Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*Z*,*N*′*E*)-*N*′-[(2-Hydroxy-1-naphthyl)-methylidene]furan-2-carbohydrazonic acid

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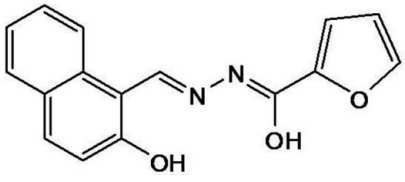
Received 18 May 2010; accepted 13 July 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.052; wR factor = 0.095; data-to-parameter ratio = 7.5.

In the title compound, $C_{16}H_{12}N_2O_3$, the dihedral angle between the mean planes of the naphthalene ring system and the furan ring is 21.3 (6)°. The molecular structure is stabilized by an intramolecular O—H···N hydrogen bond, which generates an S(6) graph-set motif.

Related literature

For historical background to aroylhydrazones, see: Arapov *et al.* (1987); Pickart *et al.* (1983); Offe *et al.* (1952); Nagaraju *et al.* (2009); Ghosh *et al.* (2007). For related structures, see: Monfared *et al.* (2010); Ali *et al.* (2005); Qian *et al.* (2006); Tarafder *et al.* (2002); Prathapachandra Kurup & Bessy Raj (2007). For graph-set analysis of hydrogen-bond networks, see: Bernstein *et al.* (1995); Etter *et al.* (1990). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{12}N_2O_3$
M_r = 280.28
Orthorhombic, $Pna2_1$
a = 9.7427 (8) Å
b = 21.4182 (8) Å
c = 6.445 (2) Å
V = 1344.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.31 × 0.27 × 0.15 mm

Data collection

STOE IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.970, T_{max} = 0.985
7278 measured reflections
1440 independent reflections
944 reflections with $I > 2\sigma(I)$
R_{int} = 0.097

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.095
S = 1.02
1440 reflections
191 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 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
O1—H1···N1	0.82	1.84	2.565 (5)	146

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors are grateful to Zanjan University and Ondokuz Mayis University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2034).

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supporting information

Acta Cryst. (2010). E**66**, o2073 [https://doi.org/10.1107/S1600536810027935]

(2*Z*,*N*′*E*)-*N*′-[(2-Hydroxy-1-naphthyl)methylidene]furan-2-carbohydrazonic acid

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S1. Comment

Hydrazone ligands derived from the condensation of aliphatic acid hydrazides or aromatic acid hydrazides with aromatic 2-hydroxy carbonyl compounds are important tridentate O, N,O-donor ligands. These compounds, due to their facile keto-enol tautomerization and the availability of several potential donor sites, can coordinate to metals. Furthermore, the possibility of tautomerism makes their study interesting (Ghosh *et al.*, 2007). Hydrazones have wide spread applications in coordination, analytical and bioinorganic chemistry, and display magnetic, electronic, NLO and fluorescent properties in biologically active compounds (Prathapachandra Kurup *et al.*, 2007). They find applications in the treatment of diseases such as anti-tumor, tuberculosis, leprosy and mental disorder (Nagaraju *et al.*, 2009). As part of our studies on the synthesis and characterization of aroylhydrazone derivatives, we report here the crystal structure of $C_{16}H_{12}N_2O_3$.

In the title compound, $C_{16}H_{12}N_2O_3$, the dihedral angle between the mean planes of the naphthalene and furan rings is 21.3 (6)° (Fig.1). The angle formed between the menn planes of the naphthalene substituted hydroxy group (C11/C10/C1/O1/H1) and the 2-carbohydrazonic acid furan substituted hydroxy group (N1/N2/C12/O2/H22) is 17.9 (1)°. Bond distances and angles are in normal ranges (Allen *et al.*, 1987). Crystal packing is stabilized by O1—H1···N1 intramolecular hydrogen bonds which form an $S_1^1(6)$ graph-set motif (Bernstein *et al.*, 1995), Etter *et al.*, 1990), (Fig. 2).

S2. Experimental

All reagents were commercially available and used as received. A methanol (10 ml) solution of 2-hydroxy-1-naphtaldehyde (1.5 mmol) was drop-wise added to a methanol solution (10 ml) of 2-furanecarboxylic acid hydrazide (1.5 mmol), and the mixture was refluxed for 3 h. Then the solution was evaporated on a steam bath to 5 cm^3 and cooled to room temperature. Yellow precipitates of the title compound were separated and filtered off, washed with 3 ml of cooled methanol and then dried in air. X-ray quality crystals of the title compound were obtained from methanol by slow solvent evaporation. Yield: 82%, mp 197-198 °C.

S3. Refinement

The hydroxyl hydrogen atoms were located by Fourier analysis and refined using the riding model with d(O—H) = 0.82Å [U_{iso}(H) = 1.5U_{eq}(O)]. C-bonded H atoms were positioned geometrically (C—H = 0.93 Å) and treated as riding on their parent atoms [U_{iso}(H) = 1.2U_{eq}(C)].

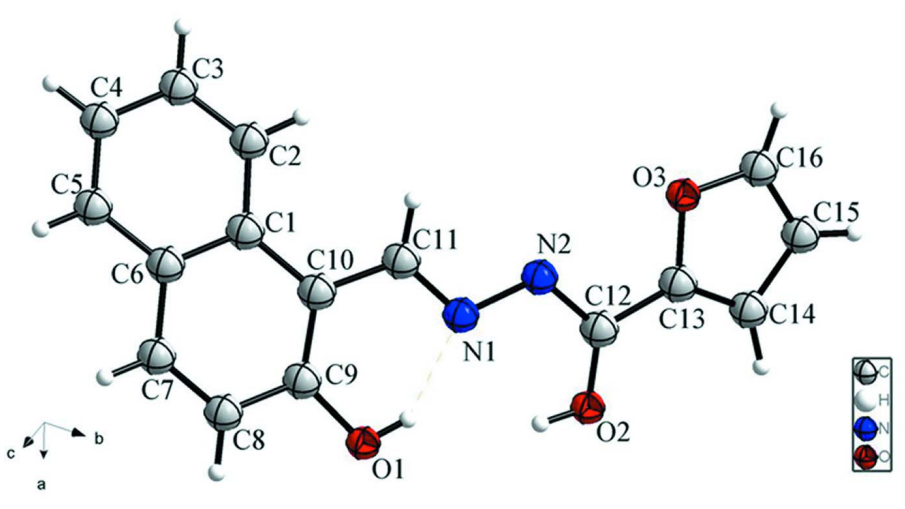

Figure 1

The molecular structure of the title compound, $C_{16}H_{12}N_2O_3$, with atom labels and anisotropic displacement ellipsoids (drawn at 30% probability level) for non-H atoms.

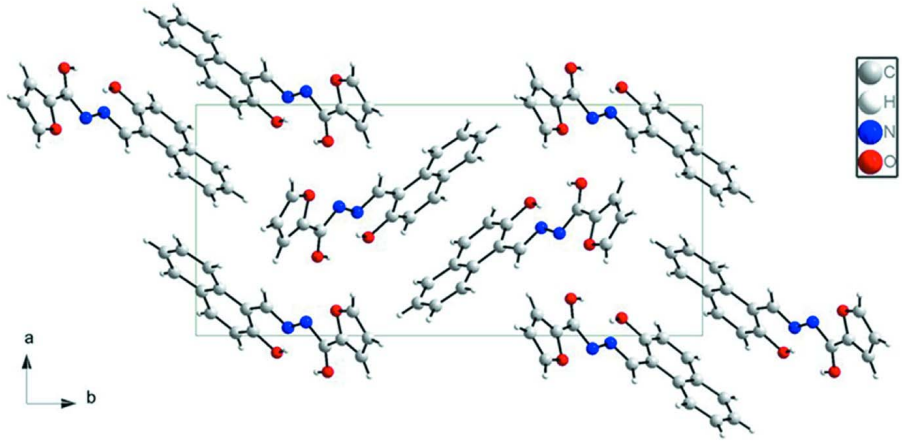

Figure 2

View of the unit cell of the title compound, $C_{16}H_{12}N_2O_3$, viewed along [110].

(2*Z*,*N*′*E*)-*N*′-[(2-Hydroxy-1- naphthyl)methylidene]furan-2-carbohydrazonic acid

Crystal data

$C_{16}H_{12}N_2O_3$
$M_r = 280.28$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 9.7427\ (8)$ Å
$b = 21.4182\ (8)$ Å
$c = 6.445\ (2)$ Å
$V = 1344.8\ (4)$ Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.384$ Mg m^{-3}
Melting point = 470–471 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8863 reflections
$\theta = 1.9$–$27.1°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism, colourless
0.31 × 0.27 × 0.15 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.970, T_{max} = 0.985
7278 measured reflections
1440 independent reflections
944 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 26.0°, θ_{min} = 1.9°
h = −12→10
k = −26→24
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.095
S = 1.02
1440 reflections
191 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0063 (17)

Special details

Experimental. 12912 Friedel pairs have been merged

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}
C1	0.2976 (5)	0.54675 (18)	0.6316 (7)	0.0451 (11)
C2	0.2057 (5)	0.5256 (2)	0.4789 (8)	0.0522 (12)
H2	0.1969	0.5479	0.3559	0.063*
C3	0.1290 (6)	0.4730 (2)	0.5070 (8)	0.0706 (16)
H3	0.0688	0.4601	0.4036	0.085*
C4	0.1400 (7)	0.4384 (2)	0.6892 (10)	0.0786 (18)
H4	0.0883	0.4022	0.7065	0.094*
C5	0.2262 (6)	0.4574 (2)	0.8410 (10)	0.0714 (16)
H5	0.2320	0.4347	0.9636	0.086*
C6	0.3079 (5)	0.51178 (19)	0.8155 (7)	0.0499 (12)
C7	0.4022 (6)	0.5297 (2)	0.9729 (7)	0.0591 (14)
H7	0.4051	0.5078	1.0974	0.071*
C8	0.4882 (5)	0.5788 (2)	0.9420 (8)	0.0552 (13)

H8	0.5516	0.5897	1.0436	0.066*
C9	0.4814 (5)	0.61298 (19)	0.7575 (7)	0.0474 (11)
C10	0.3861 (5)	0.6002 (2)	0.6042 (6)	0.0406 (10)
C11	0.3758 (5)	0.63934 (18)	0.4226 (6)	0.0440 (11)
H11	0.3027	0.6340	0.3314	0.053*
C12	0.5461 (5)	0.7550 (2)	0.1419 (7)	0.0488 (11)
C13	0.5167 (5)	0.78815 (19)	−0.0481 (7)	0.0513 (12)
C14	0.5895 (6)	0.8270 (2)	−0.1646 (8)	0.0631 (14)
H14	0.6764	0.8425	−0.1343	0.076*
C15	0.5117 (7)	0.8404 (3)	−0.3412 (9)	0.0810 (19)
H15	0.5371	0.8661	−0.4511	0.097*
C16	0.3952 (7)	0.8095 (3)	−0.3215 (9)	0.0783 (18)
H16	0.3240	0.8102	−0.4178	0.094*
N1	0.4666 (4)	0.68174 (16)	0.3852 (6)	0.0488 (10)
N2	0.4425 (4)	0.71739 (15)	0.2109 (6)	0.0495 (10)
O1	0.5751 (3)	0.65972 (14)	0.7404 (5)	0.0632 (10)
H1	0.5641	0.6779	0.6296	0.095*
O2	0.6585 (3)	0.76014 (14)	0.2278 (5)	0.0658 (10)
H22	0.6598	0.7385	0.3328	0.099*
O3	0.3934 (3)	0.77680 (15)	−0.1422 (6)	0.0675 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (3)	0.037 (2)	0.048 (3)	0.008 (2)	0.011 (2)	0.001 (2)
C2	0.052 (3)	0.048 (3)	0.056 (3)	0.002 (2)	0.008 (3)	−0.001 (2)
C3	0.075 (4)	0.056 (3)	0.081 (4)	−0.017 (3)	0.005 (3)	−0.006 (3)
C4	0.084 (5)	0.052 (3)	0.100 (5)	−0.015 (3)	0.023 (4)	0.005 (4)
C5	0.076 (4)	0.058 (3)	0.080 (4)	0.001 (3)	0.015 (4)	0.009 (3)
C6	0.052 (3)	0.040 (2)	0.057 (3)	0.010 (2)	0.011 (2)	0.002 (2)
C7	0.073 (4)	0.057 (3)	0.047 (3)	0.023 (3)	0.002 (3)	0.013 (2)
C8	0.055 (3)	0.060 (3)	0.050 (3)	0.016 (3)	−0.007 (2)	−0.011 (3)
C9	0.046 (3)	0.042 (2)	0.054 (3)	0.008 (2)	−0.001 (2)	−0.003 (2)
C10	0.036 (3)	0.043 (2)	0.043 (2)	0.011 (2)	0.003 (2)	0.001 (2)
C11	0.037 (3)	0.047 (2)	0.049 (3)	0.001 (2)	0.000 (2)	−0.002 (2)
C12	0.036 (3)	0.054 (3)	0.056 (3)	−0.002 (2)	0.005 (2)	−0.008 (2)
C13	0.044 (3)	0.047 (2)	0.063 (3)	0.000 (2)	0.007 (3)	0.005 (2)
C14	0.059 (3)	0.060 (3)	0.070 (3)	−0.018 (3)	0.012 (3)	0.009 (3)
C15	0.087 (5)	0.075 (4)	0.081 (4)	0.011 (4)	0.027 (4)	0.034 (3)
C16	0.060 (4)	0.087 (4)	0.088 (5)	0.022 (3)	0.011 (3)	0.033 (4)
N1	0.038 (2)	0.050 (2)	0.058 (3)	−0.002 (2)	0.0096 (18)	0.0013 (19)
N2	0.043 (2)	0.0485 (19)	0.057 (2)	−0.0082 (18)	0.0117 (19)	0.0134 (19)
O1	0.056 (2)	0.060 (2)	0.074 (2)	−0.0063 (18)	−0.0109 (19)	−0.0017 (18)
O2	0.056 (2)	0.078 (2)	0.064 (2)	−0.0186 (18)	0.001 (2)	0.0063 (19)
O3	0.040 (2)	0.078 (2)	0.085 (3)	0.0037 (18)	0.0047 (19)	0.0323 (19)

Geometric parameters (Å, º)

C1—C2	1.406 (6)	C10—C11	1.443 (6)
C1—C6	1.406 (6)	C11—N1	1.291 (5)
C1—C10	1.444 (6)	C11—H11	0.9300
C2—C3	1.364 (7)	C12—O2	1.232 (5)
C2—H2	0.9300	C12—N2	1.366 (5)
C3—C4	1.393 (8)	C12—C13	1.444 (6)
C3—H3	0.9300	C13—C14	1.326 (6)
C4—C5	1.352 (8)	C13—O3	1.367 (5)
C4—H4	0.9300	C14—C15	1.398 (7)
C5—C6	1.420 (7)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.321 (8)
C6—C7	1.422 (7)	C15—H15	0.9300
C7—C8	1.359 (7)	C16—O3	1.352 (6)
C7—H7	0.9300	C16—H16	0.9300
C8—C9	1.397 (6)	N1—N2	1.379 (5)
C8—H8	0.9300	O1—H1	0.8200
C9—O1	1.359 (5)	O2—H22	0.8200
C9—C10	1.384 (6)		
C2—C1—C6	117.6 (4)	C9—C10—C11	120.7 (4)
C2—C1—C10	123.4 (4)	C9—C10—C1	118.1 (4)
C6—C1—C10	118.9 (4)	C11—C10—C1	121.2 (4)
C3—C2—C1	121.5 (5)	N1—C11—C10	120.8 (4)
C3—C2—H2	119.3	N1—C11—H11	119.6
C1—C2—H2	119.3	C10—C11—H11	119.6
C2—C3—C4	120.6 (5)	O2—C12—N2	124.3 (4)
C2—C3—H3	119.7	O2—C12—C13	120.9 (4)
C4—C3—H3	119.7	N2—C12—C13	114.8 (4)
C5—C4—C3	119.8 (5)	C14—C13—O3	109.3 (4)
C5—C4—H4	120.1	C14—C13—C12	133.0 (5)
C3—C4—H4	120.1	O3—C13—C12	117.6 (4)
C4—C5—C6	120.8 (6)	C13—C14—C15	107.5 (5)
C4—C5—H5	119.6	C13—C14—H14	126.3
C6—C5—H5	119.6	C15—C14—H14	126.3
C1—C6—C5	119.6 (5)	C16—C15—C14	106.5 (5)
C1—C6—C7	120.3 (4)	C16—C15—H15	126.7
C5—C6—C7	120.1 (5)	C14—C15—H15	126.7
C8—C7—C6	120.2 (5)	C15—C16—O3	110.7 (6)
C8—C7—H7	119.9	C15—C16—H16	124.7
C6—C7—H7	119.9	O3—C16—H16	124.7
C7—C8—C9	120.0 (5)	C11—N1—N2	115.1 (4)
C7—C8—H8	120.0	C12—N2—N1	117.7 (4)
C9—C8—H8	120.0	C9—O1—H1	109.5
O1—C9—C10	122.6 (4)	C12—O2—H22	109.5
O1—C9—C8	115.0 (5)	C16—O3—C13	106.0 (4)
C10—C9—C8	122.4 (5)		

C6—C1—C2—C3	−0.1 (7)	C6—C1—C10—C9	2.6 (6)
C10—C1—C2—C3	176.6 (4)	C2—C1—C10—C11	6.2 (6)
C1—C2—C3—C4	−0.2 (8)	C6—C1—C10—C11	−177.3 (4)
C2—C3—C4—C5	0.9 (9)	C9—C10—C11—N1	9.5 (6)
C3—C4—C5—C6	−1.3 (8)	C1—C10—C11—N1	−170.6 (4)
C2—C1—C6—C5	−0.3 (6)	O2—C12—C13—C14	−0.1 (8)
C10—C1—C6—C5	−177.1 (4)	N2—C12—C13—C14	−178.3 (5)
C2—C1—C6—C7	178.0 (4)	O2—C12—C13—O3	175.5 (4)
C10—C1—C6—C7	1.2 (6)	N2—C12—C13—O3	−2.6 (6)
C4—C5—C6—C1	1.0 (7)	O3—C13—C14—C15	−0.9 (5)
C4—C5—C6—C7	−177.3 (5)	C12—C13—C14—C15	175.0 (5)
C1—C6—C7—C8	−3.5 (7)	C13—C14—C15—C16	0.7 (6)
C5—C6—C7—C8	174.8 (5)	C14—C15—C16—O3	−0.1 (7)
C6—C7—C8—C9	1.8 (7)	C10—C11—N1—N2	−177.8 (4)
C7—C8—C9—O1	−177.9 (4)	O2—C12—N2—N1	−1.6 (6)
C7—C8—C9—C10	2.2 (7)	C13—C12—N2—N1	176.5 (4)
O1—C9—C10—C11	−4.3 (6)	C11—N1—N2—C12	−168.4 (4)
C8—C9—C10—C11	175.5 (4)	C15—C16—O3—C13	−0.5 (6)
O1—C9—C10—C1	175.7 (4)	C14—C13—O3—C16	0.9 (5)
C8—C9—C10—C1	−4.5 (6)	C12—C13—O3—C16	−175.7 (4)
C2—C1—C10—C9	−173.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.84	2.565 (5)	146