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N-(2-Nitrobenzylidene)aniline

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
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.

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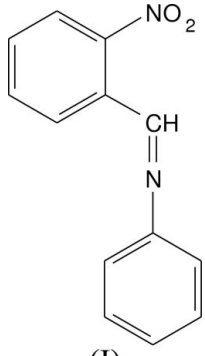
In the title compound, $C_{34}H_{10}N_2O_2$, the dihedral angle between the two six-membered aromatic rings is 60.49 (9)°. The molecule adopts an *E* configuration with respect to the imine C=N bond.

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.



(I)

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)°. As (I) crystallizes in a centrosymmetric space group, $P2_1/c$, there is no spontaneous resolution. The C12—N11—C10—C3 torsion angle of 175.05 (14)° indicates that the molecule adopts an *E* configuration with respect to the imine C=N bond. This is comparable with the corresponding value of 176.2 (3)° reported earlier (Akitsu *et al.*, 2004). The nitro group deviates from the plane of the phenyl ring, as indicated by the O9—N7—C4—C3 and O8—N7—C4—C5 torsion angles of −35.0 (2)° and −36.2 (2)°, 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.

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 $KHSO_4$. The solvent was removed under reduced pressure and the resulting product was recrystallized using methanol.

Crystal data

$C_{13}H_{10}N_2O_2$	$Z = 4$
$M_r = 226.23$	$D_x = 1.321$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 11.178$ (13) Å	$\mu = 0.09$ mm^{-1}
$b = 7.718$ (5) Å	$T = 295$ (2) K
$c = 13.217$ (16) Å	Block, pale yellow
$\beta = 94.064$ (3)°	0.25 × 0.23 × 0.22 mm
$V = 1137$ (2) Å^3	

Data collection

MacScience DIPLabo 32001 diffractometer	1923 independent reflections
ω scans	1555 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.020$
3583 measured reflections	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1279P)^2 + 0.0772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.172$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.16$ e Å^{-3}
1923 reflections	Extinction correction: *SHELXL97* (Sheldrick, 1997)
155 parameters	Extinction coefficient: 0.081 (12)
H-atom parameters constrained	

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

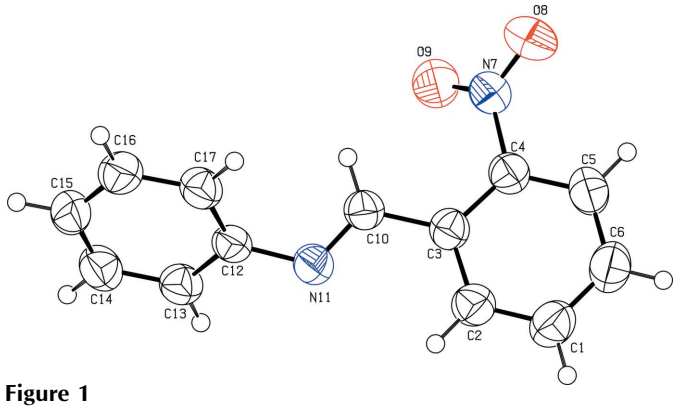


Figure 1
A view of (I), with 50% probability displacement ellipsoids.

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