Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[2-(1-Naphthyl)vinyl]-*N*,*N*-diphenylaniline

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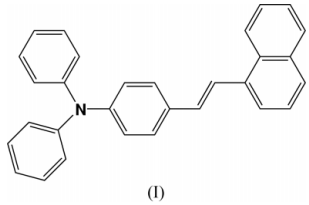
Received 10 October 2003
Accepted 3 November 2003
Online 29 November 2003

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.121
Data-to-parameter ratio = 13.5

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

The title compound, $C_{30}H_{23}N$, was synthesized *via* the Ullmann reaction. The plane of the vinyl linkage almost coincides with the plane of the directly attached aromatic ring of the triarylamine group [dihedral angle 6.2 (2)°] and forms a dihedral angle of 41.07 (4)° with the mean plane of the naphthalene group.



(I)

Experimental

0.01 mol of 4-(2-naphthalen-1-ylvinyl)aniline, 0.026 mol of iodobenzene, 0.002 mol of CuCl, 0.001 mol of 1,10-phenanthroline and 24 g of KOH were dissolved in toluene (30 ml). The mixture was refluxed for 6 h, then the toluene was removed by evaporation. The residue was dissolved in dichloromethane (8 ml) and separated by column chromatography (silica gel, ethyl acetate/petroleum ether = 1:200) to give (I) (Pautmeier *et al.*, 1990). Its structure was identified by IR and MS. Single crystals were obtained by slow evaporation of a petroleum ether solution over a period of 15 d. M.p: 413 K; MS (*m*/*z*): 397.2, 228.1, 198.5, 153.1, 77.

Crystal data

$C_{30}H_{23}N$
M_r = 397.49
Triclinic, $P\overline{1}$
a = 8.883 (3) Å
b = 9.446 (3) Å
c = 13.466 (4) Å
α = 88.416 (5)°
β = 83.527 (4)°
γ = 74.129 (4)°
V = 1079.9 (6) Å^3
Z = 2
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1023 reflections
θ = 2.4–26.3°
μ = 0.07 mm^{-1}
T = 293 (2) K
Block, yellow
0.22 × 0.20 × 0.16 mm

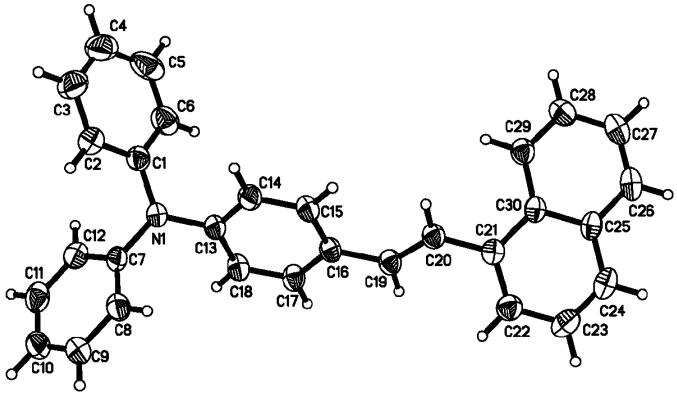


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer	3781 independent reflections
φ and ω scans	2384 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	$R_{int} = 0.018$
$T_{min} = 0.874$, $T_{max} = 0.990$	$\theta_{max} = 25.0^\circ$
5593 measured reflections	$h = -8 \rightarrow 10$
	$k = -8 \rightarrow 11$
	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.1151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	
$wR(F^2) = 0.121$	
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.003$
3781 reflections	$\Delta\rho_{max} = 0.12$ e Å^{-3}
280 parameters	$\Delta\rho_{min} = -0.14$ e Å^{-3}
H-atom parameters constrained	

H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined in a riding model, with $U_{iso}(H) = 1.2U_{eq}$(carrier).

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*.

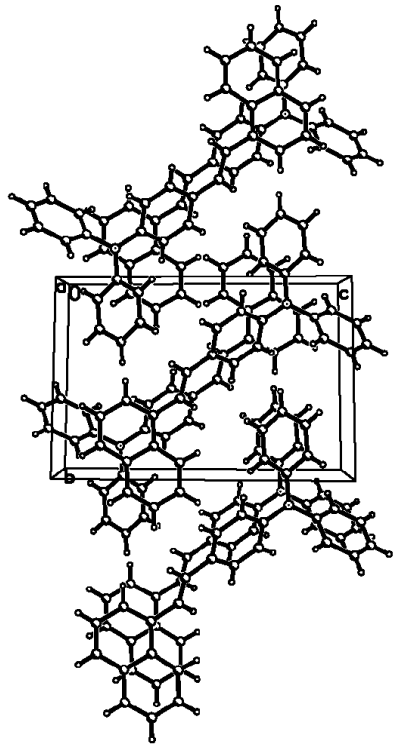


Figure 2
The crystal structure of (I), viewed along the *a* axis.

References

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