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N-(2,4-Dinitrophenyl)-*N*′-(4-methoxybenzylidene)hydrazine

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In the crystal structure of the title compound, $C_{14}H_{12}N_4O_5$, molecules are connected *via* weak intermolecular N—H···O and C—H···O hydrogen bonds, forming a three-dimensional network.

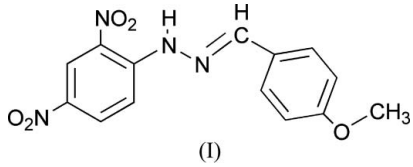
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.096
Data-to-parameter ratio = 11.6

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

Comment

Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands (Yu *et al.*, 2005; Deng *et al.*, 2005; Jing, Fan *et al.*, 2005*a*,*b*; Jing, Wang *et al.*, 2005), we report the synthesis and structure of the title compound, (I).



(I)

The molecular structure of (I) is approximately planar (Fig. 1); the central chromophore (C1–C6/N1–N4) and the 4-methoxybenzaldehyde group (C7—C13/O5) are planar with r.m.s. deviations of 0.0288 (2) and 0.0051 (5) Å, respectively; the dihedral angle between these two planes is 1.29 (7)°. An intramolecular N—H···O hydrogen bond stabilizes the molecular structure, while intermolecular N—H···O and C—H···O hydrogen bonds stabilize the crystal structure (Table 2 and Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-methoxybenzaldehyde (1.36 g, 10 mmol) was added to an anhydrous ethanol solution

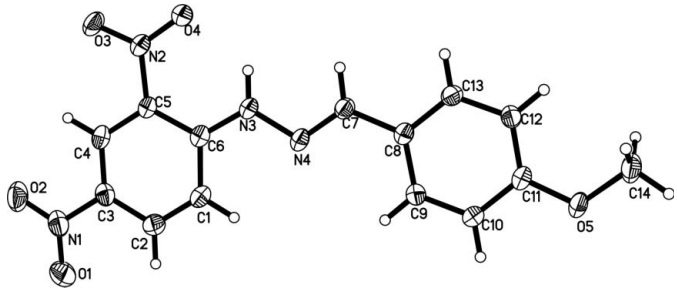


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

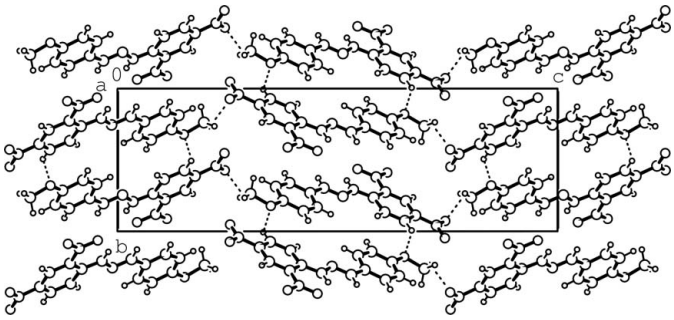


Figure 2
The packing of (I), viewed down the *a* axis, showing intermolecular hydrogen bonds (dashed lines).

(50 ml) of (2,4-dinitrophenyl)hydrazine (2.03 g, 10 mmol) and the mixture was stirred at 330 K for 6 h under N_2, whereupon a red solution appeared. The solvent was removed and the residue was recrystallized from *N*,*N*-dimethylformamide. The product was isolated and then dried *in vacuo* to give the title compound in 82% yield. Red single crystals suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution of (I).

Crystal data

$C_{14}H_{12}N_4O_5$
M_r = 316.28
Monoclinic, $P2_1/n$
a = 6.189 (2) Å
b = 8.581 (3) Å
c = 26.669 (11) Å
β = 96.392 (5)°
V = 1407.5 (9) Å^3
Z = 4
D_x = 1.492 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2340 reflections
θ = 3.1–26.1°
μ = 0.12 mm^{-1}
T = 294 (2) K
Block, red
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.979
7349 measured reflections
2481 independent reflections
1914 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°
$h = -7 \rightarrow 6$
$k = -10 \rightarrow 9$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.03
2481 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.1714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O5—C11	1.3614 (15)	N3—C6	1.3457 (18)
N1—C3	1.4500 (19)	N3—N4	1.3782 (15)
N2—C5	1.4462 (18)	N4—C7	1.2746 (18)
C6—N3—N4	119.99 (12)	C7—N4—N3	114.37 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O4	0.869 (18)	1.984 (17)	2.6189 (17)	129.0 (14)
N3—H3···O4^{i}	0.869 (18)	2.620 (18)	3.4419 (19)	158.2 (14)
C2—H2···O5^{ii}	0.93	2.59	3.375 (2)	143
C14—H14*B*···O2^{iii}	0.96	2.56	3.188 (3)	123

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $-x+2, -y+1, -z$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{3}{2}$.

The H atom attached to N atom was located in a difference Fourier map and refined freely. C-bound H atoms were included in calculated positions and refined using a riding model approximation, with C—H = 0.93 Å (aromatic) and 0.96 Å (methyl), and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C), respectively.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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