

## (*E*)-*N'*-(2-Hydroxynaphthalen-1-yl)-methylidene]-4-methylbenzohydrazide

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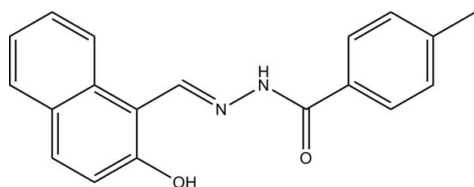
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.068;  $wR$  factor = 0.192; data-to-parameter ratio = 15.7.

In the title compound,  $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_2$ , the benzene ring and the naphthyl ring system form a dihedral angle of  $8.7(3)^\circ$  and an intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond generates an  $S(6)$  ring. In the crystal, molecules are linked by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming  $C(4)$  chains propagating in  $[001]$ .

### Related literature

For hydrazones we have reported previously and background references, see: Liu & You (2010*a,b,c*); Liu & Wang (2010*a,b*). For a related structure, see: Cao (2009).



### Experimental

#### Crystal data

$\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_2$   
 $M_r = 304.34$   
Monoclinic,  $P2_1/c$   
 $a = 11.014(2)$  Å  
 $b = 15.487(2)$  Å

$c = 9.150(1)$  Å  
 $\beta = 93.503(3)^\circ$   
 $V = 1557.8(4)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation

$\mu = 0.09$  mm<sup>-1</sup>  
 $T = 298$  K

$0.20 \times 0.17 \times 0.15$  mm

#### Data collection

Bruker SMART CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{\min} = 0.983$ ,  $T_{\max} = 0.987$

12464 measured reflections  
3335 independent reflections  
1515 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.065$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.192$   
 $S = 0.93$   
3335 reflections  
213 parameters  
1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O2}^i$	0.90 (1)	2.02 (1)	2.897 (3)	164 (3)
$\text{O1}-\text{H1}\cdots\text{N1}$	0.82	1.86	2.586 (3)	146

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

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: HB5818).

### References

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**supplementary materials**

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**(E)-N'-[(2-Hydroxynaphthalen-1-yl)methylidene]-4-methylbenzohydrazide**

**S.-Y. Liu, S.-S. Sun, T.-T. Zheng, X.-L. Zheng, X.-F. Zhao and X.-F. Li**

**Comment**

As a continuation of our structural studies of hydrazones (Liu & You, 2010*a,b,c*; Liu & Wang, 2010*a,b*), we report herein the crystal structure of the title compound, (I) (Fig. 1).

The dihedral angle between the C1—C10 benzene ring and the C13—C18 naphthyl ring is 8.7 (3)°. All the bond lengths are comparable to those observed in related structures (Cao, 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 *c* axis (Fig. 2 and Table 1).

**Experimental**

The title compound was prepared by the condensation reaction of 2-hydroxy-1-naphthaldehyde (0.05 mol, 8.6 g) and 4-methylbenzohydrazide (0.05 mol, 7.5 g) in anhydrous methanol (200 ml) at ambient temperature. Colourless blocks were obtained by slow evaporation of the solution for a period of a week.

**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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $1.5U_{\text{eq}}(\text{O and C19})$ .

**Figures**

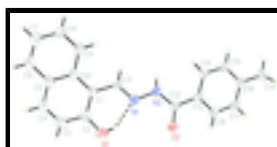


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are shown as spheres of arbitrary radius and the intramolecular hydrogen bond is drawn as a dashed line.

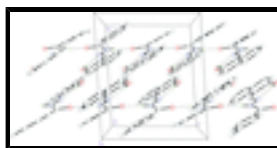


Fig. 2. The packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted.

**(E)-N'-[(2-Hydroxynaphthalen-1-yl)methylidene]- 4-methylbenzohydrazide**

*Crystal data*

C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>

$F(000) = 640$

# supplementary materials

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$$M_r = 304.34$$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$$a = 11.014 (2) \text{ \AA}$$

$$b = 15.487 (2) \text{ \AA}$$

$$c = 9.150 (1) \text{ \AA}$$

$$\beta = 93.503 (3)^\circ$$

$$V = 1557.8 (4) \text{ \AA}^3$$

$$Z = 4$$

$$D_x = 1.298 \text{ Mg m}^{-3}$$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1270 reflections

$$\theta = 2.3\text{--}26.4^\circ$$

$$\mu = 0.09 \text{ mm}^{-1}$$

$$T = 298 \text{ K}$$

Block, colourless

$$0.20 \times 0.17 \times 0.15 \text{ mm}$$

## Data collection

Bruker SMART CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)

$$T_{\min} = 0.983, T_{\max} = 0.987$$

12464 measured reflections

3335 independent reflections

1515 reflections with  $I > 2\sigma(I)$

$$R_{\text{int}} = 0.065$$

$$\theta_{\max} = 27.0^\circ, \theta_{\min} = 1.9^\circ$$

$$h = -14 \rightarrow 13$$

$$k = -19 \rightarrow 19$$

$$l = -11 \rightarrow 11$$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.068$$

$$wR(F^2) = 0.192$$

$$S = 0.93$$

3335 reflections

213 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

$$w = 1/[\sigma^2(F_o^2) + (0.0921P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\min} = -0.25 \text{ e \AA}^{-3}$$

## 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.6996 (2)	0.17460 (14)	-0.0689 (2)	0.0519 (6)
N2	0.7488 (2)	0.24189 (14)	0.0157 (2)	0.0525 (7)
O1	0.5593 (2)	0.11437 (14)	-0.2818 (2)	0.0706 (7)
H1	0.5958	0.1516	-0.2329	0.106*
O2	0.75910 (18)	0.32363 (11)	-0.1872 (2)	0.0596 (6)
C1	0.6450 (2)	0.02635 (17)	-0.0848 (3)	0.0472 (7)
C2	0.5756 (3)	0.03725 (19)	-0.2161 (3)	0.0553 (8)
C3	0.5169 (3)	-0.0341 (2)	-0.2832 (4)	0.0706 (9)
H3	0.4679	-0.0261	-0.3686	0.085*
C4	0.5303 (3)	-0.1141 (2)	-0.2263 (4)	0.0702 (10)
H4	0.4897	-0.1600	-0.2731	0.084*
C5	0.6039 (3)	-0.13015 (19)	-0.0983 (4)	0.0586 (8)
C6	0.6208 (3)	-0.2140 (2)	-0.0396 (4)	0.0693 (10)
H6	0.5810	-0.2604	-0.0857	0.083*
C7	0.6934 (3)	-0.2278 (2)	0.0816 (4)	0.0761 (10)
H7	0.7041	-0.2835	0.1183	0.091*
C8	0.7527 (3)	-0.1584 (2)	0.1524 (4)	0.0721 (10)
H8	0.8030	-0.1682	0.2361	0.087*
C9	0.7375 (3)	-0.07684 (18)	0.1001 (3)	0.0575 (8)
H9	0.7780	-0.0316	0.1489	0.069*
C10	0.6618 (2)	-0.05878 (17)	-0.0264 (3)	0.0480 (7)
C11	0.6973 (2)	0.10041 (17)	-0.0080 (3)	0.0494 (7)
H11	0.7299	0.0939	0.0876	0.059*
C12	0.7759 (2)	0.31563 (17)	-0.0533 (3)	0.0464 (7)
C13	0.8249 (2)	0.38767 (17)	0.0401 (3)	0.0456 (7)
C14	0.8877 (3)	0.37590 (19)	0.1745 (3)	0.0568 (8)
H14	0.9016	0.3205	0.2110	0.068*
C15	0.9292 (3)	0.4465 (2)	0.2537 (3)	0.0639 (9)
H15	0.9706	0.4374	0.3440	0.077*
C16	0.9125 (3)	0.5301 (2)	0.2056 (3)	0.0579 (8)
C17	0.8512 (3)	0.54064 (19)	0.0705 (4)	0.0626 (9)
H17	0.8382	0.5961	0.0340	0.075*
C18	0.8091 (3)	0.47147 (18)	-0.0113 (3)	0.0577 (8)
H18	0.7694	0.4809	-0.1026	0.069*
C19	0.9554 (3)	0.6073 (2)	0.2941 (4)	0.0829 (11)
H19A	1.0096	0.6410	0.2388	0.124*
H19B	0.9973	0.5883	0.3834	0.124*
H19C	0.8867	0.6419	0.3165	0.124*
H2	0.752 (3)	0.2325 (19)	0.1132 (12)	0.080*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0629 (16)	0.0419 (13)	0.0516 (15)	-0.0017 (12)	0.0087 (12)	-0.0052 (12)

## supplementary materials

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N2	0.0786 (18)	0.0367 (13)	0.0428 (14)	-0.0055 (12)	0.0079 (13)	-0.0006 (11)
O1	0.0734 (16)	0.0762 (15)	0.0610 (15)	0.0081 (13)	-0.0060 (12)	0.0068 (12)
O2	0.0847 (16)	0.0572 (13)	0.0364 (12)	-0.0029 (10)	-0.0010 (10)	0.0036 (9)
C1	0.0443 (17)	0.0479 (17)	0.0500 (18)	-0.0007 (13)	0.0075 (14)	-0.0086 (13)
C2	0.0518 (18)	0.0588 (19)	0.055 (2)	0.0048 (15)	0.0027 (16)	-0.0034 (16)
C3	0.052 (2)	0.094 (3)	0.065 (2)	-0.0017 (19)	-0.0027 (17)	-0.019 (2)
C4	0.058 (2)	0.069 (2)	0.084 (3)	-0.0140 (18)	0.0074 (19)	-0.029 (2)
C5	0.0523 (19)	0.057 (2)	0.067 (2)	-0.0060 (15)	0.0136 (17)	-0.0147 (17)
C6	0.074 (2)	0.049 (2)	0.087 (3)	-0.0107 (17)	0.023 (2)	-0.0150 (18)
C7	0.094 (3)	0.0457 (19)	0.091 (3)	-0.0033 (19)	0.025 (2)	0.0035 (19)
C8	0.088 (3)	0.058 (2)	0.071 (2)	0.0006 (18)	0.0055 (19)	0.0081 (17)
C9	0.070 (2)	0.0435 (17)	0.060 (2)	-0.0018 (15)	0.0105 (17)	0.0001 (15)
C10	0.0438 (17)	0.0467 (17)	0.0544 (19)	-0.0039 (13)	0.0095 (14)	-0.0081 (14)
C11	0.0538 (18)	0.0454 (17)	0.0495 (17)	0.0011 (14)	0.0065 (14)	-0.0012 (14)
C12	0.0497 (17)	0.0426 (16)	0.0471 (17)	0.0046 (13)	0.0054 (13)	0.0005 (14)
C13	0.0489 (17)	0.0470 (16)	0.0414 (16)	0.0023 (13)	0.0063 (13)	0.0020 (13)
C14	0.0601 (19)	0.0570 (19)	0.0528 (19)	-0.0048 (15)	-0.0001 (16)	0.0112 (15)
C15	0.067 (2)	0.074 (2)	0.0491 (19)	-0.0151 (18)	-0.0055 (16)	0.0005 (17)
C16	0.0520 (18)	0.063 (2)	0.059 (2)	-0.0116 (15)	0.0114 (16)	-0.0079 (16)
C17	0.074 (2)	0.0442 (17)	0.070 (2)	-0.0008 (15)	0.0066 (18)	-0.0003 (16)
C18	0.066 (2)	0.0485 (18)	0.058 (2)	-0.0002 (15)	-0.0016 (16)	0.0042 (15)
C19	0.089 (3)	0.084 (2)	0.077 (2)	-0.025 (2)	0.012 (2)	-0.024 (2)

### *Geometric parameters (Å, °)*

N1—C11	1.278 (3)	C8—C9	1.358 (4)
N1—N2	1.388 (3)	C8—H8	0.9300
N2—C12	1.347 (3)	C9—C10	1.413 (4)
N2—H2	0.902 (10)	C9—H9	0.9300
O1—C2	1.344 (3)	C11—H11	0.9300
O1—H1	0.8200	C12—C13	1.486 (4)
O2—C12	1.234 (3)	C13—C14	1.386 (4)
C1—C2	1.394 (4)	C13—C18	1.388 (3)
C1—C10	1.430 (4)	C14—C15	1.375 (4)
C1—C11	1.446 (3)	C14—H14	0.9300
C2—C3	1.403 (4)	C15—C16	1.376 (4)
C3—C4	1.348 (4)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.382 (4)
C4—C5	1.405 (4)	C16—C19	1.504 (4)
C4—H4	0.9300	C17—C18	1.371 (4)
C5—C6	1.413 (4)	C17—H17	0.9300
C5—C10	1.418 (4)	C18—H18	0.9300
C6—C7	1.344 (4)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—C8	1.395 (4)	C19—H19C	0.9600
C7—H7	0.9300		
C11—N1—N2	116.7 (2)	C9—C10—C1	123.0 (2)
C12—N2—N1	117.7 (2)	C5—C10—C1	120.1 (3)
C12—N2—H2	127.2 (19)	N1—C11—C1	121.3 (3)

N1—N2—H2	114.8 (19)	N1—C11—H11	119.4
C2—O1—H1	109.5	C1—C11—H11	119.4
C2—C1—C10	119.0 (3)	O2—C12—N2	121.7 (3)
C2—C1—C11	120.3 (3)	O2—C12—C13	121.5 (2)
C10—C1—C11	120.7 (3)	N2—C12—C13	116.8 (2)
O1—C2—C1	123.0 (3)	C14—C13—C18	118.0 (3)
O1—C2—C3	117.3 (3)	C14—C13—C12	123.7 (2)
C1—C2—C3	119.7 (3)	C18—C13—C12	118.3 (3)
C4—C3—C2	121.2 (3)	C15—C14—C13	119.7 (3)
C4—C3—H3	119.4	C15—C14—H14	120.2
C2—C3—H3	119.4	C13—C14—H14	120.2
C3—C4—C5	121.9 (3)	C14—C15—C16	123.1 (3)
C3—C4—H4	119.1	C14—C15—H15	118.4
C5—C4—H4	119.1	C16—C15—H15	118.4
C4—C5—C6	122.4 (3)	C15—C16—C17	116.5 (3)
C4—C5—C10	118.0 (3)	C15—C16—C19	123.0 (3)
C6—C5—C10	119.7 (3)	C17—C16—C19	120.5 (3)
C7—C6—C5	121.2 (3)	C18—C17—C16	121.8 (3)
C7—C6—H6	119.4	C18—C17—H17	119.1
C5—C6—H6	119.4	C16—C17—H17	119.1
C6—C7—C8	119.9 (3)	C17—C18—C13	121.0 (3)
C6—C7—H7	120.1	C17—C18—H18	119.5
C8—C7—H7	120.1	C13—C18—H18	119.5
C9—C8—C7	120.6 (3)	C16—C19—H19A	109.5
C9—C8—H8	119.7	C16—C19—H19B	109.5
C7—C8—H8	119.7	H19A—C19—H19B	109.5
C8—C9—C10	121.8 (3)	C16—C19—H19C	109.5
C8—C9—H9	119.1	H19A—C19—H19C	109.5
C10—C9—H9	119.1	H19B—C19—H19C	109.5
C9—C10—C5	116.9 (3)		

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O2 <sup>i</sup>	0.90 (1)	2.02 (1)	2.897 (3)	164 (3)
O1—H1 $\cdots$ N1	0.82	1.86	2.586 (3)	146

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

Fig. 1

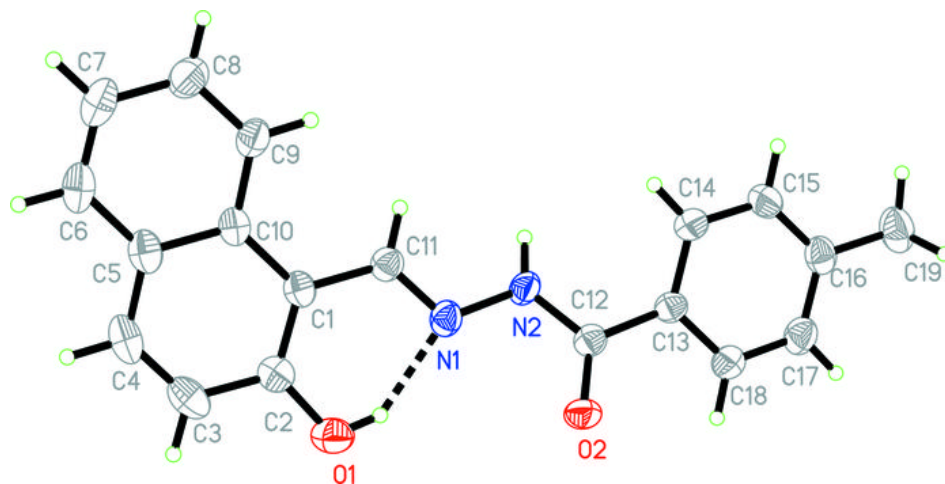




Fig. 2

