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2-(4-Methylphenyl)-1,1-diphenylethene

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In the crystal structure of the title compound, $C_{21}H_{18}$, the T-shaped molecules adopt a packing arrangement which does not display any special intermolecular interactions.

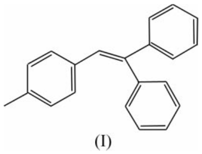
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.117
Data-to-parameter ratio = 11.8

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

Comment

The title compound, (I), was synthesized as a precursor material for a functionalized 1,4-bis(2,2-diphenylethenyl)-benzene, which can be grafted on to a polystyrene backbone in order to combine the blue electroluminescence of the molecule (Yang, Heremans *et al.*, 2000; Yang, Jin *et al.*, 2000) with the excellent processing characteristics of polystyrene.



(I)

The molecular structure of (I) is shown in Fig. 1. The bond distances and angles are normal and in the crystal structure there are no intermolecular contacts shorter than the sum of the van der Waals radii. There is only one intermolecular contact conforming to the geometrical criteria that are generally accepted for a T-shaped phenyl–phenyl interaction [see, for example, McGauchey *et al.* (1998) and Meyer *et al.* (2003)]: C5($-$H5)$\cdots$$CgC^{i}$ = 3.27 (2) Å and C5$-$H5$\cdots$$CgC^{i}$ = 147.3° [CgC is the centroid of the ring C; symmetry code: (i) $1 + x, y, z$]. There are, however, a large number of interactions that exist between the benzene rings due to their close

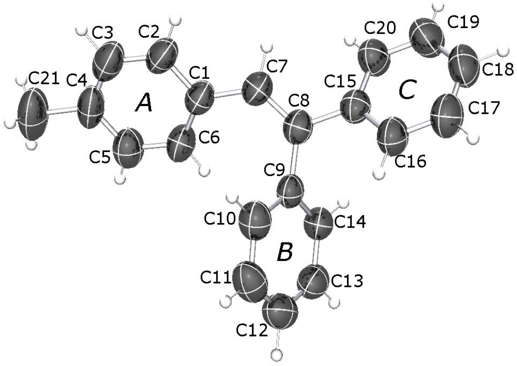


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

proximity, but these interactions do not conform to the above criteria. Of the three compounds in the Cambridge Structural Database (Version 5.25; Allen, 2002) that contain a similar 1,1-diphenyl-2-phenylethene fragment, HADCEU and HADCIY (Chiba, 1993) have additional phenyl rings in another functional group which, together, can display well defined interactions. REDFEL (Bartholomew *et al.*, 2000) displays a geometry which is very similar to the one presented here, but with two molecules in the asymmetric unit, allowing it to arrange the six symmetry-independent rings in a pattern that generates several standard phenyl–phenyl interactions. The only possible conclusion regarding the crystal structure of (I) is that the steric requirements in this molecule outweigh the additional stabilization obtained by the construction of an extended network of parallel-displaced or T-shaped phenyl–phenyl interactions. Nevertheless, the interactions that exist between the benzene rings stabilize the structure sufficiently to allow crystallization with only three symmetry-independent rings in the structure.

Experimental

All starting materials were obtained from Acros or Aldrich and used as received. Dimethylformamide (DMF) was dried over 3 A molecular sieves. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian Unity-400 apparatus in $CDCl_3$ with tetramethylsilane (TMS) as the internal reference. For the synthesis of (4-methylbenzyl)diethylphosphonate, (II), a mixture of α-chloro-*p*-xylene (21 g, 0.15 mol) and triethyl phosphite (48.1 g, 0.29 mol) was gently refluxed for 8 h. The mixture was then cooled to room temperature, the excess triethylphosphite evaporated off and the resulting liquid used without further purification. For the synthesis of 1-(2,2-diphenylethenyl)-4-methylbenzene, (I), a solution of (II) (9.6 g, 30 mmol) and benzophenone (5.5 g, 30 mmol) in 50 ml of dry DMF was stirred and refluxed under nitrogen protection. Potassium *tert*-butoxide (3.6 g, 32 mmol) was added portionwise and the mixture refluxed for 2 d. After cooling to room temperature, the solution was added to 500 ml of water. A pale yellow solid precipitated and was collected by filtration. Purification by refluxing in methanol yielded 2.3 g (28%) of the pure product [m.p. 342–343 K (uncorrected)]. ^{1}H NMR ($CDCl_3$): δ 2.24 (*s*, 3H, CH_3), 6.91 (*m*, 5H, aromatic and olefinic protons), 7.30 (*m*, 10H, aromatic and olefinic protons). ^{13}C NMR ($CDCl_3$): δ 21.13 (CH_3), 127.30, 127.31, 127.52, 128,13, 128.17, 128.63, 128.71, 129.48, 130.40, 134.57 (*q*), 136.56 (*q*), 140.64 (*q*), 141.74 (*q*), 143.57 (*q*). Irregularly shaped crystals, suitable for X-ray diffraction, were grown from hot methanol.

Crystal data

$C_{21}H_{18}$
$M_r = 270.35$
Monoclinic, $P2_1/c$
$a = 8.9060\ (10)$ Å
$b = 16.768\ (3)$ Å
$c = 10.628\ (3)$ Å
$\beta = 93.39\ (2)^\circ$
$V = 1584.4\ (6)$ Å^3
$Z = 4$
$D_x = 1.133$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 13$–22°
$\mu = 0.06$ mm^{-1}
$T = 293\ (2)$ K
Fragment, colourless
0.4 × 0.2 × 0.2 mm

Data collection

Enraf–Nonius MACH3 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
5826 measured reflections
2787 independent reflections
1355 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.051$
$\theta_{\rm max} = 25.0^\circ$
$h = 0 \rightarrow 10$
$k = -19 \rightarrow 19$
$l = -12 \rightarrow 12$
3 standard reflections every 60 reflections intensity decay: 4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.117$
$S = 0.95$
2787 reflections
237 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.13$ e Å^{-3}

H atoms were placed in calculated positions and for the majority their coordinates were refined, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. For methyl atom C21, the H atoms were constrained, allowing the methyl group to rotate and the hydrogen distances to refine, but keeping the H—C—H angles fixed at 109.5°; here $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$.

Data collection: *CAD*-4 *EXPRESS* (Enraf—Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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