

## *N*-(2-Nitrobenzylidene)aniline

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### Key indicators

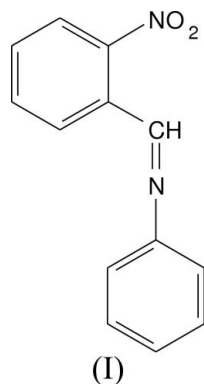
Single-crystal X-ray study  
*T* = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
*R* factor = 0.051  
*wR* factor = 0.172  
Data-to-parameter ratio = 12.4

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

In the title compound,  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$ , the dihedral angle between the two six-membered aromatic rings is  $60.49(9)^\circ$ . The molecule adopts an *E* configuration with respect to the imine  $\text{C}=\text{N}$  bond.

### Comment

Imines are synthesized by the reaction of an aldehyde or a ketone with a primary amine (Patai, 1970). In order to obtain the desired imine, the by-product, water, must be removed in order to drive the equilibrium in favour of the imine (Layer, 1963). This result can be achieved by the use of a Dean–Stark trap or molecular sieves (Bose *et al.*, 1967). As part of our work in the area of catalytic transfer hydrogenation, we required a number of imines as starting materials. With this background, the title compound, (I), was synthesized and we report its crystal structure here.



A perspective view of (I) is shown in Fig. 1. In compound (I), the dihedral angle between the two six-membered aromatic rings is  $60.49(9)^\circ$ . As (I) crystallizes in a centrosymmetric space group,  $P2_1/c$ , there is no spontaneous resolution. The  $\text{C}12-\text{N}11-\text{C}10-\text{C}3$  torsion angle of  $175.05(14)^\circ$  indicates that the molecule adopts an *E* configuration with respect to the imine  $\text{C}=\text{N}$  bond. This is comparable with the corresponding value of  $176.2(3)^\circ$  reported earlier (Akitsu *et al.*, 2004). The nitro group deviates from the plane of the phenyl ring, as indicated by the  $\text{O}9-\text{N}7-\text{C}4-\text{C}3$  and  $\text{O}8-\text{N}7-\text{C}4-\text{C}5$  torsion angles of  $-35.0(2)^\circ$  and  $-36.2(2)^\circ$ , respectively.

### Experimental

To a solution of *o*-nitrobenzaldehyde (0.75 g, 5 mmol) in dichloromethane (6 ml), aniline (0.45 ml, 5 mmol) was slowly added dropwise with constant stirring at 273 K in the presence of molecular sieves.

Received 7 August 2006  
Accepted 8 August 2006

The reaction mixture was further stirred for a further 12 h at room temperature. The molecular sieves were removed by filtration and the filtrate was washed with  $\text{KHSO}_4$ . The solvent was removed under reduced pressure and the resulting product was recrystallized using methanol.

#### Crystal data

$\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$   
 $M_r = 226.23$   
 Monoclinic,  $P2_1/c$   
 $a = 11.178$  (13) Å  
 $b = 7.718$  (5) Å  
 $c = 13.217$  (16) Å  
 $\beta = 94.064$  (3)°  
 $V = 1137$  (2) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.321$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Block, pale yellow  
 $0.25 \times 0.23 \times 0.22$  mm

#### Data collection

MacScience DIPLabo 32001  
 diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 3583 measured reflections

1923 independent reflections  
 1555 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\text{max}} = 25.0^\circ$

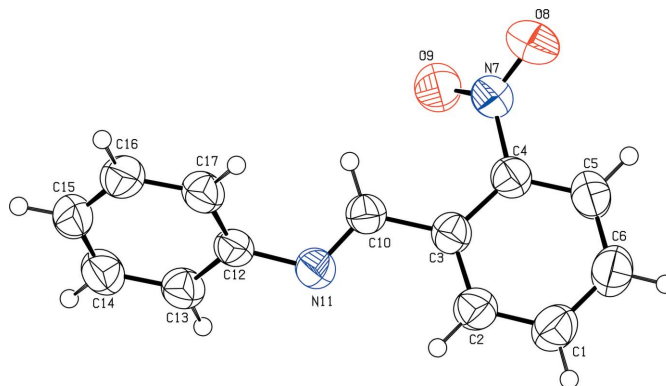
#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.051$   
 $wR(F^2) = 0.172$   
 $S = 1.00$   
 1923 reflections  
 155 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1279P)^2 + 0.0772P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97*  
 (Sheldrick, 1997)  
 Extinction coefficient: 0.081 (12)

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) 1.2U_{\text{eq}}(\text{carrier atom})$ .

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997);



**Figure 1**  
 A view of (I), with 50% probability displacement ellipsoids.

program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *PLATON*.

The authors thank the DST, Government of India, for financial assistance under project No. SP/I2/FOO/93.

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