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2,3,2′,3′-Tetramethylbiphenyl

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.135
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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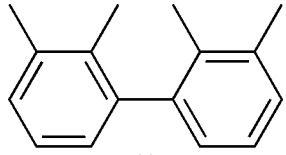
The title compound, $C_{16}H_{18}$, was synthesized by a palladium-catalyzed boronic acid cross-coupling reaction. A crystallographic twofold axis passes through the mid-point of the C—C bond connecting the two rings. In the crystal structure, two fairly close C—H···π(arene) contacts appear to be the only significant intermolecular interactions.

Comment

The title compound, (I), was synthesized using the *tert*-butyl group as a positional protective group (Tashiro & Yamato, 1979). We obtained (I) in excellent yield using a Suzuki cross-coupling reaction (Miyaura, 2002). The crystal structure of the related 2,3,3′,4′-tetramethylbiphenyl, (II), has already been reported (Robertson & Price, 2005).



(I)

The molecular structure of (I) is shown in Fig. 1. A crystallographic twofold axis passes through the mid-point of the C6—C6*A* bond. All bond distances and angles are as expected. The dihedral angle between the planes of the two benzene rings is 69.9 (3)°, compared with the value of 54.10 (7)° in (II). The larger angle in (I) may be related to the greater steric hindrance from the two 2,2′-methyl groups in (I) compared with the two 2,3′-methyl groups in (II). The molecule adopts a *cis* configuration, with all the methyl groups on the same side of the biphenyl unit.

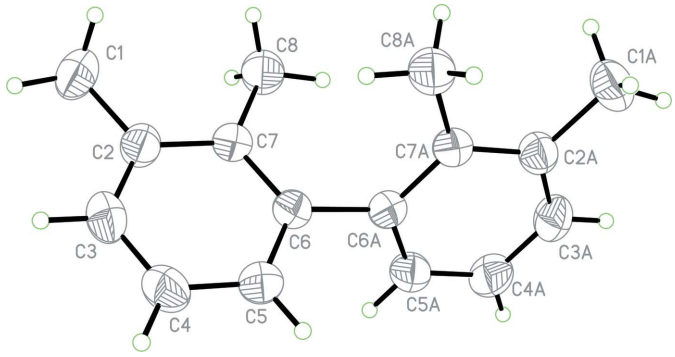


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres. Atoms labelled with the suffix A are related by the symmetry operator $(1-x, y, \frac{3}{2}-z)$.

There are no significant π–π stacking interactions, but two intermolecular weak C—H···π(arene) interactions may be effective in stabilizing the crystal structure (Table 1 and Fig. 2).

Experimental

The title compound was synthesized according to the procedure described by Robertson & Price (2005), using the same quantities but substituting 2,3-dimethylbromobenzene for 3,4-dimethylbromobenzene. Crystals were obtained by dissolving (I) (1.0 g) in petroleum ether (20 ml) and evaporating the solvent slowly at room temperature for about 25 d.

Crystal data

$C_{16}H_{18}$
M_r = 210
Monoclinic, $C2/c$
a = 13.536 (3) Å
b = 6.5150 (13) Å
c = 14.754 (3) Å
β = 106.49 (3)°
V = 1247.6 (4) Å^3
Z = 4
D_x = 1.120 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.975, T_{max} = 0.988
2438 measured reflections
1221 independent reflections
1007 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.135
S = 1.05
1221 reflections
74 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 0.4P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.087 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···$Cg1^{i}$	0.96	2.85	3.729 (2)	152
C4—H4A···$Cg1^{ii}$	0.93	2.90	3.7429 (18)	150

Symmetry codes: (i) $x+\frac{3}{2}, y+\frac{1}{2}, z+1$; (ii) $x+1, -y, z+\frac{1}{2}$.

H atoms were placed in calculated postions, with C—H = 0.93 or 0.96 Å, and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for methyl H.

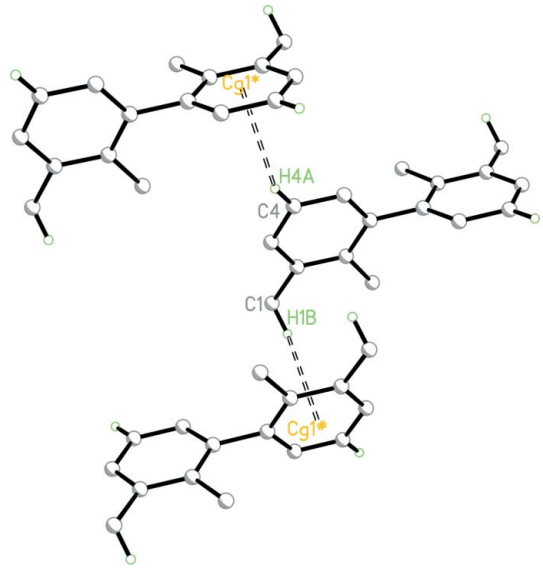


Figure 2
Part of the crystal structure of (I), with dashed lines indicating intermolecular C—H···π(arene) interactions. Only H atoms involved in the interactions are shown. [Symmetry codes: (#) $\frac{3}{2}+x, \frac{1}{2}+y, 1+z$; (*) $1+x, -y, \frac{1}{2}+z$.]

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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