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## Structure Reports

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# 4,4'-Bis(2-methoxystyryl)biphenyl

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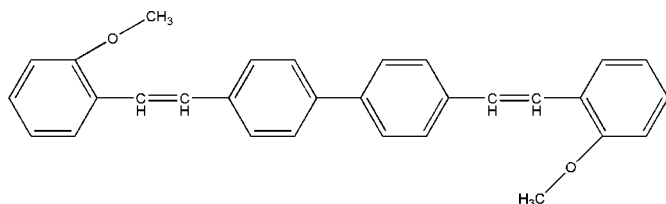
Received 24 June 2009; accepted 9 July 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.065;  $wR$  factor = 0.218; data-to-parameter ratio = 16.7.

The title compound,  $\text{C}_{30}\text{H}_{26}\text{O}_2$ , was prepared by the reaction of a Wittig reagent and 2-methoxybenzaldehyde. The molecule lies about an inversion centre located at the midpoint of the C—C bond between the inner benzene rings. The crystal structure is stabilized by C—H $\cdots\pi$  interactions.

## Related literature

For the optical properties of ethylene biphenyls, see: Song *et al.* (2003). For comparative bond lengths, see: Trueblood *et al.* (1982).



## Experimental

### Crystal data

$\text{C}_{30}\text{H}_{26}\text{O}_2$

$M_r = 418.51$

Monoclinic,  $P2_1/c$   
 $a = 15.499$  (3) Å  
 $b = 5.5050$  (11) Å  
 $c = 13.445$  (3) Å  
 $\beta = 98.61$  (3)°  
 $V = 1134.2$  (4) Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.25 \times 0.20 \times 0.18$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: none  
2541 measured reflections

2431 independent reflections  
1144 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$   
 $wR(F^2) = 0.218$   
 $S = 1.01$   
2431 reflections

146 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C1}-\text{H1C}\cdots\text{Cg1}^i$	0.96	2.76	3.611 (3)	149
$\text{C15}-\text{H15A}\cdots\text{Cg2}^{ii}$	0.93	2.91	3.643 (3)	137

Symmetry codes: (i)  $x, y - 1, z$ ; (ii)  $-x, y + \frac{1}{2}, -z + \frac{1}{2}$ . Cg1 and Cg2 are the centroids of the C2–C7 and C10–C15 rings, respectively.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2831).

## References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Song, H. C., Xu, X. H. & Liu, G. R. (2003). *Chin. Chem. Res.* **14**, 1–5.  
Trueblood, K., Mirsky, K., Maverick, E., Knobler, C. & Grossenbacher, L. (1982). *Acta Cryst.* **B38**, 2428–2435.

**supplementary materials**

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## 4,4'-Bis(2-methoxystyryl)biphenyl

Y.-F. Li and F.-F. Jian

### Comment

Ethylene biphenyl have received considerable attention in the literature. They are attractive from several points of view, such as the optics characteristic. (Song *et al.*, 2003). As part of our search for new ethylene biphenyl compounds we synthesized the title compound (I), and describe its structure here.

As shown in Fig. 1, the molecule has an inversion centre lied on the midpoint of the C—C bond between the inner benzene rings. The C8—C9 bond length of 1.314 (4)Å is comparable with C—C double bond [1.336 (2) Å] reported (Trueblood *et al.*, 1982).

In the structure, there is no classcial hydrogen bonds. The crystal structure is stabilized by C—H... $\pi$  interactions (Table 1).

### Experimental

A mixture of the Wittig-reagent (0.1 mol), and 2-methoxybenzaldehyde (0.2 mol) was stirred in refluxing *N,N*-dimethylformamide (20 mL) for 4 h to afford the title compound (0.084 mol, yield 84%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

### Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H = 0.93 - 0.96 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C})$ .

### Figures

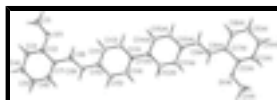


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

## 4,4'-Bis(2-methoxystyryl)biphenyl

### Crystal data

$\text{C}_{30}\text{H}_{26}\text{O}_2$

$M_r = 418.51$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 15.499$  (3) Å

$b = 5.5050$  (11) Å

$F_{000} = 444$

$D_x = 1.225$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 987 reflections

$\theta = 2.2$ – $27.5^\circ$

$\mu = 0.08$  mm<sup>-1</sup>

# supplementary materials

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$c = 13.445 (3) \text{ \AA}$   
 $\beta = 98.61 (3)^\circ$   
 $V = 1134.2 (4) \text{ \AA}^3$   
 $Z = 2$

$T = 293 \text{ K}$   
Block, yellow  
 $0.25 \times 0.20 \times 0.18 \text{ mm}$

## Data collection

Bruker SMART CCD area-detector diffractometer  
Radiation source: fine-focus sealed tube  
Monochromator: graphite  
 $T = 293 \text{ K}$   
 $\varphi$  and  $\omega$  scans  
Absorption correction: none  
2541 measured reflections  
2431 independent reflections

1144 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 27.0^\circ$   
 $\theta_{\text{min}} = 1.3^\circ$   
 $h = -18 \rightarrow 18$   
 $k = -6 \rightarrow 0$   
 $l = -16 \rightarrow 0$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.065$   
 $wR(F^2) = 0.218$   
 $S = 1.01$   
2431 reflections  
146 parameters

Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.1165P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$   
Extinction correction: SHELXL97 (Sheldrick, 2008),  
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.045 (8)

Primary atom site location: structure-invariant direct methods  
Secondary atom site location: difference Fourier map

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

$x$                        $y$                        $z$                        $U_{\text{iso}}^*/U_{\text{eq}}$

O1	0.37628 (14)	0.1134 (4)	0.17470 (14)	0.0684 (7)
C1	0.4420 (2)	-0.0626 (6)	0.1680 (2)	0.0738 (11)
H1A	0.4491	-0.1627	0.2271	0.111*
H1B	0.4961	0.0178	0.1627	0.111*
H1C	0.4254	-0.1619	0.1096	0.111*
C2	0.35652 (18)	0.2759 (5)	0.09673 (19)	0.0493 (7)
C3	0.3997 (2)	0.2830 (6)	0.0136 (2)	0.0602 (9)
H3A	0.4442	0.1727	0.0082	0.072*
C4	0.3770 (2)	0.4529 (7)	-0.0611 (2)	0.0665 (10)
H4A	0.4066	0.4568	-0.1164	0.080*
C5	0.3114 (2)	0.6160 (6)	-0.0545 (2)	0.0625 (9)
H5A	0.2963	0.7302	-0.1051	0.075*
C6	0.26746 (19)	0.6097 (6)	0.0283 (2)	0.0565 (8)
H6A	0.2233	0.7216	0.0327	0.068*
C7	0.28816 (16)	0.4391 (5)	0.10519 (19)	0.0456 (7)
C8	0.24047 (17)	0.4232 (5)	0.19277 (19)	0.0497 (8)
H8A	0.2537	0.2911	0.2354	0.060*
C9	0.18161 (18)	0.5755 (5)	0.2166 (2)	0.0493 (8)
H9A	0.1705	0.7120	0.1759	0.059*
C10	0.13109 (17)	0.5531 (5)	0.30137 (19)	0.0434 (7)
C11	0.1426 (2)	0.3639 (6)	0.3705 (2)	0.0616 (9)
H11A	0.1851	0.2472	0.3654	0.074*
C12	0.0920 (2)	0.3457 (5)	0.4468 (2)	0.0615 (9)
H12A	0.1016	0.2159	0.4914	0.074*
C13	0.02809 (16)	0.5122 (5)	0.45942 (19)	0.0406 (6)
C14	0.0180 (2)	0.7035 (5)	0.3911 (2)	0.0556 (8)
H14A	-0.0239	0.8216	0.3970	0.067*
C15	0.0683 (2)	0.7237 (6)	0.3145 (2)	0.0576 (9)
H15A	0.0596	0.8553	0.2707	0.069*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0824 (16)	0.0795 (15)	0.0477 (12)	0.0305 (13)	0.0238 (11)	0.0099 (12)
C1	0.083 (2)	0.081 (3)	0.057 (2)	0.027 (2)	0.0114 (17)	-0.0030 (18)
C2	0.0517 (16)	0.0613 (18)	0.0365 (15)	-0.0004 (15)	0.0114 (12)	-0.0031 (14)
C3	0.0571 (18)	0.082 (2)	0.0457 (17)	0.0071 (17)	0.0228 (15)	-0.0038 (17)
C4	0.0594 (19)	0.104 (3)	0.0409 (17)	-0.0055 (19)	0.0235 (14)	0.0008 (18)
C5	0.0603 (19)	0.089 (2)	0.0393 (16)	-0.0015 (19)	0.0110 (14)	0.0128 (17)
C6	0.0491 (16)	0.075 (2)	0.0465 (16)	0.0034 (16)	0.0091 (13)	0.0075 (16)
C7	0.0404 (15)	0.063 (2)	0.0350 (14)	-0.0034 (13)	0.0107 (11)	-0.0011 (13)
C8	0.0475 (16)	0.065 (2)	0.0393 (15)	0.0066 (15)	0.0136 (12)	0.0041 (14)
C9	0.0523 (17)	0.0556 (19)	0.0423 (15)	-0.0007 (15)	0.0142 (12)	0.0004 (13)
C10	0.0411 (15)	0.0501 (17)	0.0397 (15)	-0.0015 (13)	0.0081 (12)	-0.0064 (13)
C11	0.0591 (18)	0.065 (2)	0.067 (2)	0.0249 (16)	0.0306 (16)	0.0138 (17)
C12	0.067 (2)	0.063 (2)	0.0608 (19)	0.0243 (17)	0.0318 (16)	0.0209 (16)
C13	0.0403 (14)	0.0462 (15)	0.0357 (13)	-0.0002 (12)	0.0078 (10)	-0.0044 (12)
C14	0.0585 (18)	0.0579 (19)	0.0554 (17)	0.0198 (15)	0.0248 (14)	0.0066 (15)

## supplementary materials

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C15                    0.0662 (19)            0.062 (2)            0.0490 (16)            0.0172 (16)            0.0235 (15)            0.0154 (15)

### *Geometric parameters (Å, °)*

O1—C2	1.377 (3)	C8—C9	1.314 (4)
O1—C1	1.419 (4)	C8—H8A	0.9300
C1—H1A	0.9600	C9—C10	1.482 (4)
C1—H1B	0.9600	C9—H9A	0.9300
C1—H1C	0.9600	C10—C15	1.383 (4)
C2—C3	1.386 (4)	C10—C11	1.389 (4)
C2—C7	1.407 (4)	C11—C12	1.386 (4)
C3—C4	1.379 (4)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.379 (4)
C4—C5	1.370 (4)	C12—H12A	0.9300
C4—H4A	0.9300	C13—C14	1.391 (4)
C5—C6	1.390 (4)	C13—C13 <sup>i</sup>	1.500 (5)
C5—H5A	0.9300	C14—C15	1.387 (4)
C6—C7	1.398 (4)	C14—H14A	0.9300
C6—H6A	0.9300	C15—H15A	0.9300
C7—C8	1.484 (3)		
C2—O1—C1	118.4 (2)	C9—C8—C7	127.1 (3)
O1—C1—H1A	109.5	C9—C8—H8A	116.5
O1—C1—H1B	109.5	C7—C8—H8A	116.5
H1A—C1—H1B	109.5	C8—C9—C10	126.9 (3)
O1—C1—H1C	109.5	C8—C9—H9A	116.5
H1A—C1—H1C	109.5	C10—C9—H9A	116.5
H1B—C1—H1C	109.5	C15—C10—C11	116.5 (2)
O1—C2—C3	123.6 (3)	C15—C10—C9	120.3 (3)
O1—C2—C7	116.0 (2)	C11—C10—C9	123.2 (2)
C3—C2—C7	120.5 (3)	C12—C11—C10	121.3 (3)
C4—C3—C2	120.4 (3)	C12—C11—H11A	119.4
C4—C3—H3A	119.8	C10—C11—H11A	119.4
C2—C3—H3A	119.8	C13—C12—C11	122.7 (3)
C5—C4—C3	120.5 (3)	C13—C12—H12A	118.7
C5—C4—H4A	119.7	C11—C12—H12A	118.7
C3—C4—H4A	119.7	C12—C13—C14	115.7 (2)
C4—C5—C6	119.5 (3)	C12—C13—C13 <sup>i</sup>	122.4 (3)
C4—C5—H5A	120.2	C14—C13—C13 <sup>i</sup>	121.8 (3)
C6—C5—H5A	120.2	C15—C14—C13	122.1 (3)
C5—C6—C7	121.6 (3)	C15—C14—H14A	119.0
C5—C6—H6A	119.2	C13—C14—H14A	119.0
C7—C6—H6A	119.2	C10—C15—C14	121.7 (3)
C6—C7—C2	117.5 (2)	C10—C15—H15A	119.2
C6—C7—C8	122.7 (3)	C14—C15—H15A	119.2
C2—C7—C8	119.8 (3)		

Symmetry codes: (i)  $-x, -y+1, -z+1$ .

*Hydrogen-bond geometry* (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C1—H1C···Cg1 <sup>ii</sup>	0.96	2.76	3.611 (3)	149
C15—H15A···Cg2 <sup>iii</sup>	0.93	2.91	3.643 (3)	137

Symmetry codes: (ii)  $x, y-1, z$ ; (iii)  $-x, y+1/2, -z+1/2$ .

Fig. 1

