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N-(4-Ethoxyphenyl)-*N*-[3-(2-nitrophenyl)-prop-2-enylidene]amine

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Key indicators

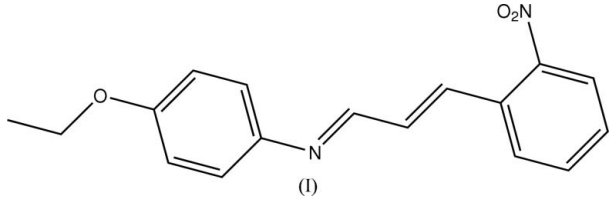
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.156
Data-to-parameter ratio = 14.6

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, $C_{17}H_{16}N_2O_3$, is non-planar, with a dihedral angle of 15.3 (1)° between the two benzene rings. An intramolecular C—H···O hydrogen bond forms a six-membered ring.

Comment

We have recently reported the structure of 2-{[3-(2-nitrophenyl)prop-2-enylidene]amino}phenol, (II) (Li *et al.*, 2005). In our ongoing studies of non-linear optical materials, the title compound, (I), was obtained. We report here its crystal structure (Fig. 1).



(I)

The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with the corresponding ones in compound (II). The molecule is non-planar, with a dihedral angle of 15.3 (1)° between the two benzene rings. An intramolecular C—H···O hydrogen bond (Table 1) forms a six-membered ring.

Experimental

Compound (I) was prepared according to the method of Li *et al.* (2005). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanol–water (3:1 *v*/*v*) solution over a period of 2 d.

Crystal data

$C_{17}H_{16}N_2O_3$
M_r = 296.32
Triclinic, $P\overline{1}$
a = 7.1103 (10) Å
b = 7.6318 (11) Å
c = 15.456 (2) Å
α = 76.803 (2)°
β = 81.767 (2)°
γ = 67.553 (2)°
V = 753.23 (18) Å^3
Z = 2
D_x = 1.307 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 (2) K
Plate, yellow
0.30 × 0.26 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.993
4201 measured reflections
2898 independent reflections
1643 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.156$
$S = 1.01$
2898 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1	0.93	2.23	2.786 (3)	117

H atoms were positioned geometrically, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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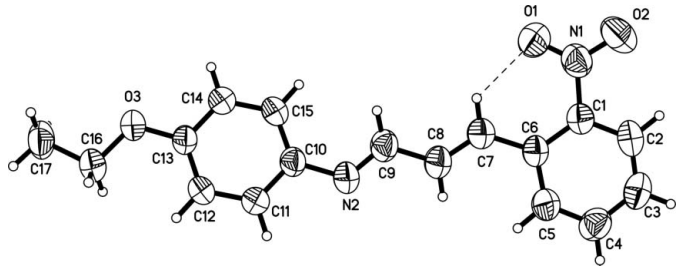

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

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