



Novel arylated chloro- and methoxy-1,3-dibutadienes: Influence of substituents on molecular conformation and crystal packing



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HIGHLIGHTS

- Three novel arylated 1,3-butadienes were prepared.
- Isomers in solution were studied by NMR and UV/Vis spectroscopy.
- Influence of the substituents (and different positions of substituents) on the molecular conformation.

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ABSTRACT

Three novel arylated chloro- and methoxy-1,3-butadienes were prepared and studied by a combination of spectroscopic (UV/vis, IR and NMR) and X-ray crystallographic methods. Influence of substituent on the molecular conformation and crystal packing (i.e. intermolecular interactions) was studied. It was predicted that the differences in electronic and steric effects of two chlorine atoms in comparison to two methoxy groups as substituents at different locations in the molecule would provide various packing of the molecules and cause different assumptions for the photochemical behaviour.

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Introduction

Synthetic organic photochemistry occasionally provides an easy access to complicated structures, difficult to obtain by a classical synthetic approach [1]. Among the most studied and used reactions are the intra- and intermolecular photocycloadditions [2]. Important precursors for these reactions are butadiene derivatives of *o*-divinylbenzenes. Under their prolonged conjugated system, these compounds could participate in photochemical reactions and give novel complex structures [3,4].

In order to study the influence of chlorine as a substituent on the photochemical behaviour of conjugated butadiene systems [5–7], dichloro derivatives of butadiene **1–2** were synthesized. The initial compounds **1–2** undergo photochemical reaction to give new polycyclic structures [4]. Their formation depends on the electronic and steric effects of two chlorine atoms, bounded as substituent on different locations in the molecule. Chlorine can

affect on dibutadiene unit by mesomeric and inductive effect. Understanding the key effects of chlorine substituent in photochemical reaction of these butadiene derivatives, makes the synthesis of these systems suitable for routing photoreaction towards various interesting structures for further transformations and functionalization.

In continuation of our interest in effect of substituent on intramolecular photocycloaddition reactions, we extended synthesis to para-methoxy substituted 1,3-butadiene derivative **3**. It could be expected that very similar compounds with different substitution may display diverse photoreactivity and consequently new type of products, interesting for further studies.

Results and discussion

Synthesis and spectroscopic characterization

Butadiene derivatives **1–3** were prepared by Wittig reaction from diphosphonium salt and the corresponding cinnamaldehydes (Scheme 1). The products were obtained in good yields (50–70%)

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as mixture of three isomers (*cis,cis*-, *cis,trans*- and *trans,trans*-), which were separated by column chromatography and completely characterised spectroscopically. Because the synthesis were performed always from the corresponding (*E*) geometric isomers of the cinnamaldehyde, the second double bond (looking from the *ortho*-substituted central benzene ring) in the products retain the (*E*) configuration. Hence, the number of the geometric isomers was reduced.

Fig. 1a shows the absorption spectra of starting *trans,trans*-isomers 1–2 in ethanol. Band absorption maxima of these compounds are found in the range of 350–375 nm. *Trans,trans*-isomer of 2, which has the same configuration but different location of chlorine atoms substitution, show a bathochromic shift in comparison to *trans,trans*-isomer of 1. This effect can be explained by better delocalization of π -electrons in the absence of the chlorine on the butadiene units.

The UV spectra of separated *cis,cis*-, *cis,trans*- and *trans,trans*-isomers of methoxy derivative 3 clearly show the configuration influence on absorption characteristic (Fig. 1b). Maxima wavelengths of these isomers are in the range of 300–400 nm. The *trans,trans*-isomer show a bathochromic shift and an increase of the molar absorption coefficient in comparison to their *cis,trans*- and *cis,cis*-isomers, as expected. The reason for this effect is increased molecular planarity of *trans,trans* configuration and the possibility of better delocalisation of π electrons.

The ^1H NMR spectra of the compounds 1–2 are presented in Fig. 2. The signals of ethenylic protons (except H_B protons of *trans,trans*-2) of both derivatives are widespread between 6.60–7.10 ppm, and have very similar chemical shift. Therefore, the effect of position of chlorine atoms is in this case negligible. The exception is H_B ethenylic proton of *trans,trans*-isomer of 2, which is drastically shifted to 7.44 ppm. The reason for this phenomenon is strong electronic effect of chlorine atoms on butadiene units to nearby protons.

Fig. 3 shows the ^1H NMR spectra of *cis,cis*-, *cis,trans*- and *trans,trans*-isomers of methoxy derivative 3 with the emphasis on ethenylic protons. These protons in all examples appear as doublet or doublet of doublets between 6.42 and 7.00 ppm. Under increased molecular planarity of *trans,trans*-isomer, the *trans*-ethenylic protons as expected are shifted to higher field, in comparison to the signals of *cis*-protons.

Crystal structures

Conformations of molecules of *trans,trans*-1 and *trans,trans*-2 are very different. Symmetry of *trans,trans*-2 is C_s (Fig. 4a), with the crystallographic mirror plane passing through the middle of

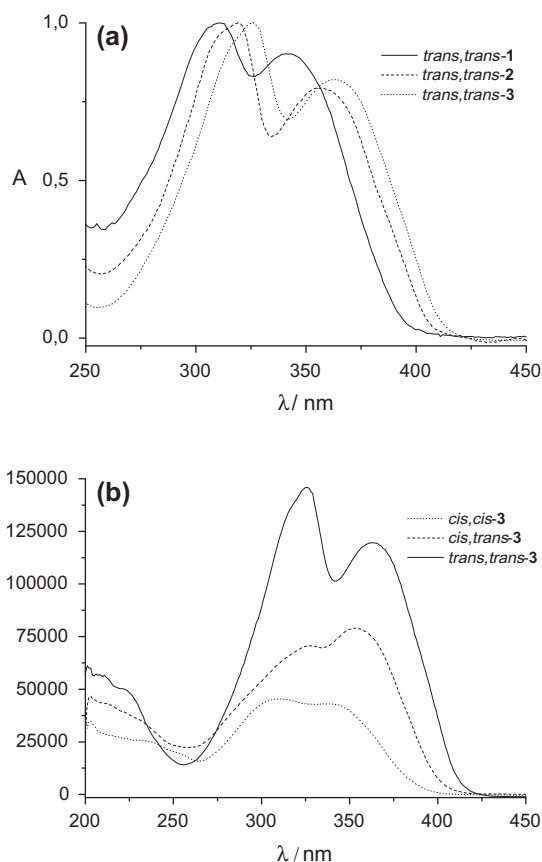
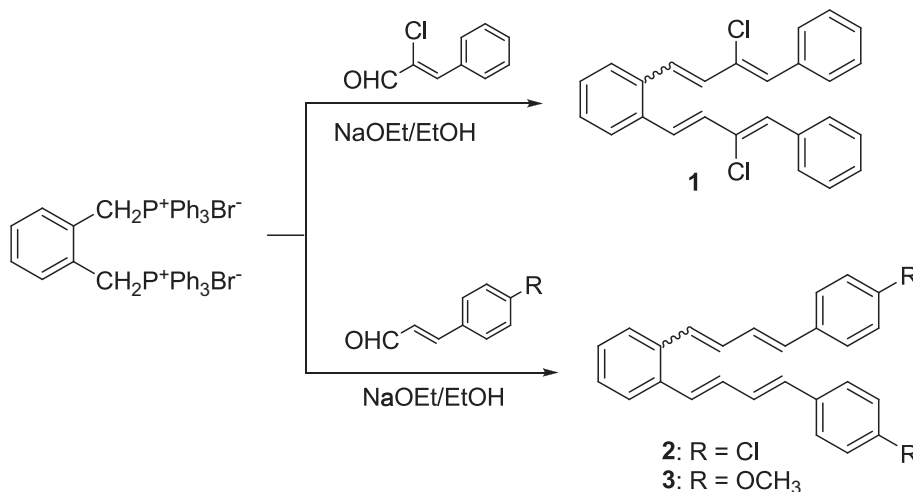


Fig. 1. UV spectra in ethanol: (a) *trans,trans* isomers of compounds 1–3; (b) *cis,cis*-, *cis,trans*- and *trans,trans*-isomers of compound 3.

the central phenyl ring (i.e. bonds $\text{C11}-\text{C11}^i$ and $\text{C13}-\text{C13}^i$, $i = x, y, 1-z$). The molecule is relatively flat (Fig. 6a), with angle between terminal phenyl groups ($\text{C1} \rightarrow \text{C6}$) of 28.8° . Molecule of *trans,trans*-1 is twisted and chiral (Figs. 4b and 5b), its molecular symmetry being C_1 . One of its chlorine atoms is disordered over two positions (designated as Cl2 and Cl2a) with respective populations of 0.63 and 0.37.

The entire molecule of each compound comprises a conjugated system, so both can be regarded as single, delocalised, π electron systems. The formally single C–C bonds in the butadienyl fragment (bonds $\text{C4}-\text{C7}$, $\text{C8}-\text{C9}$ and $\text{C10}-\text{C11}$; in *trans,trans*-1 there are also



Scheme 1. Synthesis of butadiene derivatives 1–3 by Wittig reaction.

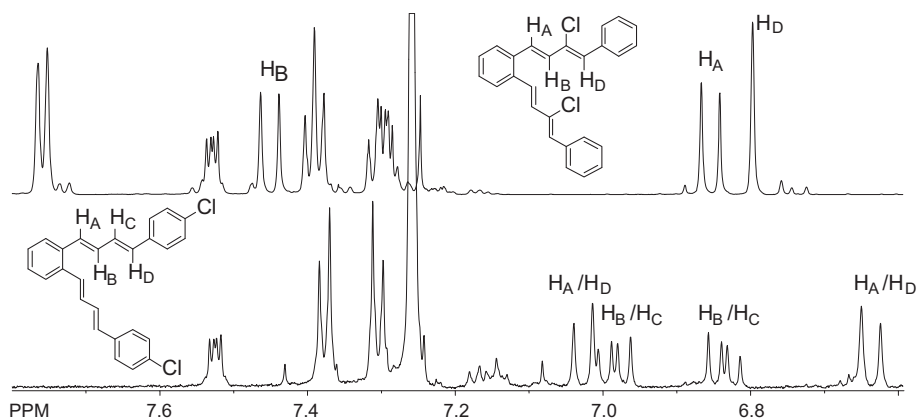


Fig. 2. ^1H NMR spectra of the *trans,trans* isomers of compounds 1–2 (CDCl_3 , 600 MHz).

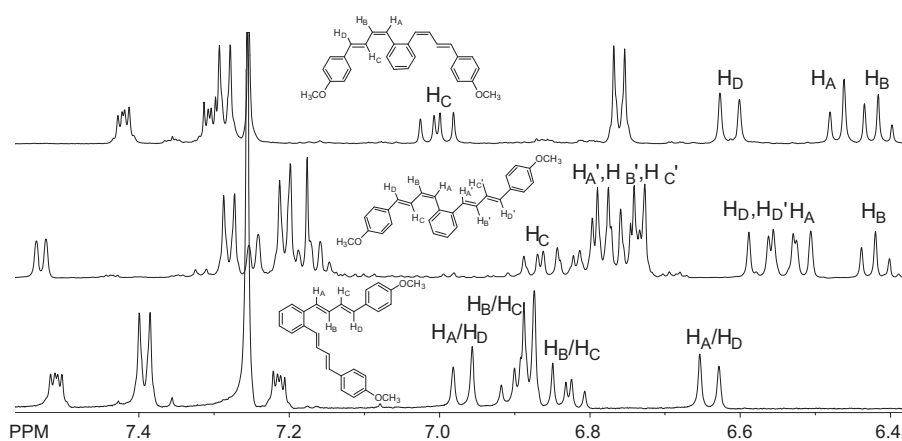


Fig. 3. ^1H NMR spectra of *cis,cis*-, *cis,trans*- and *trans,trans*-isomers of compound 3 CDCl_3 , 600 MHz).

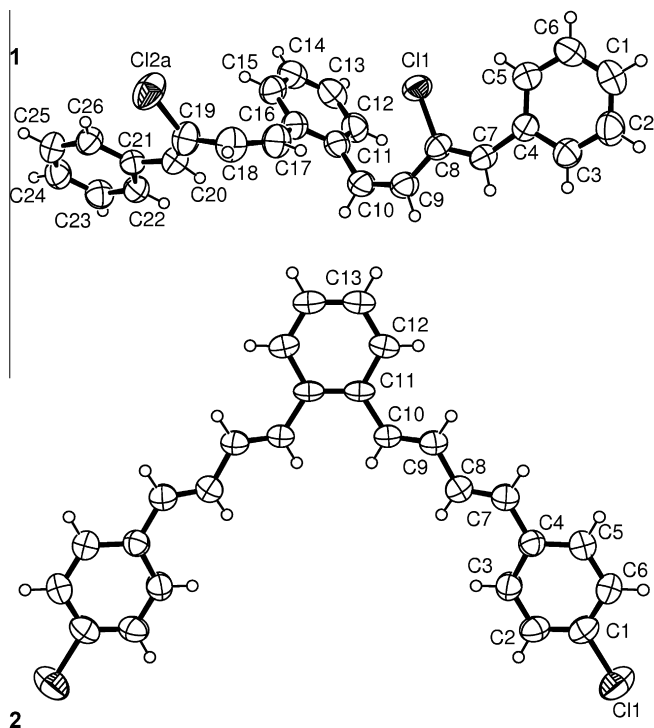


Fig. 4. Molecular structures of compounds *trans,trans*-1 and *trans,trans*-2. Displacement ellipsoids are drawn for the probability of 50% and hydrogen atoms are shown as spheres of arbitrary radii.

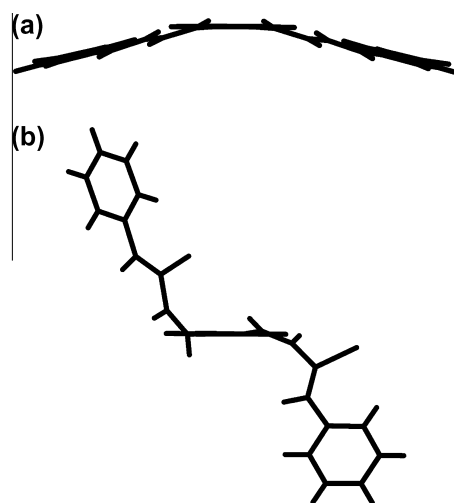


Fig. 5. Side-view showing conformations of molecules of *trans,trans*-2 (above) and *trans,trans*-1 (below).

fragments C16–C17, C18–C19 and C20–C21) are significantly shortened (Table 1), indicating a considerable electron delocalisation.

Crystal packing of *trans,trans*-2 is dominated by hydrogen bonded layers parallel to the plane (101), which are generated by a single symmetry-independent C–H...Cl hydrogen bond (Fig. 6a, and Table 2). The molecules are stacked in the direction

Table 1

Selected bond lengths (Å). There are two symmetry-independent butadienyl fragments in *trans,trans-1*, so they are listed separately.

	<i>trans,trans-2</i>	<i>trans,trans-1</i>	<i>trans,trans-1</i>	
C4–C7	1.464(9)	1.469(4)	C21–C20	1.474(4)
C7–C8	1.317(8)	1.338(4)	C20–C19	1.311(5)
C8–C9	1.462(9)	1.459(4)	C19–C18	1.476(5)
C9–C10	1.311(8)	1.341(5)	C18–C17	1.322(4)
C10–C11	1.469(7)	1.478(5)	C17–C16	1.479(4)

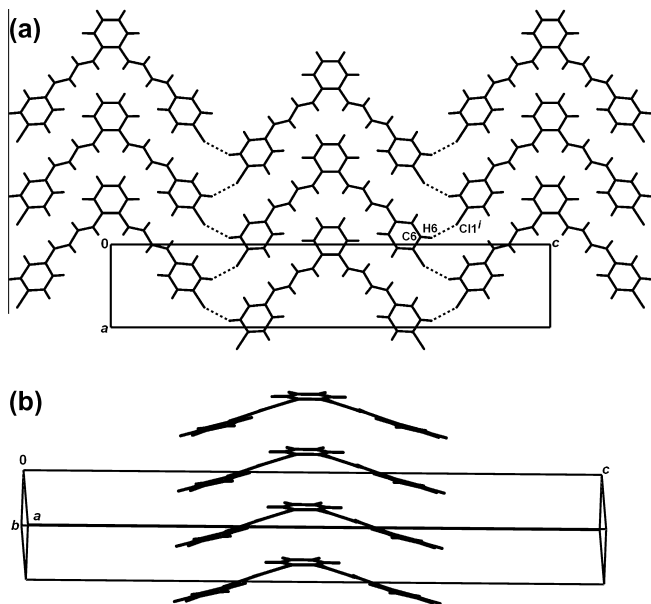


Fig. 6. Crystal packing of *trans,trans-2*: (a) layers generated by C–H...Cl hydrogen bonding, and (b) stacking of molecules which generates 3D packing.

[010] through interactions between their aromatic moieties (Fig. 6b, and Table 3). Therefore, stacking of layers produces a 3D structure.

Crystal packing of *trans,trans-1* is more complicated. C–H...Cl hydrogen bonds generate double chains running in the direction [010] (Fig. 7a); due to the disorder of Cl2 atom, there are two sym-

Table 2

Geometric parameters of hydrogen bonds.

	D–H (Å)	H...A (Å)	D...A (Å)	D–H...A (°)	Symm. op. on A
<i>trans,trans-1</i>					
C1–H1...Cl2b	0.93	3.04	3.593(5)	120	$x, -1 + y, -1 + z$
C18–H18...Cl2b	0.93	2.82	3.592(6)	141	$2 - x, -1/2 + y, 1 - z$
<i>trans,trans-2</i>					
C6–H6...Cl1	0.93	3.05	3.826(8)	142	$-1/2 + x, 1 - y, 1/2 - z$
C20–H20...Cl2a	0.93	2.89	3.617(5)	136	$x, y, -1 + z$

Table 3

Geometric parameters of the π ... π interactions in *trans,trans-2*.

π ... π	Cg ^a ...Cg (Å)	α ^b	β ^c	Cg...plane(Cg2) (Å)	Offset (Å)	Symm. op.
C1 → C6...C1 → C6	4.012(4)	0.00	22.35	3.711(2)	1.526	$x, -1 + y, 1 - z$
C11 → C11 ^d ...C11 → 11 ^d	4.012(4)	0.00	22.35	3.711(2)	1.526	$x, -1 + y, 1 - z$

^a Cg = centre of gravity of the aromatic ring.

^b α = angle between planes of two aromatic rings.

^c β = angle between Cg...Cg line and normal to the plane of the first aromatic ring.

^d Symmetry operator $x, y, 1 - z$.

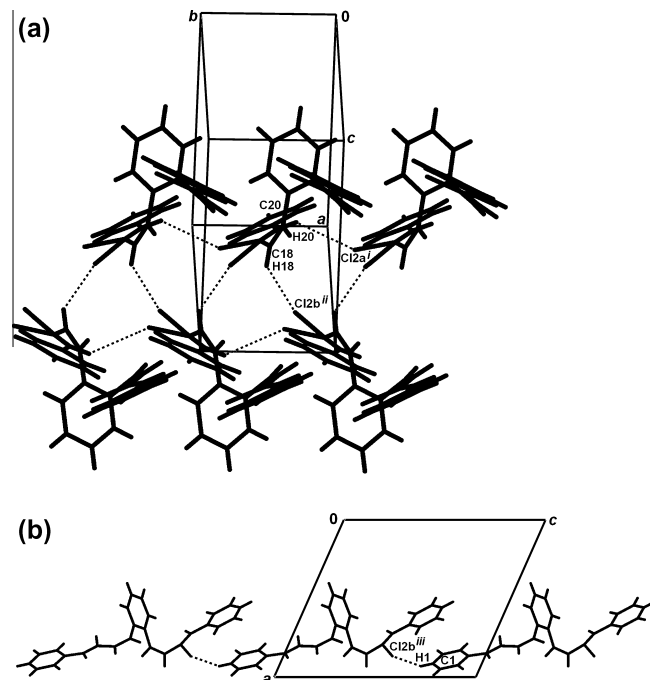


Fig. 7. Crystal packing of *trans,trans-1*: (a) double chains generated by a pair of C–H...Cl hydrogen bonds extending in the direction [010], (b) hydrogen bonded chains parallel to [001]. Symmetry operators: (i) $x, y, -1 + z$; (ii) $2 - x, -1/2 + y, 1 - z$; (iii) $x, -1 + y, -1 + z$.

metry-independent bonds: C18–H18...Cl2b and C20–H20...Cl2a (Table 2). Another hydrogen bond, C1–H1...Cl2b links the molecules into chains parallel to [001] (Fig. 7b, and Table 2); 2D motive parallel to (100) is thus formed. 3D packing is achieved through several C–H... π interactions (Table 4).

Conclusions

As it was shown, the photochemical behaviour of dichloro-substituted butadiene derivatives was studied and it was confirmed [4] that these compounds display diverse photochemical behaviour. The α -chloro derivative **1** photocyclizes to give six-

Table 4
Geometric parameters of the C–H... π interactions in *trans,trans*-1.

	H...Cg (Å)	γ (°) ^a	C–H...Cg (°)	C...Cg (Å)	Symm. operation on Cg
C6–H6...C21 → C26	2.85	14.82	128	3.495(4)	$x, y, -1 + z$
C22–H22...C21 → C26	2.84	5.58	128	3.489(3)	$1 - x, -\frac{1}{2} + y, 1 - z$
C24–H24...C11 → C16	2.91	13.18	150	3.741(4)	$1 - x, \frac{1}{2} + y, 1 - z$
C3–H3...C4–C7 ^b	2.84	–	143	3.631(5)	$2 - x, -1/2 + y, -z$

^a γ = angle defined by a line connecting centre of gravity of the aromatic ring with H atom and the normal to the aromatic ring.

^b The C–H group is directed towards a C=C bond. Therefore, Cg refers to the midpoint of the C4–C7 bond.

membered ring photoproduct. *p*-Chloro-substituted butadiene **2** undergoes intramolecular [2 + 2] cycloaddition followed by formation of benzobicyclic structures. It was proposed that the steric hindrance of chlorines in α -positions in the combination with specific weak interactions causes a greater deviation from planarity, relative to *p*-substitution, shifts conformer equilibria and affects the reaction pathways and yields. Those results are in accordance with this study by the presented X-ray crystallographic methods. Replacing the *p*-chloro substituents by *p*-methoxy functional groups probably changes the electronic influence and crystal packing and can show different sequence to the photochemical reaction.

Since no strong proton donors are present, the molecules are held together by weak intermolecular interactions: C–H...O and C–H...Cl hydrogen bonds, C–H... π interactions and dispersion interactions. Therefore, crystal packing of compounds *trans,trans*-1 and *trans,trans*-2 depends on a subtle interplay of weak interaction and steric effects.

Experimental section

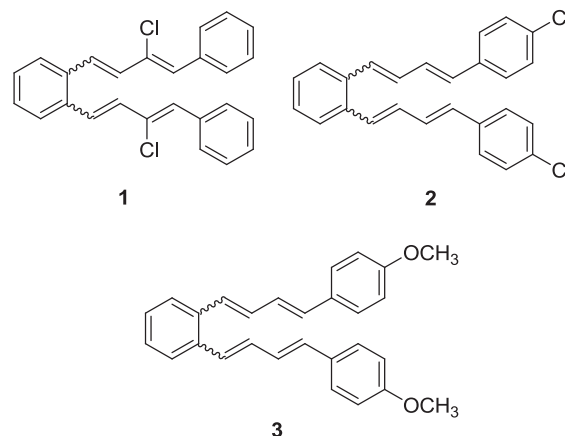
Physical measurements

The ¹H spectra were recorded on a spectrometer at 600 MHz. The ¹³C NMR spectra were registered at 150 MHz, respectively. All NMR spectra were measured in CDCl₃ using tetramethylsilane as reference. The assignment of the signals is based on 2D-CH correlation and 2D-HH-COSY experiments. UV spectra were measured on a UV/VIS Cary 50 spectrophotometer. IR spectra were recorded on a FTIR-ATR (film) with resolution of 4 cm⁻¹. Irradiation experiments were performed in a quartz vessel in toluene solution in a photochemical reactor equipped with 3000 Å lamps. All irradiation experiments were carried out in deaerated solutions by bubbling a stream of argon prior to irradiation. Melting points were obtained using microscope equipped apparatus and are uncorrected. HRMS analysis were carried out on a mass spectrometer (MALDI TOF/TOF analyzer), equipped with Nd:YAG laser operating at 355 nm with firing rate 200 Hz in the positive (H+) or negative (H-) ion reflector mode. Silica gel (0.063–0.2 mm) was used for chromatographic purifications. Thin-layer chromatography (TLC) was performed silica gel 60 F₂₅₄ plates. Solvents were purified by distillation.

Para-methoxy-cinnamaldehyde, para-chloro-cinnamaldehyde and alpha-chloro-cinnamaldehyde were obtained from a commercial source, β,β -*o*-xylyl(ditriphenylphosphonium) dibromide was prepared from *o*-xylyldibromide and triphenylphosphine in dimethylformamide.

Synthesis

To a stirred solution of the triphenylphosphonium salt (0.005 mol) and the corresponding aldehyde (0.011 mol) in absolute ethanol (100 mL) the solution of sodium ethoxide (0.253 g, 0.011 mol in 15 mL of absolute ethanol) was added dropwise. The reaction was completed within 3–4 h (usually was left to stand overnight). After removal of the solvent, the residue was worked up with water and toluene. The toluene extracts were dried (anhydrous MgSO₄) and concentrated. The crude reaction mixture was purified and the isomers of products **1** (55%), **2** (50%) and **3** (70%) were separated by repeated column chromatography on silica gel using petroleum ether/dichloromethane (9:1) as the eluent. The first fractions yielded *cis,cis*-, *cis,trans*- and the last fractions *trans,trans*-isomer. The (1*Z*,3*E*)-4-[*o*-[(1*E*,3*Z*)-3-Chloro-4-phenyl-1,3-butadienyl]phenyl]-2-chloro-1-phenyl-1,3-butadiene (**1**) and (1*E*,3*E*)-1-[*o*-[(1*E*,3*E*)-4-(*p*-Chlorophenyl)-1,3-butadienyl]phenyl]-4-(*p*-chlorophenyl)-1,3-butadiene (**2**) are described [4]. The data of the new compound **3** are given below.



(1*Z*,3*E*)-1-[*o*-[(1*E*,3*E*)-4-(*p*-Methoxyphenyl)-1,3-butadienyl]phenyl]-4-(*p*-methoxyphenyl)-1,3-butadiene (*cis,cis*-5)

18%; *R*_f 0.61 (petroleum ether/dichloromethane = 6:4); colourless oil; UV (96% EtOH) λ_{\max} 339 (4.63), 311 (4.66); ¹H NMR (CDCl₃, 600 MHz) δ 7.42 (d, *J* = 9.0 Hz, 1H), 7.31 (d, *J* = 9.0 Hz, 1H), 7.29 (d, *J* = 8.7 Hz, 2H), 7.00 (dd, *J* = 15.5; 10.9 Hz, 1H), 6.76 (d, *J* = 8.7 Hz, 2H), 6.62 (d, *J* = 15.5 Hz, 1H), 6.47 (d, *J* = 11.2 Hz, 1H), 6.42 (t, 1H, *J* = 11.2 Hz), 3.76 (s, 3H, –OCH₃); ¹³C NMR (CDCl₃, 75 MHz) δ 158.8 (s), 136.2 (s), 133.6 (d), 130.6 (d), 129.7 (s), 129.5 (d), 128.1 (d), 127.4 (2d), 126.3 (d), 123.3 (d), 113.6 (2d), 56.4 (q); IR ν_{\max} 3022, 1509, 1336, 979, 768.

(1*Z*,3*E*)-1-[*o*-[(1*E*,3*E*)-4-(*p*-Methoxyphenyl)-1,3-butadienyl]phenyl]-4-(*p*-methoxyphenyl)-1,3-butadiene (*cis,trans*-5)

47%; *R*_f 0.61 (petroleum ether/dichloromethane = 6:4); colourless oil; UV (96% EtOH) λ_{\max} 353 (4.90), 327 (4.85); ¹H NMR (CDCl₃, 600 MHz) δ 7.53 (d, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 8.7 Hz, 2H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.21 (d, *J* = 8.7 Hz, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.87 (dd, *J* = 15.6; 11.1 Hz, 1H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 6.72–6.82 (m, 3H), 6.58 (d, *J* = 15.6 Hz, 1H), 6.54 (d, *J* = 15.6 Hz, 1H), 6.52 (d, *J* = 11.1 Hz, 1H), 6.42 (t, *J* = 11.1 Hz, 1H), 3.74 (s, 3H, –OCH₃), 3.70 (s, 3H, –OCH₃); ¹³C NMR (CDCl₃, 75 MHz) δ 158.9 (s), 158.8 (s), 135.7 (s), 135.4 (s), 133.6 (d), 132.1 (d), 130.9 (d), 130.6 (d), 130.0 (d), 129.8 (s), 129.7 (s), 129.2 (d), 127.8 (d), 127.3 (2d), 127.1 (2d), 126.8 (d), 126.4 (d), 124.9 (d), 123.1 (d), 113.7 (2d), 113.6 (2d), 54.80 (q), 54.77 (q); IR ν_{\max} 3027, 1602 (C=C, ar), 1509 (C=C), 1250 (C_{ar}–O–CH₃), 1174, 1032, 751.

Table 5

Crystallographic, data collection and structure refinement details.

Compound	<i>trans,trans-1</i>	<i>trans,trans-2</i>
Empirical formula	C ₂₆ H ₂₀ Cl ₂	C ₂₆ H ₂₀ Cl ₂
Formula wt./g mol ⁻¹	403.32	403.32
Crystal dimensions/mm	0.18 × 0.14 × 0.08	0.10 × 0.06 × 0.04
Space group	P 2 ₁	P 2 ₁ n m
<i>a</i> /Å	12.9820(3)	6.8871(4)
<i>b</i> /Å	5.8510(1)	4.0120(3)
<i>c</i> /Å	15.2038(4)	36.501(3)
α /°	90	90
β /°	113.870(3)	90
γ /°	90	90
Z	2	2
<i>V</i> /Å ³	1056.07(4)	1008.57(12)
<i>D</i> _{calc} /g cm ⁻³	1.268	1.328
μ /mm ⁻¹	2.809	2.941
Θ range/°	3.18–75.80	4.85–75.40
<i>T</i> /K	293(2)	293(2)
Radiation wavelength	1.54179 (Cu K α)	1.54179 (Cu K α)
Diffractometer type	Xcalibur Nova	Xcalibur Nova
Range of <i>h, k, l</i>	–16 < <i>h</i> < 15; –7 < <i>k</i> < 5; –19 < <i>l</i> < 18	–8 < <i>h</i> < 8; –3 < <i>k</i> < 5; –45 < <i>l</i> < 34
Reflections collected	5060	2738
Independent reflections	3224	1618
Observed reflections (<i>I</i> ≥ 2 σ)	3116	1478
Absorption correction	Multi-scan	Multi-scan
<i>R</i> _{int}	0.0180	0.0622
<i>R</i> (F)	0.0447	0.0760
<i>R</i> _w (F ²)	0.1316	0.2309
Goodness of fit	0.880	1.111
H atom treatment	Constrained	Constrained
No. of parameters	164	127
No. of restraints	1	1
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (eÅ ⁻³)	0.189; –0.285	0.450; –0.313

(1*E*,3*E*)-1-*o*-[*(1E,3E)*-4-(*p*-Methoxyphenyl)-1,3-butadienyl]phenyl]-4-(*p*-methoxyphenyl)-1,3-butadiene (*trans,trans-5*)

5%; *R*_f 0.61 (petroleum ether/dichloromethane = 6:4); yellow crystals; mp 212–214 °C; UV (96% EtOH) λ_{\max} (log ϵ) 363 (5.08), 325 (5.16); ¹H NMR (CDCl₃, 600 MHz) δ 7.51 (d, *J* = 9.1 Hz, 1H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.21 (d, *J* = 9.1 Hz, 1H), 6.97 (d, *J* = 15.1 Hz, 1H), 6.90 (dd, *J* = 15.1; 10.5 Hz, 1H), 6.88 (d, *J* = 8.6 Hz, 2H), 6.83 (dd, *J* = 15.1; 10.5 Hz, 1H), 6.64 (d, *J* = 15.1 Hz, 1H), 3.83 (s, –OCH₃); ¹³C NMR (CDCl₃, 75 MHz) δ 158.9 (s), 135.2 (s), 132.1 (d), 131.2 (d), 129.7 (s), 128.7 (d), 127.2 (2d), 127.1 (d), 126.9 (d), 125.7 (d), 113.7 (2d), 54.8 (q); IR ν_{\max} . 2918, 1597 (C=C, ar), 1510 (C=C), 1252 (C_{ar}–O–CH₃), 1172, 1029, 993, 752; HRMS (TOF ES⁺) *m/z* for C₂₈H₂₆O₂: *M*_{calc}⁺ 394.1927; *M*_{found}⁺ 394.1937 (for a mixture of isomers **3**).

Crystallography

Single crystal measurements were performed on an Oxford Diffraction Xcalibur Nova R (microfocus Cu tube) at room temperature [293(2) K]. Only the symmetry-independent part of the Ewald sphere was measured; no Friedel pairs were measured in the case of non-centrosymmetric crystals. Program package CrysAlis PRO [8] was used for data reduction. The structures were solved using SHELXS97 [9] and refined with SHELXL97 [9]. The models were refined using the full-matrix least squares refinement; all non-hydrogen atoms were refined anisotropically. Hydrogen atoms were modelled as riding entities using the AFIX command.

Molecular geometry calculations were performed by PLATON [10], and molecular graphics were prepared using ORTEP-3 [11], and CCDC-Mercury [12]. Crystallographic and refinement data for the structures reported in this paper are shown in Table 5.

Appendix A. Supplementary material

Supplementary crystallographic data for this paper can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; or deposit@ccdc.cam.ac.uk). CCDC 986521 and 986522 contain the supplementary crystallographic data for this paper. Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.molstruc.2014.04.028>.

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