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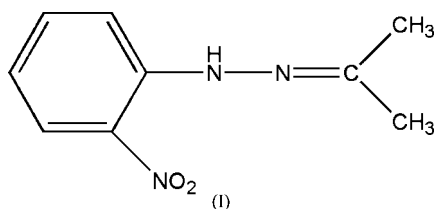
Key indicatorsSingle-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.048
 wR factor = 0.160
Data-to-parameter ratio = 16.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Acetone (2-nitrophenyl)hydrazone

The title compound, $\text{C}_9\text{H}_{11}\text{N}_3\text{O}_2$, was prepared by the reaction of 1-(2-nitrophenyl)hydrazine with acetone at room temperature. The molecule is approximately planar and exhibits a weak intramolecular hydrogen-bond interaction.

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Schiff bases have been used extensively as ligands in the field of coordination chemistry (Ogretir *et al.*, 2006). As dinegatively charged ligands, Schiff bases show potential as antimicrobial and anticancer agents (Tarafder *et al.*, 2000; Deschamps *et al.*, 2003) and so have biochemical and pharmacological applications. The recent growing interest in Schiff bases is also due to their ability to form intramolecular hydrogen bonds by electron coupling between acid–base centres (Rozwadowski *et al.*, 1999). The title compound, (I), was synthesized as part of our study of these ligands and we present its crystal structure here.



In compound (I) (Fig. 1), the six C atoms of the benzene ring and the three N atoms of the hydrazine and nitro groups are essentially planar [the greatest deviation from planarity is 0.045 (1) Å for atom N2]. The C=N bond length (Table 1) is in agreement with those observed for *N*-isonicotinamidosalicylaldehydeimine and 4-salicylaldehydylaminoantipyrene (Liu *et al.*, 2002). Atoms O1, O2, N1 and C1, and N2, N3, C7 and C8, define the mean planes $p1$ and $p2$, respectively, with a dihedral angle between $p1$ and $p2$ of 13.87 (2)°. The dihedral angles formed between the benzene ring and $p1$ and $p2$ are 8.47 (2) and 5.71 (2)°, respectively.

A possible factor promoting the approximate planarity of the molecule is the formation of a weak N–H...O intramolecular hydrogen bond (Table 2).

Experimental

A mixture of 1-(2-nitrophenyl)hydrazine (0.02 mol) and acetone (0.02 mol) was stirred in refluxing (30 ml) for 5 h at 293 K to afford the title compound (3.24 g, yield 84%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

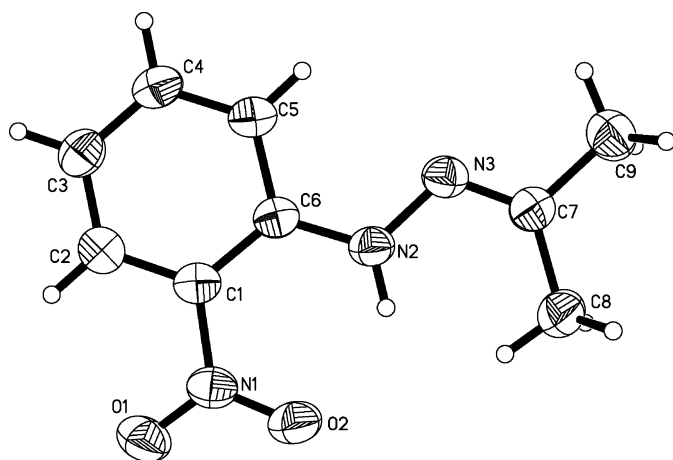


Figure 1
The molecular structure and atom-labelling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_9H_{11}N_3O_2$	$Z = 4$
$M_r = 193.21$	$D_x = 1.300 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.5080 (17) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 15.479 (3) \text{ \AA}$	$T = 295 (2) \text{ K}$
$c = 8.1420 (16) \text{ \AA}$	Block, red
$\beta = 112.96 (3)^\circ$	$0.25 \times 0.20 \times 0.18 \text{ mm}$
$V = 987.3 (4) \text{ \AA}^3$	

Data collection

Enraf–Nonius CAD-4 diffractometer	1244 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.019$
Absorption correction: none	$\theta_{\text{max}} = 27.0^\circ$
2257 measured reflections	3 standard reflections
2111 independent reflections	every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 0.0868P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.160$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
2111 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
130 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	(Sheldrick, 1997)
	Extinction coefficient: 0.022 (5)

Table 1

Selected bond lengths (\AA).

N2–C6	1.363 (2)	N3–C7	1.281 (2)
N2–N3	1.388 (2)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H2A \cdots O2	0.86	2.00	2.622 (2)	128

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N–H and C–H distances of 0.86 and 0.93–0.96 \AA , respectively, and with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C},\text{N})$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

- Deschamps, P., Kulkarni, P. P. & Sarkar, B. (2003). *Inorg. Chem.* **42**, 7366–7368.
- Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
- Liu, B., Hu, R. X., Chen, Z. F., Chen, X. B. & Liang, H. (2002). *Chin. J. Struct. Chem.* **21**, 414–419.
- Ogretir, C., Dal, H., Berber, H. & Taktak, F. F. (2006). *J. Chem. Eng. Data*, **51**, 46–51.
- Rozwadowski, Z., Majewski, E., Dziembowska, T. & Hansen, P. E. (1999). *J. Chem. Soc. Perkin Trans. 2*, pp. 2809–2817.
- Sheldrick, G. M. (1990). *SHELXTL/PC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Tarafder, M. T. H., Ali, M. A., Wee, D. J., Azahari, K., Silong, S. & Crouse, K. A. (2000). *Transition Met. Chem.* **25**, 456–460.