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N-(3-Nitrobenzylidene)-*p*-toluidine

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.084
Data-to-parameter ratio = 9.9

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

The title compound, $C_{14}H_{12}N_2O_2$, is non-planar. The dihedral angle between the two benzene rings is 32.1 (2)° and the nitro group is at an angle of 13.2 (2)° with respect to its attached benzene ring. In the crystal structure, the molecules are stacked through π–π interactions. The stacks are arranged through π–π and C—H$\cdots\pi$ interactions, forming chains along [001], which are further connected by C—H$\cdots$O and C—H$\cdots$N hydrogen bonds, forming networks along [100]. The networks are connected by C—H$\cdots$O hydrogen bonds along [010].

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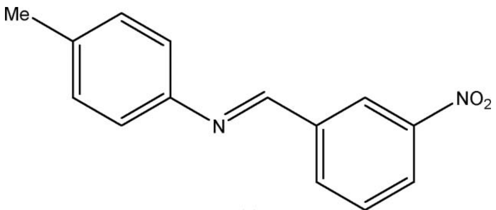
Comment

For the purpose of developing non-linear optical materials for second harmonic generators (SHG), a series of benzylidene–aniline derivatives (BA) (Tetsuya *et al.*, 1990; Sun *et al.*, 1994; Zhang, 2002) have been synthesized. To be a SHG crystal, the crystal structure must be non-centrosymmetric and the molecule should have a relatively large first superpolarizability (β), usually deriving from a large conjugated system substituted on one side by a donor and on the opposite side by an acceptor, the so-called *D*–π–*A* structure.



(I)

During our systematic research on BA compounds, we synthesized the title compound, (I), and confirmed its structure by X-ray diffraction methods.

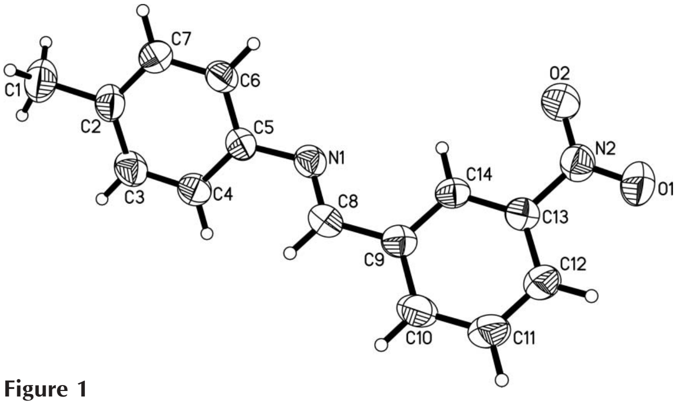


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids

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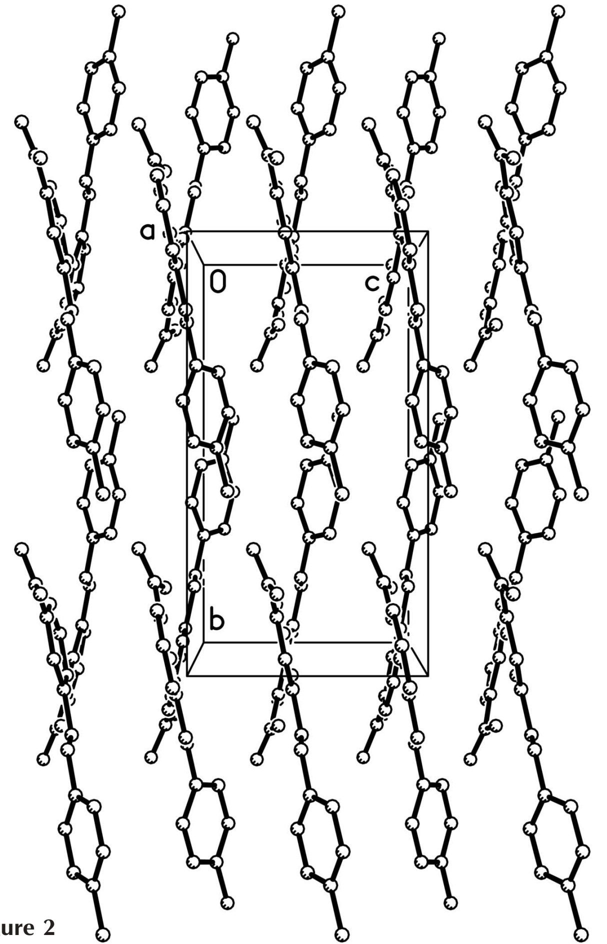

Figure 2
Packing diagram of (I), viewed down the *a* axis. H atoms have been omitted.

As expected, the title compound crystallized in a non-centrosymmetric space group, $Pca2_1$. The title molecule (Fig. 1) is not planar, as demonstrated by the dihedral angle of 32.1 (2)° between the benzene rings. In the crystal structure, the molecules are stacked through π–π interactions along [001] (Desiraju, 1995); the distances between the parallel molecular planes (C2–C14/N1) are 3.359 (3) and 3.565 (3) Å, and the distances between the two centroids are 3.587 (3) and 3.587 (3) Å [symmetry relationships $(-x + \frac{3}{2}, y, z - \frac{1}{2})$ and $(-x + \frac{3}{2}, y, z + \frac{1}{2})$, respectively]. The chains further interact through C—H···O and C—H···N hydrogen bonds (Table 1), forming networks along [100]. The networks are then packed through C—H···O hydrogen bonds along [010], forming a three-dimensional ordered crystal structure.

Experimental

3-Nitrobenzaldehyde (1.51 g, 10 mmol) and 4-methylbenzenamine (1.07 g, 10 mmol) in ethanol (10 ml) were heated at 363 K with stirring for thirty minutes. The product was recrystallized from 85 percent ethanol, and a white–yellow crystal was grown from methylcyclohexane (m.p. 368–369 K). Spectroscopic analysis: IR: 1635, 1586, 1501, 1334, 845, 783, 687 cm^{-1}. Elemental analysis: found C 69.84, H 5.08, N 11.70%; $C_{14}H_{12}N_2O_2$ requires: C 69.99, H 5.03, N 11.66%.

Crystal data

$C_{14}H_{12}N_2O_2$
$M_r = 240.26$
Orthorhombic, $Pca2_1$
$a = 13.413$ (2) Å
$b = 13.115$ (2) Å
$c = 7.1040$ (10) Å
$V = 1249.7$ (3) Å^3
$Z = 4$
$D_x = 1.277$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 23 reflections
$\theta = 3.0$–15.8°
$\mu = 0.09$ mm^{-1}
$T = 291$ (2) K
Granular, white–yellow
0.56 × 0.52 × 0.40 mm

Data collection

Siemens P4 diffractometer
ω scans
Absorption correction: ψ scan (*XSCANS*; Siemens, 1990)
$T_{\min} = 0.950$, $T_{\max} = 0.970$
1953 measured reflections
1629 independent reflections
1086 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.008$
$\theta_{\max} = 28.0°$
$h = -1 \rightarrow 17$
$k = -17 \rightarrow 0$
$l = 0 \rightarrow 9$
3 standard reflections every 97 reflections intensity decay: 3.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.084$
$S = 0.93$
1629 reflections
165 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.027 (2)

Table 1
Selected geometric parameters (Å, °).

O1—N2	1.213 (2)	N2—C13	1.466 (3)
O2—N2	1.213 (2)	C1—C2	1.511 (3)
N1—C8	1.263 (2)	C8—C9	1.466 (3)
N1—C5	1.420 (3)		
C8—N1—C5	120.42 (18)	C4—C5—N1	124.04 (19)
O1—N2—O2	123.0 (2)	N1—C8—C9	121.67 (19)
O1—N2—C13	118.92 (19)	C14—C9—C10	118.42 (19)
O2—N2—C13	118.13 (18)	C14—C9—C8	120.73 (17)
C7—C2—C3	117.5 (2)	C10—C9—C8	120.84 (19)
C7—C2—C1	120.8 (2)	C12—C13—C14	122.6 (2)
C3—C2—C1	121.7 (2)	C12—C13—N2	118.90 (19)
C6—C5—C4	118.76 (19)	C14—C13—N2	118.53 (17)
C6—C5—N1	117.18 (18)		
C8—N1—C5—C6	146.0 (2)	C5—N1—C8—C9	179.9 (2)
C8—N1—C5—C4	−35.6 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1^{i}—H1C^{i}···O2	0.96	2.81	3.703 (3)	155
C3^{i}—H3^{i}···O1	0.93	2.94	3.777 (2)	150
C10^{ii}—H10^{ii}···O2	0.93	2.50	3.351 (3)	152
C11^{ii}—H11^{ii}···N1	0.93	2.82	3.696 (3)	158
C6^{iii}—H6^{iii}···O2	0.93	2.68	3.485 (3)	145

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

H atoms attached to C atoms were positioned geometricaly (C—H = 0.96 Å for methyl and C—H = 0.93 Å for others) and treated as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *XSCANS* (Siemens, 1990); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997b); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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