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(*E*)-*N*′-[(2-Hydroxy-1-naphthalen-1-yl)-methylidene]-3-methylbenzohydrazide

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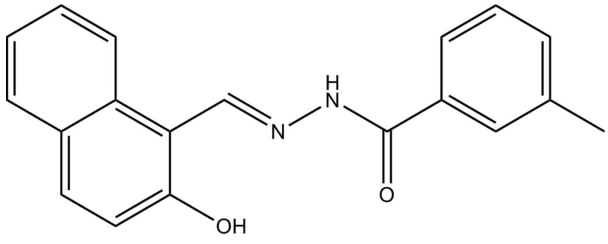
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.166; data-to-parameter ratio = 15.4.

In the title compound, $C_{19}H_{16}N_2O_2$, the benzene ring and naphthyl ring system are inclined at a dihedral angle of 16.1 (3)°. An intramolecular O—H···N hydrogen bond influences the molecular conformation. In the crystal, molecules are linked through N—H···O hydrogen bonds into chains running along the *a* axis.

Related literature

For the medicinal applications of hydrazone compounds, see: Hillmer *et al.* (2010); Raj *et al.* (2007). For hydrazones we have reported previously, see: Liu & You (2010); Liu & Wang (2010). For the crystal structures of other similar hydrazone compounds, see: Vijayakumar *et al.* (2009). For related structures, see: Xu *et al.* (2009); Shafiq *et al.* (2009).



Experimental

Crystal data

$C_{19}H_{16}N_2O_2$
M_r = 304.34
Monoclinic, $P2_1/n$
a = 7.1927 (11) Å
b = 31.042 (4) Å
c = 7.3557 (11) Å
β = 108.455 (2)°
V = 1557.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.983, T_{max} = 0.985
8247 measured reflections
3295 independent reflections
1736 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.166
S = 1.04
3295 reflections
214 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 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
N2—H2···O2^{i}	0.90 (1)	2.00 (1)	2.869 (3)	163 (3)
O1—H1···N1	0.82	1.85	2.567 (3)	146

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5120).

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supporting information

Acta Cryst. (2011). E**67**, o965 [doi:10.1107/S1600536811010361]

(*E*)-*N*′-[(2-Hydroxy-1-naphthalen-1-yl)methylidene]-3-methylbenzohydrazide

Shi-Yong Liu, Shan-Shan Sun, Ting-Ting Zheng, Xiang-Lei Zheng, Xiao-Feng Zhao and Xiao-Fang Li

S1. Comment

Considerable attention has been focused on hydrazones and their medicinal applications (Hillmer *et al.*, 2010; Raj *et al.*, 2007). The crystal structures of such compounds are of particular interest (Vijayakumar *et al.*, 2009). As a continuation of our work on similar compounds (Liu & You, 2010; Liu & Wang, 2010), we report herein the crystal structure of the title compound a new hydrazone.

The molecular structure of the title compound is shown in Fig. 1. The benzene ring and the naphthyl ring system are inclined at a dihedral angle of 16.1 (3) °. The dihedral angle between the C1—C10 benzene ring and the C13—C18 naphthyl ring is 16.1 (3)°. All the bond lengths are comparable to those observed in related structures (Xu *et al.*, 2009; Shafiq *et al.*, 2009) and those we reported previously.

In the crystal structure, molecules are linked through N–H···O hydrogen bonds, to form one-dimensional chains running along the *a* axis (Fig. 2 and Table 1).

S2. Experimental

The title compound was prepared by the condensation reaction of 2-hydroxy-1-naphthaldehyde (0.05 mol, 8.6 g) and 3-methylbenzohydrazide (0.05 mol, 7.5 g) in anhydrous methanol (200 ml) at ambient temperature. Colourless block-shaped single crystals suitable for X-ray structural determination were obtained by slow evaporation of the solution for a period of a week.

S3. Refinement

H2 was located from a difference Fourier map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å. The remaining H atoms were positioned geometrically and constrained to ride on their parent atoms, with C–H distances of 0.93–0.96 Å, O–H distance of 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O and C19).

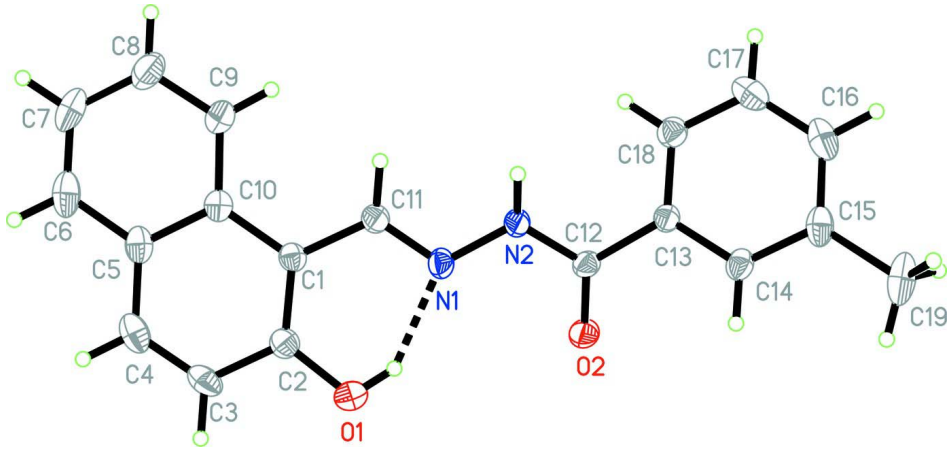

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are shown as spheres of arbitrary radius and the intramolecular hydrogen bond is drawn as a dashed line.

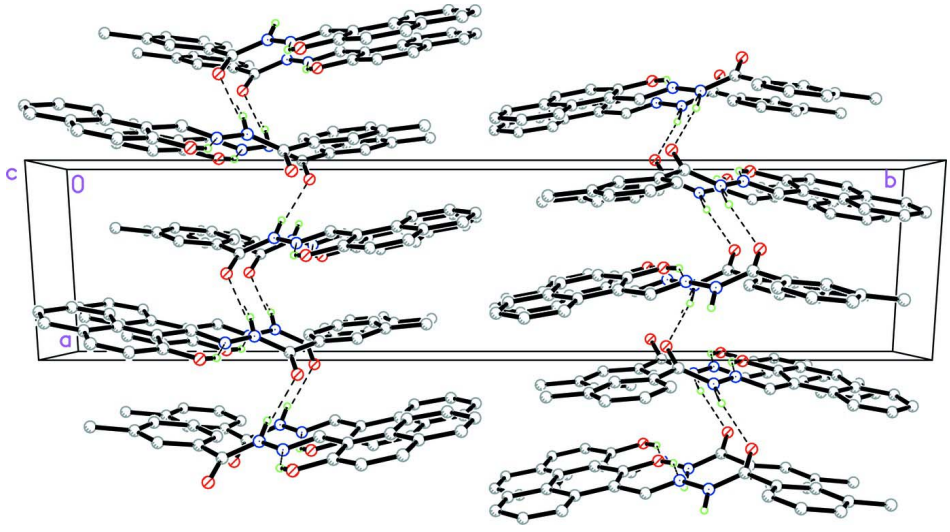

Figure 2

The molecular packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted.

(*E*)-*N*′-[(2-Hydroxy-1-naphthalen-1-yl)methylidene]- 3-methylbenzohydrazide

Crystal data

$C_{19}H_{16}N_2O_2$
$M_r = 304.34$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.1927\ (11)$ Å
$b = 31.042\ (4)$ Å
$c = 7.3557\ (11)$ Å
$\beta = 108.455\ (2)°$
$V = 1557.9\ (4)$ Å^3
$Z = 4$

$F(000) = 640$
$D_x = 1.298$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2077 reflections
$\theta = 2.6–28.2°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.20 × 0.20 × 0.18 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, 2001)
T_{min} = 0.983, T_{max} = 0.985
8247 measured reflections
3295 independent reflections
1736 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.0°, θ_{min} = 2.6°
h = −8→9
k = −33→39
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.166
S = 1.04
3295 reflections
214 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 1.2072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.9044 (4)	0.21446 (7)	0.1747 (4)	0.0379 (6)
N2	0.8759 (4)	0.24304 (8)	0.0245 (4)	0.0390 (7)
O1	0.9690 (4)	0.19721 (7)	0.5307 (3)	0.0551 (7)
H1	0.9671	0.2122	0.4383	0.083*
O2	1.0611 (3)	0.29377 (6)	0.2203 (3)	0.0471 (6)
C1	0.8618 (4)	0.14411 (9)	0.2810 (4)	0.0337 (7)
C2	0.9202 (5)	0.15626 (10)	0.4718 (4)	0.0400 (8)
C3	0.9317 (5)	0.12581 (12)	0.6167 (5)	0.0525 (9)
H3	0.9674	0.1347	0.7439	0.063*
C4	0.8914 (5)	0.08380 (12)	0.5729 (5)	0.0542 (10)
H4	0.9004	0.0642	0.6707	0.065*
C5	0.8357 (5)	0.06922 (10)	0.3811 (5)	0.0422 (8)
C6	0.7989 (5)	0.02510 (11)	0.3339 (6)	0.0587 (11)
H6	0.8090	0.0052	0.4312	0.070*
C7	0.7494 (6)	0.01134 (11)	0.1513 (7)	0.0654 (12)

H7	0.7285	−0.0178	0.1234	0.079*
C8	0.7298 (6)	0.04084 (11)	0.0046 (6)	0.0622 (11)
H8	0.6937	0.0313	−0.1216	0.075*
C9	0.7629 (5)	0.08375 (10)	0.0430 (5)	0.0497 (9)
H9	0.7481	0.1029	−0.0577	0.060*
C10	0.8191 (4)	0.09950 (9)	0.2322 (4)	0.0358 (7)
C11	0.8430 (4)	0.17606 (9)	0.1302 (4)	0.0360 (7)
H11	0.7864	0.1685	0.0023	0.043*
C12	0.9562 (5)	0.28269 (9)	0.0607 (4)	0.0355 (7)
C13	0.9074 (4)	0.31232 (9)	−0.1072 (4)	0.0330 (7)
C14	0.8915 (4)	0.35600 (9)	−0.0735 (5)	0.0385 (8)
H14	0.9137	0.3654	0.0517	0.046*
C15	0.8436 (5)	0.38593 (10)	−0.2206 (5)	0.0456 (9)
C16	0.8164 (5)	0.37093 (12)	−0.4034 (5)	0.0551 (10)
H16	0.7840	0.3904	−0.5048	0.066*
C17	0.8357 (5)	0.32802 (12)	−0.4401 (5)	0.0560 (10)
H17	0.8191	0.3190	−0.5648	0.067*
C18	0.8798 (5)	0.29812 (10)	−0.2929 (5)	0.0421 (8)
H18	0.8906	0.2690	−0.3180	0.051*
C19	0.8209 (6)	0.43299 (10)	−0.1815 (6)	0.0701 (12)
H19A	0.9126	0.4496	−0.2228	0.105*
H19B	0.8456	0.4372	−0.0466	0.105*
H19C	0.6899	0.4421	−0.2501	0.105*
H2	0.782 (3)	0.2362 (10)	−0.085 (3)	0.048 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0403 (16)	0.0307 (14)	0.0373 (15)	0.0000 (12)	0.0046 (12)	0.0056 (12)
N2	0.0448 (17)	0.0299 (14)	0.0311 (16)	−0.0027 (12)	−0.0040 (13)	0.0032 (12)
O1	0.0730 (18)	0.0479 (14)	0.0415 (14)	−0.0114 (13)	0.0139 (14)	−0.0084 (11)
O2	0.0525 (15)	0.0393 (13)	0.0358 (13)	−0.0018 (11)	−0.0055 (11)	−0.0021 (10)
C1	0.0314 (17)	0.0342 (17)	0.0336 (17)	0.0031 (13)	0.0074 (14)	0.0037 (13)
C2	0.039 (2)	0.0409 (19)	0.0386 (19)	0.0010 (15)	0.0110 (16)	0.0014 (15)
C3	0.059 (2)	0.065 (2)	0.0294 (19)	0.0026 (19)	0.0086 (17)	0.0098 (17)
C4	0.053 (2)	0.057 (2)	0.053 (2)	0.0070 (18)	0.0164 (19)	0.0223 (19)
C5	0.0315 (18)	0.0382 (19)	0.056 (2)	0.0047 (14)	0.0121 (16)	0.0126 (16)
C6	0.049 (2)	0.041 (2)	0.087 (3)	0.0041 (17)	0.021 (2)	0.022 (2)
C7	0.067 (3)	0.033 (2)	0.094 (3)	−0.0100 (19)	0.023 (3)	−0.005 (2)
C8	0.071 (3)	0.042 (2)	0.072 (3)	−0.0121 (19)	0.021 (2)	−0.012 (2)
C9	0.056 (2)	0.0386 (19)	0.052 (2)	−0.0084 (16)	0.0147 (19)	−0.0020 (16)
C10	0.0284 (18)	0.0361 (17)	0.042 (2)	0.0035 (13)	0.0104 (15)	0.0034 (14)
C11	0.0352 (19)	0.0351 (17)	0.0339 (18)	0.0015 (14)	0.0056 (15)	0.0023 (14)
C12	0.0378 (19)	0.0307 (17)	0.0336 (19)	0.0043 (14)	0.0051 (15)	−0.0026 (14)
C13	0.0312 (17)	0.0301 (16)	0.0345 (18)	−0.0003 (13)	0.0056 (14)	0.0007 (13)
C14	0.0356 (19)	0.0314 (16)	0.045 (2)	−0.0033 (14)	0.0074 (15)	−0.0004 (14)
C15	0.0315 (19)	0.0367 (19)	0.066 (3)	−0.0003 (14)	0.0114 (17)	0.0126 (17)
C16	0.043 (2)	0.058 (2)	0.059 (3)	−0.0010 (18)	0.0089 (19)	0.0244 (19)

C17	0.055 (2)	0.073 (3)	0.039 (2)	−0.003 (2)	0.0122 (18)	0.0092 (19)
C18	0.042 (2)	0.0399 (18)	0.043 (2)	−0.0014 (15)	0.0107 (16)	−0.0012 (15)
C19	0.059 (3)	0.036 (2)	0.114 (4)	0.0054 (18)	0.027 (3)	0.019 (2)

Geometric parameters (Å, º)

N1—C11	1.277 (4)	C8—C9	1.367 (4)
N1—N2	1.380 (3)	C8—H8	0.9300
N2—C12	1.350 (4)	C9—C10	1.408 (4)
N2—H2	0.898 (10)	C9—H9	0.9300
O1—C2	1.353 (4)	C11—H11	0.9300
O1—H1	0.8200	C12—C13	1.490 (4)
O2—C12	1.227 (3)	C13—C18	1.388 (4)
C1—C2	1.384 (4)	C13—C14	1.390 (4)
C1—C10	1.439 (4)	C14—C15	1.384 (4)
C1—C11	1.462 (4)	C14—H14	0.9300
C2—C3	1.407 (4)	C15—C16	1.377 (5)
C3—C4	1.352 (5)	C15—C19	1.508 (4)
C3—H3	0.9300	C16—C17	1.375 (5)
C4—C5	1.413 (5)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.385 (4)
C5—C6	1.417 (5)	C17—H17	0.9300
C5—C10	1.419 (4)	C18—H18	0.9300
C6—C7	1.346 (5)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—C8	1.388 (5)	C19—H19C	0.9600
C7—H7	0.9300		

C11—N1—N2	116.3 (3)	C9—C10—C1	123.5 (3)
C12—N2—N1	118.8 (2)	C5—C10—C1	119.1 (3)
C12—N2—H2	123 (2)	N1—C11—C1	119.8 (3)
N1—N2—H2	116 (2)	N1—C11—H11	120.1
C2—O1—H1	109.5	C1—C11—H11	120.1
C2—C1—C10	119.2 (3)	O2—C12—N2	122.7 (3)
C2—C1—C11	120.7 (3)	O2—C12—C13	122.2 (3)
C10—C1—C11	120.2 (3)	N2—C12—C13	115.2 (3)
O1—C2—C1	123.0 (3)	C18—C13—C14	119.4 (3)
O1—C2—C3	116.2 (3)	C18—C13—C12	122.8 (3)
C1—C2—C3	120.8 (3)	C14—C13—C12	117.7 (3)
C4—C3—C2	120.7 (3)	C15—C14—C13	122.0 (3)
C4—C3—H3	119.7	C15—C14—H14	119.0
C2—C3—H3	119.7	C13—C14—H14	119.0
C3—C4—C5	121.2 (3)	C16—C15—C14	117.4 (3)
C3—C4—H4	119.4	C16—C15—C19	121.6 (3)
C5—C4—H4	119.4	C14—C15—C19	121.1 (3)
C4—C5—C6	121.7 (3)	C17—C16—C15	121.8 (3)
C4—C5—C10	119.1 (3)	C17—C16—H16	119.1
C6—C5—C10	119.2 (3)	C15—C16—H16	119.1

C7—C6—C5	121.4 (3)	C16—C17—C18	120.6 (3)
C7—C6—H6	119.3	C16—C17—H17	119.7
C5—C6—H6	119.3	C18—C17—H17	119.7
C6—C7—C8	119.8 (3)	C17—C18—C13	118.8 (3)
C6—C7—H7	120.1	C17—C18—H18	120.6
C8—C7—H7	120.1	C13—C18—H18	120.6
C9—C8—C7	120.9 (4)	C15—C19—H19A	109.5
C9—C8—H8	119.5	C15—C19—H19B	109.5
C7—C8—H8	119.5	H19A—C19—H19B	109.5
C8—C9—C10	121.3 (3)	C15—C19—H19C	109.5
C8—C9—H9	119.3	H19A—C19—H19C	109.5
C10—C9—H9	119.3	H19B—C19—H19C	109.5
C9—C10—C5	117.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.90 (1)	2.00 (1)	2.869 (3)	163 (3)
O1—H1···N1	0.82	1.85	2.567 (3)	146

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