# trans-2-[4-(Diethylamino)styryl]pyridine

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**Key indicators**

Single-crystal X-ray study
$T = 298$ K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.038
$wR$ factor = 0.097
Data-to-parameter ratio = 7.9

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

The molecule of the title compound, $C_{17}H_{20}N_2$, is roughly planar and displays a *trans* configuration with respect to the C=C double bond. The dihedral angle between the pyridine and benzene rings is 2.52 (9)°.

## Comment

After the experimental verification of two-photon absorption in $Eu^{2+}$-doped $CaF_2$ crystals (Kaiser & Garrett, 1961), materials showing two-photon absorption effects have been widely exploited in up-converted lasing (He, Bhawalkar *et al.*, 1995), optical limiting devices (He, Xu *et al.*, 1995), two-photon fluorescence microscopy and three-dimensional optical data storage (Dimitri & Rentzepis, 1989). In the course of our study aimed at the design of new materials with strong two-photon absorption, the title compound, (I), has been synthesized and its crystal structure is reported here.



(I)
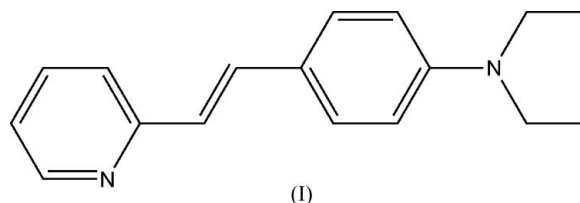
In the title compound, the C5—C6 and C7—C8 bond lengths (Table 1) are intermediate between single and double bonds, indicating significant conjugation of the aromatic $\pi$ systems. All other bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The molecule is roughly planar, with a dihedral angle between the benzene and pyridine rings of 2.52 (9)°. The crystal structure is stabilized by intra- and intermolecular hydrogen-bonding interactions (Table 2).

## Experimental

Potassium (2 mmol, 78 mg) and *tert*-butyl alcohol (12 mmol, 888 mg) were introduced into a round-bottomed flask at room temperature and stirred for 2.5 h. 4-(Diethylamino)benzaldehyde (1.0 mmol, 177 mg) and 2-methylpyridine (1.0 mmol, 93 mg) were added to the mixture, which was stirred for 2 h at 343 K. The *tert*-butyl alcohol was gradually removed under reduced pressure. The solution was then cooled to room temperature and poured into a mixture of dichloromethane (10 ml) and ice–water (10 ml) with stirring. The aqueous phase was extracted with dichloromethane (2 × 5 ml). After evaporation of dichloromethane, the crude product was obtained. Crystals of the title compound suitable for the X-ray diffraction analysis were obtained by slow evaporation of an ethanol solution. Elemental analysis found: C 80.96, H 7.91, N 11.13%; calculated for $C_{17}H_{20}N_2$: C 80.91, H 7.91, N 11.13%.

# organic papers

## Crystal data

$C_{17}H_{20}N_2$
$M_r = 252.35$
Orthorhombic, $P2_12_12_1$
$a = 7.594 (2)$ Å
$b = 9.604 (3)$ Å
$c = 19.932 (6)$ Å
$V = 1453.6 (7)$ Å$^3$

$Z = 4$
$D_x = 1.153$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm$^{-1}$
$T = 298 (2)$ K
Block, yellow
$0.52 \times 0.43 \times 0.19$ mm

## Data collection

Bruker SMART CCD
  diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan
  (SADABS; Sheldrick, 1996)
  $T_{min} = 0.966$, $T_{max} = 0.987$

7665 measured reflections
1506 independent reflections
1081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$

## Refinement

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.097$
$S = 1.06$
1506 reflections
191 parameters
H atoms treated by a mixture of
  independent and constrained
  refinement

$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.4698P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.13$ e Å$^{-3}$
Extinction correction: SHELXL97
Extinction coefficient: 0.0140 (14)

## Table 1
Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|---|---|---|---|
| C7—H7$\cdots$N1 | 1.01 (2) | 2.48 (2) | 2.864 (3) | 102.0 (13) |
| C2—H2$\cdots$N1$^i$ | 0.95 (3) | 2.52 (3) | 3.443 (4) | 165 (2) |

Symmetry code: (i) $-x + 2, y - \frac{1}{2}, -z - \frac{1}{2}$.

The H atoms on C1, C2, C6 and C7 were located in a difference Fourier map and refined freely [C—H =0.94 (3)–1.01 (3) Å]. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 or 0.96 Å (methyl C) and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).
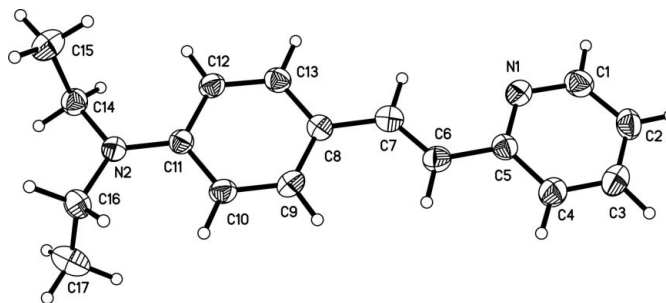


**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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