

**{4-[(1-Naphthyl)vinyl]phenyl}di-*p*-tolylamine**

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**Key indicators**

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$

$R$  factor = 0.056

$wR$  factor = 0.154

Data-to-parameter ratio = 7.1

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

The title compound,  $\text{C}_{32}\text{H}_{27}\text{N}$ , was synthesized *via* the Ullmann reaction. The structure has a pseudo-twofold axis approximately parallel to the  $b$  axis, and hence the pseudo-space group  $C2/c$ . The crystal packing is stabilized by weak  $\text{C}-\text{H}\cdots\pi$  and van der Waals interactions.

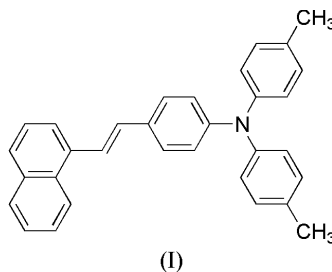
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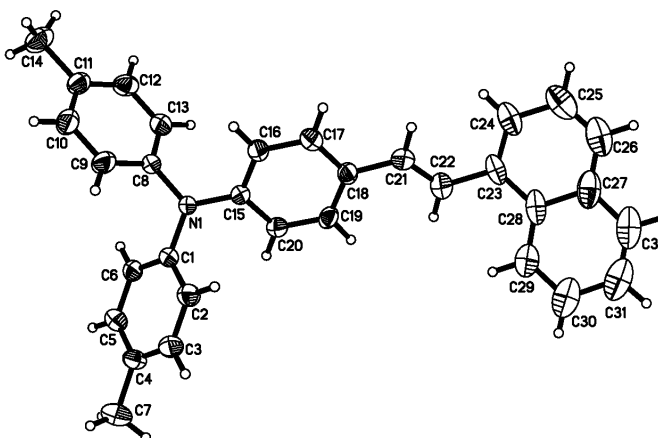
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**Comment**

Organic photoconductive materials are a new type of high technology information material which can generate electron-hole pairs upon illumination. They have been extensively used in copier applications, laser printing and digital xerography (Yang & Geize, 1992). The title compound, (I), a triarylamine, is a charge transfer material which can be used in double-layered photoconductive devices. We describe its structure here.

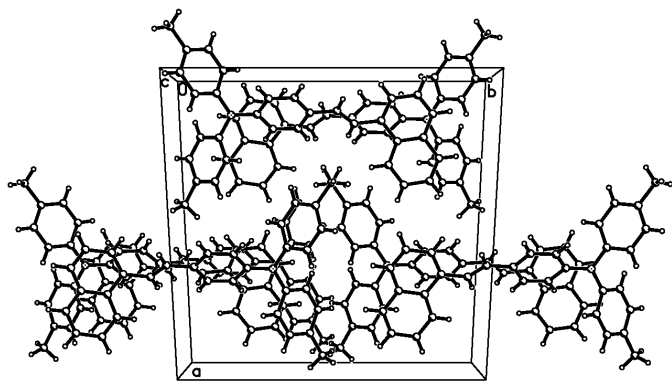


The molecular structure of (I) is illustrated in Fig. 1. The structure has a pseudo-twofold axis passing through the atoms N1, C15, C18, C21, C23 and C26, approximately parallel to the  $b$  axis, and hence it has the pseudo-space group  $C2/c$ . The two



**Figure 1**

The molecular structure of (I), showing 30% probability ellipsoids.



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

toluene rings (C1–C6 and C8–C13) are oriented at angles 62.7 (3) and 68.0 (3)°, respectively, to the central aromatic ring (C15–C20). The dihedral angle between the naphthalene ring system [planar within 0.035 (1) Å] and the C15–C20 ring is 33.7 (2)°. The molecular packing in the crystal is stabilized by weak C–H··· $\pi$  interactions (Table 1) and van der Waals interactions.

## Experimental

4-(1-Naphthylvinyl)phenylamine (0.01 mol), 4-methyliodobenzene (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 and, after evaporation of the solvent, the residue was separated by column chromatography (silica gel, ethyl acetate/petroleum ether = 1:200) to give the title compound (Pautmeier *et al.*, 1990). The compound was identified by IR and MS. Single crystals were obtained by slow evaporation of a petroleum ether solution; m.p: 383–386 K; MS: 425.3, 286.2, 244.1, 91.7, 51.6.

### Crystal data

$C_{32}H_{27}N$	$D_x = 1.167 \text{ Mg m}^{-3}$
$M_r = 425.55$	Mo $K\alpha$ radiation
Monoclinic, <i>Cc</i>	Cell parameters from 724 reflections
$a = 18.482$ (7) Å	$\theta = 2.4$ – $21.7^\circ$
$b = 17.045$ (7) Å	$\mu = 0.07 \text{ mm}^{-1}$
$c = 8.635$ (3) Å	$T = 293$ (2) K
$\beta = 117.094$ (5)°	Block, yellow
$V = 2421.9$ (16) Å <sup>3</sup>	$0.40 \times 0.34 \times 0.28 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	2130 independent reflections
$\omega$ scans	1453 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$R_{\text{int}} = 0.028$
$T_{\text{min}} = 0.973$ , $T_{\text{max}} = 0.981$	$\theta_{\text{max}} = 25.0^\circ$
5052 measured reflections	$h = -21 \rightarrow 21$
	$k = -20 \rightarrow 10$
	$l = -10 \rightarrow 7$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0877P)^2 + 0.2832P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.154$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
2130 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
300 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H2···Cg3 <sup>i</sup>	0.93	3.09	3.835 (7)	138
C10–H10···Cg1 <sup>ii</sup>	0.93	3.26	4.107 (8)	153
C16–H16···Cg2 <sup>i</sup>	0.93	3.15	3.586 (6)	111
C20–H20···Cg2 <sup>iii</sup>	0.93	3.03	3.592 (6)	121
C30–H30···Cg1 <sup>iv</sup>	0.93	3.30	4.079 (11)	142

Symmetry codes: (i)  $x, 1 - y, \frac{1}{2} + z$ ; (ii)  $x, -y, \frac{1}{2} + z$ ; (iii)  $x, 1 - y, z - \frac{1}{2}$ ; (iv)  $\frac{1}{2} + x, \frac{1}{2} + y, z$ . Notes: Cg1, Cg2 and Cg3 denote the centroids of the C8–C13, C23–C28 and C27–C32 rings, respectively.

H atoms were positioned geometrically, with C–H = 0.93–0.96 Å, and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Restraints for similarity and approximate isotropy were applied to the  $U_{ij}$  components of some of the naphthalene ring atoms. The Friedel pairs were merged during the final cycles of refinement.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1997); 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*.

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