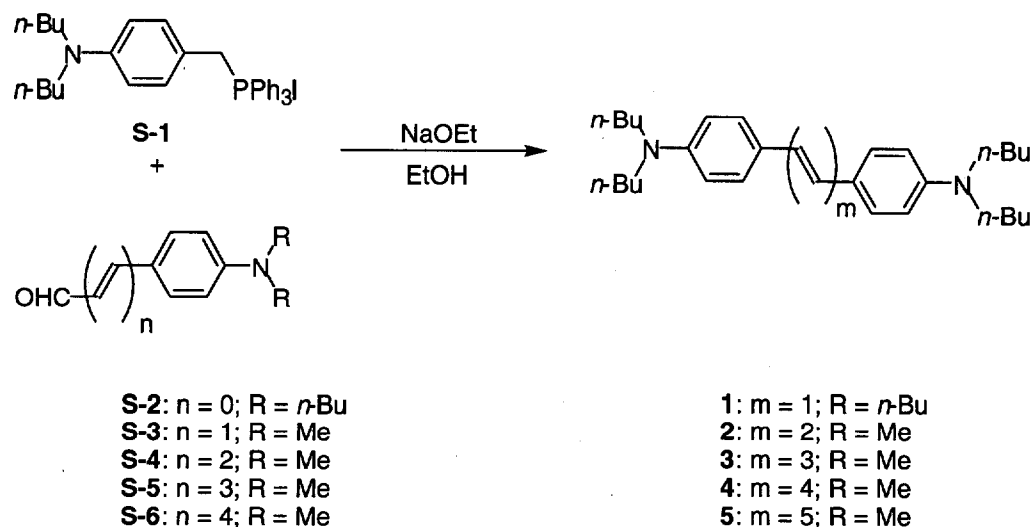
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Materials. All solvents, common reagents, (N,N-di-*n*-butylamino)benzaldehyde (**S-2**), and terephthalaldehyde (**S-8**) were purchased as reagent grade and used without further purification. 1,2-*Bis*[4-(diphenylamino)phenyl]ethene (**6**) was prepared according to the literature.¹ The following starting materials were prepared according to the literature: [[4-(dibutylamino)phenyl]methylene]triphenylphosphonium iodide (**S-1**);² polyenals **S-3** through **S-6**, **S-14**;³ [(2,5-dimethoxy-1,4-phenylene)bis-(methylene)]bistriphenylphosphonium dichloride (**S-9**);⁴ 1-bromo-4-(*m*-tolylphenyl-amino)benzene (**S-10**);⁵ tetramethyl *p*-xylylenediphosphonate (**S-12**);⁶ [[2,5-bis-(dodecyloxy)-1,4-phenylene]bis(methylene)] bis-triphenyl phosphonium dibromide (**S-13**);⁷ and 4-bromo-2,5-dimethoxybenzaldehyde (**S-15**).⁸

Instrumentation. ¹H-NMR were recorded on a General Electric QE-300 FT NMR spectrometer using the proton of the solvent as the internal standard. Chemical shifts are reported in parts per million (ppm). When peak multiplicities are given, the following

abbreviations are used: s, singlet; d, doublet; t, triplet; q, quartet; sx, sextet; m, multiplet; br, broad. ^{13}C -NMR spectra were proton decoupled and recorded on a QE-300 or Bruker AMX-500 using the carbon signal of the deuterated solvent as the internal standard. Electron Impact (EI) and Fast Atom Bombardment (FAB) mass spectra were performed on Finnigan-MAT CH-5 and 311-A spectrometers at the Caltech Mass Spectrometry Facility. Elemental analyses were performed by the Caltech Micro Analytical Service Laboratory. UV spectra were taken using a Hewlett Packard UV spectrophotometer operating between 190-820 nm. Flash chromatography was performed with EM science 37-75 μm silica gel. Analytical thin layer chromatography was performed on EM Science silica plates with F-254 indicator and the visualization was accomplished by UV lamp or using the ammonium molybdate stain mixture.

General Procedure for the Wittig Reaction (Scheme 1). Sodium (3 equivalents) was slowly dissolved in 100 mL of absolute ethanol and added to a solution of the aldehyde (1 equivalent) and the phosphonium salt (1 to 2 equivalents) in 300 mL of absolute ethanol. The resulting mixture was heated under reflux for 15 hours. After cooling to room temperature, either methanol or water was added to precipitate the *trans*-stilbene or diphenyl polyene, respectively. Usually, the triphenylphosphine oxide and *cis*-stilbene did not precipitate in the solvent mixture. When a mixture of *trans* and *cis* did precipitate, the crude mixture was isomerized to all *trans* by dissolution in toluene and refluxing with a fleck of iodine for 1 h. Further purification can be accomplished by filtration through Florisil. To achieve correct elemental analysis, the products were either chromatographed on silica gel or recrystallized from ethanol (stilbene **1**) or acetone (polyenes **2-5**).



Scheme 1

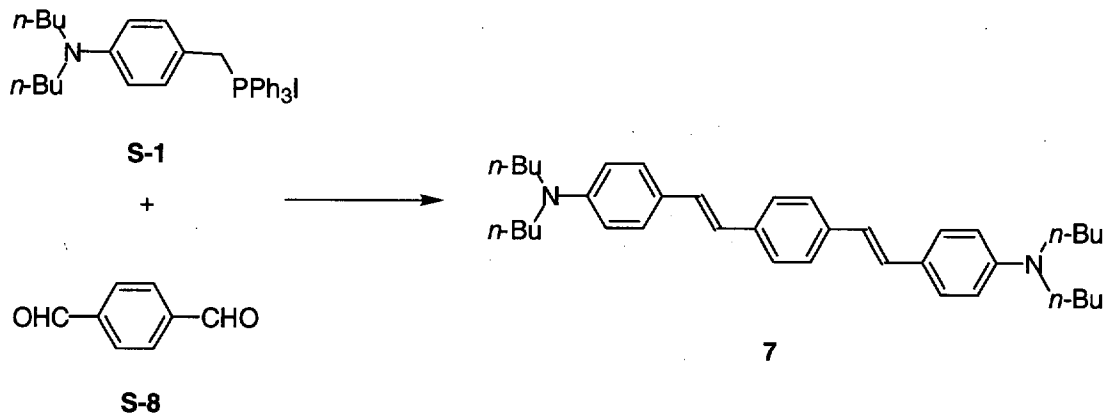
***E*-4,4'-Bis(*N,N*-di-*n*-butylamino)stilbene (1).** Prepared from **S-1** and dibutylaminobenzaldehyde (**S-2**) by the general Wittig procedure. ^1H NMR (300 MHz, acetone- d_6) δ (ppm) 7.31 (d, $J = 8.7$ Hz, 4H), 6.81 (s, 2H), 6.64 (d, $J = 8.7$ Hz, 4H), 3.32 (t, $J = 7.5$ Hz, 8H), 1.57 (m, 8H), 1.36 (m, 8H), 0.94 (t, $J = 7.27$, 12H); ^{13}C NMR (75 MHz, acetone- d_6) δ (ppm) 148.122, 127.82, 126.50, 124.77, 112.73, 51.28, 30.27, 20.87, 14.26; HRMS (FAB) m/z calcd: 434.3661; found: 434.3673. Anal. Calcd for $\text{C}_{30}\text{H}_{48}\text{N}_2$: C, 82.89; H, 10.67; N 6.44. Found: C, 82.55; H, 9.20; N 6.37.

***E,E*-1-(4-*N,N*-di-*n*-butylaminophenyl)-4-(4'-*N,N*-dimethylaminophenyl)-1,3-butadiene (2).** Prepared from **S-1** and 3-[4-(dimethylamino)phenyl]-2-propenal (**S-3**) by the general Wittig procedure. ^1H NMR (300 MHz, benzene- d_6) δ (ppm) 7.45 (d, $J = 4.4$ Hz, 2H), 7.42 (d, $J = 4.3$ Hz, 2H), 7.04-6.95 (m, 2H), 6.74-6.55 (m, 6H), 3.06 (t, $J = 7.5$ Hz, 4H), 2.51 (s, 6H), 1.44 (p, $J = 7.3$ Hz, 4H), 1.16 (s, $J = 7.5$ Hz, 4H), 0.84 (t, $J = 7.3$ Hz, 6H); HRMS (FAB) m/z calcd: 376.2878, found: 376.2880. Anal. Calcd for $\text{C}_{26}\text{H}_{36}\text{N}_2$: C, 82.93; H, 9.64; N 7.44. Found: C, 82.72; H, 9.78; N, 7.44.

***E,E,E*-1-(4-*N,N*-di-*n*-butylaminophenyl)-6-(4'-*N,N*-dimethylaminophenyl)-1,3,5-hexatriene (3).** Prepared from **S-1** and 5-[4-(dimethylamino)phenyl]-2,4-pentadienal (**S-4**) by the general Wittig procedure. ^1H NMR (300 MHz, benzene- d_6) δ (ppm) 7.42-7.37 (m, 4H), 6.97-6.89 (m, 2H), 6.68-6.54 (m, 8H), 3.04 (t, $J = 7.5$ Hz, 4H), 2.49 (s, 6H), 1.42 (p, $J = 7.5$ Hz, 4H), 1.15 (s, $J = 7.3$ Hz, 4H), 0.83 (t, $J = 7.3$ Hz, 6H); ^{13}C NMR (75 MHz, benzene- d_6) δ (ppm) 150.11, 147.91, 132.93, 132.53 (2), 132.24, 128.16, 127.83, 126.99, 126.26, 126.05, 125.69, 50.93, 40.03, 29.82, 20.55, 14.16; HRMS (FAB) m/z calcd: 402.3035, found: 402.3041. Anal. Calcd for $\text{C}_{28}\text{H}_{38}\text{N}_2$: C, 83.53; H, 9.51; N 6.96. Found: C, 83.18; H, 9.63; N, 6.79.

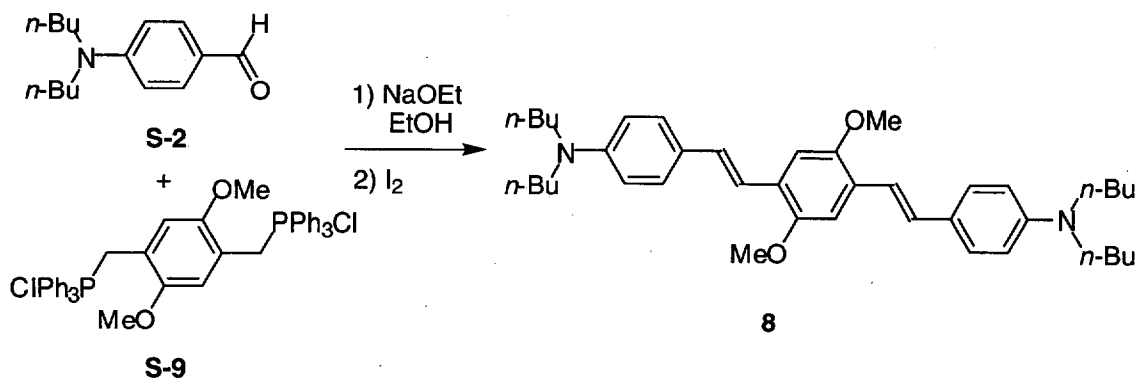
***E,E,E,E*-1-(4-*N,N*-di-*n*-butylaminophenyl)-8-(4'-*N,N*-dimethylaminophenyl)-1,3,5,7-octatetraene (4).** Prepared from **S-1** and 7-[4-(dimethylamino)phenyl]-2,4,6-heptatrienal (**S-5**) by the general Wittig procedure. ^1H NMR (300 MHz, benzene- d_6) δ (ppm) 7.50-7.30 (m, 4H), 6.95-6.78 (m, 2H), 6.75-6.38 (m, 10H), 3.05 (t, $J = 7.1$ Hz, 4H), 2.50 (s, 6H), 1.50-1.30 (m, 4H), 1.15 (q, $J = 7.2$ Hz, 4H) 0.84 (t, $J = 7.1$ Hz, 6H); HRMS (FAB) m/z calcd: 428.3191, found: 428.3176. Anal. Calcd for $\text{C}_{30}\text{H}_{40}\text{N}_2$: C, 84.06; H, 9.41; N, 6.54. Found: C, 83.86; H, 9.20; N, 6.28.

***E,E,E,E,E*-1-(4-*N,N*-di-*n*-butylaminophenyl)-10-(4'-*N,N*-dimethylaminophenyl)-1,3,5,7,9-decapentaene (5).** Prepared from **S-1** and 9-[4-(dimethylamino)phenyl]-2,4,6,8-nonatetraenal (**S-6**) by the general Wittig procedure. ^1H NMR (300 MHz, benzene- d_6) δ (ppm) 7.45-7.32 (m, 4H), 6.95-6.80 (m, 2H), 6.68-6.37 (m, 12 H), 3.03 (t, $J = 7.4$ Hz, 4H), 2.48 (s, 6H), 1.50-1.28 (m, 4H), 1.20-1.05 (m, 4H), 0.83 (t, $J = 7.3$ Hz, 6H); HRMS (FAB) m/z calcd: 454.3348, found: 454.3332. Anal. Calcd for $\text{C}_{32}\text{H}_{42}\text{N}_2$: C, 84.53; H, 9.31; N, 6.16. Found: C, 84.51; H, 9.23; N, 6.02.



Scheme 2

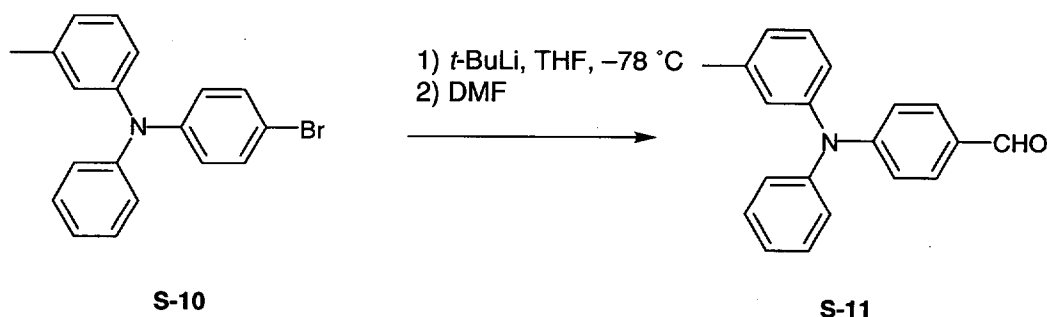
***E,E*-1,4-Bis[4'-(*N,N*-di-*n*-butylamino)styryl]benzene (7, Scheme 2).** Compound 7 was prepared from the reaction of terephthalaldehyde (S-8) (1.34 g, 0.01 mol) and S-1 (14.06 g, 0.023 mol) and lithium/ethanol (0.32g, 0.053 mol / 100 mL). Recrystallized from ethanol, yield 40.7%; Mp: 130-32°C; IR (KBr) ν , cm^{-1} : 2955, 2870, 1603, 1520, 1367, 1187, 962, 823; UV-Vis (acetone) λ_{max} , nm: 402; ^1H NMR (300 MHz, CDCl_3) δ (ppm) 7.42 (s, 4H), 7.01 (d, $J = 16.21$ Hz, 2H), 7.36-6.61 (m, 8H), 6.85 (d, $J = 16.2$ Hz, 2H), 3.28 (t, $J = 7.5$ Hz, 8H), 1.56 (m, 8H), 1.35 (m, 8H), 0.932 (t, $J = 7.2$ Hz, 12H); MS (FAB, *m*-NBA matrix): m/z 536.5. Anal. Calcd for $\text{C}_{38}\text{H}_{52}\text{N}_2$: C, 85.02; H, 9.76; N, 5.22. Found: C, 84.79; H, 9.93; N, 5.32.



Scheme 3

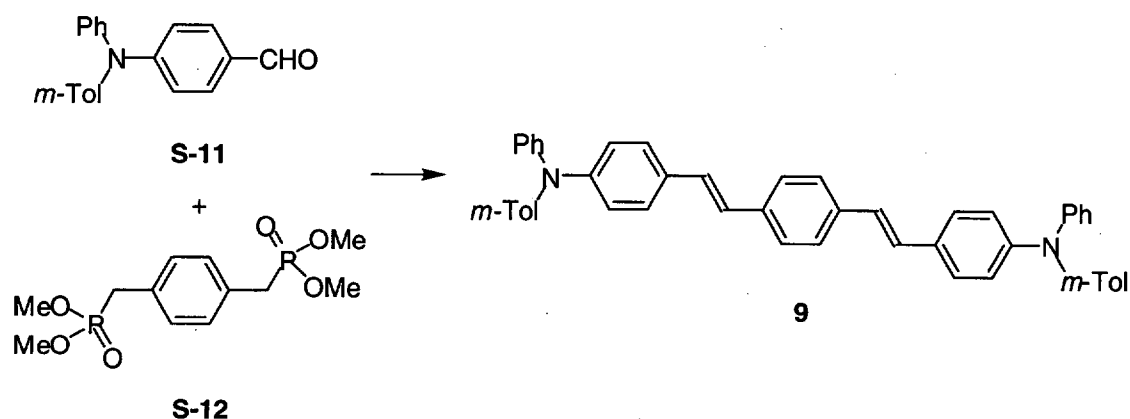
***E,E*-1,4-Bis[4'-(*N,N*-di-*n*-butylamino)styryl]-2,5-dimethoxybenzene (8, Scheme 3).**

Prepared from **S-2** and **S-9** by the general Wittig procedure followed by the double bond isomerization in 22.4 % yield. ^1H NMR (300 MHz, acetone- d_6) δ (ppm) 7.37 (d, $J = 8.73$ Hz, 2H), 7.24 (d, $J = 16.4$ Hz, 2H), 7.24 (s, 2H), 7.12 (d, $J = 16.5$ Hz, 2H), 6.68 (d, $J = 8.79$ Hz, 2H), 3.89 (s, 6H), 3.35 (t, $J = 7.56$ Hz, 8H), 1.58 (p, $J = 7.40$ Hz, 8H), 1.36 (sx, $J = 7.40$ Hz, 8H), 0.95 (t, $J = 7.30$ Hz, 12H); ^{13}C NMR (125 MHz, acetone- d_6) δ (ppm) 152.3, 148.9, 129.6, 128.6, 127.4, 126.3, 118.8, 112.8, 109.4, 56.7, 51.4, 30.2, 21.0, 14.4; UV (toluene) λ_{max} 429 ($\epsilon_{429} = 67000$) nm; HRMS (LSI) calcd: 596.434, found 596.434. Anal. Calcd for $\text{C}_{40}\text{H}_{56}\text{N}_2\text{O}_2$: C, 80.48; H, 9.46; N, 4.70. Found: C, 80.37; H, 9.39; N, 4.58.

**Scheme 4**

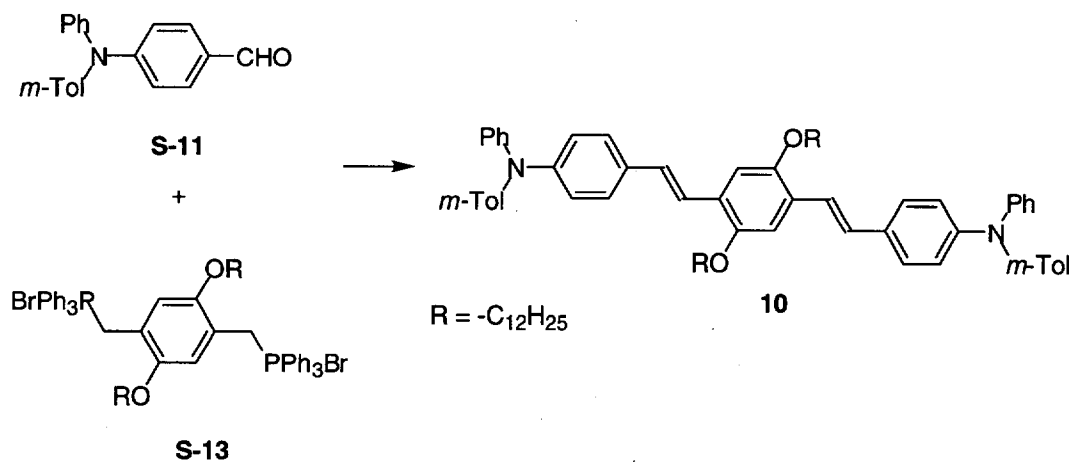
Synthesis of 4(*m*-tolylphenylamino)benzaldehyde (S-11) from 1-bromo-4-*m*-tolylphenylamino)benzene (S-10) (Scheme 4). To the bromo compound **S-10** (20 g, 59.130 mmol) in THF (480 mL) at -78°C was added *t*-BuLi (85.6 mL, 1.45 M solution in pentane, 124.17 mmol) and stirred for 10 minutes at this temperature. To this solution at -78°C was added DMF (15.50 mL, 0.200 mol) and stirred for 6 hours while warming up to room temperature. The solution was poured into water (400 mL) and extracted with ether (2 x 400 mL). The combined ether layer was washed with water (500 mL), dried over Na_2SO_4 , concentrated in vacuo. The resultant residue was purified using silica gel

column chromatography using 9/1 hexane / ethyl acetate followed by 4/1 hexane / ethyl acetate mixture as the mobile phase to obtain 15.53 g (91%) of product **S-11** as a fluorescent viscous oil. ^1H NMR (300 MHz, acetone- d_6) δ (ppm) 9.85 (s, 1H); 7.74 (d, 2H, $J = 8.7$ Hz); 7.43 (t, 2H, $J = 7.5$ Hz); 7.32 (t, 1H, $J = 8.0$ Hz); 7.24 (t, 3H); 7.09-6.97 (m, 4H); 2.32 (s, 3H); ^{13}C NMR (75 MHz, acetone- d_6) δ (ppm) 190.6, 147.1, 147.0, 140.6, 131.8, 130.6, 130.5, 130.1, 127.9, 127.3, 127.2, 127.0, 126.0, 124.5, 119.6, 21.3. HRMS calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}$: 287.131014; found: 287.130999.



***E,E*-1,4-Bis[4'-(*N,N*-*m*-tolylphenylamino)styryl]benzene (9, Scheme 5).** A solution of **S-12** (10.7 g, 33.3 mmol) in dry *N,N*-dimethylformamide (200 mL) was added dropwise to a stirred suspension of sodium hydride (*ca.* 10 g, 420 mmol) in dry *N,N*-dimethylformamide (250 mL). After 1 h stirring at room temperature a solution of **S-11** (20.6 g, 71.5 mmol) in *N,N*-dimethylformamide (200 mL) was added dropwise. After 48 h water (200 mL) was added *cautiously*. The mixture was transferred to a separating funnel together with more water and dichloromethane. The aqueous layer was extracted with dichloromethane until the extracts were almost colorless. The combined organics were dried over magnesium sulfate. After filtration silica gel was added and the solvent

removed under reduced pressure leaving the product absorbed onto the silica. The mixture was transferred to the top of a silica gel column which was eluted with toluene. Evaporation of the first fraction under reduced pressure afforded a yellow powder (16.3 g, 25.3 mmol, 76%) which was found to be NMR-pure **9**. The compound can be conveniently recrystallized from a hot mixture of heptane and toluene. ^1H NMR (300 MHz, CD_2Cl_2) δ (ppm) 7.49 (s, 4H), 7.41 (d, $J = 8.6$ Hz, 4H), 7.30–6.88 (m, 26H), 2.27 (s, 6H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ (ppm) 147.9, 147.8, 147.7, 139.7, 137.0, 131.6, 129.6, 129.4, 128.2, 127.6, 126.9, 126.7, 125.7, 124.8, 124.5, 123.6, 123.3, 122.2, 21.5; UV (THF) λ_{max} 305 ($\epsilon_{305} = 34000$), 405 ($\epsilon_{405} = 65000$) nm; T_m (DSC) 215 °C; HRMS (LSI) m/z calcd: 644.3192, found 644.3177. Anal. Calcd for $\text{C}_{48}\text{H}_{40}\text{N}_2$: C, 89.40; H, 6.25; N, 4.34. Found: C, 89.29; H, 6.43; N, 4.31.



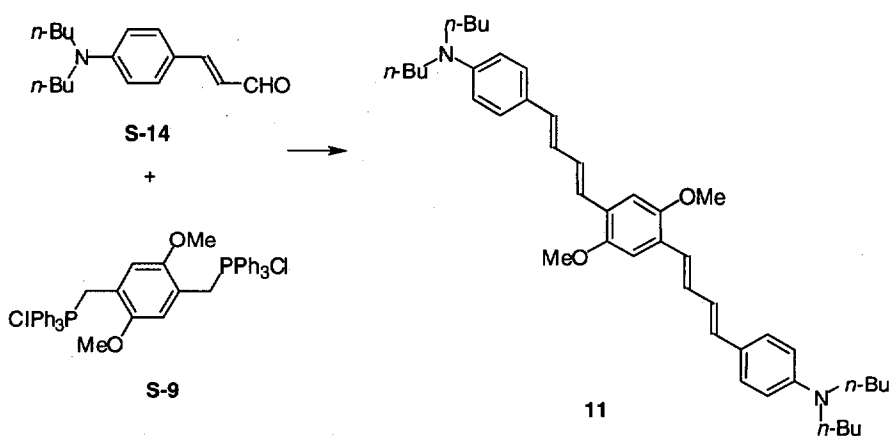
Scheme 6

***E,E*-1,4-Bis[4'-(*N,N*-*m*-tolylphenylamino)styryl]-2,5-di(*n*-dodecyloxy)benzene (10, Scheme 6).** *n*-Butyl-lithium (2.3 mL of a 2.5 M hexane solution, 5.75 mmol) was added dropwise to 2,5-*bis*(triphenylmethylphosphonium)-1,4-di(*n*-dodecyloxy)benzene dibromide (2.498 g, 2.15 mmol) in dry tetrahydrofuran (50 mL) at -78 °C; the reaction mixture immediately became very dark. The cooling bath was removed and the reaction

mixture was allowed to warm to room temperature over 2 h before recooling to $-78\text{ }^{\circ}\text{C}$ and adding a solution of 4-(*m*-tolylphenylamino)benzaldehyde **S-11** (1.637 g, 5.70 mmol) in dry THF (30 mL) dropwise. The reaction mixture was allowed to warm to room temperature and then stirred at room temperature for 2.5 h before *cautiously* adding water (150 mL). The mixture was extracted with diethyl ether ($3 \times 50\text{ mL}$) and the combined ether layers were dried over magnesium sulfate. After filtration, the solvent was removed under reduced pressure; the residue was dissolved in the minimum amount of dichloromethane and the resulting solution was transferred to the top of a silica gel column which was eluted with hexane / ethyl acetate (7 : 1). The first fraction was found to be a mixture of the geometric isomers of 1,4-*bis*[4'-(*N,N*-*m*-tolylphenylamino)styryl]-2,5-di(*n*-dodecoxy)benzene. The mixed isomers were dissolved in toluene (200 mL) and heated under nitrogen with a few crystals of iodine. After 3 d the solution was passed through a silica plug. The solvent was removed under reduced pressure to afford a yellow oil (*ca.* 2.7 g) which was recrystallized from acetone to afford the pure *E,E* isomer as a bright yellow powder (925 mg, 0.927 mmol, 43%). ^1H NMR (300 MHz, CD_2Cl_2) δ (ppm) 7.42 (d, $J = 8.6\text{ Hz}$, 4H), 7.35 (app. s, 2H), 7.27 (t, $J = \text{ca. } 8\text{ Hz}$, 4H), 7.19–7.01 (m, *ca.* 16H), 6.95 (s, 2H), 6.89 (br 3-line m, 4H), 4.05 (t, $J = 7.2\text{ Hz}$, 4H), 2.27 (s, 6H), 1.86 (app. quin., $J = \text{ca. } 7\text{ Hz}$, 4H), 1.53 (m, 4H), 1.48–1.19 (overlapping multiplets, 32H), 0.87 (t, $J = \text{ca. } 6.5\text{ Hz}$, 6H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ (ppm) 151.3, 148.0, 147.8, 147.7, 139.6, 132.4, 129.6, 129.4, 128.3, 127.6, 127.0, 125.7, 124.7, 124.4, 123.7, 123.2, 122.2, 121.9, 110.5, 69.8, 32.3, 30.0 (several overlapping peaks), 29.9, 29.8, 29.7, 26.7, 23.1, 21.5, 14.3; HRMS (LSI) m/z calcd: 1012.6845, found: 1012.6874. Anal. Calcd for $\text{C}_{72}\text{H}_{88}\text{N}_2\text{O}_2$: C, 85.33; H, 8.75; N, 2.76. Found: C, 85.51; H, 8.69; N, 2.71.

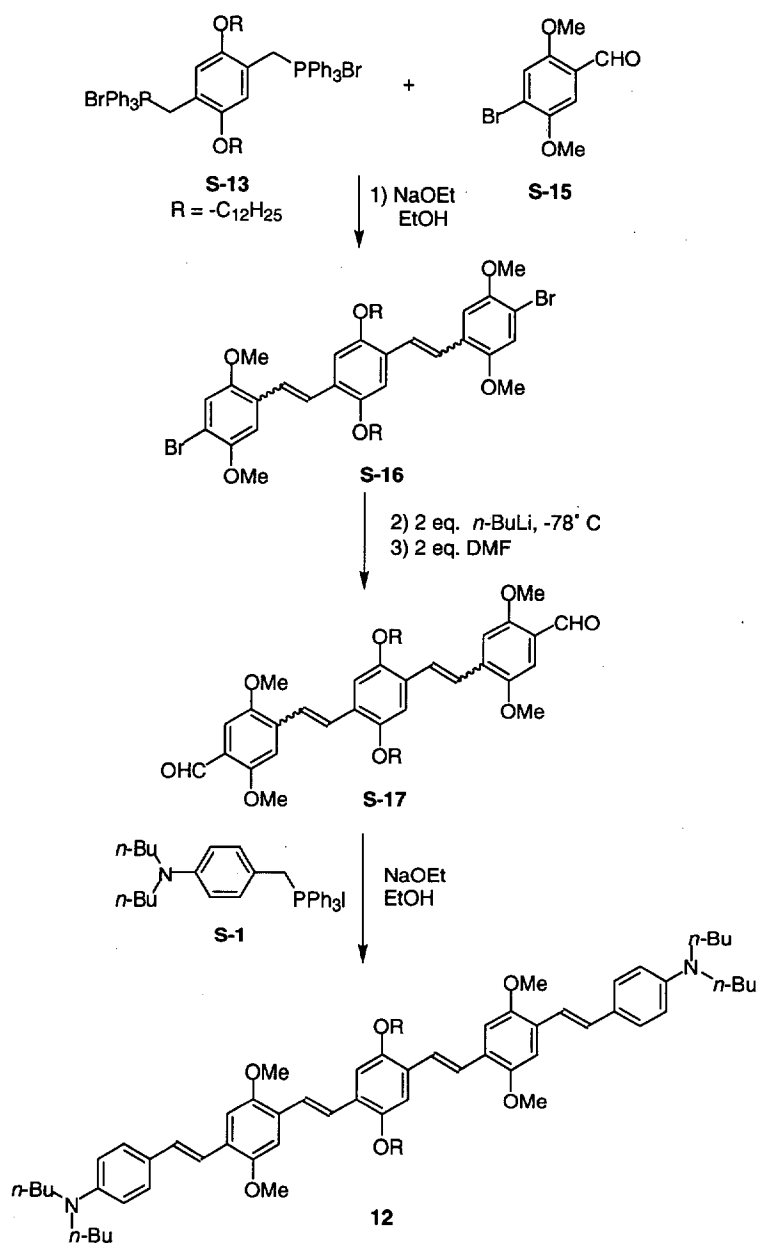
***E,E,E,E*-1,4-Bis[4-[4'-(*N,N*-di-*n*-butylamino)phenyl]-1,3-butadienyl]-2,5-dimethoxybenzene (11, Scheme 7).** Prepared from 3-[4-(di-*n*-butylamino)phenyl]-2-propenal (**S-14**) and **S-9** by the general Wittig procedure followed by the double bond isomerization

in 15.3 % yield. ^1H NMR (300 MHz, acetone- d_6) δ (ppm) 7.31 (d, $J = 8.60$ Hz, 4H), 7.18 (s, 2H), 6.60-6.55 (m, 2H), 6.64 (d, $J = 8.70$ Hz, 4H), 7.13-6.79 (m, 6H), 3.89 (s, 6H), 3.34 (t, $J = 7.50$ Hz, 8H), 1.57 (p, $J = 7.40$ Hz, 8H), 1.36 (sx, $J = 7.40$ Hz, 8H), 0.94 (t, $J = 7.29$ Hz, 12H); ^{13}C NMR (75 MHz, acetone- d_6) δ (ppm) 152.0, 148.7, 133.9, 131.3, 128.5, 127.2, 126.0, 125.6, 125.0, 112.6, 109.1, 56.4, 51.2, 30.2, 20.8, 14.2; UV (toluene) λ_{max} 456 ($\epsilon_{456} = 93000$) nm; HRMS (LSI) calcd: 648.465, found 648.465. Anal. Calcd for $\text{C}_{44}\text{H}_{60}\text{N}_2\text{O}_2$: C, 81.42; H, 9.32; N, 4.32. Found: C, 81.26; H, 9.31; N, 4.26.



Scheme 7

***E,E,E,E*-1,4-Bis[4'-[4''-(*N,N*-di-*n*-butylamino)styryl]-2',5'-dimethoxystyryl]-2,5-di(*n*-dodecoxy)benzene (12, Scheme 8).** The general procedure for the double Wittig reaction was used with **S-13** and **S-15** to give the dibromide **S-16** as a yellow oil that was a mixture of *cis* and *trans* isomers in an overall yield of 94.9% that was used directly in the next step. Low Resolution LSIMS calcd. for $\text{C}_{50}\text{H}_{72}\text{Br}_2\text{O}_6$: M^+ 928.4, found 928.4. A THF (35 mL) solution of **S-16** (1.40 g, 1.51 mmol) was chilled to -78°C and was then treated with *n*-BuLi (2.64 mL, 4.22 mmol). The mixture was allowed to react at -78°C with stirring for 1 h, and then DMF (0.93 mL, 12.1 mmol) was added in one portion. Upon addition of DMF a fluorescent viscous solution formed. The cooling bath was removed, and the reaction mixture was allowed to warm to ambient temperature over a



Scheme 8

period of 2 h. The mixture was diluted with water (200 mL) and stirred for 1h. Upon the addition of water, a bright orange precipitate formed. The precipitate (pure *trans* isomer of the bisaldehyde **S-17**) was collected by filtration and was rinsed with diethylether (200 mL). The organic layer (that contained the *cis* / *trans* isomeric mixture of the

bisaldehyde) was collected and extracted with water (2x), extracted with brine (1x), and dried over Na_2SO_4 . The solvents were removed *in vacuo*, and the crude product was purified by column chromatography on silica using hexanes/EtOAc (9:1) as the eluent. 0.193 g of the pure *trans* isomer was obtained, and 0.561 g of the purified isomeric mixture was obtained. 60.4% yield total. ^1H NMR (300 MHz, CD_2Cl_2) δ (ppm) 10.40 (s, 2H), 7.63 (d overlapping, $J = 14.54$ Hz, 2H), 7.57 (d overlapping, $J = 14.42$ Hz, 2H), 7.33 (s, 2H), 7.27 (s, 2H), 7.19 (s, 2H), 4.09 (t, $J = 6.04$ Hz, 4H), 3.97 (s, 6H), 3.91 (s, 6H), 1.88 (p, $J = 6.80$ Hz, 4H), 1.54-1.24 (m, 36H), 0.87 (t, $J = 6.02$ Hz, 6H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ (ppm) 188.8, 157.0, 151.8, 151.6, 134.9, 127.5, 124.3, 123.2, 111.1, 109.8, 109.3, 69.8, 56.4, 56.3, 32.3, 30.0-29.6 (overlapping m), 26.7, 23.0, 14.2; UV (toluene) λ_{max} ($\epsilon_{445} = 52000$) nm; High Resolution LSIMS M^+ calcd: 826.538, found: 826.538. Anal. Calcd for $\text{C}_{52}\text{H}_{74}\text{O}_8$: C, 75.49; H, 9.02. Found: C, 75.38; H, 9.12.

Compound **12** was synthesized from **S-17** and **S-1** using the general Wittig procedure followed by double bond isomerization and recrystallization using acetone, EtOAc, and/or toluene with hexanes afforded orange crystals (Mp: 146-149°C). ^1H NMR (300 MHz, benzene- d_6) δ (ppm) 8.14-7.86 (m, 8H), 7.61 (d, $J = 8.52$ Hz, 4H), 7.50-7.38 (m, 8H), 7.26 (s, 2H), 6.65 (d, $J = 8.60$ Hz, 4H), 3.77 (t, $J = 6.07$ Hz, 4H), 3.58 (s, 6H), 3.50 (s, 6H), 3.04 (t, $J = 7.40$ Hz, 8H), 1.74-1.69 (m, 4H), 1.47-0.81 (m, 70H); ^{13}C NMR (75 MHz, benzene- d_6) δ (ppm) 152.2, 151.8, 151.9, 148.1, 129.7 (overlapping m), 126.7, 123.8, 119.1, 112.4, 110.8, 109.2, 108.7, 69.2, 55.7 (overlapping m), 50.9, 32.3, 29.6 (overlapping m), 26.7, 23.1, 20.5, 14.4, 14.2; UV (toluene) λ_{max} 468 ($\epsilon_{468} = 110000$) nm; MS (LSI) m/z calcd: 1228.9, found 1228.9. Anal. Calcd for $\text{C}_{82}\text{H}_{120}\text{N}_2\text{O}_6$: C, 80.07; H, 9.84; N, 2.28. Found: C, 80.00; H, 9.89; N, 2.22.

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