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1-(2-Furylmethylene)-2-(2-nitrophenyl)-hydrazine

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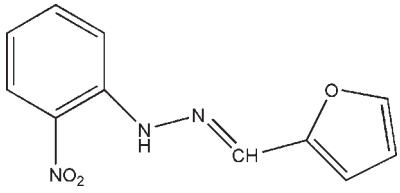
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.070; wR factor = 0.195; data-to-parameter ratio = 13.2.

The title Schiff base compound, $C_{11}H_9N_3O_3$, was obtained from a condensation reaction of furan-2-carbaldehyde and 2-nitrophenylhydrazine. The molecule is roughly planar, the largest deviation from the mean plane defined by all non-H atoms being 0.097 (4). An in ntramolecular N—H···O hydrogen bond might influence the planar conformation of the molecule. In the crystal, weak C—H···O hydrogen bonds link the molecules, forming a chain.

Related literature

For the role played by Schiff base compounds in the development of various proteins and enzymes, see: Kahwa *et al.* (1986); Santos *et al.* (2001).



Experimental

Crystal data

$C_{11}H_9N_3O_3$
M_r = 231.21
Monoclinic, $P2_1/n$
a = 15.852 (3) Å
b = 3.8000 (12) Å
c = 17.721 (4) Å
β = 97.89 (2)°
V = 1057.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.21 × 0.19 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.979, T_{max} = 0.982
3497 measured reflections
2033 independent reflections
619 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.195
S = 0.73
2033 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	0.86	1.98	2.599 (5)	128
C2—H2A···O2^{i}	0.93	2.48	3.360 (7)	158

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2486).

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supporting information

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S1. Comment

The chemistry of Schiff base has attracted a great deal of interest in recent years. These compounds play an important role in the development of various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of our interest in the study of the coordination chemistry of Schiff bases, we synthesized the title compound and determined its crystal structure.

The whole molecule is roughly planar with the largest deviations from the mean plane being -0.0973 (0.0041) at O3 (Fig. 1). The phenyl and the furan rings are slightly twisted from each other making a dihedral angle of 4.8 (3)°.

The intramolecular N—H···O hydrogen bond might influence the planar conformation of the molecule. Weak intermolecular C-H···O hydrogen bonds link the molecule forming a chain parallel to the (1 0 1) plane (Table 1, Fig. 2).

S2. Experimental

2-Nitrophenylhydrazine (1 mmol, 0.153 g) was dissolved in anhydrous ethanol (15 ml), The mixture was stirred for several minitutes at 351k, furan-2-carbaldehyde (1 mmol, 0.096 g) in ethanol (8 mm l) was added dropwise and the mixture was stirred at refluxing temperature for 2 h. The product was isolated and recrystallized from methanol, red single crystals of (I) was obtained after 3 d.

S3. Refinement

All H atoms were positioned geometrically and refined as riding with C—H=0.93 (aromatic), N—H=0.86 Å, and U_{iso}(H)=1.2U_{eq}(C).

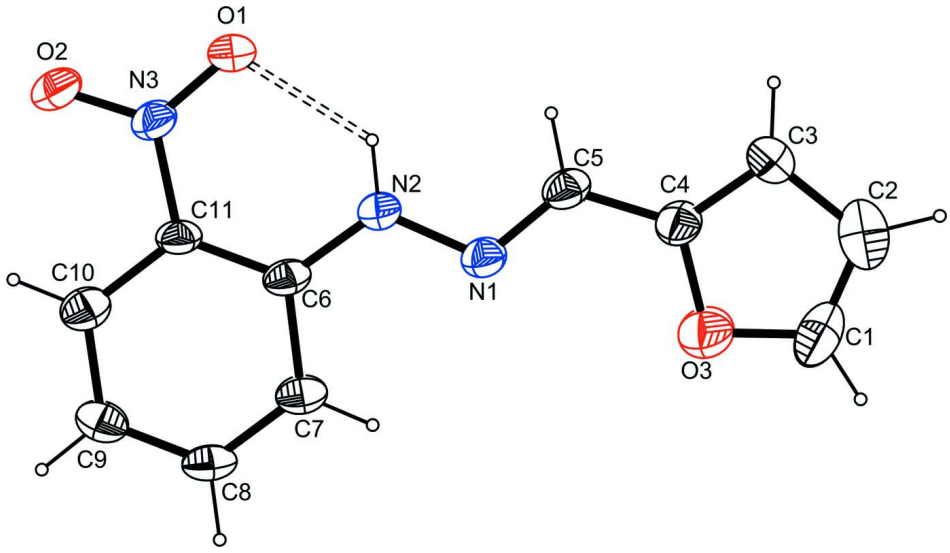

Figure 1

Molecular view of (I) with the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen are represented as small sphere of arbitrary radii. Intramolecular N-H···O hydrogen bond is shown as dashed lines.

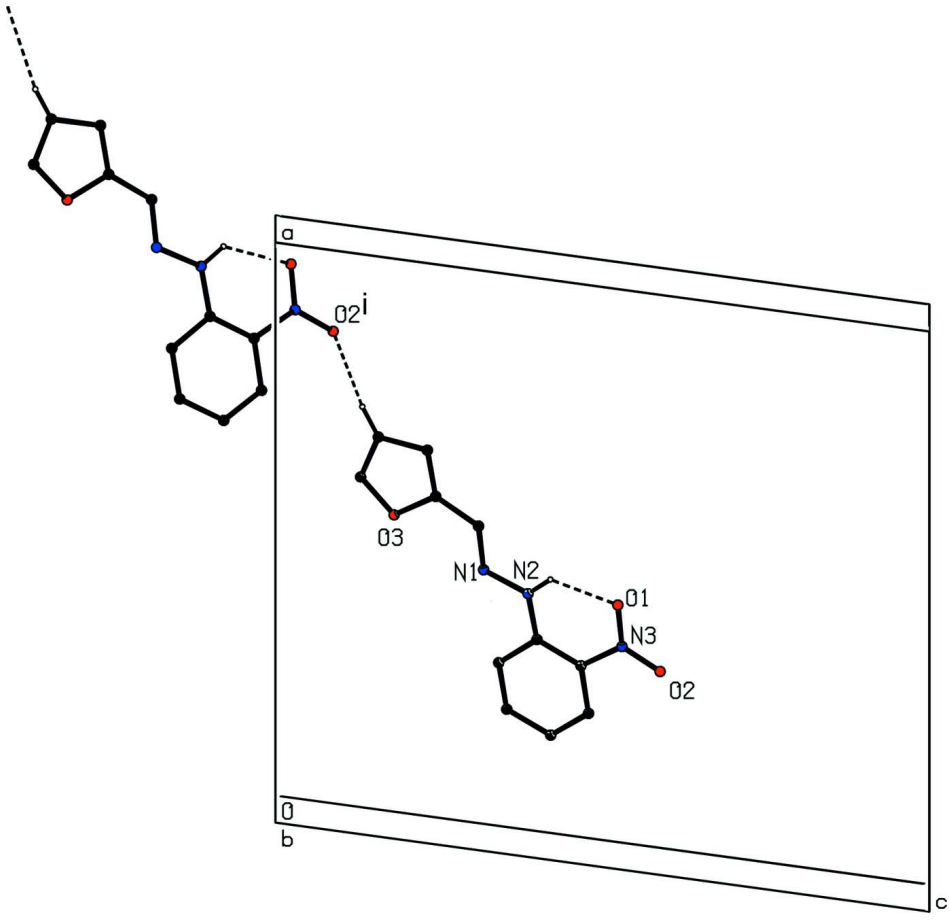

Figure 2

Partial packing view showing the chain formed by C-H···O hydrogen bonds.H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) x+1/2, -y+1/2, z-1/2]

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Crystal data

$C_{11}H_9N_3O_3$
$M_r = 231.21$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.852$ (3) Å
$b = 3.8000$ (12) Å
$c = 17.721$ (4) Å
$\beta = 97.89$ (2)°
$V = 1057.4$ (5) Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1960 reflections
$\theta = 3.2$–28.2°
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Block, red
0.21 × 0.19 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.979$, $T_{max} = 0.982$
3497 measured reflections
2033 independent reflections

619 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.2°$
$h = -12 \rightarrow 19$
$k = -4 \rightarrow 4$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.195$
$S = 0.73$
2033 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0948P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5620 (4)	−0.1566 (18)	0.1304 (3)	0.089 (2)
H1	0.5467	−0.2470	0.0817	0.107*
C2	0.6396 (4)	−0.0571 (18)	0.1574 (4)	0.085 (2)
H2A	0.6878	−0.0666	0.1328	0.103*
C3	0.6342 (3)	0.0688 (15)	0.2323 (3)	0.0609 (16)
H3	0.6781	0.1673	0.2659	0.073*
C4	0.5541 (3)	0.0181 (15)	0.2450 (3)	0.0554 (14)
C5	0.5169 (3)	0.1022 (14)	0.3106 (2)	0.0508 (14)
H5	0.5500	0.2188	0.3502	0.061*
C6	0.3320 (2)	0.0389 (13)	0.3999 (2)	0.0447 (13)
C7	0.2756 (2)	−0.1246 (13)	0.3415 (3)	0.0521 (14)
H7	0.2938	−0.1806	0.2952	0.063*
C8	0.1937 (3)	−0.2002 (14)	0.3537 (3)	0.0560 (14)
H8	0.1574	−0.3116	0.3154	0.067*
C9	0.1634 (3)	−0.1163 (15)	0.4210 (3)	0.0591 (15)
H9	0.1071	−0.1636	0.4269	0.071*
C10	0.2168 (3)	0.0365 (14)	0.4787 (3)	0.0555 (14)
H10	0.1979	0.0861	0.5250	0.067*
C11	0.3009 (2)	0.1184 (13)	0.4672 (2)	0.0446 (12)
N1	0.4392 (2)	0.0254 (11)	0.3182 (2)	0.0509 (11)
N2	0.4128 (2)	0.1163 (11)	0.3862 (2)	0.0499 (11)
H2	0.4473	0.2227	0.4205	0.060*

N3	0.3518 (2)	0.2903 (12)	0.5299 (2)	0.0535 (12)
O1	0.42600 (19)	0.3693 (10)	0.52361 (17)	0.0679 (11)
O2	0.32065 (19)	0.3559 (12)	0.58821 (19)	0.0776 (13)
O3	0.5066 (2)	−0.1130 (12)	0.1815 (2)	0.0797 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.111 (5)	0.101 (6)	0.059 (4)	0.020 (5)	0.027 (4)	−0.012 (4)
C2	0.081 (4)	0.086 (5)	0.095 (5)	0.018 (4)	0.035 (4)	0.020 (5)
C3	0.046 (3)	0.072 (4)	0.065 (4)	−0.005 (3)	0.008 (2)	−0.002 (3)
C4	0.048 (3)	0.073 (4)	0.042 (3)	0.014 (3)	−0.003 (2)	−0.003 (3)
C5	0.052 (3)	0.055 (4)	0.042 (3)	0.010 (3)	−0.006 (2)	−0.007 (3)
C6	0.044 (2)	0.047 (3)	0.039 (3)	0.005 (3)	−0.009 (2)	−0.003 (3)
C7	0.051 (3)	0.057 (4)	0.044 (3)	0.000 (3)	−0.011 (2)	−0.001 (3)
C8	0.051 (3)	0.059 (4)	0.051 (3)	−0.004 (3)	−0.016 (2)	−0.008 (3)
C9	0.040 (2)	0.070 (4)	0.064 (3)	−0.002 (3)	−0.006 (2)	−0.001 (3)
C10	0.056 (3)	0.061 (4)	0.045 (3)	0.003 (3)	−0.005 (2)	0.001 (3)
C11	0.040 (2)	0.053 (3)	0.037 (3)	−0.003 (3)	−0.0077 (19)	−0.002 (3)
N1	0.046 (2)	0.063 (3)	0.042 (2)	0.004 (2)	−0.0018 (16)	−0.008 (2)
N2	0.042 (2)	0.067 (3)	0.039 (2)	−0.003 (2)	−0.0005 (16)	−0.007 (2)
N3	0.046 (2)	0.077 (3)	0.035 (2)	0.005 (2)	−0.0035 (18)	−0.007 (2)
O1	0.0486 (18)	0.107 (3)	0.045 (2)	−0.016 (2)	−0.0029 (14)	−0.015 (2)
O2	0.0599 (19)	0.127 (4)	0.043 (2)	−0.003 (2)	−0.0027 (15)	−0.024 (2)
O3	0.072 (2)	0.104 (4)	0.060 (2)	0.006 (2)	−0.0034 (18)	−0.006 (3)

Geometric parameters (Å, º)

C1—C2	1.313 (8)	C7—C8	1.376 (5)
C1—O3	1.355 (6)	C7—H7	0.9300
C1—H1	0.9300	C8—C9	1.383 (6)
C2—C3	1.426 (7)	C8—H8	0.9300
C2—H2A	0.9300	C9—C10	1.363 (6)
C3—C4	1.334 (6)	C9—H9	0.9300
C3—H3	0.9300	C10—C11	1.412 (5)
C4—O3	1.360 (5)	C10—H10	0.9300
C4—C5	1.409 (5)	C11—N3	1.437 (5)
C5—N1	1.292 (5)	N1—N2	1.373 (4)
C5—H5	0.9300	N2—H2	0.8600
C6—N2	1.367 (5)	N3—O2	1.230 (4)
C6—C11	1.386 (6)	N3—O1	1.234 (4)
C6—C7	1.415 (6)		
C2—C1—O3	112.5 (6)	C7—C8—C9	122.3 (4)
C2—C1—H1	123.7	C7—C8—H8	118.8
O3—C1—H1	123.7	C9—C8—H8	118.8
C1—C2—C3	105.2 (5)	C10—C9—C8	119.4 (4)
C1—C2—H2A	127.4	C10—C9—H9	120.3

C3—C2—H2A	127.4	C8—C9—H9	120.3
C4—C3—C2	106.8 (5)	C9—C10—C11	119.2 (5)
C4—C3—H3	126.6	C9—C10—H10	120.4
C2—C3—H3	126.6	C11—C10—H10	120.4
C3—C4—O3	110.2 (4)	C6—C11—C10	122.0 (4)
C3—C4—C5	128.4 (5)	C6—C11—N3	122.5 (4)
O3—C4—C5	121.2 (4)	C10—C11—N3	115.5 (4)
N1—C5—C4	123.3 (4)	C5—N1—N2	116.5 (4)
N1—C5—H5	118.4	C6—N2—N1	120.4 (4)
C4—C5—H5	118.4	C6—N2—H2	119.8
N2—C6—C11	123.9 (4)	N1—N2—H2	119.8
N2—C6—C7	118.6 (4)	O2—N3—O1	121.6 (4)
C11—C6—C7	117.5 (4)	O2—N3—C11	119.6 (4)
C8—C7—C6	119.4 (5)	O1—N3—C11	118.8 (4)
C8—C7—H7	120.3	C1—O3—C4	105.2 (4)
C6—C7—H7	120.3		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.98	2.599 (5)	128
C2—H2*A*···O2^{i}	0.93	2.48	3.360 (7)	158

Symmetry code: (i) $x+1/2, -y+1/2, z-1/2$.