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2-Nitrobenzaldehyde salicylhydrazone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.049
wR factor = 0.125
Data-to-parameter ratio = 13.0

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

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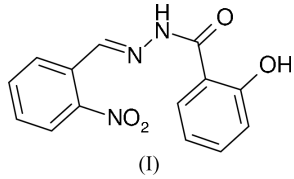
The molecule of the title compound, 2-nitrobenzaldehyde (2-hydroxybenzoyl)hydrazone, $C_{14}H_{11}N_3O_4$, is roughly planar and displays a *trans* configuration with respect to the C=N double bond. The crystal strucuture is stabilized by intermolecular N—H···O hydrogen bonds.

Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

In the title compound, (I), all the bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C8=N2 bond length of 1.261 (2) Å conforms to the value for a double bond. The dihedral angle between the two benzene rings is 1.8 (1)°.

The crystal strucuture is stabilized by intermolecular N—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

2-Nitrobenzaldehyde (0.2 mmol, 30.2 mg) and 2-hydroxybenzoic acid hydrazine (0.2 mmol, 30.4 mg) were dissolved in methanol (10 ml).

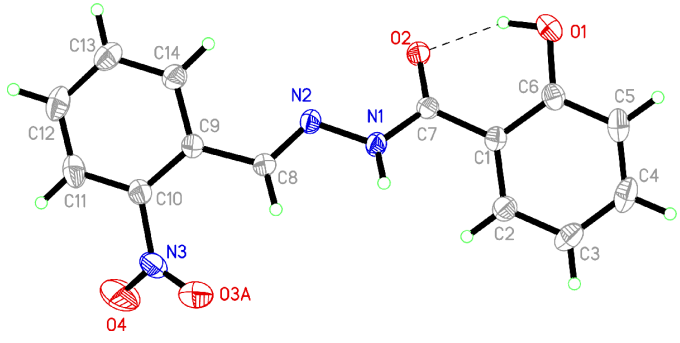


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate intramolecular hydrogen bonds. Only the major component of the disordered O atom of the nitryl group is shown.

The mixture was stirred at room temperature for 10 min to give a clear yellow solution. After keeping the solution in air for 8 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$C_{14}H_{11}N_3O_4$
M_r = 285.26
Monoclinic, $P2_1/n$
a = 7.070 (3) Å
b = 25.214 (9) Å
c = 7.870 (3) Å
β = 113.541 (5)°
V = 1286.2 (9) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1426 reflections
θ = 3.1–23.2°
μ = 0.11 mm^{-1}
T = 298 (2) K
Block, yellow
0.32 × 0.27 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.976
7466 measured reflections
2657 independent reflections
1826 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.5°
$h = -8 \rightarrow 7$
$k = -31 \rightarrow 31$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.125
S = 1.02
2657 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.1087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2	0.92 (2)	1.83 (2)	2.6817 (19)	153 (2)
N1—H1···O2^{i}	0.89 (2)	2.11 (2)	2.978 (2)	164 (2)

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

Atoms H1 and H1*A* were located in a difference Fourier map and refined isotropically, with U_{iso}(H) values fixed at 0.08 Å^2. All other 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}(C). The occupancies of the disordered positions O3A/O3B were fixed at 80/20% after refinement gave values close to these.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

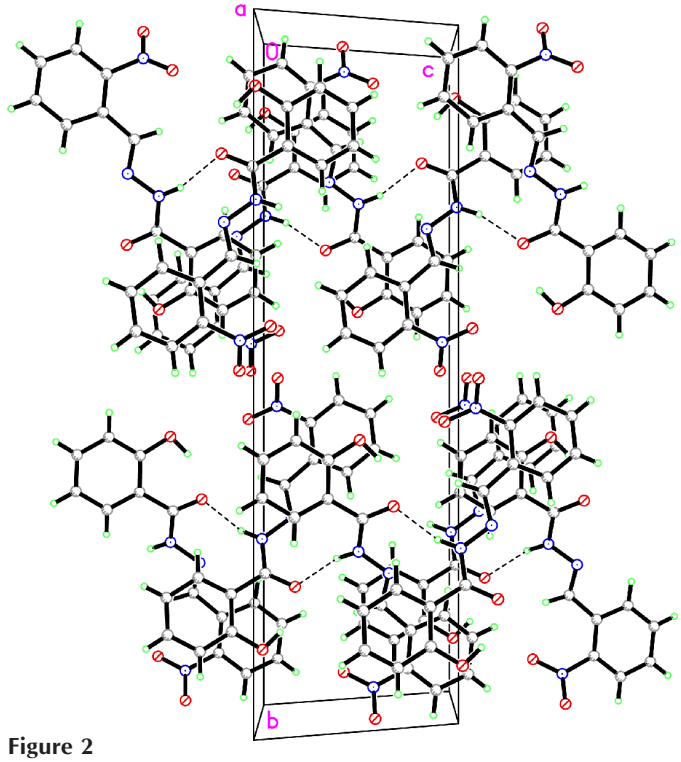


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines show intermolecular hydrogen bonds.

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