Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

N,*N*-Bis(4-chlorophenyl)-4-(2-naphthalen-1-ylvinyl)aniline

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.104
Data-to-parameter ratio = 13.9

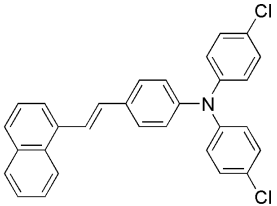
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{30}H_{21}Cl_2N$, crystallizes in the monoclinic space group $P2_1/n$. This study confirms the *trans* configuration about the double bond.

Received 9 March 2004
Accepted 7 April 2004
Online 17 April 2004

Comment

Organic photoconductive materials represent a new type of high technology capable of generating e/h pairs upon illumination. This technology has been extensively used in copier applications, laser printing and digital xerography (Yang *et al.*, 1992). The title compound, (I), a triarylamine, is a charge-transfer material which can be used in double-layered photoconductive devices and its structure is reported here.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The dihedral angle between the naphthalene ring system and the C1–C6 ring is 45.81 (8)°. The three benzene rings attached to the N atom are oriented in a propeller-type arrangement. If we denote the C1–C6 ring as *A*, the C19–C24 ring as *B* and the C25–C30 ring as *C* then the various dihedral angles are: *A*/*B* 63.72 (7)°, *A*/*C* 72.67 (6)° and *B*/*C* 74.45 (6)°. Fig. 1 shows that the C═C double bond has a *trans* configuration, the torsion angle C4—C7—C8—C9 being −178.5 (2)°. The C═C bond

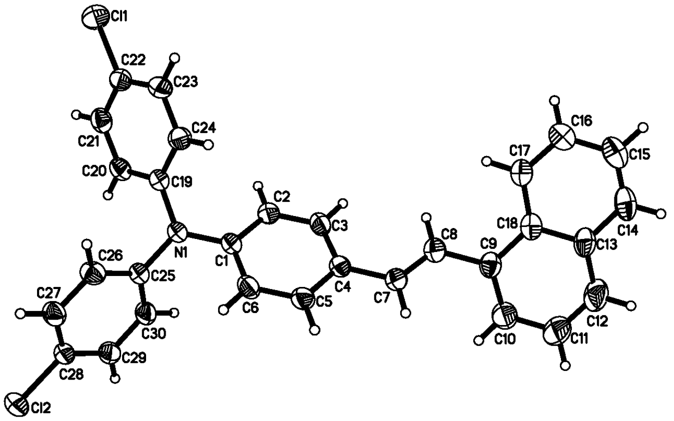


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

DOI: 10.1107/S160053680400844X

length is 1.312 (3)Å, shorter than that of a typical double bond. This value is similar to that in {4-[(1-naphthyl)vinyl]phenyl}di-*p*-tolylamine (Cao *et al.*, 2003), but shorter than that in an oxadiazole-subsitituted triarylamine (Yu *et al.*, 2002). The other bond lengths and angles are unexceptional. The molecular packing in the crystal is stabilized by Cl···Cl interactions.

Experimental

4-(2-Naphthalen-1-ylvinyl)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 and the solvent was then evaporated. The residue was separated by column chromatography (silica gel; ethyl acetate–petroleum ether, 1:200) to yield the product (Pautmeier *et al.*, 1990). The structure of the product was identified by MS. Single crystals of the product were obtained by slow evaporation of the petroleum ether solutionover a period of 12 d (m.p. 397–401 K). MS $[M - H]^+$: 465.

Crystal data

$C_{30}H_{21}Cl_2N$
$M_r = 466.38$
Monoclinic, $P2_1/n$
$a = 9.519$ (3) Å
$b = 12.924$ (4) Å
$c = 19.027$ (6) Å
$\beta = 90.744$ (5)°
$V = 2340.5$ (12) Å^3
$Z = 4$
$D_x = 1.324$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 864 reflections
$\theta = 2.7$–24.5°
$\mu = 0.30$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.792$, $T_{\max} = 0.937$
11795 measured reflections
4133 independent reflections
2562 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.037$
$\theta_{\max} = 25.0°$
$h = -11 \rightarrow 11$
$k = -15 \rightarrow 8$
$l = -21 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.104$
$S = 1.01$
4133 reflections
298 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.6497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

H atoms were positioned geometrically, with C—H = 0.93 Å, and refined in a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$(carrier atom).

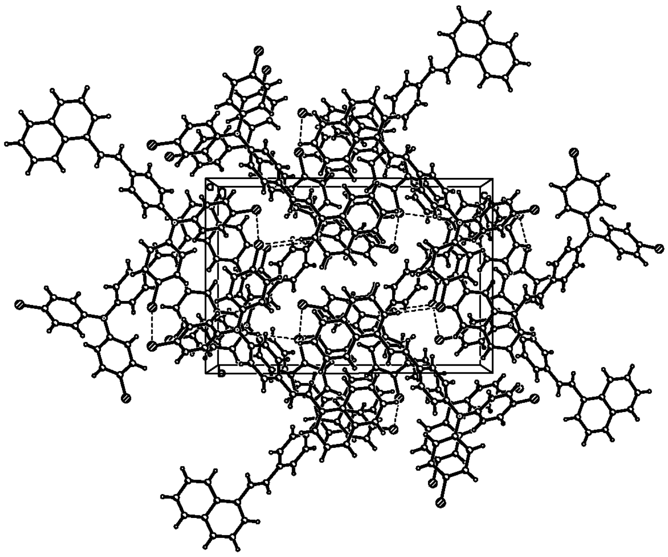


Figure 2
The crystal structure of (I), viewed along the *a* axis. Dashed lines indicate Cl···Cl interactions.

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*.

We thank Song Haibin of Nankai University for the data collection. This work was supported by a grant from the Tianjin Natural Science Foundation (No. 023801711).

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