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1,1-Diphenyl-2,2-bis(trimethylsilylethynyl)ethene

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Key indicators

Single-crystal X-ray study
T = 143 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.124
Data-to-parameter ratio = 17.1

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

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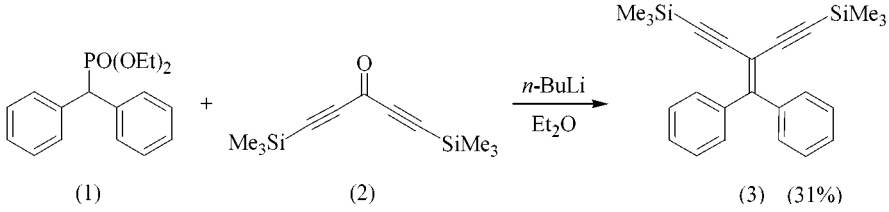
In the title compound, $C_{24}H_{28}Si_2$, the interplanar angle between the groups on the ends of the central double bond is 7.3 (4)° and the length of this bond is 1.361 (3) Å. The molecules form layers parallel to ($\bar{1}$12).

Comment

In our studies of the preparation and chemical (Eshdat *et al.*, 2002) and structural (Jones *et al.*, 2004) properties of cross-conjugated diethynylethenes, we were interested in the title compound, 1,1-diphenyl-2,2-bis(trimethylsilylethynyl)ethene, (3), a derivative easily prepared in fair yield (31%) by the reaction of the phosphonate (1) with the diethynyl ketone (2) and *n*-butyllithium in diethyl ether at 233 K (see Scheme). We report here the structure of (3). Spectroscopic and analytical data will be reported elsewhere (Berger, 2005).



The molecule of (3) is shown in Fig. 1. Molecular dimensions (Table 1) may be regarded as normal [*e.g.* the central double bond length C1═C2 of 1.361 (3) Å]. The angles C3—

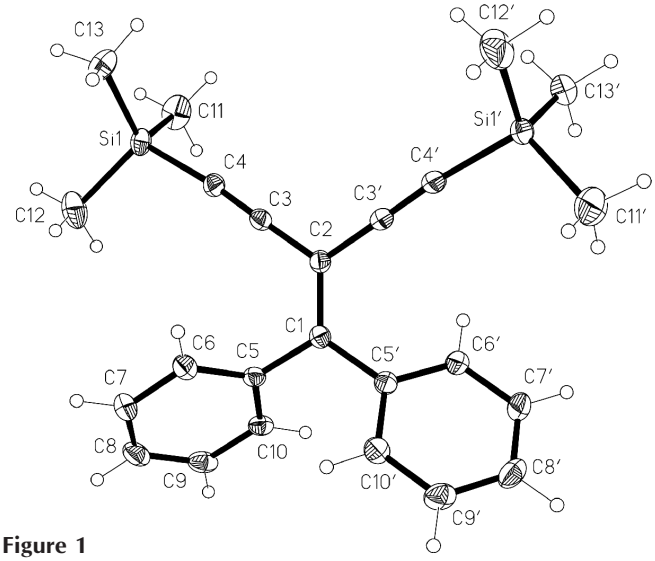


Figure 1
The molecule of the title compound in the crystal structure. Displacement ellipsoids are drawn at the 30% probability level. H-atom radii are arbitrary.

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C2—C3′ and C5—C1—C5′ are narrowed from the usual sp^2 values. The geometry around C1═C2 is essentially planar, although the groups on the ends of this double bond are slightly rotated [interplanar angle between C2/C3/C3′ and C1/C5/C5′ = 7.3 (4)°] with respect to each other. The phenyl rings subtend interplanar angles of 55.89 (8) (unprimed) and 44.39 (8)° (primed) with the central mean plane.

The packing (Fig. 2) involves layers of molecules parallel to ($\bar{1}$12).

Experimental

Details are given by Berger (2005). Single crystals were obtained by sublimation.

Crystal data

$C_{24}H_{28}Si_2$
M_r = 372.64
Triclinic, $P\bar{1}$
a = 10.026 (3) Å
b = 10.123 (3) Å
c = 12.363 (4) Å
α = 95.51 (3)°
β = 107.26 (3)°
γ = 98.19 (3)°
V = 1173.3 (6) Å^3
Z = 2
D_x = 1.055 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 54 reflections
θ = 10–11.5°
μ = 0.16 mm^{-1}
T = 143 (2) K
Tablet, colourless
0.5 × 0.5 × 0.2 mm

Data collection

Stoe Stadi-4 diffractometer
ω/θ scans
Absorption correction: none
8570 measured reflections
4131 independent reflections
3165 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.1°
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 11$
$l = -14 \rightarrow 14$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.124
S = 1.02
4131 reflections
241 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.5199P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.361 (3)	C3′—C4′	1.202 (3)
C3—C4	1.202 (3)		
C5′—C1—C5	116.58 (18)	C3′—C2—C3	115.91 (19)
C5—C1—C2—C3	−8.5 (3)	C2—C1—C5′—C6′	−43.6 (3)
C2—C1—C5—C6	−54.1 (3)		

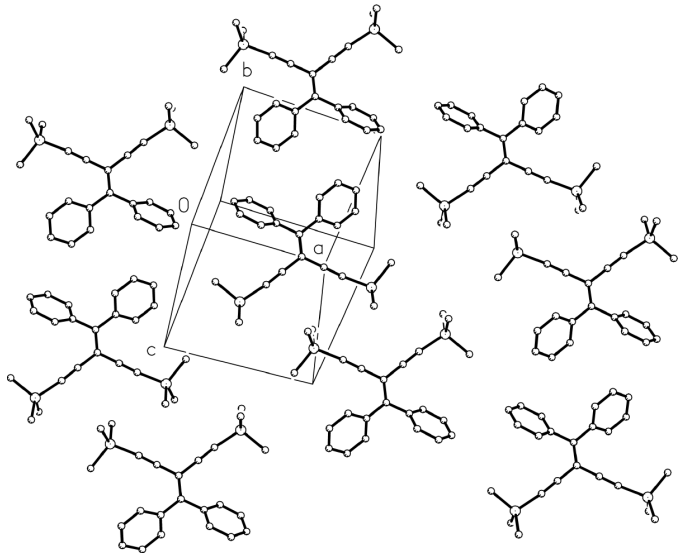

Figure 2
Packing diagram of the title compound; view of one layer [view direction perpendicular to ($\bar{1}$12)]. Radii are arbitrary and H atoms have been omitted.

Methyl H atoms were located in difference syntheses, idealized (C—H = 0.98 Å and H—C—H = 109.5°) and refined on the basis of rigid groups allowed to rotate but not tip. Other H atoms were included at calculated positions and refined using a riding model with fixed C—H bond lengths of 0.95 Å; U_{iso}(H) values were fixed at 1.2U_{eq}(parent atom).

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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