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2′-Hydroxyacetophenone furan-2-carbohydrazide

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In the crystal structure of the title compound, $C_{13}H_{12}N_2O_3$, intramolecular O—H···N and intermolecular N—H···O hydrogen bonds occur.

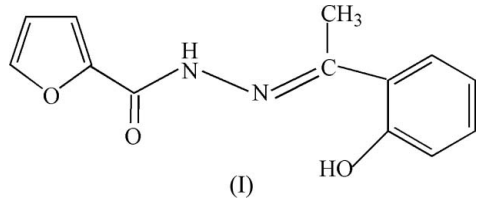
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.007 Å
R factor = 0.060
wR factor = 0.133
Data-to-parameter ratio = 9.5

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

Comment

As part of our ongoing studies of the coordination chemistry of aroylhydrazones ligands (Tai *et al.*, 2003), we now report the synthesis and structure of the title compound, (I) (Fig. 1).



(I)

In the molecule of (I), the bond lengths of C7—N1 [1.285 (5) Å] and N1—N2 [1.380 (4) Å] are close to double-bond values, indicating that the Lewis structure shown in the scheme is only an approximation to the electron distribution in the molecule. Otherwise, the geometrical parameters for (I) are normal. The dihedral angle between the furan and benzene ring mean planes is 26.0 (3)°, perhaps because of the intramolecular O—H···N hydrogen bond (Table 1). An intermolecular N—H···O link also occurs.

Experimental

2′-Hydroxyacetophenone (10 mmol) was added to a solution of furan-2-carbohydrazide (10 mmol) in ethanol (10 ml). The mixture was stirred continuously for 3 h at refluxing temperature, with evaporation of some ethanol. Upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 68%). Clear blocks of (I) were obtained by evaporation of a methanol solution after two weeks.

Crystal data

$C_{13}H_{12}N_2O_3$
M_r = 244.25
Orthorhombic, $Pca2_1$
a = 15.602 (3) Å
b = 7.7795 (14) Å
c = 9.9721 (18) Å
V = 1210.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 291 (2) K
0.32 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
7244 measured reflections
1583 independent reflections
1328 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.133$
$S = 1.08$
1583 reflections
166 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.21	2.923 (4)	140
O1—H1···N1	0.82	1.84	2.522 (4)	140

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

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. The H atoms were positioned geometrically (C—H = 0.93–0.96, O—H = 0.82 and N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

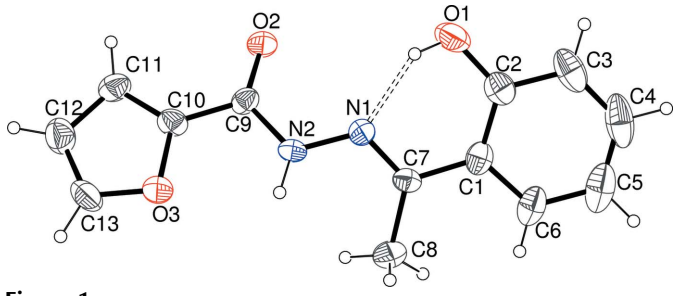


Figure 1
The molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bond is indicated by a double dashed line.

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References

Bruker (2000). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Tai, X.-S., Yin, X.-H., Tan, M.-Y. & Li, Y.-Z. (2003). *Acta Cryst.* E**59**, o681–o682.