organic papers

Bis(4-chlorophenyl)[4-(2,2-diphenylvinyl)-phenyl]amine

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The title compound, $C_{32}H_{23}Cl_2N$, was synthesized *via* the Ullmann reaction. The orientations of the three aromatic rings attached to the vinyl group are determined by the sp^2 state of the vinyl C atoms. The crystal packing is stabilized by weak C—H$\cdots\pi$ interactions.

Comment

Organic photoconductive materials constitute a new type of high-technology information materials, which can generate e/h pairs upon illumination. These materials have been extensively used in copier applications, laser printers and digital xerography (Yang & Geize, 1992).

The title compound, (I), is a charge-transfer material, which can be used in double-layered photoconductive devices. In this paper, the structure of (I), as derived from a triarylamine, is reported. The molecular structure of the crystal is illustrated in Fig. 1. The dihedral angle between the C9–C14 and C15–C20 phenyl rings is 75.6 (2)°. The orientations of the three aromatic rings attached to the vinyl group are determined by the sp^2 state of the vinyl C atoms.

(I)
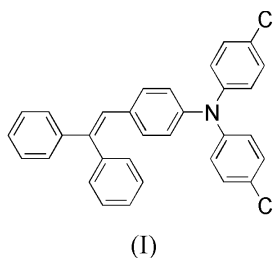
The crystal packing is stabilized by weak C—H$\cdots\pi$ interactions whose geometry is given in Table 1, where C1g, C2g, C3g and C5g are the centroids of the C1–C6, C9–C14, C15–C20 and C27–C32 phenyl rings, respectively.

Experimental

4-(2,2-Diphenylvinyl)phenylamine (0.01 mol), 1-chloro-4-iodobenzene (0.026 mol), CuCl (0.002 mol), 1,10-phenanthroline (0.001 mol) and KOH (24 g) were dissolved in toluene (30 ml). The mixture was refluxed for 6 h. After evaporation of the solvent, the residue was separated by column chromatography (silica gel, EA/PE = 1/200) to give the title compound (Pautmeier *et al.*, 1990), whose structure was identified by IR and MS. Single crystals of (I) were obtained by slow evaporation of the PE solution over a period of 10 d. M.p. 395–399 K. IR (KBr): ν 3036, 2925, 1588, 1488, 1310, 1281, 1173, 1090, 1006, 877, 826, 763, 694, MS: 491, 457, 423, 165, 77 cm^{-1}.
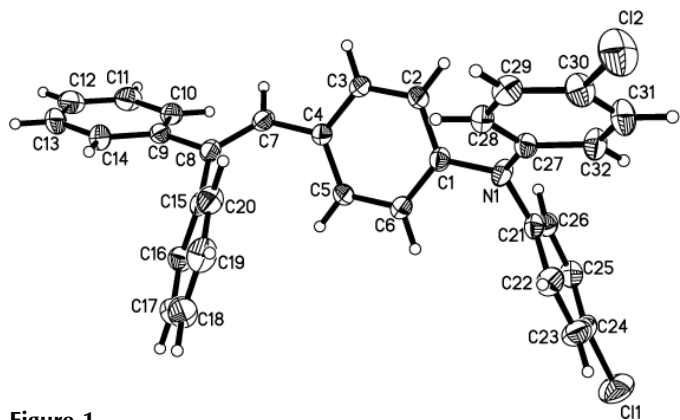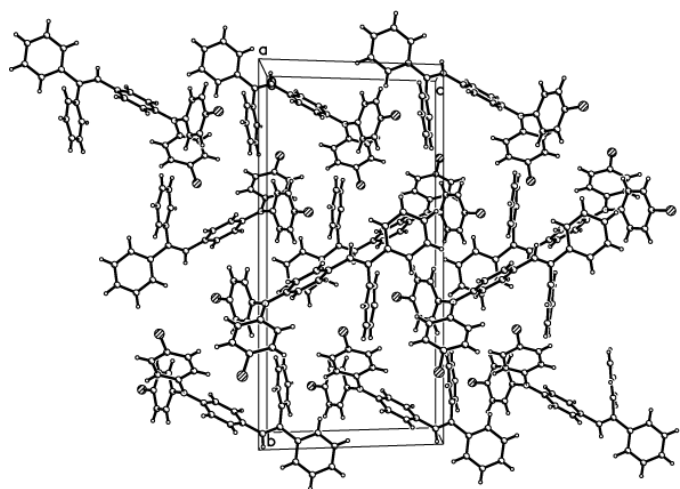
Figure 1
The molecular structure of (I), drawn with 30% probability displacement ellipsoids.

Figure 2
The crystal structure of (I), viewed along the *a* axis

Crystal data

$C_{32}H_{23}Cl_2N$	$D_x = 1.248$ Mg m^{-3}
$M_r = 492.41$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 728
$a = 9.784$ (3) Å	reflections
$b = 23.620$ (7) Å	$\theta = 2.2–22.7°$
$c = 11.752$ (4) Å	$\mu = 0.27$ mm^{-1}
$\beta = 105.228$ (5)°	$T = 293$ (2) K
$V = 2620.5$ (14) Å^3	Plate, colourless
$Z = 4$	$0.36 \times 0.28 \times 0.10$ mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer	5355 independent reflections
	2565 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.071$
Absorption correction: multi-scan	$\theta_{max} = 26.4°$
(*SADABS*; Bruker, 1997)	$h = -11 \rightarrow 12$
$T_{min} = 0.799$, $T_{max} = 0.970$	$k = -17 \rightarrow 29$
14 866 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.084P)^2]$
$wR(F^2) = 0.123$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.001$
5355 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$C2—H2\cdots C2g^{i}$	0.93	2.85	3.622 (4)	141
$C19—H19\cdots C5g^{ii}$	0.93	2.87	3.776 (5)	164
$C25—H25\cdots C1g^{iii}$	0.93	2.65	3.553 (4)	163
$C32—H32\cdots C3g^{iv}$	0.93	2.95	3.812 (4)	155

Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $x, -\frac{3}{2} - y, z - \frac{1}{2}$; (iii) $2 - x, 1 - y, 2 - z$; (iv) $x, y, 1 + z$.

H atoms were positioned geometrically, with C—H distance of 0.93–0.98 Å, and treated as riding [U_{iso}(H) = 1.2U_{eq}(C)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Versions 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Pautmeier, L., Bussiler, H. & Richert, R. (1990). *Synth. Met.* **37**, 271–278.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Yang, Z., Geize, H. J. (1992). *Synth. Met.* **47**, 111–112.