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N′-[1-(2-Furyl)ethylidene]acetohydrazide

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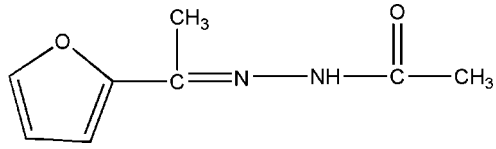
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 15.0.

In the molecule of the title compound, $C_8H_{10}N_2O_2$, the dihedral angle between the planar furyl ring and the planar N—N=C(—CH_3)—C unit is 3.57 (3)°. Intermolecular N—H···O hydrogen bonds are present in the crystal structure.

Related literature

For general background, see: Cimerman *et al.* (1997); Allen *et al.* (1987). For related literature, see: Tucker *et al.* (1975); Sutherland & Hoy (1968).



Experimental

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $C2/c$
a = 23.865 (6) Å
b = 4.3199 (10) Å
c = 16.829 (4) Å
β = 103.845 (4)°
V = 1684.5 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.18 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.992
4474 measured reflections
1729 independent reflections
1153 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.127
S = 1.03
1729 reflections
115 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.897 (9)	2.076 (10)	2.968 (2)	172.7 (17)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2265).

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supplementary materials

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N'-[1-(2-Furyl)ethylidene]acetohydrazide

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Comment

Schiff bases have received considerable attention in the literature. They are attractive from several points of view, such as the possibility of analytical application (Cimerman *et al.*, 1997). As part of our ongoing studies on new Schiff base compounds, the title compound, (I), was synthesized and we herein report its crystal structure.

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The bonds C5—N1 [1.282 (2) Å] and C7—O2 [1.231 (2) Å] are reported as 1.287 Å (Tucker *et al.*, 1975) and 1.298 Å (Sutherland & Hoy, 1968), respectively. The dihedral angle between the planar ring A (O1/C1—C4) and the planar moiety B (N1/N2/C4—C6) is A/B = 3.57 (3)°.

The intermolecular N—H···O hydrogen bonds (Table 1) seem to be effective in the stabilization of the crystal structure.

Experimental

A mixture of acetyl furan (100 mmol) and acetohydrazide (100 mmol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound (yield; 87 mmol, 87%). Single crystals suitable for X-ray analysis were obtained by recrystallization from ethanol at room temperature.

Refinement

H atom of NH group was located in difference syntheses and refined isotropically [N—H = 0.897 (9) Å and U_{iso}(H) = 0.048 (5) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for aromatic H atoms.

Figures

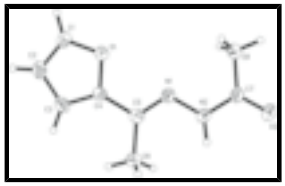

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

N'-[1-(2-Furyl)ethylidene]acetohydrazide

Crystal data

$C_8H_{10}N_2O_2$	F_{000} = 704
M_r = 166.18	D_x = 1.311 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 876 reflections
a = 23.865 (6) Å	θ = 2.5–26.4º
b = 4.3199 (10) Å	μ = 0.10 mm^{-1}
c = 16.829 (4) Å	*T* = 294 (2) K
β = 103.845 (4)º	Block, colorless
V = 1684.5 (7) Å^3	0.18 × 0.12 × 0.08 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	1153 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 26.4º
T = 294(2) K	θ_{min} = 2.5º
φ and ω scans	*h* = −22→29
Absorption correction: none	*k* = −5→5
4474 measured reflections	*l* = −20→21
1729 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.127	$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.2316P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
1729 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
115 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.05967 (5)	0.5388 (3)	0.56109 (7)	0.0488 (4)
O2	0.20044 (6)	−0.3371 (4)	0.40832 (9)	0.0627 (5)
N1	0.13897 (6)	0.1667 (3)	0.52494 (9)	0.0400 (4)
N2	0.17937 (6)	−0.0211 (4)	0.50190 (9)	0.0438 (4)
C1	0.02654 (8)	0.7266 (5)	0.59583 (13)	0.0538 (6)
H1	−0.0103	0.7947	0.5702	0.065*
C2	0.05448 (9)	0.7991 (5)	0.67200 (13)	0.0564 (6)
H2	0.0410	0.9236	0.7085	0.068*
C3	0.10853 (8)	0.6499 (5)	0.68635 (11)	0.0483 (5)
H3	0.1375	0.6580	0.7343	0.058*
C4	0.11038 (7)	0.4942 (4)	0.61803 (10)	0.0376 (4)
C5	0.15346 (8)	0.2949 (4)	0.59558 (11)	0.0388 (4)
C6	0.20992 (8)	0.2627 (5)	0.65683 (13)	0.0568 (6)
H6A	0.2223	0.0508	0.6589	0.085*
H6B	0.2055	0.3247	0.7098	0.085*
H6C	0.2382	0.3919	0.6412	0.085*
C7	0.16446 (8)	−0.1763 (4)	0.43065 (11)	0.0434 (5)
C8	0.10414 (9)	−0.1486 (5)	0.38123 (12)	0.0595 (6)
H8A	0.1003	−0.2565	0.3303	0.089*
H8B	0.0948	0.0659	0.3705	0.089*
H8C	0.0783	−0.2372	0.4109	0.089*
H2A	0.2161 (5)	−0.046 (4)	0.5298 (10)	0.048 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0460 (8)	0.0577 (9)	0.0400 (7)	0.0106 (6)	0.0049 (6)	−0.0099 (6)
O2	0.0556 (9)	0.0730 (10)	0.0607 (9)	0.0218 (8)	0.0162 (7)	−0.0114 (8)
N1	0.0415 (8)	0.0403 (8)	0.0390 (8)	0.0076 (7)	0.0112 (6)	0.0013 (7)
N2	0.0384 (9)	0.0457 (9)	0.0463 (9)	0.0112 (7)	0.0085 (7)	−0.0015 (7)
C1	0.0435 (11)	0.0627 (13)	0.0563 (13)	0.0127 (10)	0.0141 (10)	−0.0122 (11)
C2	0.0527 (12)	0.0689 (14)	0.0521 (13)	0.0002 (11)	0.0214 (10)	−0.0195 (11)

C3	0.0477 (11)	0.0603 (13)	0.0362 (10)	−0.0054 (9)	0.0088 (8)	−0.0088 (9)
C4	0.0387 (10)	0.0383 (10)	0.0349 (9)	−0.0012 (8)	0.0073 (7)	0.0009 (8)
C5	0.0408 (10)	0.0361 (10)	0.0389 (10)	−0.0021 (8)	0.0081 (8)	0.0022 (8)
C6	0.0460 (11)	0.0628 (13)	0.0560 (13)	0.0085 (10)	0.0009 (9)	−0.0110 (11)
C7	0.0467 (11)	0.0445 (11)	0.0413 (10)	0.0106 (9)	0.0151 (9)	0.0009 (9)
C8	0.0574 (13)	0.0734 (15)	0.0434 (11)	0.0186 (11)	0.0038 (9)	−0.0121 (11)

Geometric parameters (Å, °)

O1—C1	1.359 (2)	C3—C4	1.342 (2)
O1—C4	1.366 (2)	C3—H3	0.9300
O2—C7	1.231 (2)	C4—C5	1.458 (2)
N1—C5	1.282 (2)	C5—C6	1.494 (3)
N1—N2	1.385 (2)	C6—H6A	0.9600
N2—C7	1.345 (2)	C6—H6B	0.9600
N2—H2A	0.897 (9)	C6—H6C	0.9600
C1—C2	1.333 (3)	C7—C8	1.485 (3)
C1—H1	0.9300	C8—H8A	0.9600
C2—C3	1.410 (3)	C8—H8B	0.9600
C2—H2	0.9300	C8—H8C	0.9600
C1—O1—C4	106.95 (14)	N1—C5—C6	126.74 (17)
C5—N1—N2	117.48 (15)	C4—C5—C6	116.84 (16)
C7—N2—N1	119.22 (15)	C5—C6—H6A	109.5
C7—N2—H2A	115.1 (12)	C5—C6—H6B	109.5
N1—N2—H2A	125.6 (12)	H6A—C6—H6B	109.5
C2—C1—O1	110.20 (17)	C5—C6—H6C	109.5
C2—C1—H1	124.9	H6A—C6—H6C	109.5
O1—C1—H1	124.9	H6B—C6—H6C	109.5
C1—C2—C3	106.50 (17)	O2—C7—N2	119.89 (17)
C1—C2—H2	126.8	O2—C7—C8	121.87 (18)
C3—C2—H2	126.8	N2—C7—C8	118.24 (16)
C4—C3—C2	107.38 (17)	C7—C8—H8A	109.5
C4—C3—H3	126.3	C7—C8—H8B	109.5
C2—C3—H3	126.3	H8A—C8—H8B	109.5
C3—C4—O1	108.98 (15)	C7—C8—H8C	109.5
C3—C4—C5	133.45 (17)	H8A—C8—H8C	109.5
O1—C4—C5	117.57 (15)	H8B—C8—H8C	109.5
N1—C5—C4	116.42 (16)		
C5—N1—N2—C7	175.53 (16)	N2—N1—C5—C4	179.36 (14)
C4—O1—C1—C2	−0.3 (2)	N2—N1—C5—C6	−0.2 (3)
O1—C1—C2—C3	0.2 (2)	C3—C4—C5—N1	175.81 (19)
C1—C2—C3—C4	−0.1 (2)	O1—C4—C5—N1	−2.9 (2)
C2—C3—C4—O1	0.0 (2)	C3—C4—C5—C6	−4.6 (3)
C2—C3—C4—C5	−178.84 (19)	O1—C4—C5—C6	176.71 (16)
C1—O1—C4—C3	0.2 (2)	N1—N2—C7—O2	177.92 (16)
C1—O1—C4—C5	179.20 (15)	N1—N2—C7—C8	−2.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.897 (9)	2.076 (10)	2.968 (2)	172.7 (17)

Symmetry codes: (i) −*x*+1/2, −*y*−1/2, −*z*+1.

Fig. 1