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Key indicators

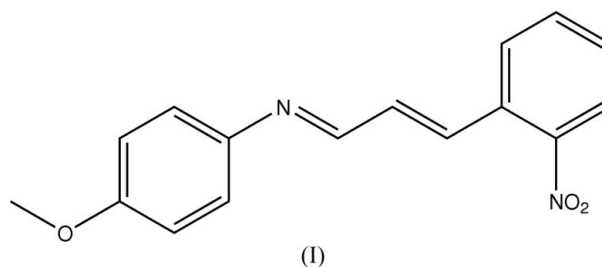
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.056
 wR factor = 0.144
Data-to-parameter ratio = 13.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4-Methoxy-*N*-[3-(2-nitrophenyl)allylidene]aniline

The molecule of the title compound, $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_3$, is slightly non-planar, with a dihedral angle of $4.01(1)^\circ$ between the two benzene rings. In the crystal structure, molecules are linked into chains by $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds. The crystal structure is stabilized by $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions.

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Comment

We have reported the synthesis and crystal structure of 2-[[3-(2-nitrophenyl)prop-2-enylidene]amino]phenol, (II) (Li *et al.*, 2005). As part of our ongoing studies of push-pull Schiff base compounds, the title compound, (I), was synthesized and the structure was determined.



The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The bonds between the two benzene rings in (I) show a characteristic length intermediate between those of single and double bonds, and comparable to those in (II). The molecule is slightly non-planar, with a dihedral angle of $4.01(1)^\circ$ between the two benzene rings, in contrast to that of $83.0(1)^\circ$ in (II). There exists an intramolecular $\text{C}9-\text{H}9\text{A}\cdots\text{O}2$ hydrogen bond (Table 1), forming a six-membered ring (Fig. 1).

In the crystal structure, molecules are linked into chains along the c axis by $\text{C}13-\text{H}13\text{A}\cdots\text{O}1$ and $\text{C}14-\text{H}14\text{A}\cdots\text{O}3$ intermolecular hydrogen bonds (Table 1 and Fig. 2). The

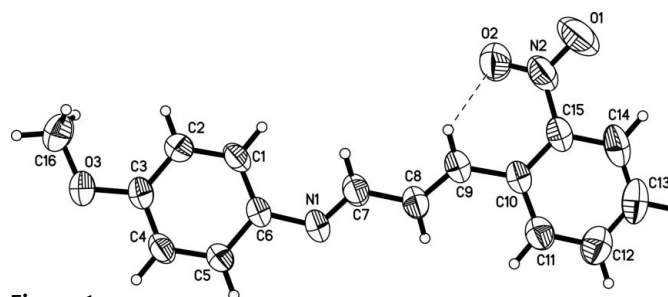


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme. The dashed line indicates a hydrogen bond.

crystal structure is stabilized by C—H $\cdots\pi$ interactions (Table 1). The packing is further stabilized by π – π interactions, with Cg1 \cdots Cg2 ($-x, 1 - y, -z$) = 3.849 Å (Cg1 and Cg2 denote the centroids of the C1–C6 and C10–C15 rings, respectively).

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 (4:1 *v/v*) solution over a period of 4 d.

Crystal data

C ₁₆ H ₁₄ N ₂ O ₃	$Z = 4$
$M_r = 282.29$	$D_x = 1.329 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 7.4308 (15) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 7.8556 (16) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 24.569 (5) \text{ \AA}$	Block, yellow
$\beta = 100.322 (6)^\circ$	$0.37 \times 0.16 \times 0.09 \text{ mm}$
$V = 1411.0 (5) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	7494 measured reflections
ω scans	2767 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1626 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.966, T_{\max} = 0.992$	$R_{\text{int}} = 0.039$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.1719P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.144$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
2767 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
205 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.0088 (16)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9–H9A \cdots Cg1 ⁱ	0.93	3.16	3.656	115
C16–H16B \cdots Cg2 ⁱ	0.96	2.82	3.586	137
C9–H9A \cdots O2	0.93	2.33	2.781 (3)	109
C13–H13A \cdots O1 ⁱⁱ	0.93	2.55	3.450 (4)	162
C14–H14A \cdots O3 ⁱⁱⁱ	0.93	2.54	3.403 (3)	154

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x + 1, y - \frac{1}{2}, -z - \frac{1}{2}$; (iii) $x + 1, -y - \frac{1}{2}, z - \frac{1}{2}$. Cg1 and Cg2 denote the centroids of the C1–C6 and C10–C15 rings, respectively.

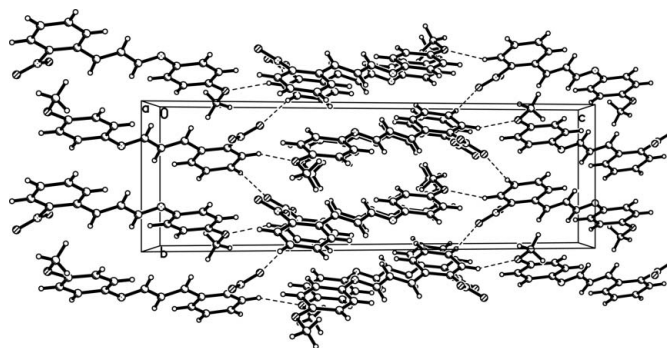


Figure 2

Packing diagram of (I), showing the hydrogen-bonded (dashed lines) chains.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ and $1.5 U_{\text{eq}}(\text{methyl C})$ H atoms.

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

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