2-{[3-(2-Nitrophenyl)prop-2-enylidene]amino}phenol

Ying Li, Xiao-Yan Yang, Shu-Sheng Zhang* and Xue-Mei Li

College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.127
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 title compound, $C_{15}H_{12}N_2O_3$, is non-planar, with a dihedral angle of 83.0 (1)° between the two benzene rings. The molecules are linked into a ribbon along the *b* axis by intermolecular C—H···O and O—H···N hydrogen bonds. The packing is further stabilized by C—H···π and π–π interactions.

Comment

For several decades, much attention has been paid to the search for new nonlinear optical (NLO) materials, because these materials have been widely applied or have great potential in modern laser technology, optical communication and information storage (Long, 1995). Some Schiff base compounds are new organic NLO materials, which have been investigated during recent years because many of them have NLO behavior and are easy to synthesize (Unver *et al.*, 2004; Jalali-Heravi *et al.*, 2000). We have recently prepared the novel push–pull Schiff base, (I), containing benzene rings, and C=N and C=C aliphatic bonds. We report here its crystal structure (Fig. 1).

(I)
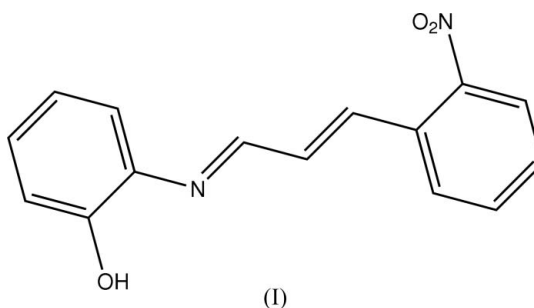
The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The bonds between the two benzene rings show a characteristic intermediate length between single and
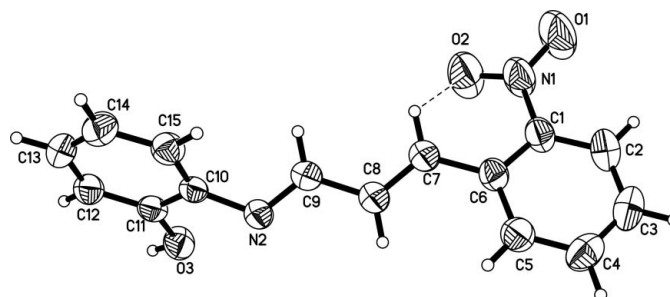

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.
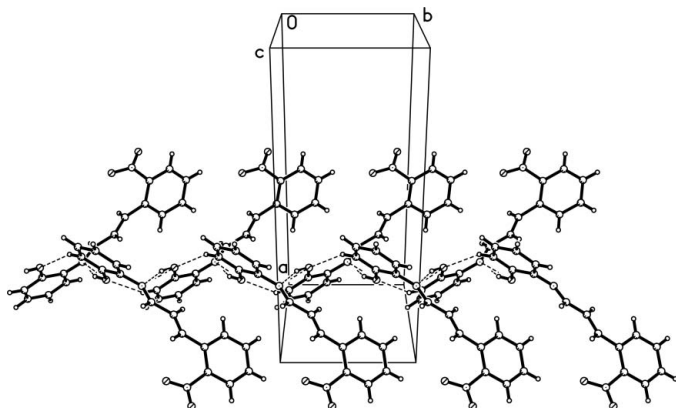
Figure 2
Packing diagram of (I), showing the ribbons along the *b* axis, viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

double bonds because of the conjugated C=C and C=N double bonds (Table 1). The whole molecule is non-planar, with a dihedral angle of 83.0 (1)° between the two benzene rings. There exists an intramolecular C—H···O hydrogen bond (Table 2), forming a six-membered ring. In the crystal structure, molecules are linked into a ribbon along the *b* axis by weak C—H···O and O—H···N intermolecular hydrogen bonds (Fig. 2). The packing is further stabilized by C—H···π and π–π interactions involving the benzene rings [$Cg1$···$Cg1(-x, -1 - y, -z)$ = 3.711 (2) Å, where $Cg1$ is the centroid of the C1–C6 ring].

Experimental

To a solution of cinnamaldehyde (13.2 g, 0.1 ml) in acetic anhydride was added concentrated nitric acid (3.6 ml) and acetic acid (12.0 ml) over a period of 3 h, keeping the temperature below 278 K. The reaction mixture was allowed to stand for 2 d at room temperature. 20% HCl was added and *o*-nitrocinnamaldehyde was obtained as a yellow solid. To a solution of *o*-nitrocinnamaldehyde (0.25 g, 1.4 mmol) in water (20 ml) was added a solution of *o*-aminophenol (0.15 g, 1.4 mmol) in ethanol (20 ml). The mixture was heated under reflux for 4 h, yielding quantities of precipitate. Yellow single crystals suitable for X-ray diffraction study were obtained by slow evaporation of an ethanol solution over a period of 3 d.

Crystal data

$C_{15}H_{12}N_2O_3$	$D_x = 1.332$ Mg m^{-3}
$M_r = 268.27$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2347
$a = 22.654$ (3) Å	reflections
$b = 7.5464$ (10) Å	$\theta = 2.6$–25.7°
$c = 18.816$ (2) Å	$\mu = 0.10$ mm^{-1}
$\beta = 123.692$ (2)°	$T = 293$ (2) K
$V = 2676.5$ (6) Å^3	Block, yellow
$Z = 8$	$0.38 \times 0.22 \times 0.14$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2635 independent reflections
	2111 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.022$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 26.0°$
$T_{min} = 0.965$, $T_{max} = 0.987$	$h = -15 \rightarrow 27$
7282 measured reflections	$k = -9 \rightarrow 9$
	$l = -23 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.048$	$+ 1.5459P]$
$wR(F^2) = 0.127$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2635 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
181 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

O1—N1	1.217 (2)	N2—C9	1.278 (2)
O2—N1	1.211 (2)	N2—C10	1.416 (2)
O3—C11	1.360 (2)	C7—C8	1.327 (2)
N1—C1	1.468 (3)	C8—C9	1.442 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···N2^i	0.82	2.01	2.761 (2)	151
C7—H7A···O2	0.93	2.38	2.707 (3)	100
C12—H12A···O3^i	0.93	2.55	3.418 (2)	155
C2—H2B···$Cg2^{ii}$	0.93	2.69	3.591 (2)	162
C14—H14A···$Cg1^{iii}$	0.93	2.80	3.628 (3)	149

Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + \frac{1}{2}, -y - \frac{1}{2}, -z$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5U_{eq}(O).

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).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Jalali-Heravi, M., Khandar, A. A. & Sheikshoaie, I. (2000). *Spectrochim. Acta Part A*, **56**, 1575–1581.
Long, N. J. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 826.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART*, *SAINT* and *SHELXTL* (Version 5.1). Siemens Analytical X-ray Systems Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Unver, H., Karakas, A. & Elmali, A. (2004). *J. Mol. Struct.* **702**, 49–54.