SUPPORTING INFORMATION FOR

A Practical Synthesis of Unsymmetrical Tetraarylethylenes and its Application for the Preparation of [Triphenylethylene-Spacer-Triphenylethylene] Triads

*Moloy Banerjee, Susanna J. Emond, Sergey V. Lindeman, and Rajendra Rathore**

Marquette University, Department of Chemistry, P.O. Box 1881,

Milwaukee, WI 53201-1881

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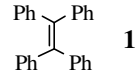
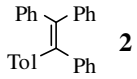
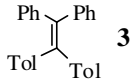
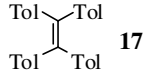
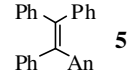
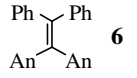
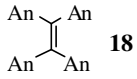
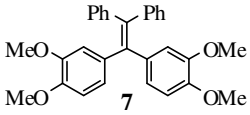
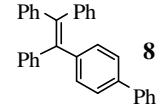
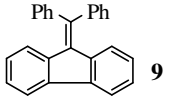
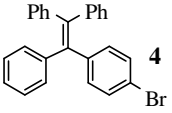
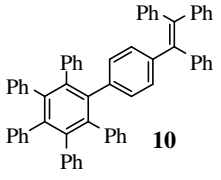
General Experimental Methods and Materials.

All reactions were performed under argon atmosphere unless otherwise noted. All commercial reagents were used without further purification unless otherwise noted. Dichloromethane 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 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 h). After distillation from CaH_2, the solvents were stored in Schlenk flasks under an argon atmosphere. Tetrahydrofuran (THF) was dried initially by distilling over lithium aluminum hydride under an argon atmosphere. The THF was further refluxed over metallic sodium in the presence of benzophenone until a persistent blue color was obtained and then it was distilled under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. NMR spectra were recorded on 300 and 400 MHz NMR spectrometers.

Cyclic Voltammetry (CV).

The CV cell was of an air-tight design with high vacuum Teflon valves and Viton O-ring seals to allow an inert atmosphere to be maintained without contamination by grease. The working electrode consisted of an adjustable platinum disk embedded in a glass seal to allow periodic polishing (with a fine emery cloth) without changing the surface area (~1 mm2) significantly. The reference SCE electrode (saturated calomel electrode) and its salt bridge were separated from the catholyte by a sintered glass frit. The counter electrode consisted of a platinum gauze that was separated from the working electrode by ~3 mm. The CV measurements were carried out in a solution of 0.1 to 0.2 M supporting electrolyte (tetra-*n*-butylammonium hexafluorophosphate, TBAH) and 2-5 x 10^{-3} M substrate in dry dichloromethane under an argon atmosphere. All the cyclic voltammograms were recorded at a sweep rate of 200 mV sec^{-1}, unless otherwise specified and were IR compensated. The oxidation potentials ($E_{1/2}$) were referenced to SCE, which was calibrated with added (equimolar) ferrocene ($E_{1/2}$ = 0.450 V *vs*. SCE). The $E_{1/2}$ values were calculated by taking the average of anodic and cathodic peak potentials in the reversible cyclic voltammograms.

Table S1. Electrochemical Oxidation Potentials of the Tetraarylethylene Derivatives[a]

Tetraethylene Derivative	E^0_{ox} (I) (V *vs.* SCE)	E^0_{ox} (II) (V *vs.* SCE)	△(mV) E^0_{ox} (II)-E^0_{ox} (I)
 **1**	1.362	1.67	350
 **2**	1.29	1.566	276
 **3**	1.226	1.526	300
 **17**	1.114	1.386	272
 **5**	1.174	1.406	232
 **6**	1.062	1.33	268
 **18**	0.79	0.91	120
 **7**	1.026	1.442[b]	416
 **8**	1.306	1.566	260
 **9**	1.434	1.782	348
 **4**	1.402	1.686	284
 **10**	1.27	1.53	260

[a]In anhydrous dichloromethane as a 0.2 mM solution containing 0.2 M TBAHP at a scan rate of 200mV/s and at 25°C. [b]CVshows complex behavior due to electrochemically induced oxidative cyclisation to the diphenylmethylidenefluorene.

General procedure for the preparation of monoethylenic compounds.

To a solution of diphenylmethane (2.02 g, 12 mmol) in dry tetrahydrofuran (20mL) was added 4 mL of a 2.5 M solution of *n*-butyllithium in hexane (10 mmol) at 0 ^{o}C under an argon atmosphere. The resulting orange-red solution was stirred for 30 min at that temperature. To this solution was added the appropriate monoketone (9 mmol), and the reaction mixture was allowed to warm to room temperature with stirring during a 6 h period. The reaction was quenched with addition of an aqueous solution of ammonium chloride and the organic layer was extracted with dichloromethane (3 X 50 mL) and the combined organic layers were washed with saturated brine solution and dried over anhydrous $MgSO_4$. The solvent was evaporated and the resulting crude alcohol (containing excess diphenylmethane) was subjected to acid catalysed dehydration as follows.

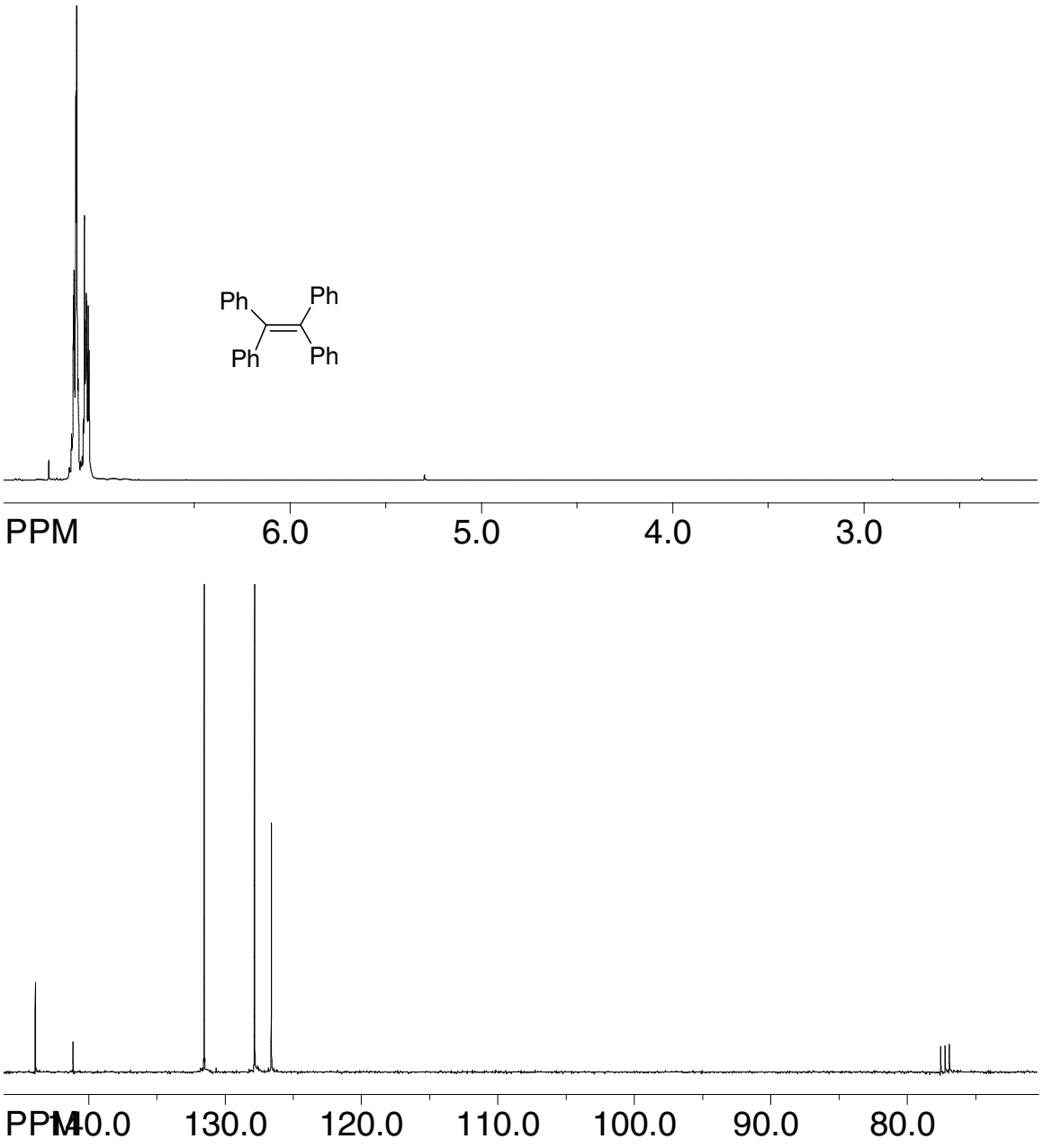
The crude alcohol was dissolved in about 80 mL of toluene in a 100-mL Schlenk flask fitted with a Dean-Stark trap. A catalytic amount of *p*-toluenesulphonic acid (342 mg, 1.8 mmol) was added and the mixture was refluxed for 3 h and cooled to room temperature. The toluene layer was washed with 10% aqueous $NaHCO_3$ solution (2 x 25 mL) and dried over anhydrous magnesium sulfate and evaporated to afford the crude tetraphenylethylene derivative. The crude product was purified either by recrystallization from a mixture of dichloromethane/methanol or dichloromethane/acetonitrile or by column chromatography on silica gel using an ethyl acetate/hexanes (2:98) mixture to afford pure compound.

General procedure for the preparation of bis-ethylenic compounds.

To a solution of diphenylmethane (2.02 g, 12 mmol) in dry tetrahydrofuran (20mL) was added 4 mL of a 2.5 M solution of *n*-butyllithium in hexane (10 mmol) at 0 ^{o}C under an argon atmosphere. The resulting orange-red solution was stirred for 30 min at that temperature. To this solution was added the appropriate diketone (4 mmol), and the reaction mixture was allowed to warm to room temperature with stirring during a 6 h period. The reaction was quenched with addition of an aqueous solution of ammonium chloride and the organic layer was extracted with dichloromethane (3 X 50 mL) and the combined organic layers were washed with saturated brine solution and dried over anhydrous $MgSO_4$. The solvent was evaporated and the resulting crude alcohol (containing excess diphenylmethane) was subjected to acid catalyzed dehydration as follows.

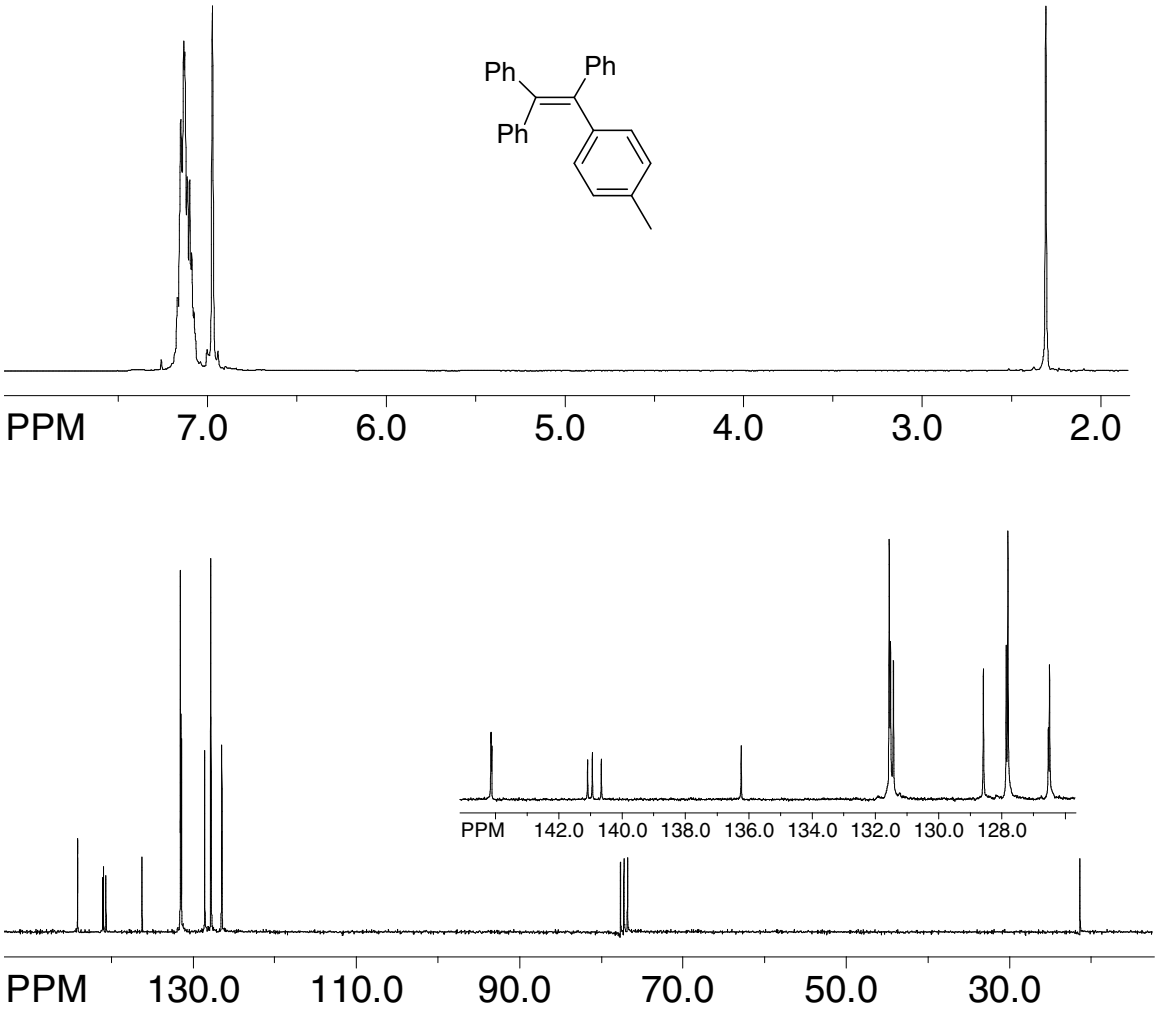
The crude alcohol was dissolved in about 80 mL of toluene in a 100 mL Schlenk flask fitted with a Dean-Stark trap. A catalytic amount of *p*-toluenesulphonic acid (342 mg, 1.8 mmol) was added and the mixture was refluxed for 3 h and cooled to room temperature. The toluene layer was washed with 10% aqueous $NaHCO_3$ solution (2 x 25 mL) and dried over anhydrous magnesium sulfate and evaporated to afford the crude tetraphenylethylene derivative. The crude product was purified either by recrystallization from a mixture of dichloromethane/methanol or dichloromethane/acetonitrile or by column chromatography on silica gel using an ethyl acetate/hexanes (2:98) mixture to afford pure compound.

1,1,2,2-tetraphenylethylene (1):



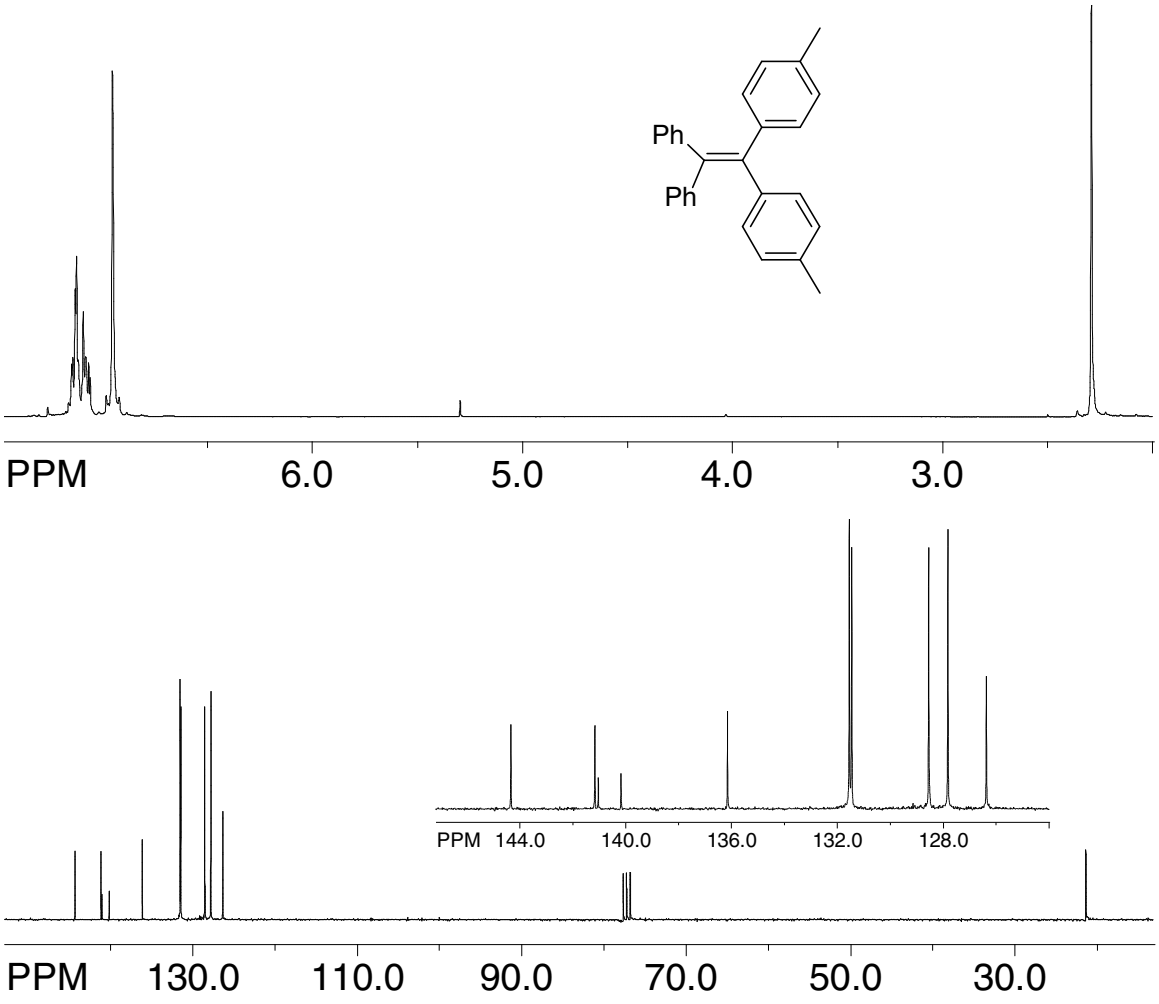
White Solid, mp 222-224 $^{\circ}$C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.05-7.08 (m, 8H), 7.10-7.13 (m, 12H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 126.6, 127.8, 131.5, 141.1, 143.9.

1-(4-Methylphenyl)-l,2,2-triphenylethylene (2):



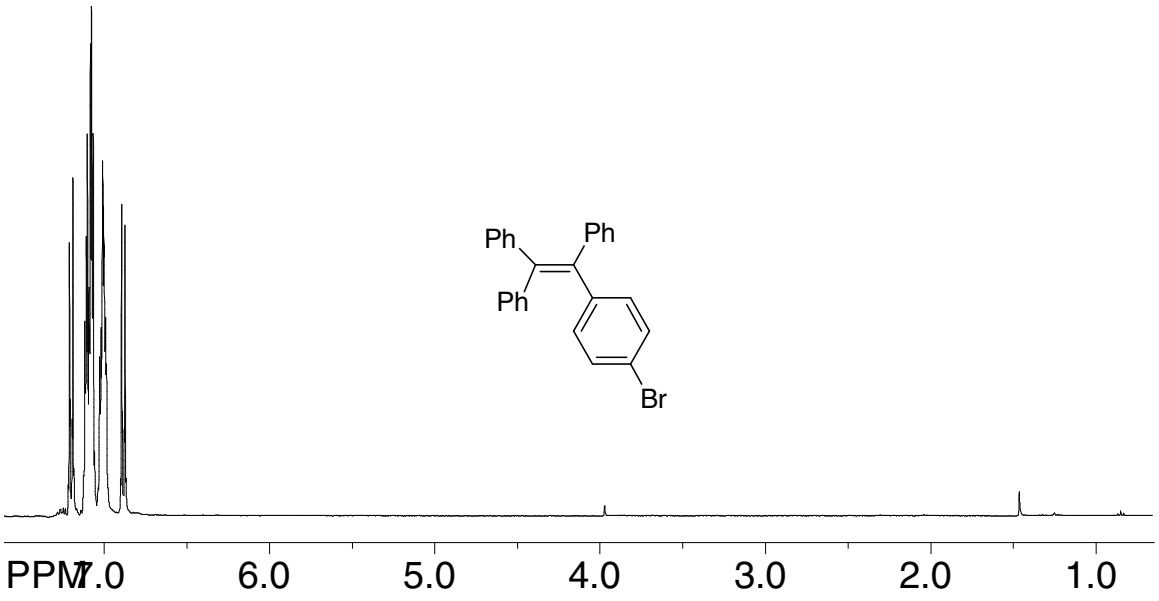
White Solid, mp 153-155 °C (lit.[1] mp 146-148 ºC); ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.31 (s, 3H), 6.97 (s, 4H), 7.07-7.17 (m, 15H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 21.4, 126.48, 126.52, 127.80, 127.86, 128.6, 131.4, 131.51, 131.55, 136.2, 140.6, 140.9, 141.1, 144.10, 144.13, 144.14.

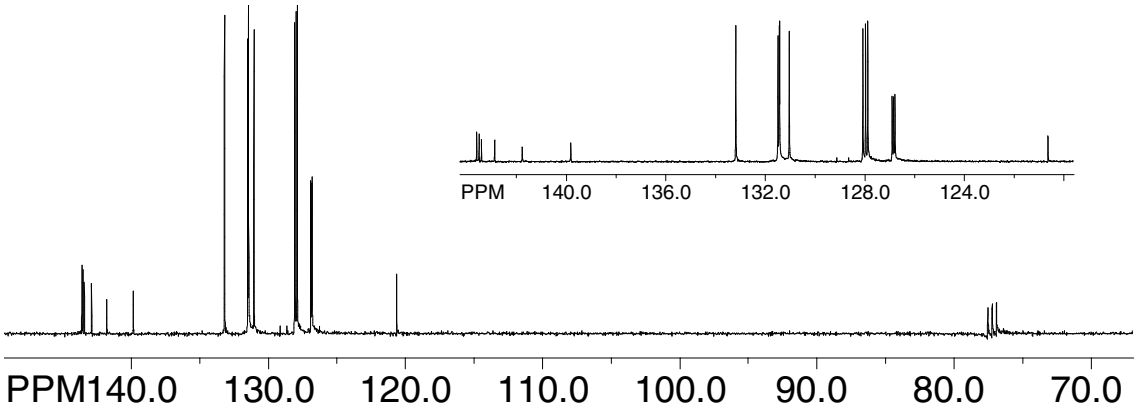
1,1-Diphenyl-2,2-di-p-tolylethylene (3):



White Solid, mp 161-163 °C (lit.[2] mp 152-154 ºC); ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.29 (s, 6H), 6.95 (s, 8H), 7.06-7.15 (m, 10H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 21.4, 127.8, 128.5, 131.45, 131.53, 136.1, 140.2, 141.0, 141.1, 144.3.

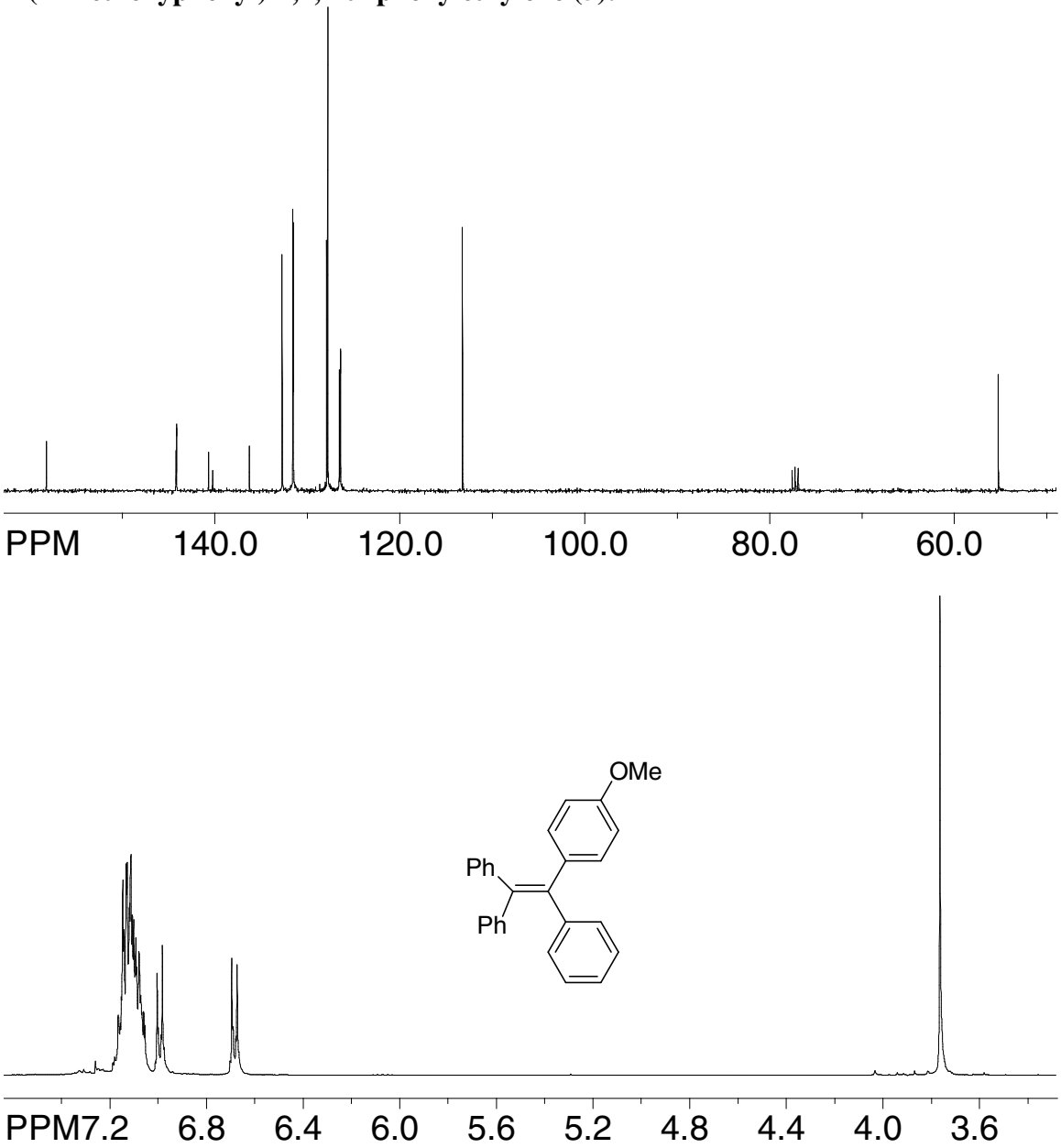
1-(4-bromophenyl)-1,2,2-triphenylethylene (4):





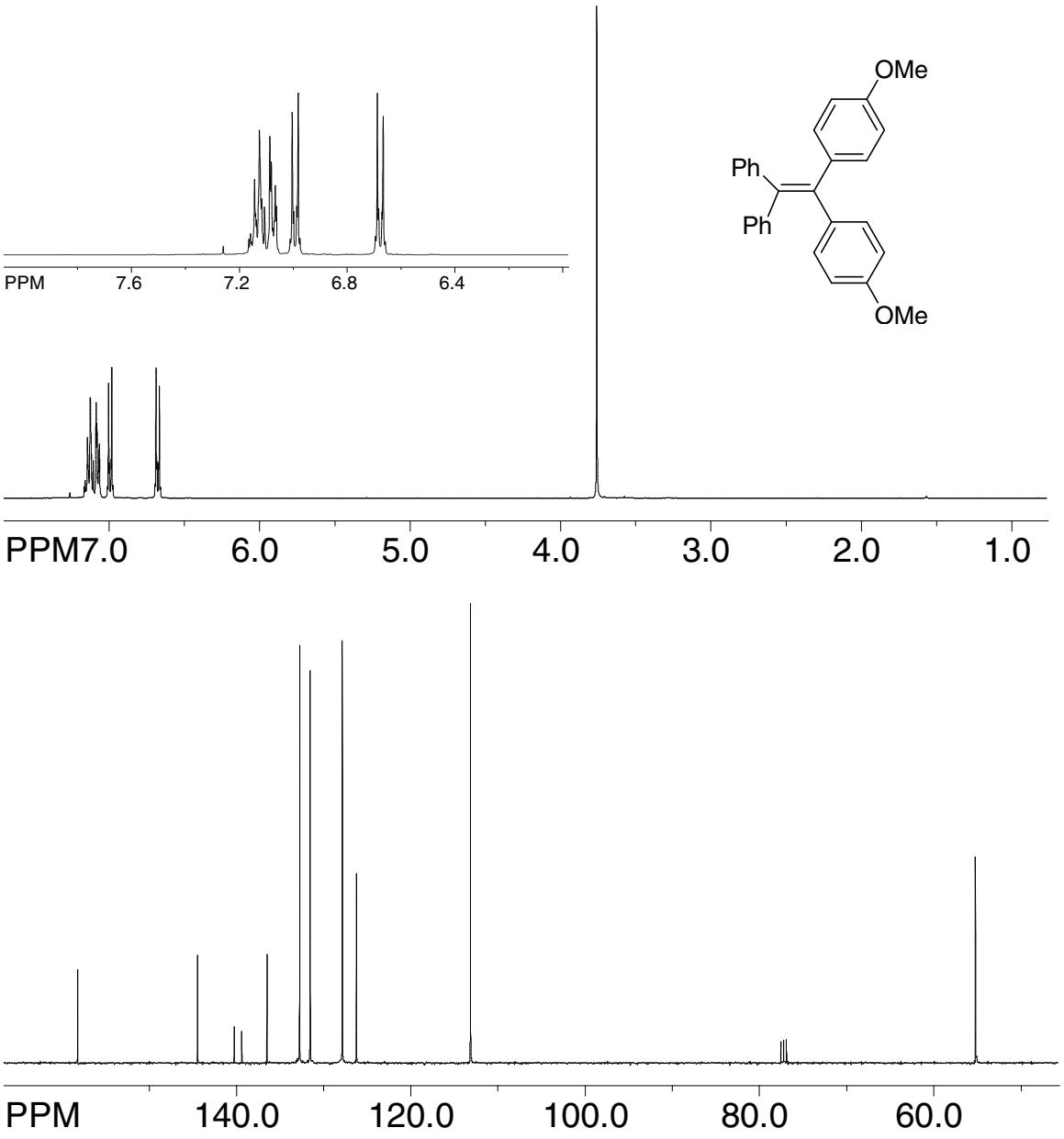
White Solid, mp 148-150 °C (lit.[3] mp 151-152 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.88 (d, J = 8.52 Hz, 2H), 6.99-7.03 (m, 6H), 7.07-7.12 (m, 9H), 7.20 (d, J = 8.52 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 120.6, 126.8, 126.8, 126.9, 127.9, 128.0, 128.1, 131.0, 131.42, 131.44, 131.5, 133.2, 139.8, 141.8, 142.9, 143.4, 143.5, 143.6.

1-(4-Methoxyphenyl)-1,2,2-triphenylethylene (5):



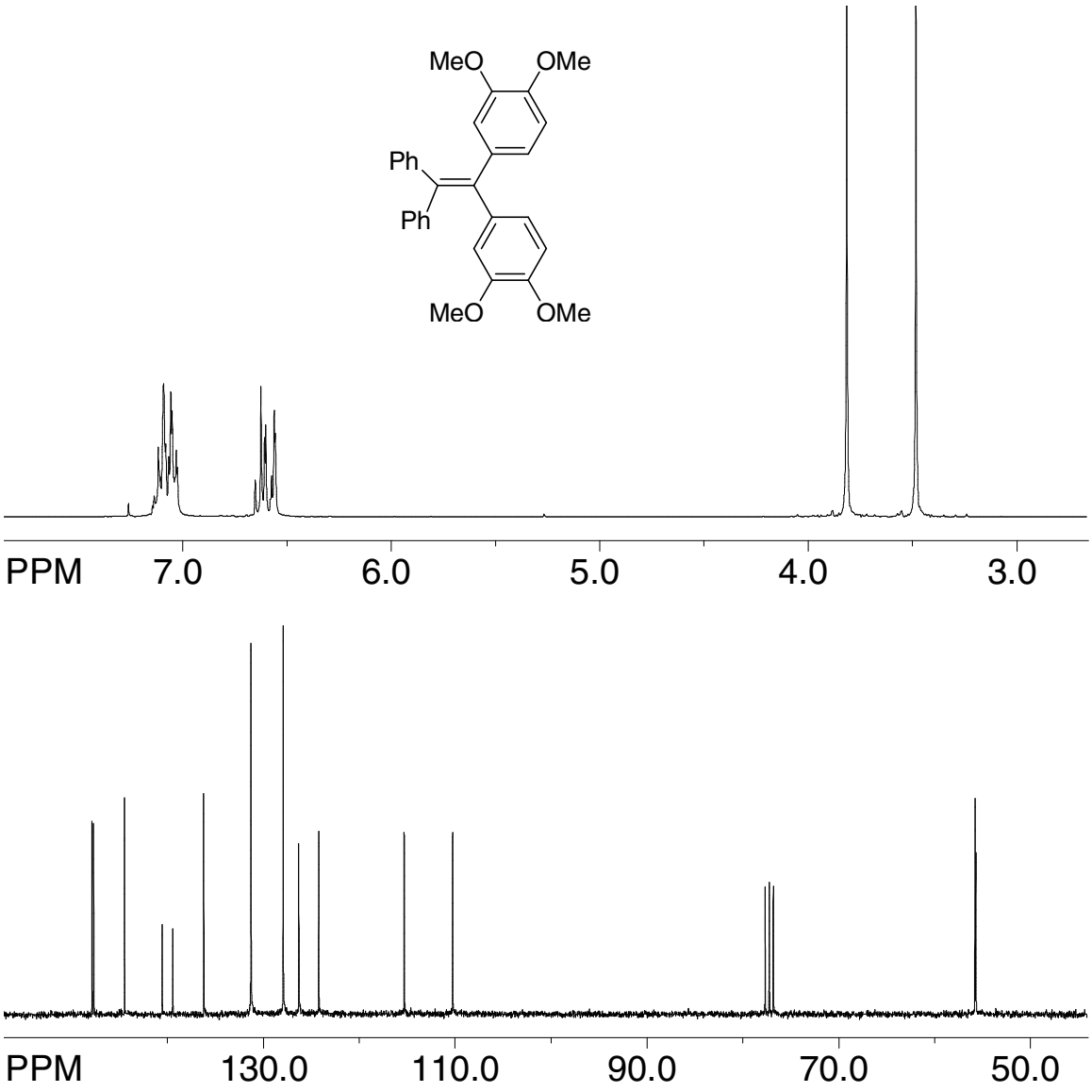
Light Yellow Solid, mp 130-132 °C (lit.[1] mp 132-134 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.76 (s, 3H), 6.68 (d, *J* = 8.88 Hz, 2H), 6.99 (d, *J* = 8.88 Hz, 2H), 7.05-7.17 (m, 10H);^{13}C NMR ($CDCl_3$, 100 MHz) δ 55.2, 113.2, 126.42, 126.43, 126.5, 127.8, 127.9, 131.52, 131.55, 131.57, 132.7, 136.3, 140.2, 140.7, 144.16, 144.21, 158.2.

1,1-Diphenyl-2,2-di-(p-methoxyphenyl)ethylene (6):



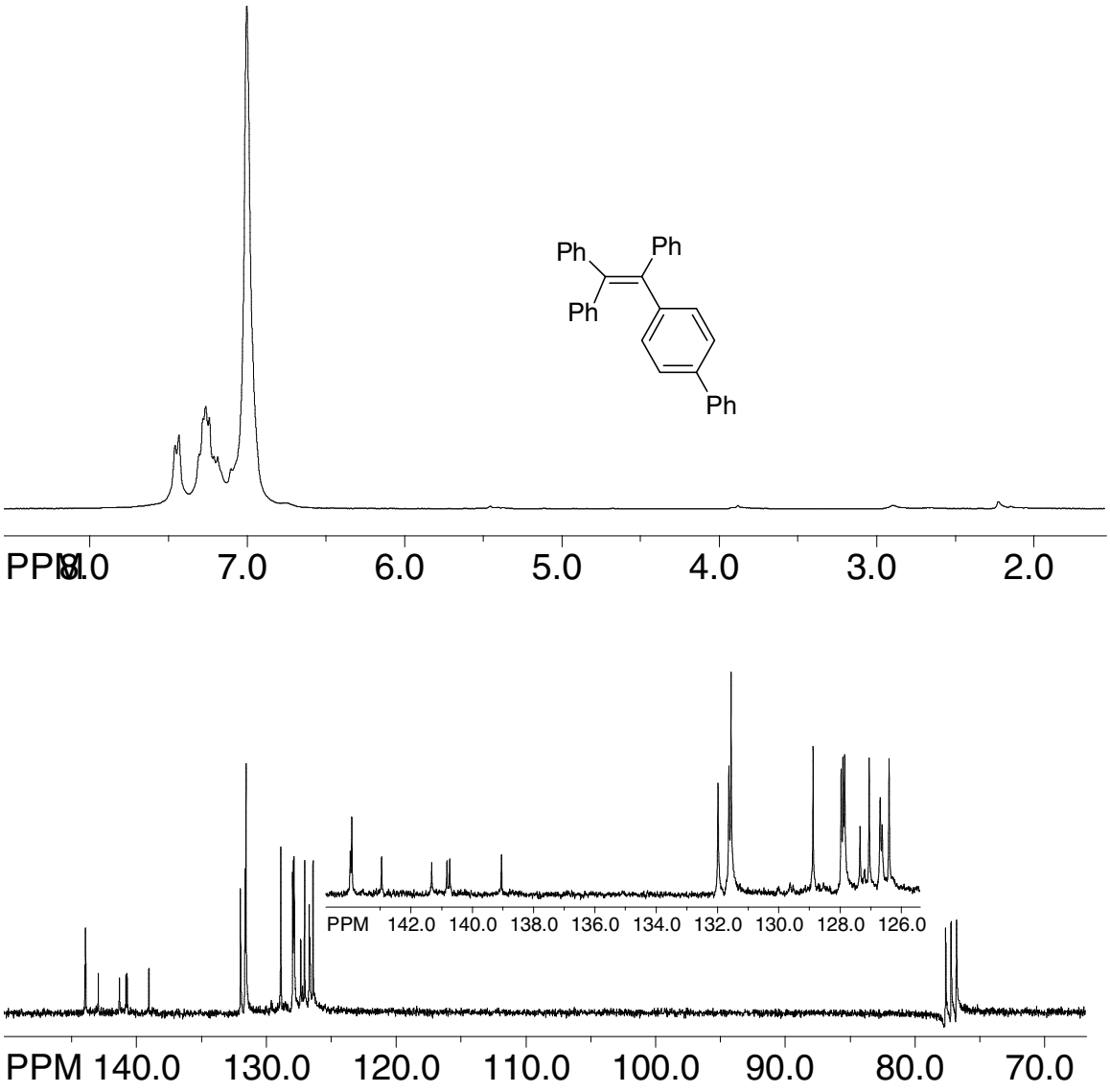
Light Yellow Solid, mp 156-158 °C (lit.[2] mp 154-158 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.76 (s, 6H), 6.68 (d, *J* = 8.84 Hz, 4H), 6.99 (d, *J* = 8.84 Hz, 4H), 7.06-7.16 (m, 10H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 55.2, 113.1, 126.2, 127.8, 131.5, 132.8, 136.5, 139.4, 140.2, 144.5, 158.2.

1,1-Diphenyl-2,2-di-(3,4-dimethoxyphenyl)ethylene (7):



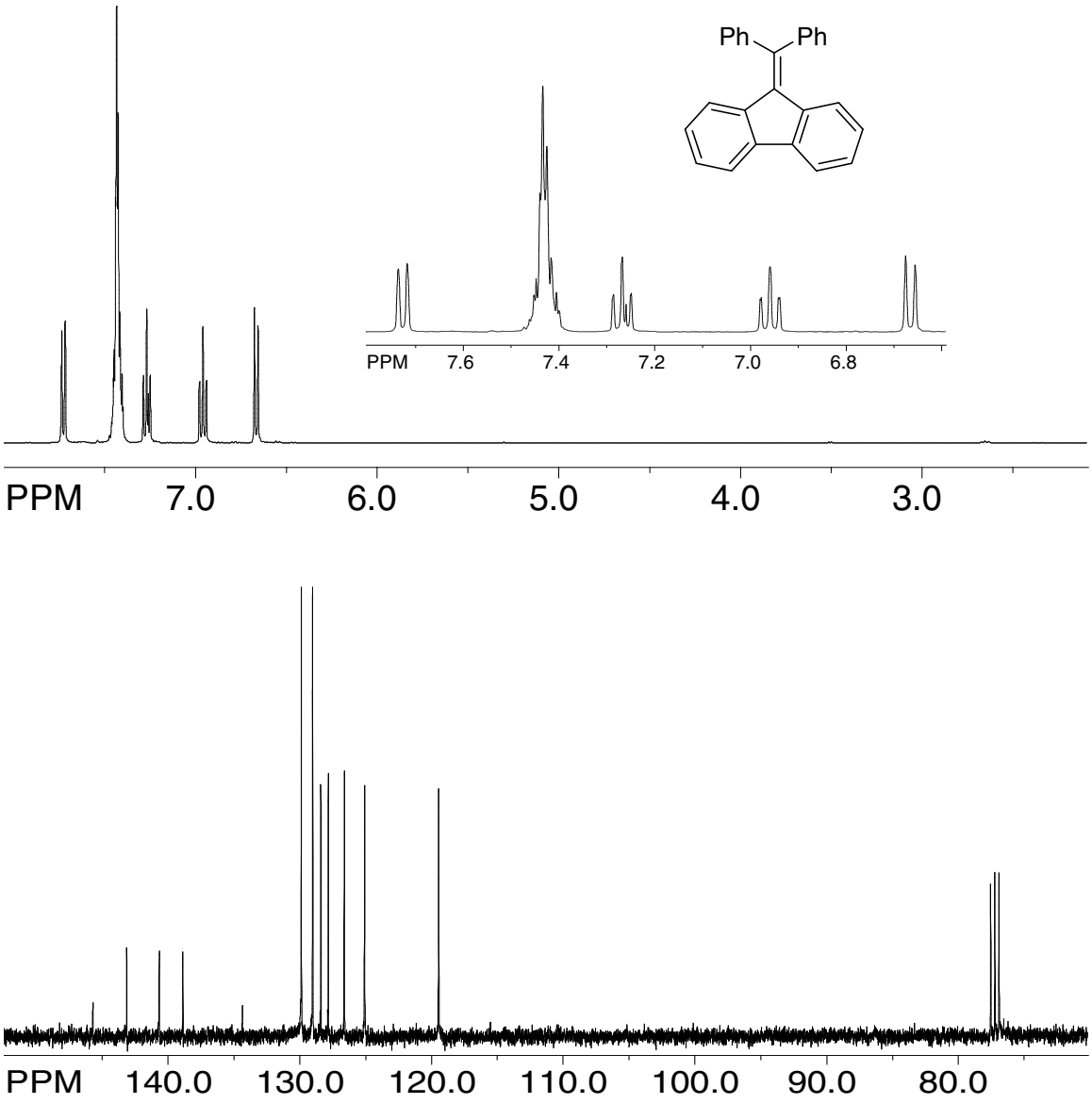
Yellow Solid, mp 167-168 $^{\circ}$C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.48 (s, 6H), 3.82 (s, 6H), 6.56-6.65 (m, 6H), 7.02-7.14 (m, 10H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 55.7, 55.8, 110.3, 115.3, 124.2, 126.3, 127.9, 131.3, 136.2, 139.5, 140.6, 144.5, 147.7, 147.9.

1-(4-Biphenyl)-l,2,2-triphenylethylene (8):



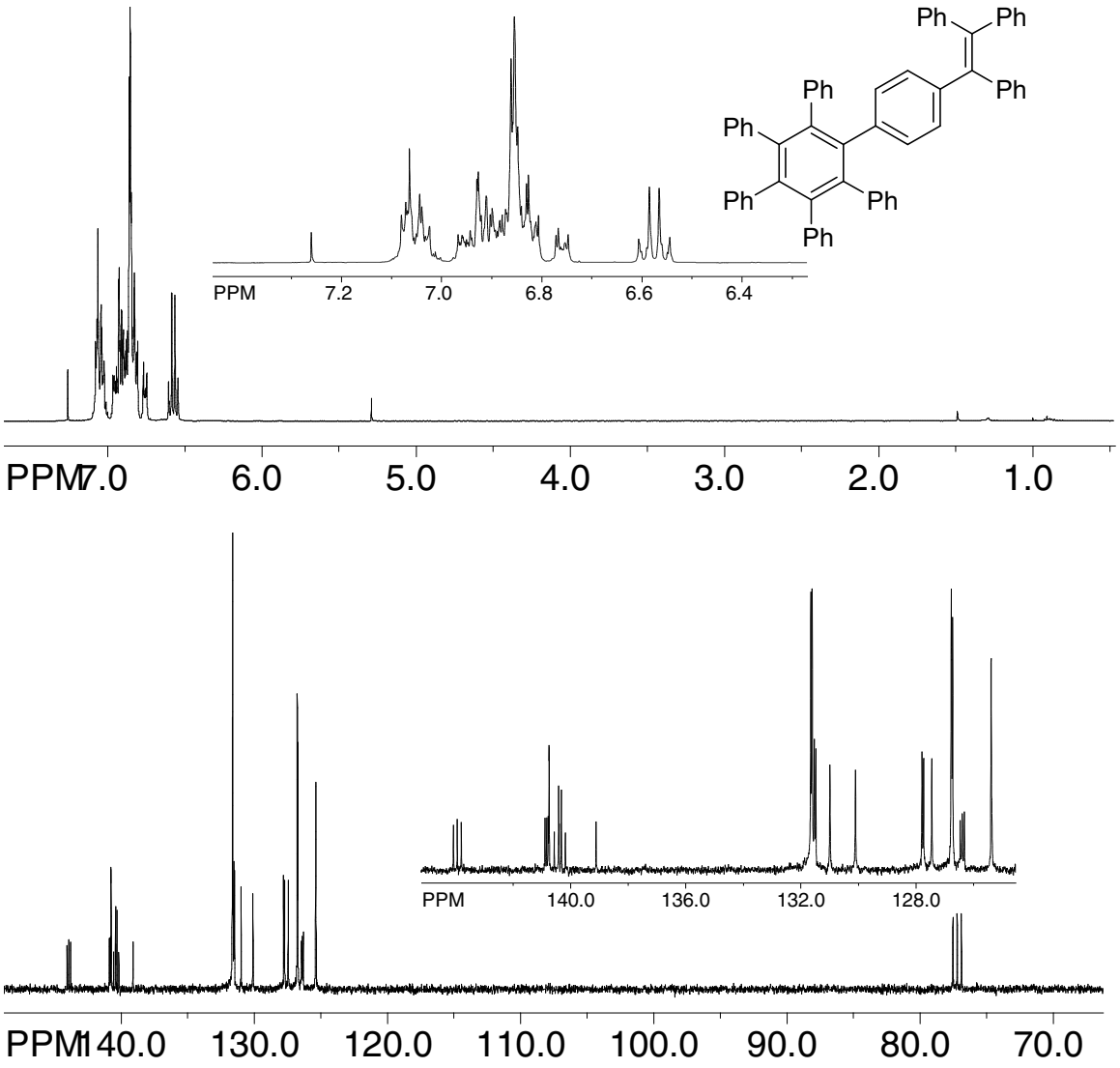
White Solid, mp 187-189 °C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.00-7.46 (m, 24H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 126.4, 126.63, 126.69, 127.0, 127.3, 127.85, 127.90, 127.96, 128.9, 131.55, 131.63, 132.0, 139.0, 140.7, 140.8, 141.3, 143.0, 143.93, 143.97.

Diphenylmethylidenefluorene (9):



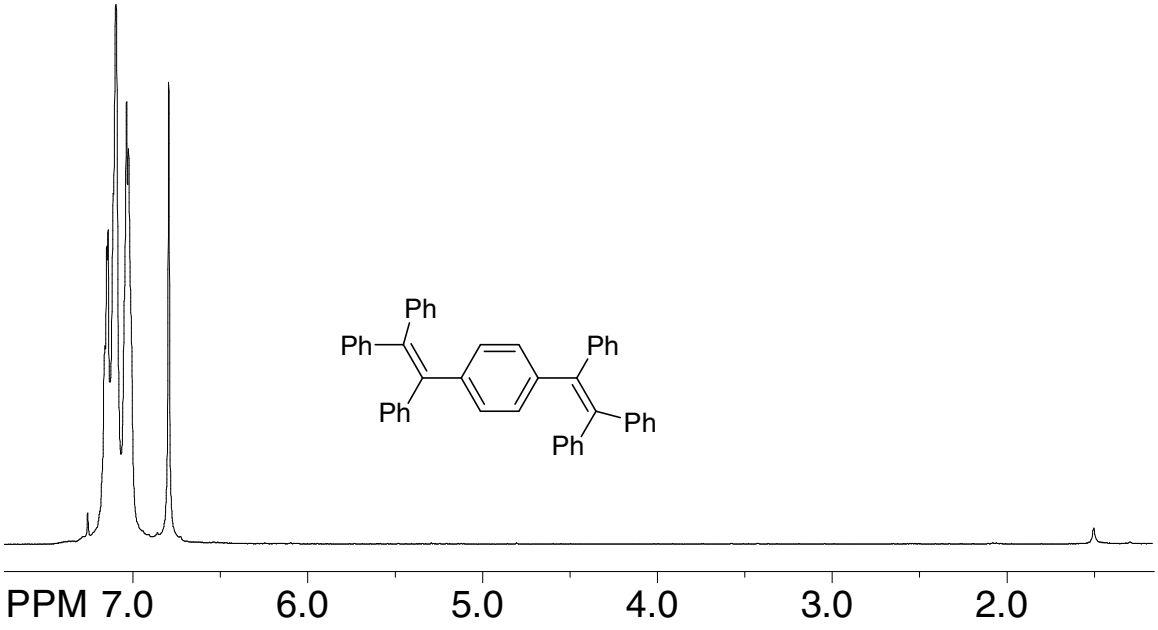
Pale yellow solid, mp 232-234 °C (lit.[4] mp 235 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.66 (d, *J* = 7.96 Hz, 2H), 6.96 (t, *J* = 6.96 Hz, 2H), 6.27 (t, *J* = 7.1 Hz, 2H), 7.41-7.45 (m, 10H), 7.73 (d, *J* = 7.36 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 119.5, 125.1, 126.6, 127.8, 128.4, 129.0, 129.9, 134.4, 138.9, 140.7, 143.1, 145.7.

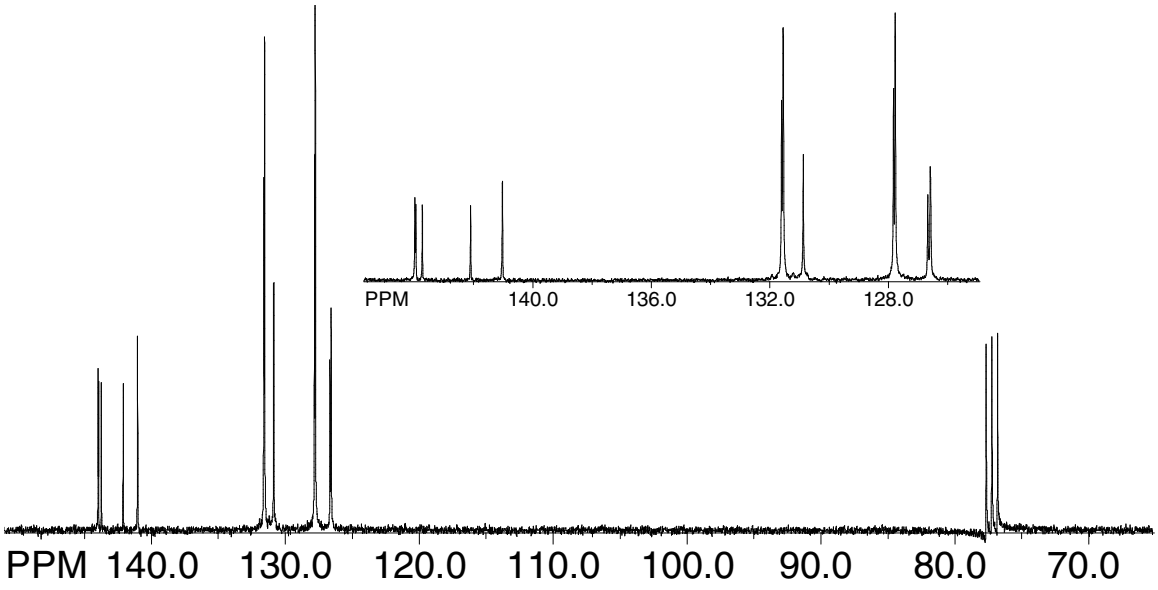
(4-Triphenylethenylphenyl)pentaphenylbenzene (10):



White Solid, mp 342-344 °C (lit.[5] mp >350 °C);^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.54-6.61 (m, 4H), 6.75-7.08 (m, 40H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 125.4, 126.33, 126.40, 126.46, 126.73, 126.78, 127.5, 127.7, 127.8, 130.1, 131.0, 131.49, 131.54, 131.61, 131.66, 139.1, 140.2, 140.3, 140.40, 140.42, 140.6, 140.76, 140.78, 140.83, 140.89, 143.8, 143.9, 144.1.

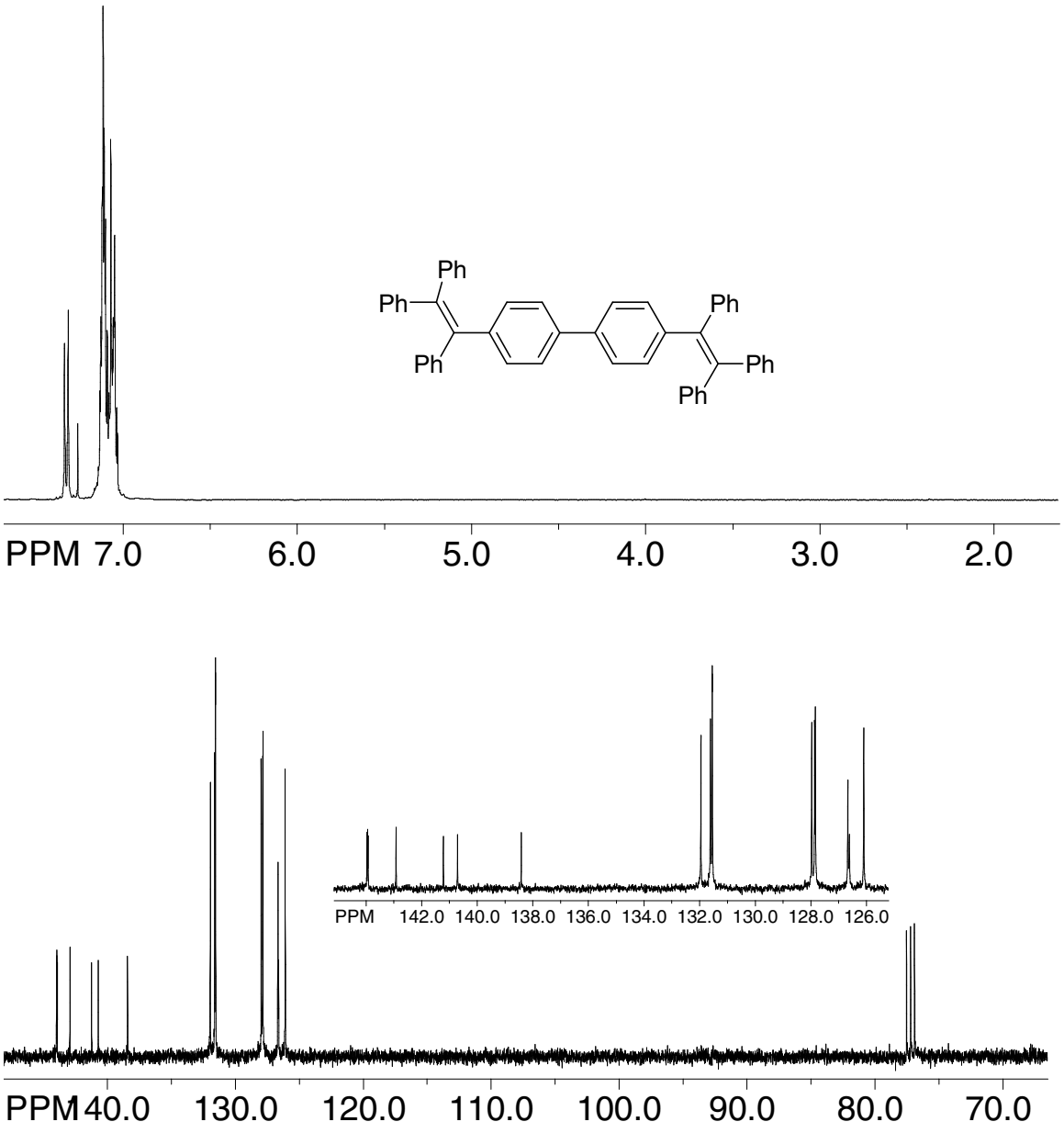
1,4-bis(triphenylethenyl)benzene (11):





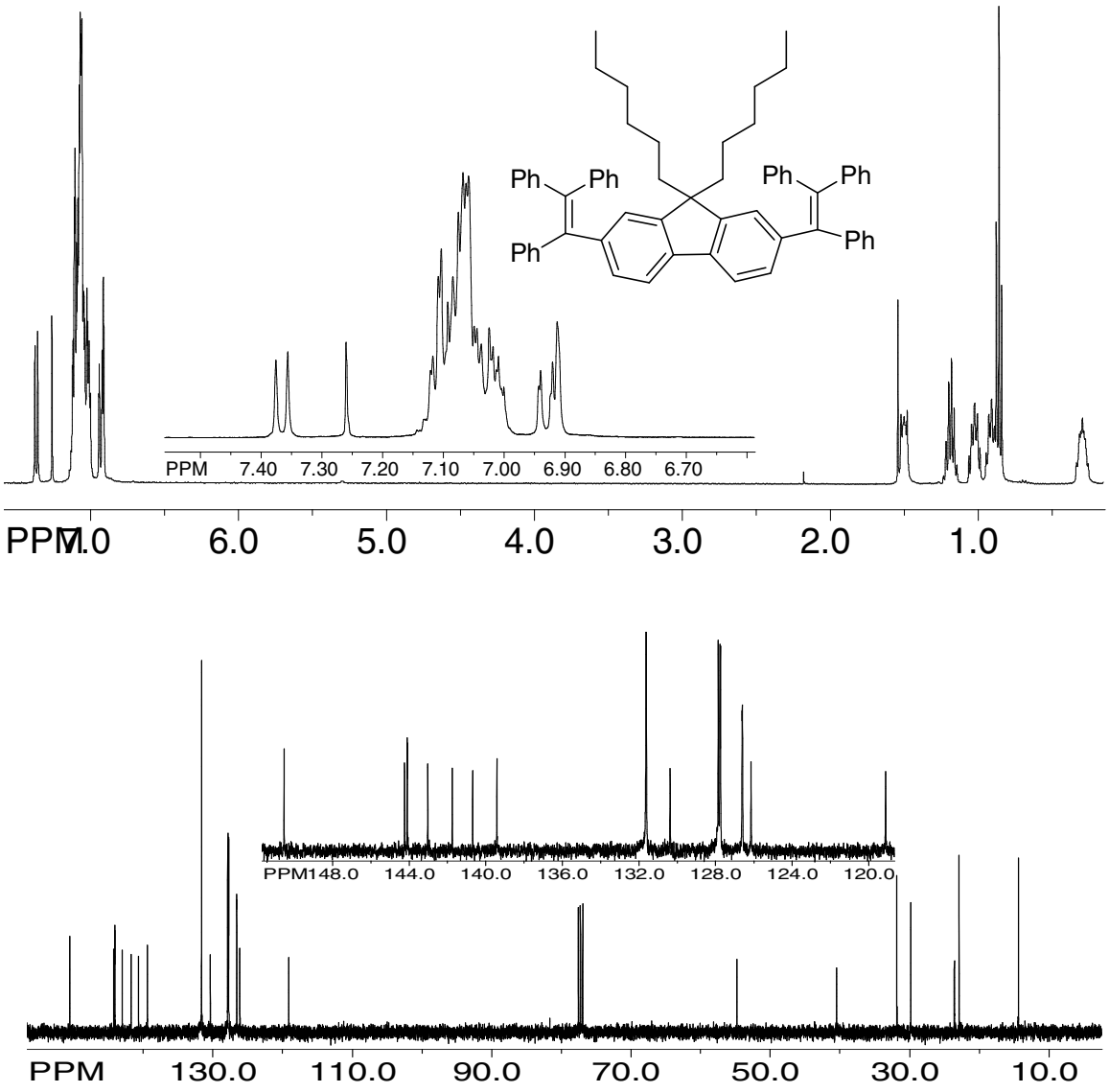
White solid, mp 242-244 $^{\circ}$C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 6.80 (s, 4H), 7.03-7.15 (m, 30H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 126.57, 126.65, 127.75, 127.81, 130.9, 131.54, 131.59, 141.0, 142.1, 143.7, 143.94, 143.97.

4,4'-bis(triphenylethenyl)-1,1'-Biphenyl (12):



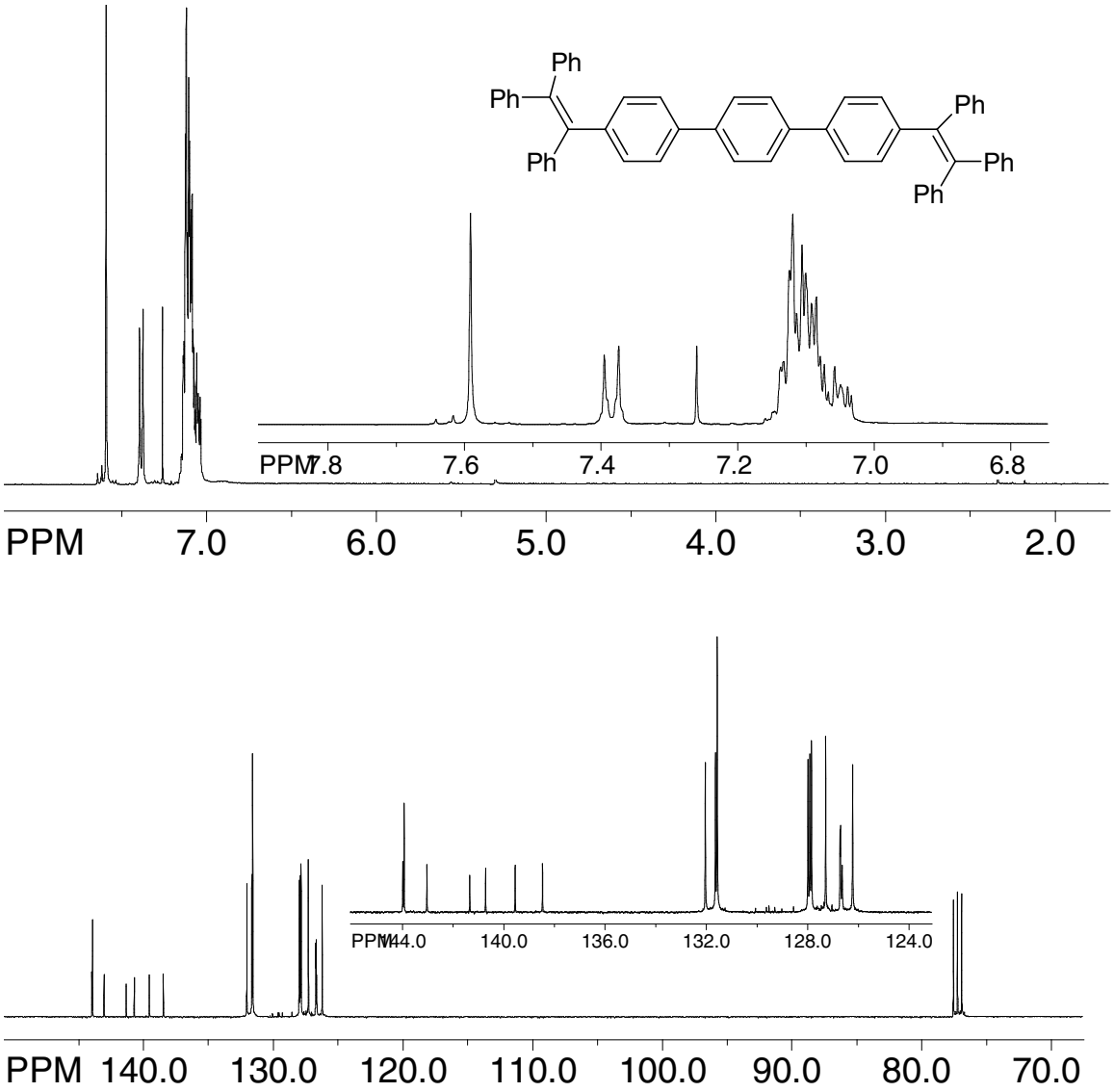
White solid, mp 288-290 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.03-7.14 (m, 34H), 7.33 (d, J = 8.44 Hz, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 126.1, 126.6, 126.67, 127.8, 127.9, 128.0, 131.55, 131.6, 131.9, 138.4, 140.7, 141.2, 142.9, 143.92, 143.94, 143.97.

2,7-bis(triphenylethenyl)- 9,9-dihexylfluorene (13):



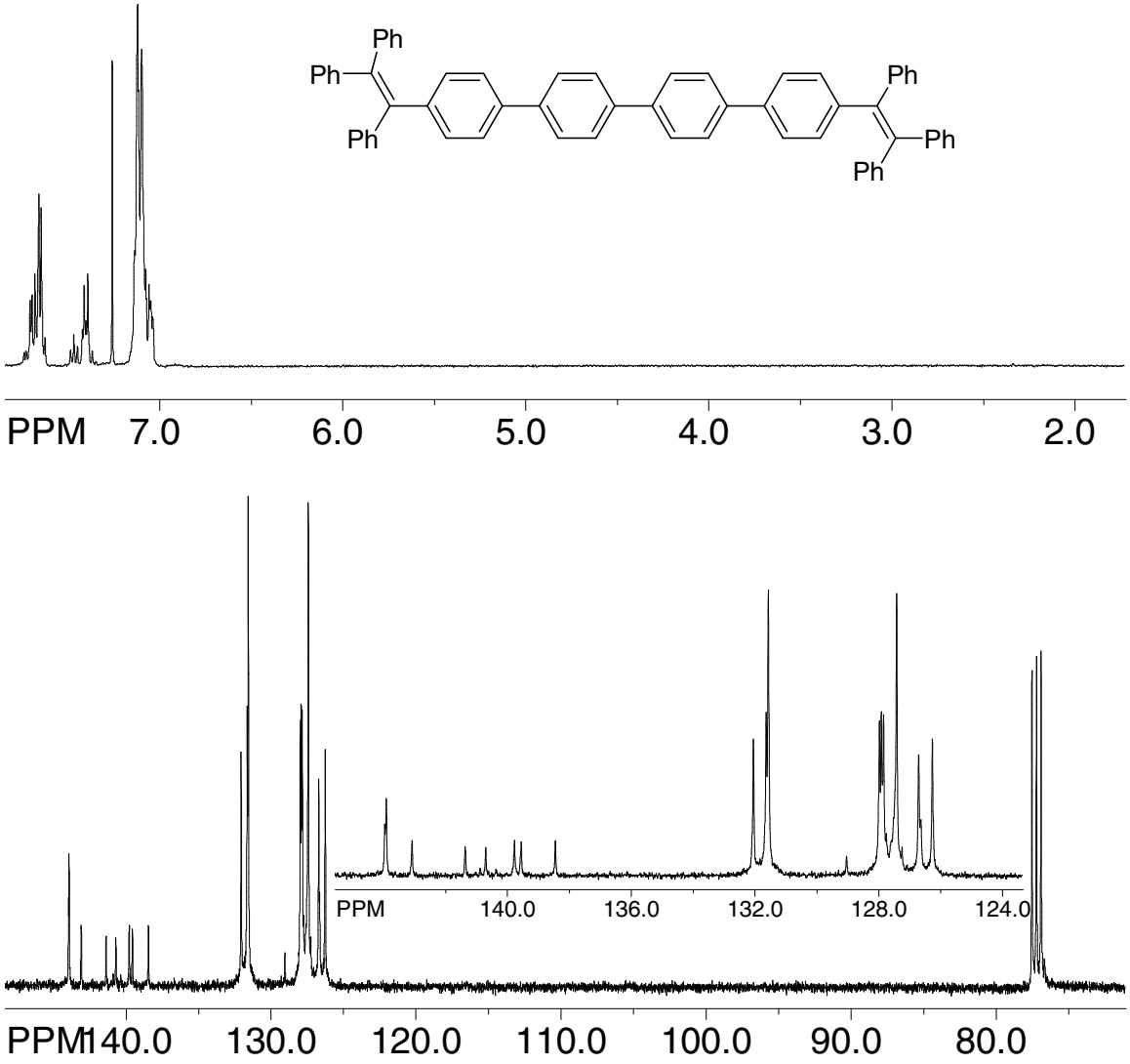
Yellow solid, mp 174-176 $^{\circ}$C;^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.26-0.33 (m, 4H), 0.84-0.95 (m, 10H), 0.99-1.06 (m, 4H), 1.14-1.22 (m, 4H), 1.48-1.52 (m, 4H), 6.91-6.94 (m, 4H), 7.00-7.12 (m, 30H), 7.36-7.38 (m, 2H).; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.4, 22.9, 23.6, 29.8, 31.8, 40.5, 54.8, 119.1, 126.1, 126.56, 126.60, 127.74, 127.76, 127.86, 130.4, 131.6, 139.4, 140.7, 141.7, 143.0, 144.1, 144.2, 150.5.

4,4''-bis(triphenylethenyl)- 1,1':4',1''-Terphenyl (14):



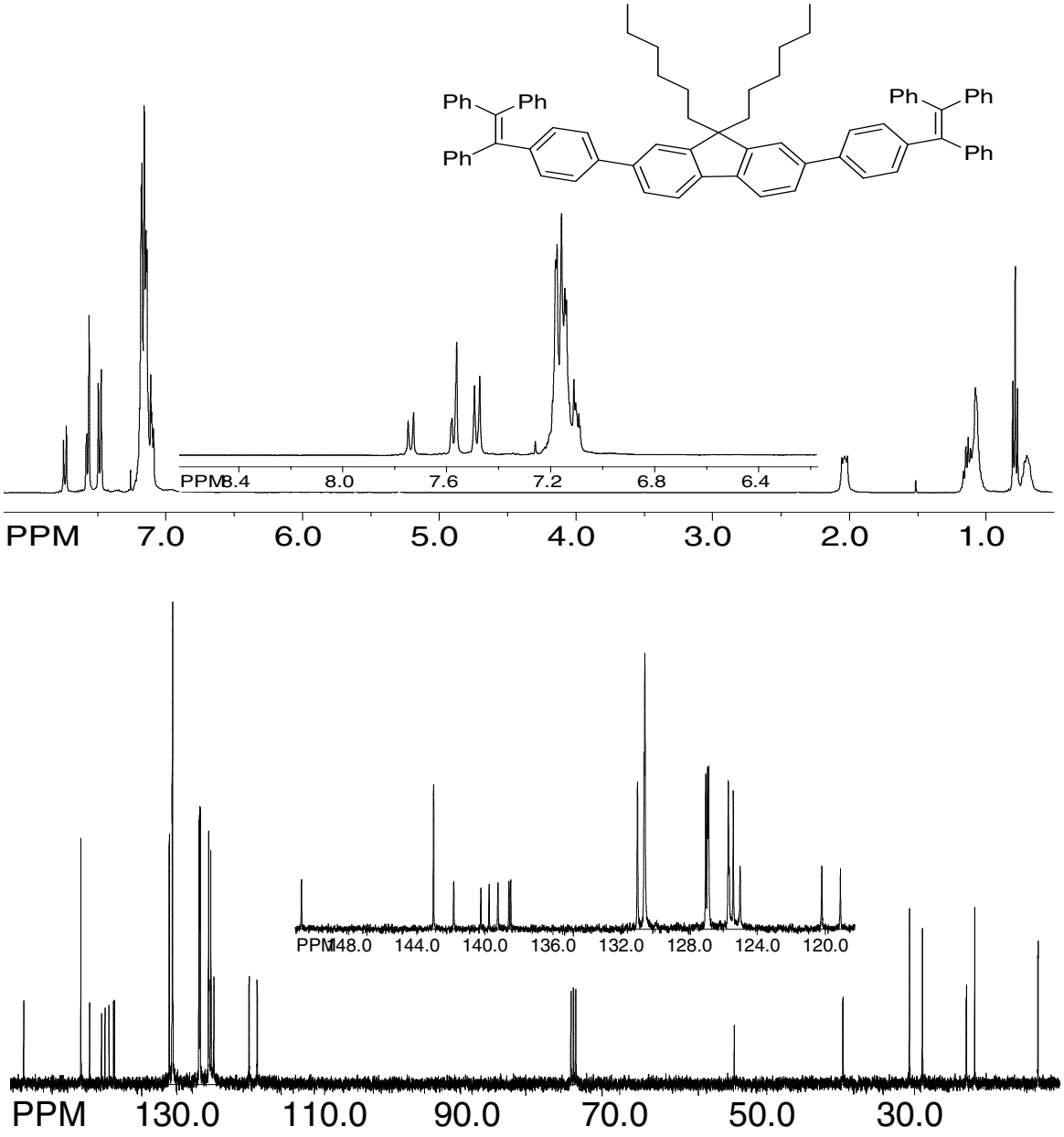
White Solid, mp 294-296 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.03-7.14 (m, 34H), 7.38 (d, *J* = 8.48 Hz, 4H), 7.59 (s, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 126.2, 126.63, 126.69, 126.71, 127.3, 127.84, 127.90, 127.98, 131.56, 131.63, 132.0, 138.5, 139.5, 140.7, 141.3, 143.0, 143.92, 143.97.

4,4'''-bis(triphenylethenyl)- 1,1':4',1'':4'',1'''-Quaterphenyl (15):



Pale yellow solid, mp 320-324 $^{\circ}$C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.03-7.14 (m, 38H), 7.39-7.41 (m 4H), 7.65-7.71 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 126.3, 126.7, 127.4, 127.85, 127.92, 127.98, 131.57, 131.6, 132.1, 138.5, 139.56, 139.77, 140.7, 141.4, 143.1, 143.92, 143.96.

2,7-bis(tetraphenylethenyl)- 9,9-dihexylfluorene (16):



Yellow solid, mp 207-209 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.71 (m, 4H), 0.79 (t, *J* = 7.06 Hz, 6H), 1.04-1.17 (m, 12H), 2.02-2.06 (m, 4H), 7.09-7.20 (m, 34H), 7.47-7.49 (m, 4H), 7.56-7.58 (m, 4H), 7.73-7.75 (m, 2H).; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.2, 21.8, 22.9, 28.9, 30.7, 39.7, 54.4, 119.1, 120.2, 125.0, 125.4, 125.7, 126.8, 126.9, 127.0, 130.6, 131.0, 138.5, 139.2, 139.7, 141.8, 143.0, 150.8.

References:

(1) Zhou, C.; Emrich, D. E.; Larock, R. C. *Org. Lett.* **2003**, *5*, 1579.

(2) Mills, N. C.; Tirla, C.; Benish, M. A.; Rakowitz, A. J.; Bebell, L. M.; Hurd, C. M. M.; Bria, A. L. M. *J. Org. Chem.* **2005**, *70*, 10709.

(3) Forrester, A. R.; Hepburn, S. P. *J. Chem. Soc.* **1971**, *20*, 3322.

(4) Franco, M. L. T. M. B.; Herold, B. J.; Evans, J. C.; Rowlands, C. C. *J. Chem. Soc., Perkin Trans. 1*, **1998**, 443.

(5) Rathore, R.; Burns, C. L.; Abdelwahed, S. A. *Org. Lett.* **2004**, *6*, 1689.

Crystal data and structure refinement for 1,1-Diphenyl-2,2-di-(*p*-methoxyphenyl)ethylene (6)

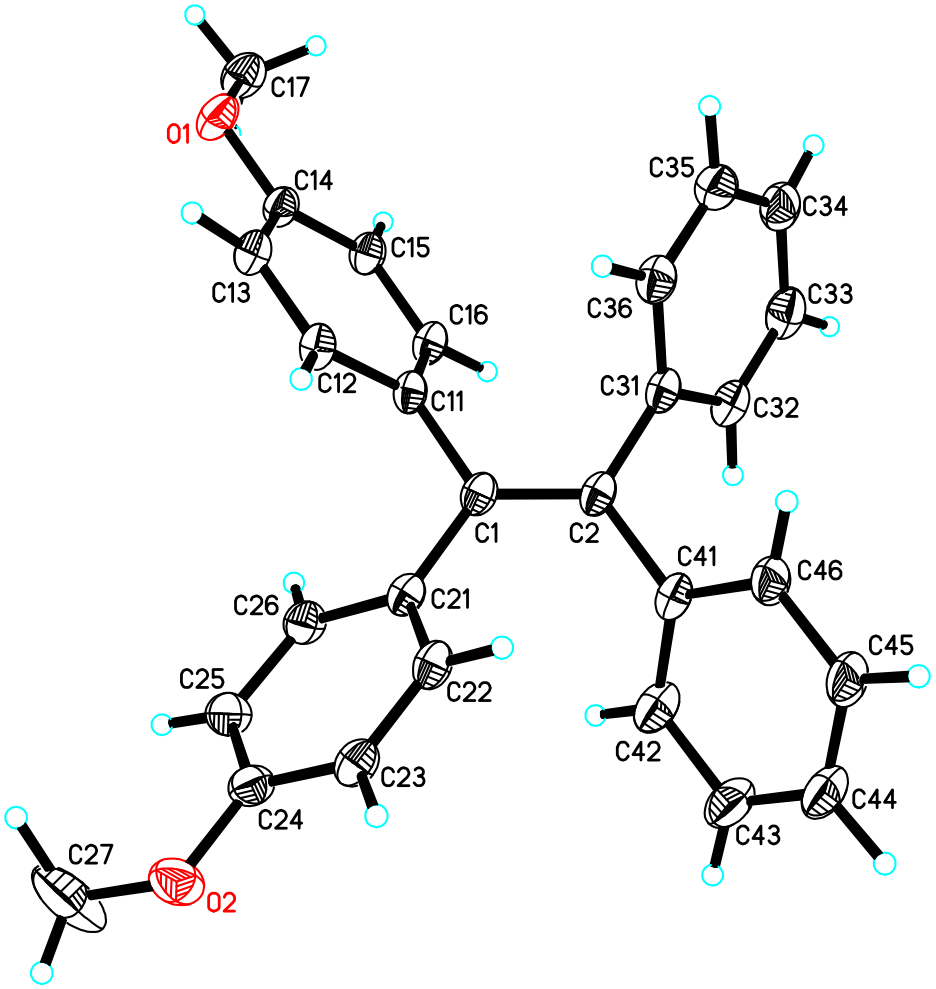


Table 1.

Identification code	raj2r	
Empirical formula	C28 H24 O2	
Formula weight	392.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 9.7502(9) Å	α= 90°.
	b = 10.4517(10) Å	β= 92.5470(10)°.
	c = 10.5257(10) Å	γ = 90°.
Volume	1071.57(18) Å^3	

Z	2
Density (calculated)	1.216 Mg/m^3
Absorption coefficient	0.075 mm^{-1}
F(000)	416
Crystal size	0.35 x 0.32 x 0.15 mm^3
Theta range for data collection	1.94 to 31.89°.
Index ranges	-14<=h<=14, -14<=k<=15, 0<=l<=15
Reflections collected	17512
Independent reflections	6840 [R(int) = 0.0279]
Completeness to theta = 31.89°	95.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9888 and 0.9742
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6840 / 1 / 367
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1139
R indices (all data)	R1 = 0.0491, wR2 = 0.1170
Absolute structure parameter	0.6(8)
Largest diff. peak and hole	0.475 and -0.168 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for raj2r. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2313(1)	6319(1)	2001(1)	29(1)
O(2)	6771(1)	7420(1)	9964(1)	34(1)
C(1)	7079(1)	5213(1)	5076(1)	21(1)
C(2)	8175(1)	4577(1)	4636(1)	21(1)
C(11)	5811(1)	5441(1)	4261(1)	20(1)
C(12)	5250(1)	6676(1)	4199(1)	23(1)
C(13)	4085(1)	6942(1)	3449(1)	24(1)
C(14)	3439(1)	5966(1)	2742(1)	22(1)
C(15)	3954(1)	4728(1)	2814(1)	23(1)
C(16)	5136(1)	4479(1)	3573(1)	22(1)
C(17)	1622(1)	5339(1)	1281(1)	31(1)

C(21)	7031(1)	5757(1)	6379(1)	21(1)
C(22)	8131(1)	6402(1)	6986(1)	23(1)
C(23)	8028(1)	6918(1)	8188(1)	25(1)
C(24)	6795(1)	6829(1)	8808(1)	25(1)
C(25)	5684(1)	6193(1)	8231(1)	27(1)
C(26)	5815(1)	5666(1)	7027(1)	25(1)
C(27)	5494(2)	7403(3)	10565(2)	68(1)
C(31)	8191(1)	4110(1)	3298(1)	22(1)
C(32)	8349(1)	2803(1)	3070(1)	27(1)
C(33)	8325(1)	2329(1)	1832(1)	32(1)
C(34)	8173(1)	3154(2)	811(1)	32(1)
C(35)	8037(1)	4459(1)	1027(1)	31(1)
C(36)	8042(1)	4933(1)	2259(1)	26(1)
C(41)	9449(1)	4295(1)	5420(1)	23(1)
C(42)	9433(1)	3665(1)	6589(1)	30(1)
C(43)	10648(2)	3434(2)	7292(2)	37(1)
C(44)	11889(1)	3825(2)	6839(2)	39(1)
C(45)	11926(1)	4435(2)	5672(1)	35(1)
C(46)	10714(1)	4658(1)	4961(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for raj2r.

O(1)-C(14)	1.3690(13)	C(13)-C(14)	1.3966(16)
O(1)-C(17)	1.4252(16)	C(13)-H(13)	0.946(18)
O(2)-C(24)	1.3659(15)	C(14)-C(15)	1.3890(15)
O(2)-C(27)	1.4213(19)	C(15)-C(16)	1.3970(15)
C(1)-C(2)	1.3582(14)	C(15)-H(15)	0.94(2)
C(1)-C(21)	1.4874(15)	C(16)-H(16)	0.966(18)
C(1)-C(11)	1.4923(15)	C(17)-H(17A)	0.99(2)
C(2)-C(41)	1.4895(15)	C(17)-H(17B)	0.96(2)
C(2)-C(31)	1.4913(16)	C(17)-H(17C)	0.959(19)
C(11)-C(16)	1.3883(15)	C(21)-C(26)	1.3964(15)
C(11)-C(12)	1.4019(15)	C(21)-C(22)	1.3978(15)
C(12)-C(13)	1.3826(16)	C(22)-C(23)	1.3825(17)
C(12)-H(12)	0.940(18)	C(22)-H(22)	0.928(18)

C(23)-C(24)	1.3961(16)	C(21)-C(1)-C(11)	114.18(9)
C(23)-H(23)	0.932(19)	C(1)-C(2)-C(41)	123.88(10)
C(24)-C(25)	1.3880(16)	C(1)-C(2)-C(31)	121.59(9)
C(25)-C(26)	1.3929(17)	C(41)-C(2)-C(31)	114.53(9)
C(25)-H(25)	0.914(19)	C(16)-C(11)-C(12)	117.91(10)
C(26)-H(26)	0.888(19)	C(16)-C(11)-C(1)	123.05(10)
C(27)-H(27A)	0.89(5)	C(12)-C(11)-C(1)	119.03(10)
C(27)-H(27B)	0.87(4)	C(13)-C(12)-C(11)	121.39(10)
C(27)-H(27C)	1.06(3)	C(13)-C(12)-H(12)	119.4(11)
C(31)-C(36)	1.3935(16)	C(11)-C(12)-H(12)	119.1(11)
C(31)-C(32)	1.3965(17)	C(12)-C(13)-C(14)	119.77(10)
C(32)-C(33)	1.3931(19)	C(12)-C(13)-H(13)	123.5(10)
C(32)-H(32)	0.938(19)	C(14)-C(13)-H(13)	116.6(10)
C(33)-C(34)	1.381(2)	O(1)-C(14)-C(15)	124.13(11)
C(33)-H(33)	0.95(2)	O(1)-C(14)-C(13)	115.96(10)
C(34)-C(35)	1.390(2)	C(15)-C(14)-C(13)	119.91(10)
C(34)-H(34)	0.930(18)	C(14)-C(15)-C(16)	119.45(10)
C(35)-C(36)	1.3885(18)	C(14)-C(15)-H(15)	118.5(13)
C(35)-H(35)	0.98(2)	C(16)-C(15)-H(15)	122.0(13)
C(36)-H(36)	0.97(2)	C(11)-C(16)-C(15)	121.54(10)
C(41)-C(42)	1.3966(17)	C(11)-C(16)-H(16)	121.0(10)
C(41)-C(46)	1.3971(15)	C(15)-C(16)-H(16)	117.4(10)
C(42)-C(43)	1.3895(18)	O(1)-C(17)-H(17A)	109.0(12)
C(42)-H(42)	0.946(19)	O(1)-C(17)-H(17B)	112.3(15)
C(43)-C(44)	1.382(2)	H(17A)-C(17)-H(17B)	113(2)
C(43)-H(43)	0.93(2)	O(1)-C(17)-H(17C)	105.7(12)
C(44)-C(45)	1.386(2)	H(17A)-C(17)-H(17C)	110.7(17)
C(44)-H(44)	1.02(2)	H(17B)-C(17)-H(17C)	105.7(18)
C(45)-C(46)	1.3899(17)	C(26)-C(21)-C(22)	117.43(10)
C(45)-H(45)	0.96(2)	C(26)-C(21)-C(1)	119.09(9)
C(46)-H(46)	0.942(19)	C(22)-C(21)-C(1)	123.44(9)
		C(23)-C(22)-C(21)	121.39(10)
C(14)-O(1)-C(17)	117.24(10)	C(23)-C(22)-H(22)	118.0(11)
C(24)-O(2)-C(27)	116.20(11)	C(21)-C(22)-H(22)	120.6(11)
C(2)-C(1)-C(21)	124.02(10)	C(22)-C(23)-C(24)	120.04(10)
C(2)-C(1)-C(11)	121.79(10)	C(22)-C(23)-H(23)	120.4(12)

C(24)-C(23)-H(23)	119.6(12)	C(36)-C(35)-C(34)	120.39(12)
O(2)-C(24)-C(25)	124.19(10)	C(36)-C(35)-H(35)	120.7(12)
O(2)-C(24)-C(23)	115.84(10)	C(34)-C(35)-H(35)	118.9(12)
C(25)-C(24)-C(23)	119.95(11)	C(35)-C(36)-C(31)	120.59(12)
C(24)-C(25)-C(26)	119.07(10)	C(35)-C(36)-H(36)	120.5(12)
C(24)-C(25)-H(25)	121.0(12)	C(31)-C(36)-H(36)	118.7(12)
C(26)-C(25)-H(25)	119.7(12)	C(42)-C(41)-C(46)	118.50(10)
C(25)-C(26)-C(21)	122.11(10)	C(42)-C(41)-C(2)	122.68(10)
C(25)-C(26)-H(26)	120.9(11)	C(46)-C(41)-C(2)	118.82(10)
C(21)-C(26)-H(26)	116.9(11)	C(43)-C(42)-C(41)	120.57(12)
O(2)-C(27)-H(27A)	118(3)	C(43)-C(42)-H(42)	121.0(11)
O(2)-C(27)-H(27B)	104(2)	C(41)-C(42)-H(42)	118.4(11)
H(27A)-C(27)-H(27B)	104(3)	C(44)-C(43)-C(42)	120.25(13)
O(2)-C(27)-H(27C)	106.6(17)	C(44)-C(43)-H(43)	121.0(12)
H(27A)-C(27)-H(27C)	102(3)	C(42)-C(43)-H(43)	118.6(12)
H(27B)-C(27)-H(27C)	124(3)	C(43)-C(44)-C(45)	119.97(12)
C(36)-C(31)-C(32)	118.53(11)	C(43)-C(44)-H(44)	121.5(13)
C(36)-C(31)-C(2)	122.26(11)	C(45)-C(44)-H(44)	118.4(13)
C(32)-C(31)-C(2)	119.20(11)	C(44)-C(45)-C(46)	119.96(12)
C(33)-C(32)-C(31)	120.72(12)	C(44)-C(45)-H(45)	115.7(13)
C(33)-C(32)-H(32)	122.5(12)	C(46)-C(45)-H(45)	124.3(13)
C(31)-C(32)-H(32)	116.7(12)	C(45)-C(46)-C(41)	120.73(12)
C(34)-C(33)-C(32)	120.19(12)	C(45)-C(46)-H(46)	120.2(12)
C(34)-C(33)-H(33)	121.3(12)	C(41)-C(46)-H(46)	119.1(12)
C(32)-C(33)-H(33)	118.4(12)		
C(33)-C(34)-C(35)	119.56(13)		
C(33)-C(34)-H(34)	122.1(12)		
C(35)-C(34)-H(34)	118.2(12)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for raj2r. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	28(1)	35(1)	-2(1)	-8(1)	5(1)
O(2)	28(1)	50(1)	26(1)	-5(1)	0(1)	-6(1)

C(1)	14(1)	20(1)	27(1)	0(1)	0(1)	-1(1)
C(2)	15(1)	21(1)	29(1)	1(1)	0(1)	1(1)
C(11)	15(1)	21(1)	25(1)	0(1)	3(1)	1(1)
C(12)	18(1)	21(1)	29(1)	-3(1)	2(1)	2(1)
C(13)	21(1)	20(1)	29(1)	0(1)	1(1)	4(1)
C(14)	16(1)	25(1)	25(1)	1(1)	0(1)	2(1)
C(15)	18(1)	22(1)	28(1)	-1(1)	1(1)	0(1)
C(16)	16(1)	19(1)	30(1)	0(1)	1(1)	1(1)
C(17)	24(1)	33(1)	35(1)	-2(1)	-7(1)	0(1)
C(21)	17(1)	22(1)	26(1)	1(1)	-1(1)	1(1)
C(22)	15(1)	23(1)	32(1)	1(1)	1(1)	0(1)
C(23)	18(1)	26(1)	31(1)	0(1)	-3(1)	-1(1)
C(24)	22(1)	30(1)	23(1)	3(1)	-2(1)	0(1)
C(25)	20(1)	36(1)	25(1)	3(1)	2(1)	-3(1)
C(26)	17(1)	30(1)	26(1)	0(1)	0(1)	-3(1)
C(27)	40(1)	130(2)	36(1)	-37(1)	15(1)	-28(1)
C(31)	14(1)	22(1)	30(1)	0(1)	1(1)	1(1)
C(32)	22(1)	24(1)	35(1)	0(1)	-1(1)	5(1)
C(33)	25(1)	29(1)	41(1)	-8(1)	-2(1)	5(1)
C(34)	21(1)	42(1)	32(1)	-7(1)	-2(1)	3(1)
C(35)	24(1)	37(1)	31(1)	4(1)	1(1)	3(1)
C(36)	21(1)	25(1)	34(1)	2(1)	3(1)	1(1)
C(41)	16(1)	20(1)	32(1)	-1(1)	-1(1)	2(1)
C(42)	21(1)	28(1)	42(1)	8(1)	-1(1)	1(1)
C(43)	29(1)	38(1)	42(1)	10(1)	-5(1)	8(1)
C(44)	22(1)	51(1)	43(1)	-3(1)	-7(1)	9(1)
C(45)	15(1)	51(1)	39(1)	-7(1)	-1(1)	2(1)
C(46)	17(1)	37(1)	30(1)	-3(1)	2(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for raj2r.

	x	y	z	U(eq)
H(12)	5708(17)	7345(18)	4639(15)	25(4)
H(13)	3728(17)	7777(17)	3326(14)	21(4)
H(15)	3510(20)	4090(20)	2319(18)	39(5)
H(16)	5470(16)	3609(17)	3601(15)	22(4)
H(17A)	1250(20)	4700(20)	1873(18)	43(5)
H(17B)	2190(20)	4970(20)	660(20)	53(6)
H(17C)	890(19)	5760(20)	807(18)	35(5)
H(22)	8947(18)	6520(18)	6579(15)	24(4)
H(23)	8780(20)	7324(19)	8590(17)	31(4)
H(25)	4850(20)	6174(19)	8597(17)	32(4)
H(26)	5137(19)	5217(18)	6654(16)	27(4)
H(27A)	5070(40)	6650(50)	10650(30)	113(13)
H(27B)	5710(30)	7630(40)	11350(30)	98(11)
H(27C)	4780(30)	7910(30)	9950(30)	75(8)
H(32)	8453(18)	2272(19)	3786(17)	32(4)
H(33)	8480(20)	1440(20)	1712(18)	42(5)
H(34)	8118(19)	2863(19)	-25(17)	31(4)
H(35)	7900(20)	5030(20)	300(20)	41(5)
H(36)	7870(20)	5840(20)	2413(19)	44(5)
H(42)	8580(20)	3417(19)	6897(17)	34(4)
H(43)	10601(19)	3065(19)	8090(18)	33(4)
H(44)	12790(20)	3640(30)	7320(20)	55(6)
H(45)	12820(20)	4700(20)	5420(20)	51(6)
H(46)	10740(20)	5048(18)	4156(18)	33(4)

Crystal data and structure refinement for 1,4-bis(triphenylethenyl)-benzene (11).

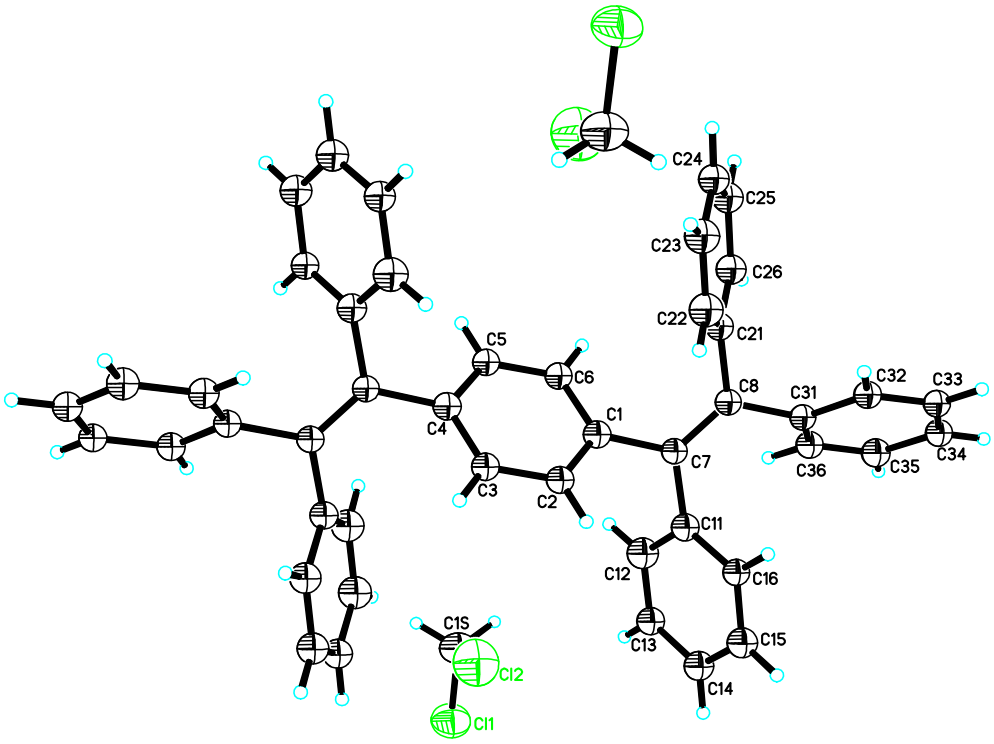


Table 1.

Identification code	raj2w	
Empirical formula	C48 H38 Cl4	
Formula weight	756.58	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P nnm	
Unit cell dimensions	a = 5.8309(2) Å	α= 90°.
	b = 15.9227(5) Å	β= 90°.
	c = 20.9840(6) Å	γ = 90°.
Volume	1948.23(11) $Å^3$	
Z	2	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	3.008 mm^{-1}	
F(000)	788	
Crystal size	0.80 x 0.65 x 0.10 mm^3	

Theta range for data collection	3.48 to 60.85°.
Index ranges	0<=h<=6, 0<=k<=18, 0<=l<=23
Reflections collected	15717
Independent reflections	1519 [R(int) = 0.0235]
Completeness to theta = 67.48°	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7530 and 0.1970
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1519 / 90 / 111
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0748, wR2 = 0.1717
R indices (all data)	R1 = 0.0768, wR2 = 0.1728
Largest diff. peak and hole	0.412 and -0.760 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for raj2w. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	16199(3)	8920(1)	5000	59(1)
Cl(2)	11928(3)	8020(1)	5000	73(1)
C(1S)	14883(11)	7931(4)	5000	52(2)
C(7)	5277(11)	5359(4)	3637(3)	23(1)
C(11)	5841(12)	6259(5)	3493(4)	28(2)
C(12)	7889(13)	6601(6)	3719(4)	37(2)
C(13)	8398(14)	7435(5)	3605(3)	29(2)
C(14)	6809(13)	7933(5)	3289(4)	32(2)
C(15)	4754(14)	7599(4)	3069(4)	33(2)
C(16)	4281(17)	6764(5)	3164(5)	25(3)
C(7A)	5277(11)	5359(4)	3637(3)	23(1)
C(1)	5114(14)	5162(4)	4339(2)	26(2)
C(2)	3850(13)	5676(5)	4750(3)	25(2)
C(3)	3754(14)	5523(4)	5398(3)	25(2)
C(4)	4886(14)	4838(4)	5661(2)	26(2)
C(5)	6150(13)	4324(5)	5250(3)	25(2)

C(6)	6246(14)	4477(4)	4602(3)	25(2)
C(8)	4857(12)	4787(3)	3186(3)	24(2)
C(21)	4036(12)	3914(4)	3336(4)	26(2)
C(22)	1933(13)	3760(6)	3632(4)	37(2)
C(23)	1158(14)	2953(6)	3732(4)	39(2)
C(24)	2421(14)	2272(5)	3523(4)	31(2)
C(25)	4502(15)	2408(4)	3222(4)	33(2)
C(26)	5228(18)	3226(5)	3129(5)	32(3)
C(8A)	4857(12)	4787(3)	3186(3)	24(2)
C(31)	5120(20)	4964(11)	2483(2)	24(2)
C(32)	3389(13)	4701(5)	2063(4)	26(2)
C(33)	3584(12)	4803(4)	1409(3)	26(2)
C(34)	5577(10)	5151(4)	1168(3)	27(2)
C(35)	7344(13)	5397(5)	1579(3)	32(2)
C(36)	7105(14)	5296(5)	2230(4)	28(2)

Table 3. Bond lengths [Å] and angles [°] for raj2w.

Cl(1)-C(1S)	1.752(6)	C(8)-C(21)	1.503(8)
Cl(2)-C(1S)	1.729(7)	C(8)-C(31)	1.509(7)
C(7)-C(8)	1.337(8)	C(21)-C(26)	1.370(9)
C(7)-C(11)	1.501(8)	C(21)-C(22)	1.396(9)
C(7)-C(1)	1.508(7)	C(22)-C(23)	1.378(10)
C(11)-C(12)	1.395(9)	C(23)-C(24)	1.382(10)
C(11)-C(16)	1.396(9)	C(24)-C(25)	1.385(11)
C(12)-C(13)	1.382(10)	C(25)-C(26)	1.383(10)
C(13)-C(14)	1.389(10)	C(31)-C(36)	1.378(11)
C(14)-C(15)	1.389(10)	C(31)-C(32)	1.405(10)
C(15)-C(16)	1.372(9)	C(32)-C(33)	1.387(10)
C(1)-C(6)	1.388(8)	C(33)-C(34)	1.383(9)
C(1)-C(2)	1.401(8)	C(34)-C(35)	1.398(8)
C(2)-C(3)	1.382(8)	C(35)-C(36)	1.383(9)
C(3)-C(4)	1.388(8)		
C(4)-C(5)	1.401(8)	Cl(2)-C(1S)-Cl(1)	111.3(4)
C(5)-C(6)	1.382(8)	C(8)-C(7)-C(11)	123.2(6)

C(8)-C(7)-C(1)	122.5(5)	C(21)-C(8)-C(31)	114.2(8)
C(11)-C(7)-C(1)	114.2(6)	C(26)-C(21)-C(22)	116.5(7)
C(12)-C(11)-C(16)	120.1(7)	C(26)-C(21)-C(8)	120.8(7)
C(12)-C(11)-C(7)	119.4(6)	C(22)-C(21)-C(8)	122.4(7)
C(16)-C(11)-C(7)	120.5(6)	C(23)-C(22)-C(21)	121.3(8)
C(13)-C(12)-C(11)	120.0(7)	C(22)-C(23)-C(24)	120.6(7)
C(14)-C(13)-C(12)	119.2(7)	C(23)-C(24)-C(25)	119.3(7)
C(13)-C(14)-C(15)	121.1(7)	C(24)-C(25)-C(26)	118.7(8)
C(16)-C(15)-C(14)	119.7(8)	C(21)-C(26)-C(25)	123.6(8)
C(15)-C(16)-C(11)	119.9(8)	C(36)-C(31)-C(32)	118.4(7)
C(6)-C(1)-C(2)	117.6(4)	C(36)-C(31)-C(8)	122.3(8)
C(6)-C(1)-C(7)	121.5(6)	C(32)-C(31)-C(8)	118.9(9)
C(2)-C(1)-C(7)	120.9(6)	C(33)-C(32)-C(31)	121.8(7)
C(3)-C(2)-C(1)	121.7(7)	C(34)-C(33)-C(32)	118.5(7)
C(2)-C(3)-C(4)	120.7(8)	C(33)-C(34)-C(35)	120.4(6)
C(3)-C(4)-C(5)	117.6(4)	C(36)-C(35)-C(34)	120.1(7)
C(6)-C(5)-C(4)	121.7(7)	C(31)-C(36)-C(35)	120.7(8)
C(5)-C(6)-C(1)	120.7(8)		
C(7)-C(8)-C(21)	122.7(5)	Symmetry transformations used to generate	
C(7)-C(8)-C(31)	123.0(7)	equivalent atoms:	

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for raj2w. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	59(1)	50(1)	67(1)	0	0	-15(1)
Cl(2)	48(1)	88(1)	83(1)	0	0	-17(1)
C(1S)	56(4)	41(3)	60(4)	0	0	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for raj2w.

	x	y	z	U(eq)
H(1SA)	15377	7613	4618	63
H(1SB)	15377	7613	5382	63
H(12)	8932	6259	3951	44
H(13)	9818	7665	3742	35
H(14)	7132	8510	3221	39
H(15)	3681	7948	2854	39
H(16)	2893	6530	3007	30
H(2)	3037	6142	4580	30
H(3)	2905	5890	5666	30
H(5)	6963	3858	5420	30
H(6)	7095	4110	4334	30
H(22)	1018	4220	3767	45
H(23)	-256	2864	3946	47
H(24)	1868	1717	3585	37
H(25)	5412	1949	3082	39
H(26)	6631	3314	2908	38
H(32)	2046	4447	2232	32
H(33)	2376	4638	1133	31
H(34)	5746	5223	721	33
H(35)	8710	5633	1410	38
H(36)	8320	5457	2506	34

Crystal data and structure refinement for 2,7-bis(triphenylethenyl)- 9,9-dihexylfluorene (13).

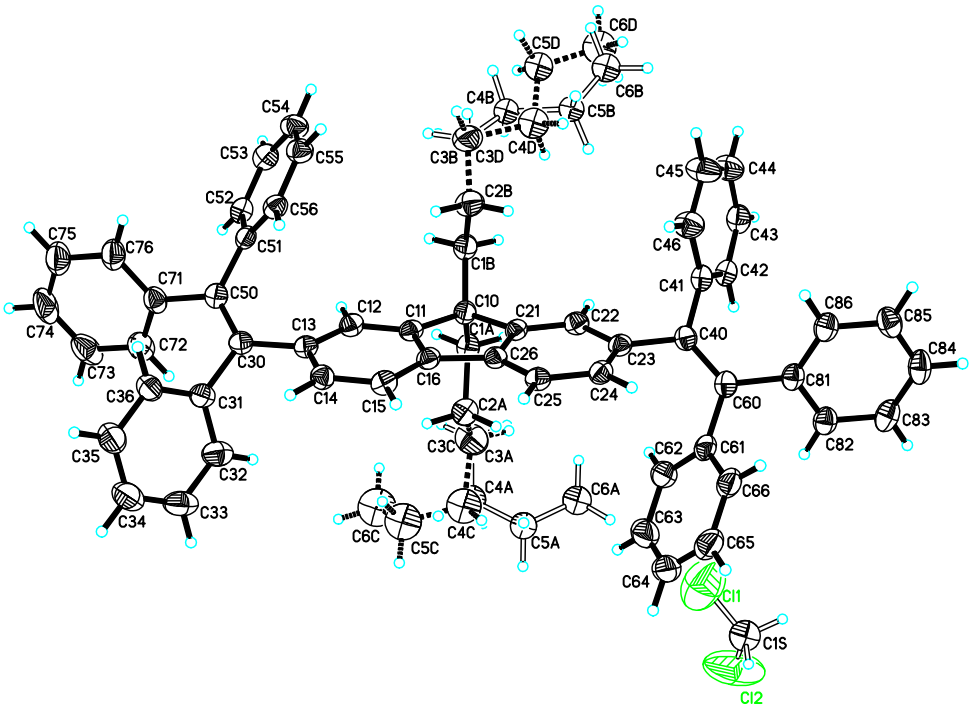


Table 1.

Identification code	raj7s	
Empirical formula	C65.10 H62.20 Cl0.20	
Formula weight	851.64	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 44.5922(14) Å	α= 90°.
	b = 9.3105(3) Å	β= 123.9420(10)°.
	c = 30.3100(9) Å	γ = 90°.
Volume	10439.7(6) $Å^3$	
Z	8	
Density (calculated)	1.084 Mg/m^3	
Absorption coefficient	0.547 mm^{-1}	
F(000)	3650	

Crystal size	0.28 x 0.06 x 0.06 mm^3
Theta range for data collection	2.39 to 67.48°.
Index ranges	-51<=h<=44, 0<=k<=11, 0<=l<=35
Reflections collected	43886
Independent reflections	9059 [R(int) = 0.0672]
Completeness to theta = 67.48°	96.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9679 and 0.8619
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9059 / 10 / 604
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0558, wR2 = 0.1221
R indices (all data)	R1 = 0.0966, wR2 = 0.1371
Extinction coefficient	0.00025(2)
Largest diff. peak and hole	0.304 and -0.280 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for raj7s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	500(1)	626(2)	1425(1)	33(1)
C(2A)	603(1)	741(2)	1994(1)	38(1)
C(3A)	685(1)	-721(3)	2264(1)	59(1)
C(4A)	800(2)	-849(9)	2815(3)	47(2)
C(5A)	1169(1)	-268(5)	3182(2)	40(1)
C(6A)	1454(1)	-900(6)	3112(2)	49(1)
C(3C)	685(1)	-721(3)	2264(1)	59(1)
C(4C)	765(3)	-519(10)	2848(3)	70(3)
C(5C)	423(2)	-457(7)	2824(3)	79(2)
C(6C)	216(2)	-1879(7)	2645(3)	90(2)
C(1B)	310(1)	1727(2)	550(1)	33(1)
C(2B)	274(1)	3019(3)	223(1)	39(1)
C(3B)	139(1)	2681(3)	-352(1)	51(1)
C(4B)	305(1)	1805(5)	-523(2)	34(1)
C(5B)	688(1)	2226(5)	-354(2)	33(1)

C(6B)	814(2)	1433(6)	-654(2)	44(2)
C(3D)	139(1)	2681(3)	-352(1)	51(1)
C(4D)	490(2)	2059(6)	-336(2)	50(1)
C(5D)	410(1)	1451(6)	-844(2)	44(1)
C(6D)	735(2)	1178(7)	-863(3)	61(2)
C(10)	431(1)	2063(2)	1126(1)	29(1)
C(11)	162(1)	3004(2)	1153(1)	27(1)
C(12)	-199(1)	2746(2)	949(1)	29(1)
C(13)	-399(1)	3735(2)	1033(1)	29(1)
C(14)	-222(1)	4955(2)	1342(1)	29(1)
C(15)	138(1)	5231(2)	1544(1)	30(1)
C(16)	329(1)	4262(2)	1446(1)	27(1)
C(21)	769(1)	3003(2)	1419(1)	26(1)
C(22)	1105(1)	2736(2)	1517(1)	29(1)
C(23)	1389(1)	3710(2)	1814(1)	26(1)
C(24)	1320(1)	4975(2)	1991(1)	28(1)
C(25)	983(1)	5258(2)	1889(1)	27(1)
C(26)	705(1)	4259(2)	1606(1)	25(1)
C(30)	-786(1)	3501(2)	829(1)	29(1)
C(31)	-895(1)	4040(2)	1186(1)	31(1)
C(32)	-721(1)	3582(3)	1710(1)	42(1)
C(33)	-825(1)	4107(3)	2036(1)	48(1)
C(34)	-1097(1)	5110(3)	1843(1)	51(1)
C(35)	-1266(1)	5598(3)	1330(1)	48(1)
C(36)	-1168(1)	5061(3)	1002(1)	38(1)
C(40)	1753(1)	3401(2)	1922(1)	27(1)
C(41)	1746(1)	2873(2)	1453(1)	29(1)
C(42)	1898(1)	1557(2)	1461(1)	31(1)
C(43)	1882(1)	1061(3)	1017(1)	37(1)
C(44)	1717(1)	1875(3)	559(1)	47(1)
C(45)	1562(1)	3178(3)	543(1)	51(1)
C(46)	1570(1)	3664(3)	980(1)	40(1)
C(50)	-1036(1)	2906(2)	351(1)	30(1)
C(51)	-978(1)	2642(2)	-81(1)	27(1)
C(52)	-1100(1)	1374(2)	-375(1)	31(1)
C(53)	-1064(1)	1151(2)	-795(1)	35(1)

C(54)	-910(1)	2189(2)	-933(1)	37(1)
C(55)	-791(1)	3456(2)	-648(1)	34(1)
C(56)	-824(1)	3681(2)	-227(1)	30(1)
C(60)	2061(1)	3560(2)	2410(1)	29(1)
C(61)	2049(1)	3824(2)	2886(1)	33(1)
C(62)	1878(1)	2855(3)	3028(1)	40(1)
C(63)	1870(1)	3100(3)	3473(1)	54(1)
C(64)	2033(1)	4299(4)	3782(1)	62(1)
C(65)	2205(1)	5259(3)	3650(1)	56(1)
C(66)	2217(1)	5023(3)	3208(1)	42(1)
C(71)	-1402(1)	2475(2)	217(1)	34(1)
C(72)	-1439(1)	1639(3)	562(1)	44(1)
C(73)	-1779(1)	1222(3)	433(1)	56(1)
C(74)	-2085(1)	1634(4)	-48(1)	63(1)
C(75)	-2054(1)	2441(3)	-400(1)	55(1)
C(76)	-1713(1)	2856(3)	-271(1)	43(1)
C(81)	2430(1)	3476(2)	2518(1)	29(1)
C(82)	2711(1)	2817(2)	2982(1)	34(1)
C(83)	3059(1)	2759(2)	3097(1)	39(1)
C(84)	3134(1)	3375(3)	2755(1)	41(1)
C(85)	2861(1)	4040(2)	2298(1)	38(1)
C(86)	2512(1)	4089(2)	2179(1)	33(1)
Cl(1)	2387(3)	-691(14)	4214(5)	131(6)
Cl(2)	2782(5)	-2305(14)	5144(5)	147(7)
C(1S)	2749(8)	-1050(30)	4807(12)	57(8)

Table 3. Bond lengths [Å] and angles [°] for raj7s.

C(1A)-C(2A)	1.519(3)	C(4C)-C(5C)	1.491(10)
C(1A)-C(10)	1.549(3)	C(5C)-C(6C)	1.530(8)
C(2A)-C(3A)	1.524(3)	C(1B)-C(2B)	1.510(3)
C(3A)-C(4A)	1.454(7)	C(1B)-C(10)	1.541(3)
C(4A)-C(5A)	1.481(9)	C(2B)-C(3B)	1.526(3)
C(5A)-C(6A)	1.519(6)	C(3B)-C(4B)	1.381(5)

C(4B)-C(5B)	1.534(6)	C(45)-C(46)	1.380(3)
C(5B)-C(6B)	1.504(6)	C(50)-C(51)	1.489(3)
C(4D)-C(5D)	1.485(6)	C(50)-C(71)	1.502(3)
C(5D)-C(6D)	1.502(7)	C(51)-C(56)	1.394(3)
C(10)-C(21)	1.525(3)	C(51)-C(52)	1.394(3)
C(10)-C(11)	1.526(3)	C(52)-C(53)	1.384(3)
C(11)-C(12)	1.385(3)	C(53)-C(54)	1.379(3)
C(11)-C(16)	1.405(3)	C(54)-C(55)	1.381(3)
C(12)-C(13)	1.401(3)	C(55)-C(56)	1.381(3)
C(13)-C(14)	1.402(3)	C(60)-C(81)	1.490(3)
C(13)-C(30)	1.492(3)	C(60)-C(61)	1.492(3)
C(14)-C(15)	1.383(3)	C(61)-C(66)	1.393(3)
C(15)-C(16)	1.384(3)	C(61)-C(62)	1.396(3)
C(16)-C(26)	1.463(3)	C(62)-C(63)	1.387(3)
C(21)-C(22)	1.380(3)	C(63)-C(64)	1.376(4)
C(21)-C(26)	1.397(3)	C(64)-C(65)	1.374(4)
C(22)-C(23)	1.402(3)	C(65)-C(66)	1.389(3)
C(23)-C(24)	1.397(3)	C(71)-C(72)	1.387(3)
C(23)-C(40)	1.493(3)	C(71)-C(76)	1.395(3)
C(24)-C(25)	1.384(3)	C(72)-C(73)	1.393(3)
C(25)-C(26)	1.395(3)	C(73)-C(74)	1.384(4)
C(30)-C(50)	1.358(3)	C(74)-C(75)	1.375(4)
C(30)-C(31)	1.496(3)	C(75)-C(76)	1.395(3)
C(31)-C(36)	1.391(3)	C(81)-C(86)	1.392(3)
C(31)-C(32)	1.391(3)	C(81)-C(82)	1.399(3)
C(32)-C(33)	1.394(3)	C(82)-C(83)	1.390(3)
C(33)-C(34)	1.374(4)	C(83)-C(84)	1.381(3)
C(34)-C(35)	1.373(4)	C(84)-C(85)	1.379(3)
C(35)-C(36)	1.382(3)	C(85)-C(86)	1.388(3)
C(40)-C(60)	1.350(3)	Cl(1)-C(1S)	1.65(3)
C(40)-C(41)	1.490(3)	Cl(2)-C(1S)	1.51(3)
C(41)-C(42)	1.393(3)		
C(41)-C(46)	1.399(3)	C(2A)-C(1A)-C(10)	116.07(18)
C(42)-C(43)	1.387(3)	C(1A)-C(2A)-C(3A)	112.1(2)
C(43)-C(44)	1.377(3)	C(4A)-C(3A)-C(2A)	121.0(4)
C(44)-C(45)	1.383(4)	C(3A)-C(4A)-C(5A)	111.4(5)

C(4A)-C(5A)-C(6A)	114.7(5)	C(25)-C(26)-C(16)	131.38(19)
C(4C)-C(5C)-C(6C)	112.5(6)	C(21)-C(26)-C(16)	108.79(18)
C(2B)-C(1B)-C(10)	114.98(18)	C(50)-C(30)-C(13)	124.81(19)
C(1B)-C(2B)-C(3B)	114.6(2)	C(50)-C(30)-C(31)	120.35(19)
C(4B)-C(3B)-C(2B)	126.8(3)	C(13)-C(30)-C(31)	114.78(18)
C(3B)-C(4B)-C(5B)	116.9(4)	C(36)-C(31)-C(32)	118.2(2)
C(6B)-C(5B)-C(4B)	113.2(4)	C(36)-C(31)-C(30)	120.19(19)
C(4D)-C(5D)-C(6D)	115.2(5)	C(32)-C(31)-C(30)	121.5(2)
C(21)-C(10)-C(11)	100.94(17)	C(31)-C(32)-C(33)	120.4(2)
C(21)-C(10)-C(1B)	112.64(17)	C(34)-C(33)-C(32)	120.0(2)
C(11)-C(10)-C(1B)	112.82(17)	C(35)-C(34)-C(33)	120.2(2)
C(21)-C(10)-C(1A)	110.28(17)	C(34)-C(35)-C(36)	120.0(3)
C(11)-C(10)-C(1A)	111.59(17)	C(35)-C(36)-C(31)	121.0(2)
C(1B)-C(10)-C(1A)	108.47(17)	C(60)-C(40)-C(41)	123.30(19)
C(12)-C(11)-C(16)	120.06(19)	C(60)-C(40)-C(23)	122.25(19)
C(12)-C(11)-C(10)	129.00(19)	C(41)-C(40)-C(23)	114.44(18)
C(16)-C(11)-C(10)	110.92(18)	C(42)-C(41)-C(46)	118.1(2)
C(11)-C(12)-C(13)	120.2(2)	C(42)-C(41)-C(40)	121.48(19)
C(12)-C(13)-C(14)	118.5(2)	C(46)-C(41)-C(40)	120.34(19)
C(12)-C(13)-C(30)	122.45(19)	C(43)-C(42)-C(41)	120.9(2)
C(14)-C(13)-C(30)	119.00(19)	C(44)-C(43)-C(42)	120.2(2)
C(15)-C(14)-C(13)	121.7(2)	C(43)-C(44)-C(45)	119.6(2)
C(14)-C(15)-C(16)	119.1(2)	C(46)-C(45)-C(44)	120.5(2)
C(15)-C(16)-C(11)	120.35(19)	C(45)-C(46)-C(41)	120.6(2)
C(15)-C(16)-C(26)	131.4(2)	C(30)-C(50)-C(51)	124.39(19)
C(11)-C(16)-C(26)	108.26(18)	C(30)-C(50)-C(71)	121.1(2)
C(22)-C(21)-C(26)	120.45(19)	C(51)-C(50)-C(71)	114.49(18)
C(22)-C(21)-C(10)	128.54(19)	C(56)-C(51)-C(52)	118.1(2)
C(26)-C(21)-C(10)	111.00(18)	C(56)-C(51)-C(50)	121.51(19)
C(21)-C(22)-C(23)	120.3(2)	C(52)-C(51)-C(50)	120.27(19)
C(24)-C(23)-C(22)	118.62(19)	C(53)-C(52)-C(51)	120.7(2)
C(24)-C(23)-C(40)	121.56(19)	C(54)-C(53)-C(52)	120.4(2)
C(22)-C(23)-C(40)	119.80(19)	C(53)-C(54)-C(55)	119.6(2)
C(25)-C(24)-C(23)	121.4(2)	C(56)-C(55)-C(54)	120.3(2)
C(24)-C(25)-C(26)	119.3(2)	C(55)-C(56)-C(51)	121.0(2)
C(25)-C(26)-C(21)	119.83(19)	C(40)-C(60)-C(81)	123.8(2)

C(40)-C(60)-C(61)	121.00(19)	C(74)-C(75)-C(76)	120.0(3)
C(81)-C(60)-C(61)	115.16(18)	C(71)-C(76)-C(75)	120.6(3)
C(66)-C(61)-C(62)	118.3(2)	C(86)-C(81)-C(82)	117.7(2)
C(66)-C(61)-C(60)	121.0(2)	C(86)-C(81)-C(60)	122.0(2)
C(62)-C(61)-C(60)	120.7(2)	C(82)-C(81)-C(60)	120.2(2)
C(63)-C(62)-C(61)	120.6(3)	C(83)-C(82)-C(81)	121.1(2)
C(64)-C(63)-C(62)	120.4(3)	C(84)-C(83)-C(82)	120.2(2)
C(65)-C(64)-C(63)	119.8(3)	C(85)-C(84)-C(83)	119.4(2)
C(64)-C(65)-C(66)	120.5(3)	C(84)-C(85)-C(86)	120.6(2)
C(65)-C(66)-C(61)	120.5(3)	C(85)-C(86)-C(81)	121.0(2)
C(72)-C(71)-C(76)	118.5(2)	Cl(2)-C(1S)-Cl(1)	124(2)
C(72)-C(71)-C(50)	121.1(2)		
C(76)-C(71)-C(50)	120.4(2)	Symmetry transformations used to generate equivalent atoms:	
C(71)-C(72)-C(73)	121.0(3)		
C(74)-C(73)-C(72)	119.7(3)		
C(75)-C(74)-C(73)	120.2(3)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for raj7s. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	30(1)	28(1)	40(1)	-3(1)	18(1)	0(1)
C(2A)	38(1)	33(1)	40(1)	2(1)	20(1)	-2(1)
C(3A)	70(2)	51(2)	62(2)	19(2)	42(2)	19(2)
C(3C)	70(2)	51(2)	62(2)	19(2)	42(2)	19(2)
C(1B)	30(1)	32(1)	34(1)	-6(1)	16(1)	-1(1)
C(2B)	43(1)	38(1)	33(1)	2(1)	19(1)	10(1)
C(3B)	43(2)	70(2)	34(1)	-2(1)	18(1)	-16(1)
C(3D)	43(2)	70(2)	34(1)	-2(1)	18(1)	-16(1)
C(10)	25(1)	30(1)	29(1)	-2(1)	14(1)	0(1)
C(11)	28(1)	29(1)	22(1)	3(1)	13(1)	1(1)
C(12)	29(1)	27(1)	27(1)	0(1)	14(1)	-2(1)
C(13)	28(1)	33(1)	25(1)	4(1)	14(1)	1(1)
C(14)	29(1)	30(1)	30(1)	2(1)	17(1)	2(1)

C(15)	32(1)	26(1)	28(1)	-1(1)	15(1)	0(1)
C(16)	26(1)	28(1)	23(1)	2(1)	12(1)	0(1)
C(21)	24(1)	27(1)	22(1)	2(1)	12(1)	3(1)
C(22)	31(1)	27(1)	27(1)	-2(1)	16(1)	3(1)
C(23)	27(1)	27(1)	23(1)	3(1)	13(1)	1(1)
C(24)	26(1)	29(1)	26(1)	0(1)	12(1)	-2(1)
C(25)	30(1)	24(1)	26(1)	-1(1)	16(1)	1(1)
C(26)	26(1)	26(1)	24(1)	2(1)	14(1)	2(1)
C(30)	29(1)	29(1)	28(1)	2(1)	16(1)	1(1)
C(31)	30(1)	36(1)	29(1)	-7(1)	17(1)	-12(1)
C(32)	46(2)	44(2)	33(1)	-3(1)	21(1)	-10(1)
C(33)	57(2)	57(2)	33(1)	-4(1)	27(1)	-15(2)
C(34)	53(2)	64(2)	48(2)	-14(1)	36(2)	-12(2)
C(35)	41(2)	59(2)	48(2)	-10(1)	29(1)	-3(1)
C(36)	34(1)	48(2)	36(1)	-6(1)	23(1)	-3(1)
C(40)	27(1)	25(1)	31(1)	1(1)	17(1)	1(1)
C(41)	24(1)	28(1)	33(1)	-1(1)	15(1)	-1(1)
C(42)	24(1)	31(1)	34(1)	0(1)	14(1)	-1(1)
C(43)	33(1)	36(1)	44(2)	-10(1)	22(1)	-3(1)
C(44)	52(2)	56(2)	38(2)	-7(1)	29(1)	-2(1)
C(45)	67(2)	53(2)	40(2)	11(1)	34(1)	10(1)
C(46)	46(2)	38(1)	38(1)	6(1)	24(1)	9(1)
C(50)	28(1)	30(1)	32(1)	-1(1)	16(1)	0(1)
C(51)	20(1)	31(1)	25(1)	-1(1)	9(1)	2(1)
C(52)	27(1)	29(1)	33(1)	1(1)	14(1)	1(1)
C(53)	36(1)	29(1)	35(1)	-6(1)	17(1)	4(1)
C(54)	44(2)	37(1)	32(1)	-1(1)	23(1)	6(1)
C(55)	38(1)	33(1)	31(1)	3(1)	19(1)	3(1)
C(56)	28(1)	29(1)	26(1)	-2(1)	12(1)	0(1)
C(60)	27(1)	25(1)	34(1)	1(1)	17(1)	1(1)
C(61)	21(1)	41(1)	30(1)	0(1)	11(1)	8(1)
C(62)	35(1)	50(2)	36(1)	6(1)	20(1)	9(1)
C(63)	42(2)	82(2)	43(2)	18(2)	27(1)	19(2)
C(64)	38(2)	113(3)	35(2)	0(2)	19(1)	25(2)
C(65)	32(2)	80(2)	42(2)	-20(2)	12(1)	10(1)
C(66)	26(1)	54(2)	38(1)	-9(1)	13(1)	4(1)

C(71)	30(1)	36(1)	38(1)	-9(1)	21(1)	-6(1)
C(72)	39(1)	53(2)	46(2)	-15(1)	26(1)	-15(1)
C(73)	57(2)	68(2)	62(2)	-26(2)	45(2)	-27(2)
C(74)	35(2)	93(2)	71(2)	-37(2)	35(2)	-25(2)
C(75)	31(2)	75(2)	55(2)	-18(2)	22(1)	-3(1)
C(76)	30(1)	50(2)	47(2)	-10(1)	21(1)	-3(1)
C(81)	26(1)	24(1)	34(1)	-5(1)	16(1)	-3(1)
C(82)	30(1)	30(1)	39(1)	-4(1)	18(1)	-2(1)
C(83)	27(1)	33(1)	46(2)	-2(1)	14(1)	2(1)
C(84)	29(1)	35(1)	59(2)	-6(1)	25(1)	1(1)
C(85)	39(1)	34(1)	50(2)	-7(1)	30(1)	-8(1)
C(86)	29(1)	29(1)	39(1)	-1(1)	17(1)	-1(1)
Cl(1)	102(9)	114(10)	138(11)	-28(8)	42(8)	-3(7)
Cl(2)	263(19)	101(9)	124(11)	-49(8)	138(13)	-69(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for raj7s.

	x	y	z	U(eq)
H(1A1)	279	33	1221	40
H(1A2)	695	107	1429	40
H(2A1)	402	1195	1993	45
H(2A2)	818	1366	2199	45
H(3A1)	465	-1316	2049	70
H(3A2)	875	-1172	2236	70
H(4A1)	796	-1873	2900	57
H(4A2)	629	-322	2867	57
H(5A1)	1243	-445	3552	48
H(5A2)	1162	785	3132	48
H(6A1)	1688	-448	3365	73
H(6A2)	1386	-722	2748	73
H(6A3)	1472	-1937	3178	73
H(3C1)	898	-1153	2292	70

H(3C2)	476	-1373	2051	70
H(4C1)	915	-1330	3077	84
H(4C2)	904	379	3007	84
H(5C1)	267	312	2575	95
H(5C2)	480	-208	3181	95
H(6C1)	-4	-1792	2644	135
H(6C2)	368	-2645	2890	135
H(6C3)	149	-2110	2285	135
H(1B1)	486	1054	562	39
H(1B2)	73	1230	369	39
H(2B1)	512	3494	397	47
H(2B2)	105	3709	223	47
H(3B1)	-107	2287	-516	61
H(3B2)	109	3623	-523	61
H(4B1)	150	1771	-916	40
H(4B2)	315	820	-392	40
H(5B1)	694	3270	-409	40
H(5B2)	858	2031	31	40
H(6B1)	1059	1746	-530	66
H(6B2)	650	1639	-1035	66
H(6B3)	814	398	-595	66
H(3D1)	45	3559	-573	61
H(3D2)	-56	1953	-502	61
H(4D1)	667	2848	-227	60
H(4D2)	606	1304	-60	60
H(5D1)	247	2119	-1136	52
H(5D2)	279	534	-912	52
H(6D1)	657	781	-1211	92
H(6D2)	896	493	-584	92
H(6D3)	864	2083	-807	92
H(12)	-311	1894	752	35
H(14)	-352	5611	1415	35
H(15)	251	6074	1747	35
H(22)	1145	1888	1381	34
H(24)	1509	5655	2184	33
H(25)	940	6125	2012	32

H(32)	-529	2906	1848	50
H(33)	-709	3771	2391	58
H(34)	-1168	5466	2065	61
H(35)	-1450	6305	1200	57
H(36)	-1288	5395	646	45
H(42)	2014	991	1776	37
H(43)	1985	158	1027	45
H(44)	1709	1543	257	56
H(45)	1448	3741	228	61
H(46)	1456	4546	960	48
H(52)	-1209	656	-286	37
H(53)	-1146	277	-990	42
H(54)	-886	2033	-1221	44
H(55)	-686	4177	-743	41
H(56)	-741	4557	-34	35
H(62)	1766	2021	2818	48
H(63)	1752	2436	3564	65
H(64)	2027	4463	4086	75
H(65)	2316	6090	3862	67
H(66)	2341	5683	3124	50
H(72)	-1230	1346	891	53
H(73)	-1801	656	675	67
H(74)	-2317	1360	-135	75
H(75)	-2264	2715	-732	66
H(76)	-1693	3404	-518	51
H(82)	2663	2403	3223	40
H(83)	3245	2294	3412	47
H(84)	3372	3341	2834	49
H(85)	2912	4468	2062	45
H(86)	2327	4548	1862	40
H(1S1)	2952	-1130	4761	68
H(1S2)	2798	-176	5025	68