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1,2-Dimethyl-4,5-bis(phenylethynyl)benzene

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.058
wR factor = 0.159
Data-to-parameter ratio = 13.6

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

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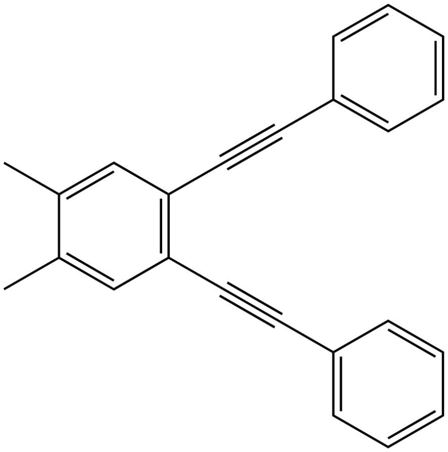
The title compound, $C_{24}H_{18}$, possesses a twofold rotation axis, which bisects the 1,2-dimethylbenzene ring. In the crystal structure, all three benzene rings are essentially coplanar, the angle between the central and terminal rings being 3.8 (1)°.

Comment

A study of the thermal cycloaromatization of enediynes led to the suggestion of a benzene 1,4-biradical intermediate (Lockhart *et al.*, 1981). 1,2-Dimethyl-4,5-bis(phenylethynyl)benzene is an important 1,4-biradical intermediate for substituted polyphenylenes. The latter have been shown to exhibit excellent thermal and chemical resilience, interesting semiconducting properties upon doping, and applications in light-emitting diodes (Kovacic & Jones, 1987; Grem *et al.*, 1992). In this paper, we present the X-ray crystallographic analysis of 1,2-dimethyl-4,5-bis(phenylethynyl)benzene, (I). The crystal structure of the isomeric compound, 1,4-bis(*p*-tolylethynyl)benzene, has been reported by Filatov & Petrukhina (2005).



(I)

The molecule of (I) possesses a twofold rotation axis, which passes through the mid-points of bonds C2—C2*a* and C4—C4*a* (Fig. 1). All three benzene rings are essentially coplanar, the angle between the central and terminal rings being 3.8 (1)°. Selected bond distances and angles are given in Table 1. In the crystal structure of (I), molecules are aligned in a herring-bone fashion (Fig. 2).

It has been shown previously that methyl groups can function as hydrogen-bond donors towards aromatic π systems (Desiraju, 2002). Weak C—H$\cdots\pi$ interactions are observed in the crystal structure (Fig. 3 and Table 2), Additionally, weak π–π stacking can be observed in the crystal structure.

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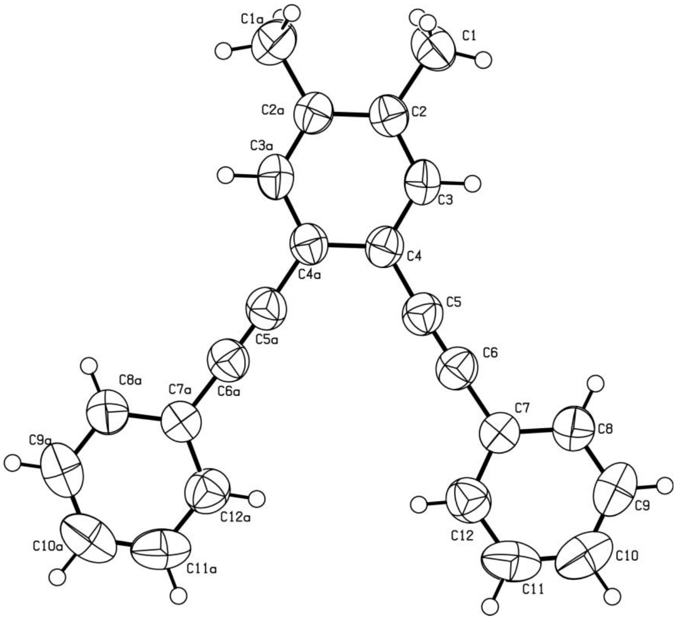

Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. The suffix a in atom labels indicates the symmetry position ($-x$, y, $\frac{3}{2} - z$).

Experimental

The title compound was synthesized according to a literature procedure (Kabalka *et al.*, 2001). Crystals appropriate for data collection were obtained by slow evaporation of a dichloromethane solution at 283 K.

Crystal data

$C_{24}H_{18}$
$M_r = 306.38$
Orthorhombic, *Pbcn*
$a = 11.735$ (2) Å
$b = 12.964$ (3) Å
$c = 11.820$ (2) Å
$V = 1798.3$ (6) Å^3
$Z = 4$
$D_x = 1.132$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 1966 reflections
$\theta = 1.0$–$27.0°$
$\mu = 0.06$ mm^{-1}
$T = 292$ (2) K
Block, colourless
$0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
9915 measured reflections
1966 independent reflections

1207 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.043$
$\theta_{\rm max} = 27.0°$
$h = -14 \rightarrow 14$
$k = -15 \rightarrow 16$
$l = -15 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.159$
$S = 1.03$
1966 reflections
145 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.2012P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.11$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.13$ e Å^{-3}

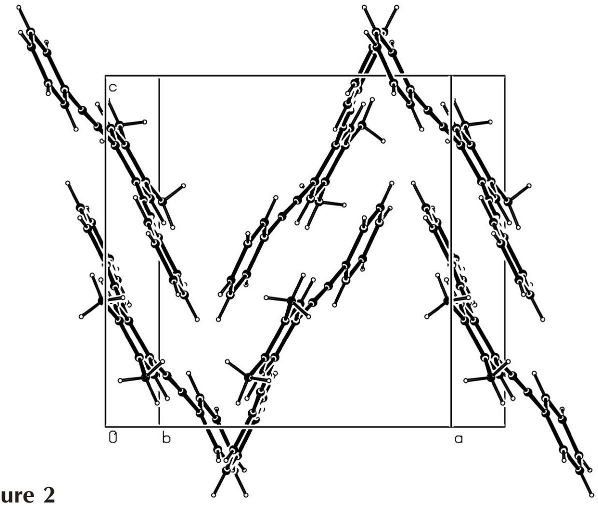

Figure 2
The packing of (I), viewed along the *b* axis.

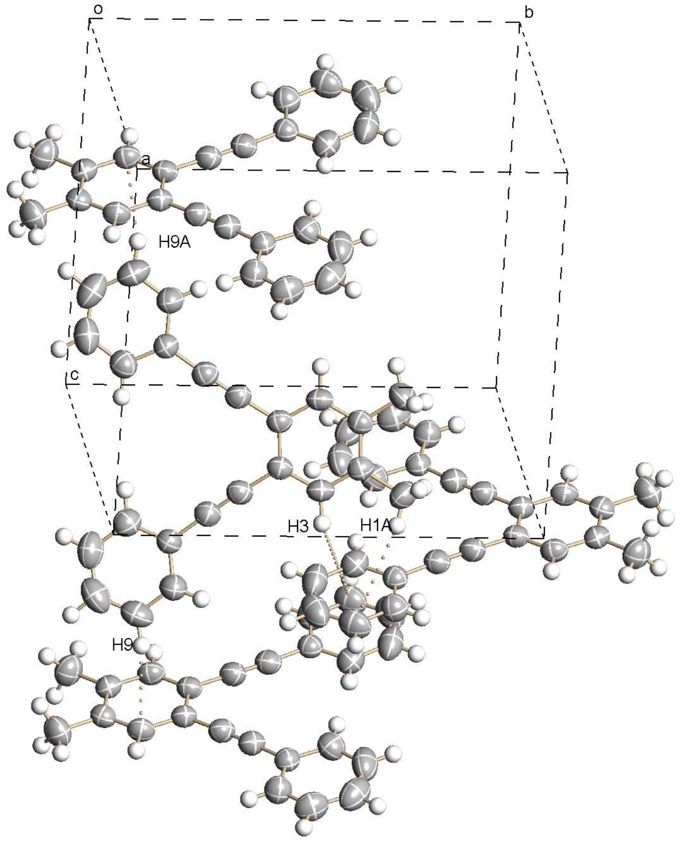

Figure 3
The C—H$\cdots\pi$(arene) interactions, indicated by dotted lines.

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.506 (3)	C6—C7	1.434 (3)
C5—C6	1.191 (2)		
C4$^{\rm i}$—C4—C5	121.48 (10)	C5—C6—C7	177.8 (2)
C6—C5—C4	177.2 (2)	C8—C7—C6	120.32 (18)

Symmetry code: (i) $-x$, y, $\frac{3}{2} - z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···*Cg*2$^{\rm ii}$	0.94 (3)	3.35 (2)	4.061 (3)	135 (2)
C3—H3···*Cg*2$^{\rm ii}$	0.990 (19)	3.035 (18)	3.849 (2)	140 (1)
C9—H9···*Cg*1$^{\rm iii}$	0.95 (3)	2.92 (2)	3.575 (3)	128 (2)
C9—H9···*Cg*1$^{\rm iv}$	0.95 (3)	2.92 (2)	3.575 (3)	128 (2)

Symmetry codes: (ii) $x, -y, z-\frac{1}{2}$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}+z$; (iv) $-x, y, \frac{5}{2}-z$. *Cg*1 and *Cg*2 are the centroids of rings C2–C4/C4*a*–C2*a* and C7–C12, respectively.

All H atoms were freely refined; C—H = 0.91 (3)–0.99 (2) Å for aromatic H atoms and 0.94 (3)–1.00 (3) Å for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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