Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-*N*′-(2-Furylmethylene)benzohydrazide

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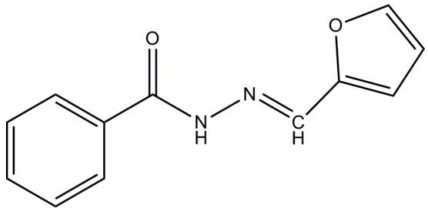
Received 13 October 2009; accepted 14 October 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 13.0.

In the title compound, $C_{12}H_{10}N_2O_2$, the dihedral angle between the benzene and furan rings is 52.54 (7)°. In the crystal, intermolecular N—H···O hydrogen bonds and C—H···π interactions link the molecules.

Related literature

For biological properties of Schiff base ligands, see: Chakraborty *et al.* (1996); Jeewoth *et al.* (1999). For related crystal structures, see: Fun *et al.* (2008); Cui *et al.* (2009); Nie (2008).



Experimental

Crystal data

$C_{12}H_{10}N_2O_2$
M_r = 214.22
Monoclinic, $P2_1/c$
a = 12.3955 (11) Å
b = 9.4777 (9) Å
c = 9.6845 (10) Å
β = 110.610 (1)°
V = 1064.93 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.43 × 0.38 × 0.30 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.973
5190 measured reflections
1882 independent reflections
1360 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
1882 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.14	2.972 (2)	163
C10—H10···$Cg1^{ii}$	0.93	2.84	3.498 (2)	128

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, y-1, z$. $Cg1$ is the centroid of the C2–C7 ring.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Foundation of Binzhou University (No. BZXYLG200609).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2168).

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supplementary materials

Acta Cryst. (2009). E**65**, o2800 [**doi:10.1107/S1600536809042251**]

(*E*)-*N*'-(2-Furylmethylene)benzohydrazide

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Comment

Conventionally, Schiff bases derived from a large number of carbonyl compounds and amines. It has been shown that Schiff base compounds have strong anticancer activity (Chakraborty *et al.*, 1996). It has been well known that a series of certain Schiff base compounds, have received considerable attention during the last decades, mainly because their structures or for their biological properties (Jeewoth *et al.*, 1999).

In the compound (I), (Fig. 1), the bond lengths an angles are normal and are comparable to the values observed in similar compounds (Nie *et al.*, 2008; Fun *et al.*, 2008; Cui *et al.*, 2009).

In the crystal structure, the C=N bond length in the molecule is 1.273 (2) ° (C8=N2), showing the double-bond character. Meanwhile, the dihedral angle between the benzene ring (C2-C7) and the furan ring (C9-C12/O2) in the Schiff base molecule is 52.54 (7)°, indicating that the two aromatic ring planes are not coplanar.

Moreover, the crystal supramolecular structure was built from the connections of intermolecular N—H···O hydrogen bonds and C-H···π hydrogen bonding interactions, as shown in Table 1.

Experimental

Benzohydrazide (5.0 mmol), 20 ml ethanol and furfural (5.0 mmol) were mixed in 50 ml flash. After refluxing 3 h, the resulting mixture was cooled to room temperature, and recrystalized from ethanol, and afforded the title compound as a crystalline solid. Elemental analysis: calculated for $C_{12}H_{10}N_2O_2$: C 67.28, H 4.71, N 13.08%; found: C 67.16, H 4.66, N 13.19%.

Refinement

All H atoms were placed in geometrically idealized positions (N—H 0.86 and C—H 0.93 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U5$_{eq}$(C) (C,*N*).

Figures

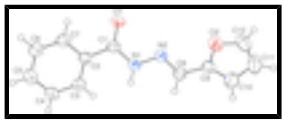

Fig. 1. A view of (I) showing the atomic numbering scheme and 50% probability displacement ellipsoids.

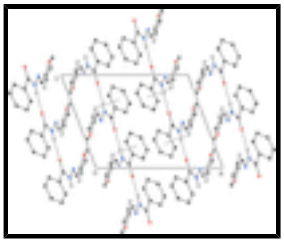

Fig. 2. A packing of (I) viewed down b-axis showing the N-H..O and C-H···π H-bond interactions with dashed lines. Symmetry codes: (i) x, -y+1/2, z+1/2; (ii) x, y-1, z.

(*E*)-*N*'-(2-Furylmethylene)benzohydrazide

Crystal data

$C_{12}H_{10}N_2O_2$	F_{000} = 448
M_r = 214.22	D_x = 1.336 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1760 reflections
a = 12.3955 (11) Å	θ = 2.8–25.6º
b = 9.4777 (9) Å	μ = 0.09 mm^{-1}
c = 9.6845 (10) Å	T = 298 K
β = 110.6100 (10)º	Needle, green
V = 1064.93 (18) Å^3	0.43 × 0.38 × 0.30 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1882 independent reflections
Radiation source: fine-focus sealed tube	1360 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 298 K	θ_{max} = 25.0º
phi and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→14
T_{min} = 0.961, T_{max} = 0.973	k = −11→5
5190 measured reflections	l = −11→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.103	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.2066P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1882 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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}
N1	0.23549 (11)	0.22758 (14)	0.10288 (15)	0.0393 (4)
H1	0.2462	0.2263	0.1956	0.047*
N2	0.18065 (12)	0.11622 (15)	0.01303 (15)	0.0394 (4)
O1	0.26227 (11)	0.34211 (13)	−0.08757 (13)	0.0525 (4)
O2	0.05357 (11)	−0.11197 (14)	−0.14345 (14)	0.0552 (4)
C1	0.27183 (14)	0.33810 (18)	0.04323 (18)	0.0369 (4)
C2	0.32908 (13)	0.45449 (17)	0.14650 (18)	0.0357 (4)
C3	0.31657 (15)	0.47508 (18)	0.28218 (19)	0.0439 (4)
H3	0.2698	0.4148	0.3122	0.053*
C4	0.37320 (17)	0.5846 (2)	0.3724 (2)	0.0539 (5)
H4	0.3642	0.5982	0.4628	0.065*
C5	0.44318 (17)	0.6740 (2)	0.3290 (2)	0.0576 (6)
H5	0.4822	0.7468	0.3908	0.069*
C6	0.45522 (16)	0.6555 (2)	0.1942 (2)	0.0553 (5)
H6	0.5019	0.7161	0.1646	0.066*
C7	0.39802 (15)	0.5469 (2)	0.1033 (2)	0.0460 (5)
H7	0.4057	0.5354	0.0118	0.055*
C8	0.17622 (14)	0.00187 (18)	0.07975 (19)	0.0407 (4)
H8	0.2088	−0.0011	0.1821	0.049*
C9	0.12239 (14)	−0.12242 (18)	0.00150 (19)	0.0406 (4)
C10	0.12911 (17)	−0.2579 (2)	0.0460 (2)	0.0574 (5)
H10	0.1701	−0.2924	0.1398	0.069*
C11	0.06160 (19)	−0.3374 (2)	−0.0779 (3)	0.0693 (6)
H11	0.0504	−0.4346	−0.0818	0.083*
C12	0.01745 (18)	−0.2464 (3)	−0.1875 (3)	0.0635 (6)
H12	−0.0316	−0.2708	−0.2817	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0512 (9)	0.0397 (8)	0.0276 (7)	−0.0026 (7)	0.0147 (6)	−0.0027 (6)

N2	0.0459 (8)	0.0386 (8)	0.0341 (8)	−0.0018 (7)	0.0146 (6)	−0.0038 (7)
O1	0.0821 (9)	0.0482 (8)	0.0309 (7)	−0.0056 (7)	0.0245 (6)	−0.0012 (6)
O2	0.0565 (8)	0.0579 (9)	0.0459 (8)	−0.0045 (7)	0.0116 (6)	−0.0062 (7)
C1	0.0414 (9)	0.0386 (10)	0.0318 (9)	0.0061 (8)	0.0142 (7)	0.0030 (8)
C2	0.0383 (9)	0.0362 (9)	0.0332 (9)	0.0047 (7)	0.0134 (7)	0.0017 (8)
C3	0.0554 (11)	0.0432 (10)	0.0381 (10)	−0.0067 (9)	0.0225 (8)	−0.0012 (8)
C4	0.0699 (13)	0.0579 (13)	0.0391 (11)	−0.0131 (10)	0.0257 (10)	−0.0102 (9)
C5	0.0634 (12)	0.0576 (13)	0.0502 (12)	−0.0191 (11)	0.0180 (10)	−0.0126 (10)
C6	0.0571 (12)	0.0598 (13)	0.0522 (12)	−0.0185 (10)	0.0233 (10)	−0.0014 (10)
C7	0.0509 (11)	0.0534 (11)	0.0386 (10)	−0.0041 (9)	0.0218 (9)	0.0008 (9)
C8	0.0451 (10)	0.0430 (10)	0.0338 (9)	0.0013 (8)	0.0136 (8)	−0.0006 (8)
C9	0.0428 (10)	0.0429 (11)	0.0378 (10)	0.0015 (8)	0.0162 (8)	−0.0012 (8)
C10	0.0647 (13)	0.0460 (12)	0.0627 (13)	0.0011 (10)	0.0241 (11)	0.0039 (11)
C11	0.0781 (15)	0.0457 (12)	0.0926 (19)	−0.0118 (12)	0.0406 (14)	−0.0163 (13)
C12	0.0560 (12)	0.0711 (15)	0.0633 (14)	−0.0171 (12)	0.0210 (11)	−0.0292 (13)

Geometric parameters (Å, °)

N1—C1	1.348 (2)	C5—C6	1.376 (3)
N1—N2	1.3844 (19)	C5—H5	0.9300
N1—H1	0.8600	C6—C7	1.377 (3)
N2—C8	1.273 (2)	C6—H6	0.9300
O1—C1	1.2306 (19)	C7—H7	0.9300
O2—C9	1.366 (2)	C8—C9	1.432 (2)
O2—C12	1.368 (2)	C8—H8	0.9300
C1—C2	1.490 (2)	C9—C10	1.348 (3)
C2—C7	1.387 (2)	C10—C11	1.415 (3)
C2—C3	1.390 (2)	C10—H10	0.9300
C3—C4	1.379 (2)	C11—C12	1.327 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.380 (3)	C12—H12	0.9300
C4—H4	0.9300		
C1—N1—N2	119.16 (13)	C5—C6—H6	120.1
C1—N1—H1	120.4	C7—C6—H6	120.1
N2—N1—H1	120.4	C6—C7—C2	120.79 (17)
C8—N2—N1	115.43 (14)	C6—C7—H7	119.6
C9—O2—C12	105.68 (16)	C2—C7—H7	119.6
O1—C1—N1	122.65 (16)	N2—C8—C9	121.81 (16)
O1—C1—C2	121.24 (15)	N2—C8—H8	119.1
N1—C1—C2	116.08 (14)	C9—C8—H8	119.1
C7—C2—C3	118.82 (16)	C10—C9—O2	110.11 (16)
C7—C2—C1	117.59 (15)	C10—C9—C8	130.51 (17)
C3—C2—C1	123.59 (15)	O2—C9—C8	119.36 (15)
C4—C3—C2	120.22 (17)	C9—C10—C11	106.54 (19)
C4—C3—H3	119.9	C9—C10—H10	126.7
C2—C3—H3	119.9	C11—C10—H10	126.7
C3—C4—C5	120.23 (18)	C12—C11—C10	106.65 (19)
C3—C4—H4	119.9	C12—C11—H11	126.7
C5—C4—H4	119.9	C10—C11—H11	126.7

C6—C5—C4	120.03 (18)	C11—C12—O2	111.01 (18)
C6—C5—H5	120.0	C11—C12—H12	124.5
C4—C5—H5	120.0	O2—C12—H12	124.5
C5—C6—C7	119.89 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.14	2.972 (2)	163
C10—H10···Cg1^{ii}	0.93	2.85	3.498 (2)	128

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

Fig. 1

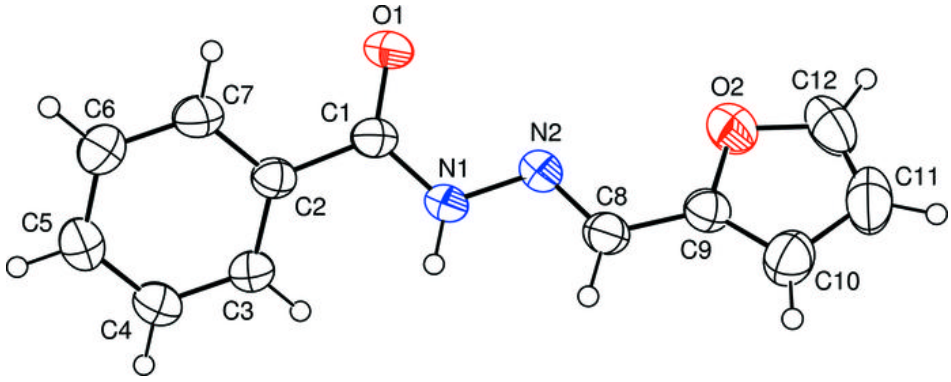

Fig. 2