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[4-(2,2-Diphenylvinyl)phenyl]diphenylamine *n*-hexane 0.25 solvate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.069
wR factor = 0.243
Data-to-parameter ratio = 13.8

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

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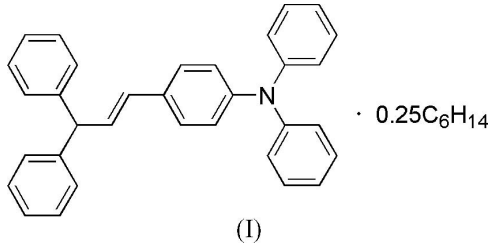
The title compound, $C_{33}H_{25}N{\cdot}0.25C_6H_{14}$, was synthesized *via* the Ullmann reaction. The dihedral angles between the planes of the phenyl rings of the diphenylamine group and the plane of the central benzene ring are 109.2 (3) and 114.1 (8)°.

Comment

Organic photoconductive materials are new high-technology information materials which can generate electron/hole (e/h) pairs upon illumination. These materials have been extensively used in copier applications, laser printing and digital xerography (Yang & Geise, 1992). The title compound is a charge transfer compound that can be used in double-layered photoconductive devices. In this paper, its structure, as derived from triarylamine, is reported. The molecular structure and the unit-cell contents of the crystal structureare illustrated in Figs. 1 and 2.



(I)

Experimental

4-(2,2-Diphenylvinyl)phenylamine (1.95 g, 0.01 mol), iodobenzene (5.34 g, 0.026 mol), CuCl (0.199 g, 0.002 mol), 1,10-phenanthroline (0.18 g, 0.001 mol) and KOH (24 g, 0.43 mol) were dissolved in toluene (30 ml). The mixture was refluxed for 6 h and filtered. The filtrate was evaporated and the residue was separated by column chromatography (silica gel, ethyl acetate/*n*-hexane 1:200) to give the

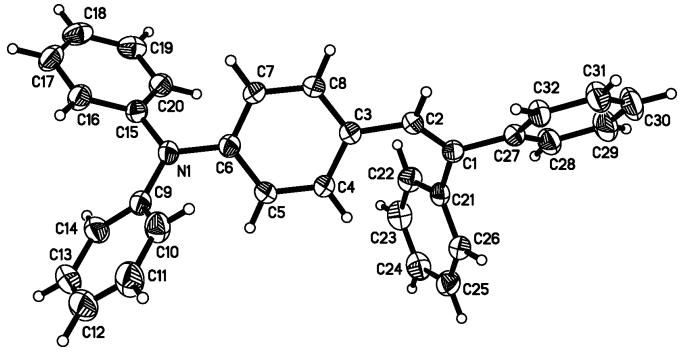


Figure 1
The molecular structure of (I), drawn with 30% probability displacement ellipsoids.

product (Pautmeier *et al.*, 1990). The structure of the product was identified by IR spectroscopy and mass spectrometry. Single crystals of the product as a hexane solvate were obtained by slow evaporation of a solution of dichloromethane/*n*-hexane (5:95) for 10 d; m.p 408 K. IR (cm^{-1}): 1625, 1500, 1310, 1260. MS (*m*/*e*): 423.2.

Crystal data

$C_{33}H_{25}N{\cdot}0.25C_6H_{14}$	D_x = 1.081 Mg m^{-3}
M_r = 445.07	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1010 reflections
a = 13.228 (9) Å	θ = 2.8–22.2°
b = 19.640 (14) Å	μ = 0.06 mm^{-1}
c = 11.524 (8) Å	T = 293 (2) K
β = 114.024 (11)°	Plate, colorless
V = 2735 (3) $Å^3$	0.40 × 0.30 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2755 reflections with $I > 2\sigma(I)$
	R_{int} = 0.041
φ and ω scans	θ_{max} = 25.0°
Absorption correction: none	$h = -15 \rightarrow 10$
13 043 measured reflections	$k = -20 \rightarrow 23$
4814 independent reflections	$l = -8 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1362P)^2 + 0.210P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.069	
$wR(F^2)$ = 0.243	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.63 e $Å^{-3}$
4814 reflections	$\Delta\rho_{min}$ = −0.22 e $Å^{-3}$
349 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(carrier). The hexane molecules are disordered over two sites, with occupancy factors of 0.368 (9) and 0.132 (9), and the C—C distances were fixed at 1.54 (1) Å in the refinement.

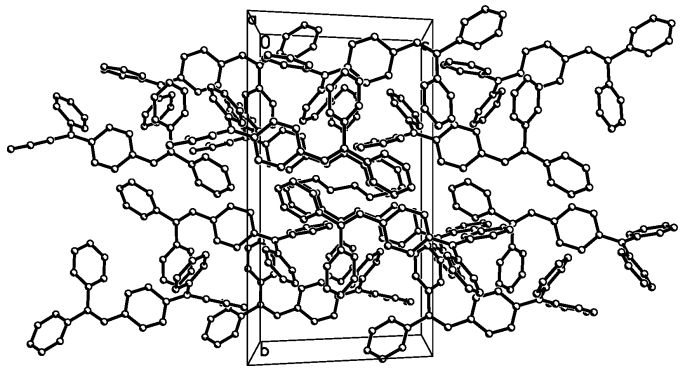


Figure 2
The crystal structure of (I), viewed along the *a* axis. H atoms have been omitted.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Pautmeier, L., Bussiler, H. & Richert, R. (1990). *Synth. Met.* **37**, 271–278.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yang, Z. & Geise, H. J. (1992). *Synth. Met.* **47**, 111–112.