

4-(4,4-Diphenylbuta-1,3-dienyl)-*N,N*-bis(4-methylphenyl)aniline

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Key indicators

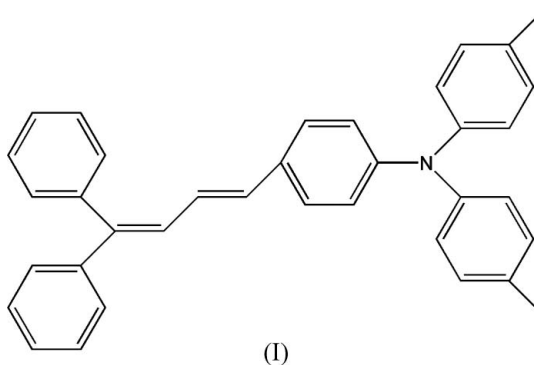
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.050
 wR factor = 0.143
Data-to-parameter ratio = 17.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_{36}\text{H}_{31}\text{N}$, was synthesized by the Wittig reaction of 1,1-diphenyl-3-cholopropylene and 4-[*N,N*-bis(4-methylphenyl)amino]benzaldehyde. The butadiene structure has a planar transoid conformation.

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Comment

Hole transporting materials (HTMs) play an important role in the fabrication of organic photoconductors (OPCs), which are widely used in xerography and holography (Wu *et al.*, 2005). Substances containing the butadiene structure have been widely investigated, because of their easy preparation by the Wittig reaction and favorable photographic performances when used as HTMs (Enokida & Hirohashi, 1991).



The title compound, (I), was synthesized by the Wittig reaction of 1,1-diphenyl-3-cholopropylene and 4-[*N,N*-bis(4-methylphenyl)aminobenzaldehyde].

Fig. 1 shows the molecular structure of (I). The butadiene structure (C1/C14–C16) is almost planar to within 0.03 Å and

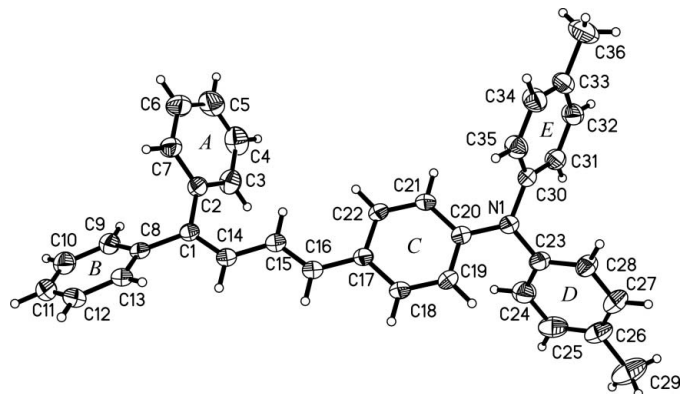


Figure 1

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

has a transoid conformation. The dihedral angles between the butadiene plane and the *A*, *B* and *C* ring planes are 53.0 (3), 40.3 (2) and 7.3 (2)°, respectively. On the other hand, the dihedral angles between the benzene rings, *C/D* = 64.3 (2)° and *C/E* = 64.4 (2)°, are essentially the same. The C1–C8 [1.477 (3) Å] and C1–C2 [1.489 (3) Å] bond distances are a little longer than C16–C17 [1.451 (3) Å], while the N1–C20 [1.410 (3) Å], N1–C23 [1.422 (3) Å] and N1–C30 [1.418 (3) Å] bond lengths are essentially the same.

Experimental

A mixture of 1,1-diphenyl-3-chloropropylene (11.4 g, 50 mmol), triethyl phosphite (18.0 ml, 50 mmol) and xylene (50 ml) was refluxed for 10 h, and then xylene was removed *in vacuo* to obtain a residue. After cooling, the residue, 4-[*N,N*-bis(4-methylphenyl)]amino-benzaldehyde (12.0 g, 40 mmol), dimethylformamide (100 ml) and potassium *tert*-butoxide (4.5 g, 40 mmol) were placed in a flask. The resulting mixture was stirred for 5 h and poured into methanol, and the resulting precipitate was separated from the liquid by filtration to obtain crude crystals. These were purified by silica gel column chromatography [eluant: toluene/ethyl acetate (2:1)], recrystallized from hexane and dried to obtain yellow crystals (yield 58.7%, m.p. 433 K).

Crystal data

$C_{36}H_{31}N$	Mo $K\alpha$ radiation
$M_r = 477.62$	Cell parameters from 4038 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 2.5\text{--}20.6^\circ$
$a = 16.629$ (2) Å	$\mu = 0.06$ mm ⁻¹
$b = 14.9729$ (19) Å	$T = 294$ (2) K
$c = 22.899$ (3) Å	Block, yellow
$V = 5701.3$ (13) Å ³	$0.24 \times 0.16 \times 0.14$ mm
$Z = 8$	
$D_x = 1.113$ Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	5830 independent reflections
φ and ω scans	2710 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 1997)	$R_{\text{int}} = 0.071$
$T_{\text{min}} = 0.975$, $T_{\text{max}} = 0.991$	$\theta_{\text{max}} = 26.4^\circ$
30699 measured reflections	$h = -16 \rightarrow 20$
	$k = -18 \rightarrow 18$
	$l = -28 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.4918P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.143$	$(\Delta/\sigma)_{\text{max}} = 0.005$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.17$ e Å ⁻³
5830 reflections	$\Delta\rho_{\text{min}} = -0.15$ e Å ⁻³
336 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically [0.93 (CH) and 0.96 Å (CH₃)] and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{CH}})$ and $1.5U_{\text{eq}}(\text{C}_{\text{CH}_3})$.

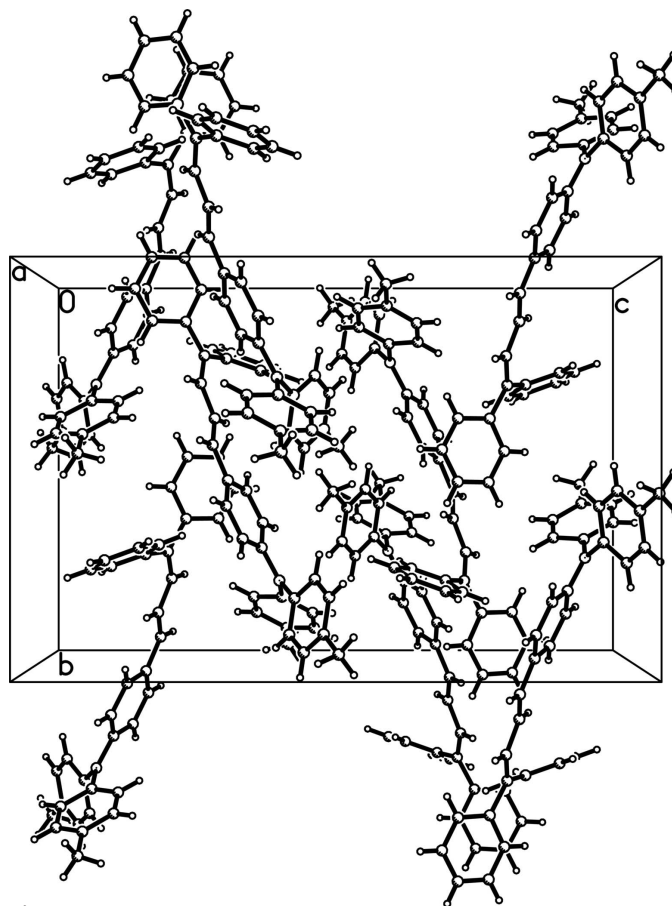


Figure 2
Packing diagram of (I).

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