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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.130
Data-to-parameter ratio = 15.2

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

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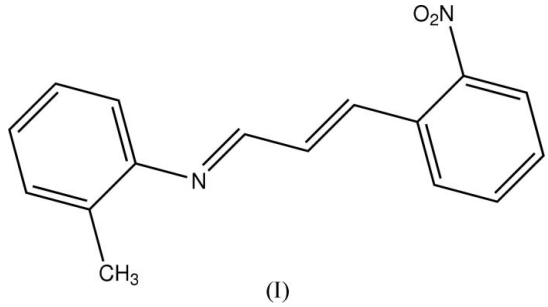
The title compound, $C_{16}H_{14}N_2O_2$, is non-planar, with a dihedral angle of 13.97 (8)° between the two benzene rings. There exists an intramolecular C—H···O hydrogen bond, forming a six-membered ring.

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 NLO (nonlinear optical) materials, the title compound, (I), was obtained. We report here its crystal structure (Fig. 1).



(I)

All bond lengths of (I) are comparable with those of (II). The molecule of (I) shows a closer approach to planarity than that of (II), the dihedral angle between the two benzene rings being 13.97 (8)° in (I) and 83.0 (1)° in (II). There exists an intramolecular C7—H7*A*···O1 hydrogen bond (Table 2), forming a six-membered ring.

Experimental

The title compound was prepared according to the method of Li *et al.* (2005).

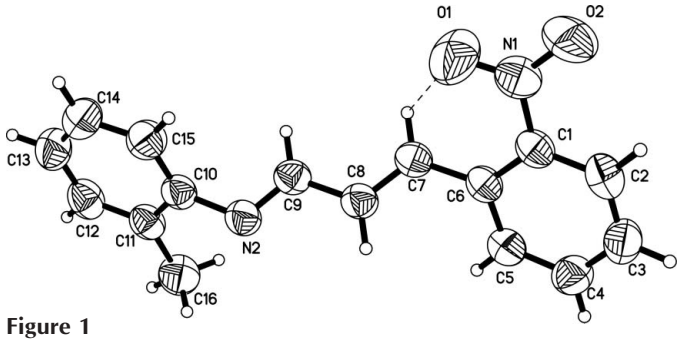


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

Crystal data

$C_{16}H_{14}N_2O_2$
M_r = 266.29
Monoclinic, $P2_1/c$
a = 11.390 (3) Å
b = 9.705 (3) Å
c = 13.072 (4) Å
β = 106.532 (4)°
V = 1385.2 (7) Å^3
Z = 4
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2769 reflections
θ = 2.6–26.1°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, yellow
0.36 × 0.25 × 0.16 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.986
7324 measured reflections
2744 independent reflections
2199 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.2°
$h = -14 \rightarrow 14$
$k = -6 \rightarrow 12$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.04
2744 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.1682P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—N1	1.2042 (19)	N2—C10	1.4159 (18)
O2—N1	1.2134 (17)	C7—C8	1.3286 (19)
N1—C1	1.472 (2)	C8—C9	1.443 (2)
N2—C9	1.2678 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1>	0.93	2.35	2.701 (2)	102

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) [U_{iso}(H) = 1.5 U_{eq}(C) for methyl H atoms].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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