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2-Methoxy-*N*-[3-(2-nitrophenyl)allylidene]aniline

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.128
Data-to-parameter ratio = 14.8

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

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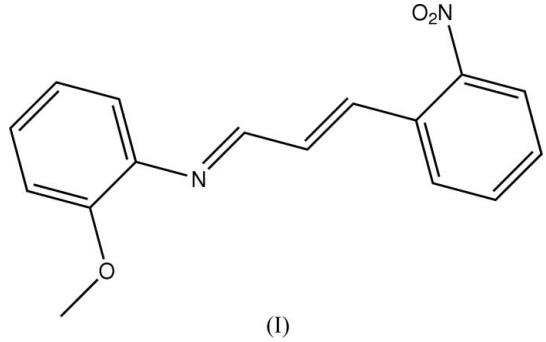
The molecule of the title compound, $C_{16}H_{14}N_2O_3$, is slightly non-planar, with a dihedral angle of 3.3 (1)° between the two benzene rings. In the crystal structure, the molecules are linked into centrosymmetric dimers by intermolecular C—H···O hydrogen bonds.

Comment

We have reported the synthesis and crystal structure of 2-{[3-(2-nitrophenyl)prop-2-enylidene]amino}phenol, (II) (Li *et al.*, 2005). In our ongoing studies of push–pull Schiff bases, the title compound, (I), was obtained. We report here its crystal structure.



(I)

The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). All the bonds in (I) show a characteristic length intermediate between those of single and double bonds, and comparable with those in (II). The molecule is slightly non-planar, with a dihedral angle of 3.3 (1)° between the two benzene rings, in contrast to that of 83.0 (1)° in (II). There exists an intramolecular C—H···O hydrogen bond (Table 2),

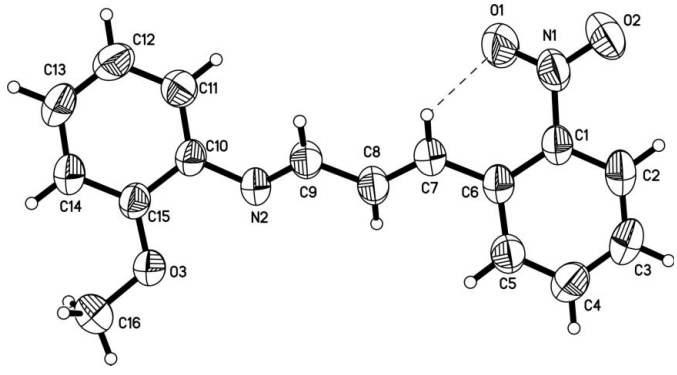


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

forming a six-membered ring (Fig. 1). In the crystal structure, molecules are linked into centrosymmetric dimers by C—H···O intermolecular hydrogen bonds (Table 1 and Fig. 2).

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 (2:1) solution over a period of 3 d.

Crystal data

$C_{16}H_{14}N_2O_3$
$M_r = 282.29$
Monoclinic, $P2_1/c$
$a = 14.0515\ (16)$ Å
$b = 5.0488\ (6)$ Å
$c = 20.118\ (2)$ Å
$\beta = 90.706\ (2)^\circ$
$V = 1427.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.314$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 294\ (2)$ K
Block, yellow
$0.41 \times 0.15 \times 0.11$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.963$, $T_{max} = 0.990$
7553 measured reflections
2807 independent reflections
2042 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.1^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.128$
$S = 1.03$
2807 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.1418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O2^{i}	0.93	2.45	3.344 (2)	162
C7—H7A···O1	0.93	2.40	2.745 (2)	102

Symmetry code: (i) $-x+1, -y-1, -z+1$.

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

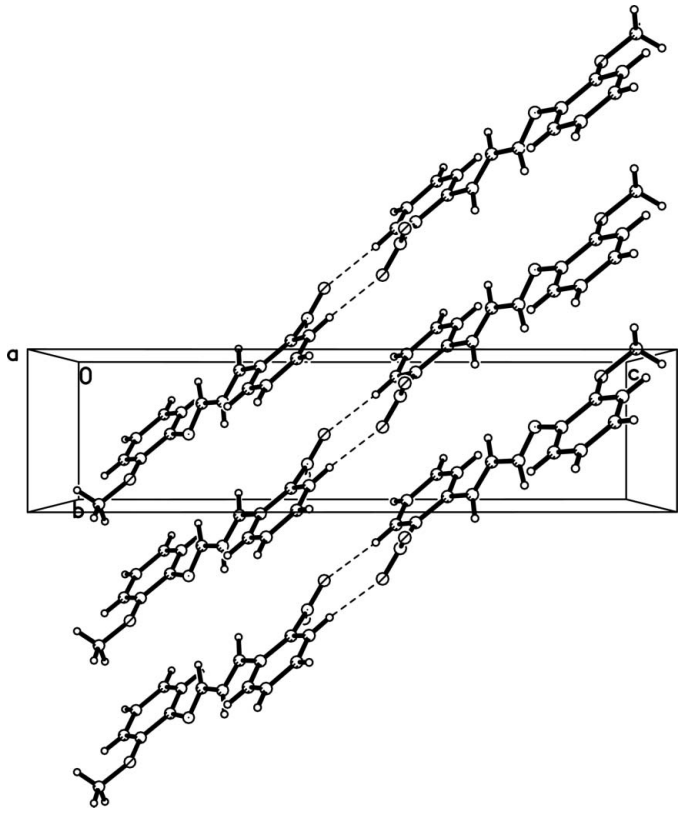


Figure 2
Packing diagram of (I), showing the centrosymmetric dimers. Hydrogen bonds are shown as dashed lines.

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