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Redetermination of *cis*,*cis*-1,2,3,4-tetraphenylbuta-1,3-diene

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Key indicators

Single-crystal X-ray study
T = 162 K
Mean σ(C–C) = 0.001 Å
R factor = 0.045
wR factor = 0.123
Data-to-parameter ratio = 19.4

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

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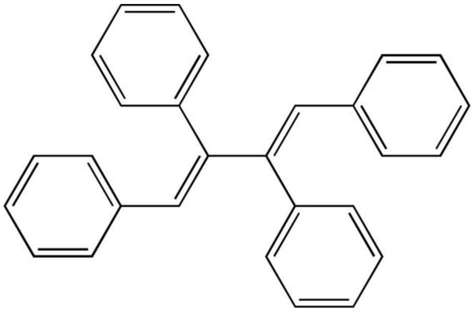
The title molecule, $C_{28}H_{22}$, is centrosymmetric with an inversion centre at the mid-point of the central C—C bond. In the crystal structure, there are two intermolecular $C_{phenyl}—H\cdots\pi_{phenyl}$ interactions.

Comment

The crystal structure of *cis*,*cis*-1,2,3,4-tetraphenylbutadiene, (I), was originally determined at room temperature by Karle & Dragonette (1965) from reflection data obtained by film methods. The present structure refinement at 162 K confirms the structure, but is an order of magnitude more precise.


(I)

The molecular structure of (I) is shown in Fig. 1. The molecule is centrosymmetric with an inversion centre at the mid-point of the central C—C bond. Consequently, the butadiene group is planar. The phenyl groups are each essentially planar,

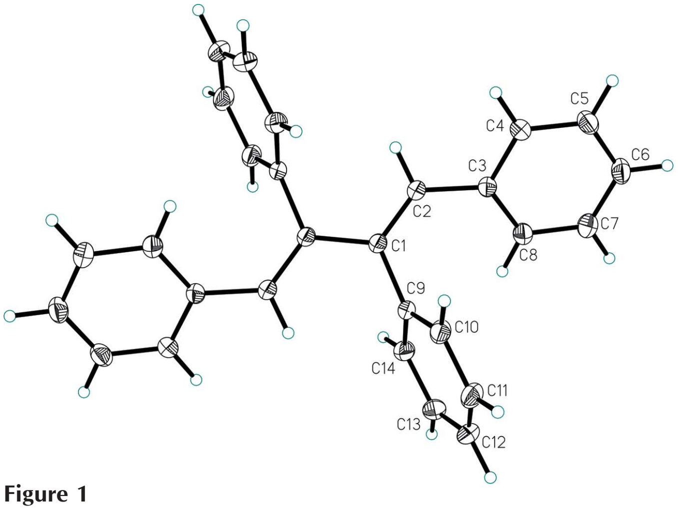


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. The H atoms are drawn as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry operator $(1 - x, 1 - y, 1 - z)$.

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the mean deviation of the C atoms from the plane of the ring being 0.006 Å for both symmetry-independent phenyl groups. The phenyl group attached to C1 makes an angle of 72.3 (1)° with the butadiene plane and the phenyl group attached to C2 makes an angle of 32.4 (1)° with the butadiene plane. The angle between the planes of these phenyl groups is 67.4 (1)°. Interplanar angles differing by up to 30° from the values observed in (I) are found in the crystal structures of 2,3-diphenyl-1,4-bis(*p*-methoxyphenyl)butadiene (Yamaguchi *et al.*, 2000) and a 1,2,3,4-tetraphenylbutadiene complex (Huan *et al.*, 1993). Thus, the interplanar angles depend on crystal packing forces.

The C2—C3 bond [1.4750 (12) Å] is significantly shorter than the corresponding C1—C9 bond [1.4993 (12) Å], due to a larger degree of resonance in the former bond. There are steric interactions between the phenyl groups; the shortest intramolecular contacts are H8···C9 = 2.56 (1) Å, H8···C14 = 2.70 (1) Å, H2···C9^{ii} = 2.48 (1) Å and H2···C14^{ii} = 2.66 (1) Å [symmetry code: (ii) $1 - x$, $1 - y$, $1 - z$]. The C2—C3—C8 angle is 5.7 (2)° larger than the corresponding C2—C3—C4 angle as a result of these steric interactions.

A thermal motion analysis of molecule (I) using the method of Schomaker & Trueblood (1998) shows the internal rotations about the C2—C3 and C1—C9 bonds not to be significant. Thus, the molecule essentially behaves as a rigid body, in agreement with an earlier observation by Burns *et al.* (1968).

The crystal packing is shown in Fig. 2. There are two intermolecular $C_{phenyl}—H\cdots\pi_{phenyl}$ interactions. Details of these interactions are given in Table 1. The C—H donors are not directed to the centre of the acceptor phenyl group but point closer to individual C—C bonds; the C6—H6 bond points to the C11—C12 bond [at $(x - 1, y, z - 1)$] and the C14—H14 bond points to the C3—C4 bond [at $(x + 1, y, z)$].

Experimental

The title compound was obtained in low yield as a by-product during the synthesis of 1-chloro-2,3,4,5-tetraphenylsilole (Schuppan *et al.*, 2001). Pale-yellow rods were obtained by recrystallization of (I) from $CDCl_3$ at room temperature.

Crystal data

$C_{28}H_{22}$
M_r = 358.46
Monoclinic, $P2_1/c$
a = 5.7873 (11) Å
b = 21.262 (3) Å
c = 7.914 (2) Å
β = 96.380 (15)°
V = 967.8 (3) Å^3
Z = 2
D_x = 1.230 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 119 reflections
θ = 3–23°
μ = 0.07 mm^{-1}
T = 162 (2) K
Rod, pale yellow
0.55 × 0.30 × 0.12 mm

Data collection

Siemens SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: none
16868 measured reflections
3325 independent reflections
2678 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 32.4°
$h = -8 \rightarrow 8$
$k = -31 \rightarrow 31$
$l = -11 \rightarrow 11$

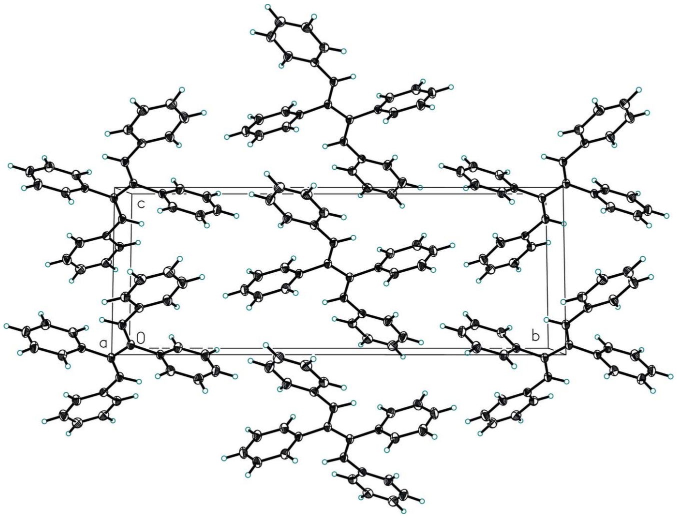

Figure 2
Crystal packing of (I), viewed along the *a* axis. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 1.10
3325 reflections
171 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the phenyl groups attached to C1 and C2.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···$Cg1^{i}$	0.99 (1)	2.96	3.747	137
C14—H14···$Cg2^{ii}$	0.97 (1)	2.74	3.595	147

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

The H atoms were located in a difference Fourier synthesis and refined with individual isotropic displacement parameters. The thermal motion analysis was performed with the *WinGX* program package (Farrugia, 1999).

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1996); software used to prepare material for publication: *SHELXL97*.

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