Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-[(2-Hydroxynaphthalen-1-yl)methylidene]-4-nitrobenzohydrazide

Yan An, Xiaofeng Li* and Yingjie Zhang

Institute of Marine Materials Science and Engineering, Shanghai Maritime University, Shanghai 201306, People's Republic of China
Correspondence e-mail: xfli@shmtu.edu.cn

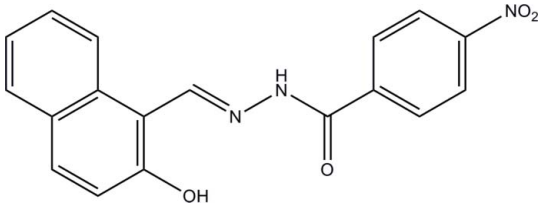
Received 25 October 2011; accepted 31 October 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.069; wR factor = 0.127; data-to-parameter ratio = 12.1.

In the title molecule, $C_{18}H_{13}N_3O_4$, the hydroxy group is involved in the formation of an intramolecular O—H···N hydrogen bond. The dihedral angle between the planes of the benzene ring and the naphthyl ring system is 9.0 (2)°. In the crystal, molecules are linked through N—H···O hydrogen bonds into chains along the *c* axis.

Related literature

For recently published crystal structures of hydrazone compounds, see: Horkaew *et al.* (2011); Fun *et al.* (2011); Su *et al.* (2011); Zhi *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{13}N_3O_4$
M_r = 335.31
Monoclinic, $P2_1/c$
a = 11.208 (3) Å
b = 15.432 (3) Å
c = 8.982 (2) Å
β = 90.701 (2)°
V = 1553.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.17 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.983
8323 measured reflections
2817 independent reflections
1564 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.127
S = 1.02
2817 reflections
232 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.86 (1)	1.85 (2)	2.599 (3)	144 (3)
N2—H2···O2^{i}	0.90 (1)	2.06 (1)	2.923 (3)	160 (3)

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: *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 thank the National Natural Science Foundation of China (21141007), Shanghai Natural Science Foundation (11ZR1414800), the 'Chen Guang' project supported by the Shanghai Municipal Education Commission and the Shanghai Education Development Foundation (09 C G52), the Project of Shanghai Municipal Education Commission (09YZ245, 10YZ111) and Shanghai Maritime University (20110017, 20110013) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5182).

References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Horkaew, J. & Chantrapromma, S. (2011). *Acta Cryst.* E**67**, o2644–o2645.
Horkaew, J., Chantrapromma, S. & Fun, H.-K. (2011). *Acta Cryst.* E**67**, o2985.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Su, F., Gu, Z.-G. & Lin, J. (2011). *Acta Cryst.* E**67**, o1634.
Zhi, F., Wang, R., Zhang, Y., Wang, Q. & Yang, Y.-L. (2011). *Acta Cryst.* E**67**, o2825.

supplementary materials

Acta Cryst. (2011). E**67**, o3278 [**doi:10.1107/S1600536811045685**]

N'-[(2-Hydroxynaphthalen-1-yl)methylidene]-4-nitrobenzohydrazide

Y. An, X. Li and Y. Zhang

Comment

As a continuation of structural studies of hydrazone compounds (Horkaew *et al.*, 2011; Fun *et al.*, 2011; Su *et al.*, 2011; Zhi *et al.*, 2011), we present here the title new hydrazone compound (I).

In (I) (Fig. 1), intramolecular O—H···N hydrogen bond (Table 1) and conjugation effects of the molecule lead to the flattening of the whole molecule. The dihedral angle between the benzene ring and the naphthyl ring is 9.0 (2)°. The bond lengths and angles are normal and comparable to those observed in the related structures (Horkaew *et al.*, 2011; Fun *et al.*, 2011; Su *et al.*, 2011; Zhi *et al.*, 2011).

In the crystal structure of the compound, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1) to form chains along the *c* axis (Fig. 2).

Experimental

Equimolar quantities (0.5 mmol each) of 2-hydroxy-1-naphthaldehyde and 4-nitrobenzohydrazide were mixed in 30 ml me thanol. The mixture was stirred at reflux for 30 min and cooled to room temperature. Yellow block-shaped single crytals were formed by slow evaporation of the solvent in air.

Refinement

The N- and O-bound H atoms were located in a difference Fourier map and were refined with distance restraints [N—H = 0.90 (1) Å, O—H = 0.85 (1) Å], and with U_{iso}(H) fixed to 0.08. The remaining H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

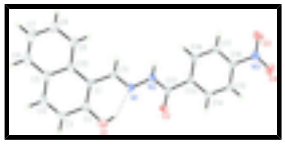


Fig. 1. The molecular structure of (I) with the displacement ellipsoids drawn at the 30% probability level. Intramolecular O—H···N hydrogen bond is shown as a dashed line.

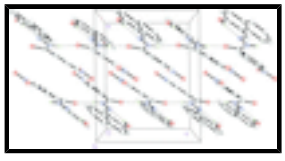


Fig. 2. A portion of the crystal packing viewed approximately along the *b* axis. Intermolecular N—H···O hydrogen bonds are shown as dashed lines. H-atoms not involved in the hydrogen bonding have been omitted.

N'-[(2-Hydroxynaphthalen-1-yl)methylidene]-4-nitrobenzohydrazide

Crystal data

$C_{18}H_{13}N_3O_4$	$F(000) = 696$
$M_r = 335.31$	$D_x = 1.434$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.208$ (3) Å	Cell parameters from 1804 reflections
$b = 15.432$ (3) Å	$\theta = 2.2$–$28.2°$
$c = 8.982$ (2) Å	$\mu = 0.10$ mm^{-1}
$\beta = 90.701$ (2)°	$T = 298$ K
$V = 1553.4$ (6) Å^3	Block, yellow
$Z = 4$	0.20 × 0.20 × 0.17 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2817 independent reflections
Radiation source: fine-focus sealed tube	1564 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.059$
ω scan	$\theta_{max} = 25.5°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -13\rightarrow13$
$T_{min} = 0.980$, $T_{max} = 0.983$	$k = -18\rightarrow16$
8323 measured reflections	$l = -10\rightarrow10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.069$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.127$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.3228P]$ where $P = (F_o^2 + 2F_c^2)/3$
2817 reflections	$(\Delta/\sigma)_{max} < 0.001$
232 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.24$ e Å^{-3}

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	0.2035 (2)	0.17748 (14)	0.5732 (2)	0.0418 (6)
N2	0.2552 (2)	0.24273 (14)	0.4891 (2)	0.0411 (6)
N3	0.4644 (2)	0.60204 (17)	0.2185 (3)	0.0537 (7)
O1	0.06218 (18)	0.12126 (14)	0.7791 (2)	0.0601 (6)
O2	0.25885 (18)	0.33099 (12)	0.6893 (2)	0.0533 (6)
O3	0.5244 (2)	0.58734 (14)	0.1093 (3)	0.0714 (7)
O4	0.4424 (2)	0.67498 (14)	0.2634 (3)	0.0884 (9)
C1	0.1483 (2)	0.02893 (16)	0.5926 (3)	0.0360 (7)
C2	0.0776 (2)	0.04214 (18)	0.7164 (3)	0.0438 (7)
C3	0.0168 (3)	−0.0276 (2)	0.7829 (3)	0.0561 (9)
H3	−0.0314	−0.0177	0.8648	0.067*
C4	0.0283 (3)	−0.1091 (2)	0.7281 (4)	0.0575 (9)
H4A	−0.0136	−0.1540	0.7724	0.069*
C5	0.1020 (2)	−0.12764 (18)	0.6053 (3)	0.0462 (8)
C6	0.1163 (3)	−0.21292 (19)	0.5488 (4)	0.0634 (10)
H6	0.0747	−0.2584	0.5920	0.076*
C7	0.1890 (3)	−0.2291 (2)	0.4333 (4)	0.0697 (10)
H7	0.1977	−0.2854	0.3981	0.084*
C8	0.2511 (3)	−0.1615 (2)	0.3673 (4)	0.0650 (10)
H8	0.3013	−0.1730	0.2879	0.078*
C9	0.2395 (3)	−0.07840 (17)	0.4173 (3)	0.0504 (8)
H9	0.2825	−0.0344	0.3718	0.060*
C10	0.1632 (2)	−0.05776 (16)	0.5373 (3)	0.0377 (7)
C11	0.2028 (2)	0.10178 (16)	0.5167 (3)	0.0377 (7)
H11	0.2380	0.0929	0.4248	0.045*
C12	0.2780 (2)	0.31916 (16)	0.5567 (3)	0.0377 (7)
C13	0.3284 (2)	0.38988 (16)	0.4623 (3)	0.0341 (6)
C14	0.3080 (2)	0.47496 (16)	0.5080 (3)	0.0416 (7)
H14	0.2641	0.4849	0.5935	0.050*
C15	0.3512 (2)	0.54420 (17)	0.4296 (3)	0.0436 (8)
H15	0.3365	0.6007	0.4604	0.052*
C16	0.4170 (2)	0.52799 (16)	0.3039 (3)	0.0386 (7)
C17	0.4401 (2)	0.44479 (17)	0.2556 (3)	0.0431 (7)
H17	0.4845	0.4355	0.1702	0.052*
C18	0.3963 (2)	0.37526 (17)	0.3363 (3)	0.0418 (7)
H18	0.4124	0.3189	0.3060	0.050*
H2	0.263 (3)	0.2326 (19)	0.3912 (13)	0.080*
H1	0.100 (3)	0.1599 (15)	0.730 (3)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0548 (16)	0.0325 (13)	0.0381 (15)	−0.0026 (11)	0.0055 (12)	0.0056 (12)
N2	0.0596 (16)	0.0313 (13)	0.0326 (14)	−0.0049 (11)	0.0078 (13)	0.0009 (12)
N3	0.0514 (17)	0.0484 (18)	0.061 (2)	−0.0082 (13)	0.0051 (15)	0.0071 (15)
O1	0.0646 (16)	0.0614 (15)	0.0547 (16)	0.0077 (12)	0.0191 (12)	−0.0034 (12)
O2	0.0846 (16)	0.0478 (12)	0.0279 (12)	−0.0042 (10)	0.0145 (11)	−0.0027 (9)
O3	0.0816 (18)	0.0724 (16)	0.0608 (16)	−0.0184 (13)	0.0259 (14)	0.0057 (13)
O4	0.106 (2)	0.0380 (13)	0.122 (2)	0.0020 (13)	0.0465 (17)	0.0116 (14)
C1	0.0366 (16)	0.0398 (17)	0.0317 (17)	0.0017 (13)	0.0015 (14)	0.0060 (13)
C2	0.0439 (18)	0.0465 (18)	0.0409 (19)	0.0049 (14)	0.0008 (16)	0.0026 (15)
C3	0.047 (2)	0.079 (2)	0.043 (2)	−0.0017 (17)	0.0121 (16)	0.0169 (18)
C4	0.053 (2)	0.052 (2)	0.067 (2)	−0.0131 (16)	−0.0026 (19)	0.0260 (18)
C5	0.0410 (18)	0.0447 (19)	0.053 (2)	−0.0038 (14)	−0.0023 (16)	0.0124 (16)
C6	0.068 (2)	0.037 (2)	0.085 (3)	−0.0094 (16)	−0.012 (2)	0.0134 (19)
C7	0.081 (3)	0.038 (2)	0.091 (3)	0.0013 (18)	−0.010 (2)	−0.006 (2)
C8	0.075 (2)	0.048 (2)	0.072 (3)	0.0029 (18)	0.005 (2)	−0.0115 (18)
C9	0.057 (2)	0.0370 (18)	0.058 (2)	−0.0003 (14)	0.0067 (17)	0.0002 (15)
C10	0.0387 (17)	0.0341 (16)	0.0402 (18)	−0.0008 (13)	−0.0045 (14)	0.0076 (14)
C11	0.0428 (17)	0.0367 (17)	0.0338 (17)	0.0012 (13)	0.0065 (13)	0.0058 (14)
C12	0.0427 (17)	0.0377 (17)	0.0329 (18)	0.0023 (13)	0.0033 (14)	−0.0011 (14)
C13	0.0376 (16)	0.0339 (16)	0.0307 (17)	−0.0016 (13)	0.0018 (13)	−0.0022 (13)
C14	0.0487 (18)	0.0394 (17)	0.0370 (18)	0.0017 (13)	0.0126 (14)	−0.0052 (14)
C15	0.0482 (18)	0.0344 (16)	0.048 (2)	0.0036 (13)	0.0071 (16)	−0.0034 (14)
C16	0.0380 (16)	0.0349 (16)	0.0428 (18)	−0.0053 (13)	0.0020 (14)	0.0011 (14)
C17	0.0462 (18)	0.0490 (18)	0.0344 (18)	−0.0047 (14)	0.0109 (14)	−0.0030 (15)
C18	0.0478 (18)	0.0369 (16)	0.0408 (19)	−0.0023 (13)	0.0053 (15)	−0.0082 (14)

Geometric parameters (Å, °)

N1—C11	1.274 (3)	C6—C7	1.351 (4)
N1—N2	1.390 (3)	C6—H6	0.9300
N2—C12	1.350 (3)	C7—C8	1.392 (4)
N2—H2	0.898 (10)	C7—H7	0.9300
N3—O3	1.218 (3)	C8—C9	1.365 (4)
N3—O4	1.222 (3)	C8—H8	0.9300
N3—C16	1.479 (3)	C9—C10	1.420 (4)
O1—C2	1.357 (3)	C9—H9	0.9300
O1—H1	0.859 (10)	C11—H11	0.9300
O2—C12	1.227 (3)	C12—C13	1.496 (3)
C1—C2	1.388 (4)	C13—C18	1.391 (3)
C1—C10	1.437 (3)	C13—C14	1.395 (3)
C1—C11	1.453 (3)	C14—C15	1.371 (3)
C2—C3	1.411 (4)	C14—H14	0.9300
C3—C4	1.357 (4)	C15—C16	1.379 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.415 (4)	C16—C17	1.381 (3)

C4—H4A	0.9300	C17—C18	1.388 (3)
C5—C10	1.420 (3)	C17—H17	0.9300
C5—C6	1.420 (4)	C18—H18	0.9300
C11—N1—N2	116.7 (2)	C7—C8—H8	119.5
C12—N2—N1	117.8 (2)	C8—C9—C10	121.4 (3)
C12—N2—H2	125 (2)	C8—C9—H9	119.3
N1—N2—H2	117 (2)	C10—C9—H9	119.3
O3—N3—O4	123.6 (3)	C5—C10—C9	117.0 (2)
O3—N3—C16	118.7 (3)	C5—C10—C1	120.0 (3)
O4—N3—C16	117.7 (3)	C9—C10—C1	123.0 (2)
C2—O1—H1	110 (2)	N1—C11—C1	121.6 (3)
C2—C1—C10	118.9 (2)	N1—C11—H11	119.2
C2—C1—C11	120.6 (2)	C1—C11—H11	119.2
C10—C1—C11	120.5 (2)	O2—C12—N2	122.2 (2)
O1—C2—C1	122.8 (3)	O2—C12—C13	120.9 (2)
O1—C2—C3	116.5 (3)	N2—C12—C13	117.0 (2)
C1—C2—C3	120.7 (3)	C18—C13—C14	119.0 (2)
C4—C3—C2	120.3 (3)	C18—C13—C12	123.8 (2)
C4—C3—H3	119.9	C14—C13—C12	117.1 (2)
C2—C3—H3	119.9	C15—C14—C13	121.5 (3)
C3—C4—C5	122.0 (3)	C15—C14—H14	119.3
C3—C4—H4A	119.0	C13—C14—H14	119.3
C5—C4—H4A	119.0	C14—C15—C16	118.3 (2)
C4—C5—C10	118.1 (3)	C14—C15—H15	120.8
C4—C5—C6	122.4 (3)	C16—C15—H15	120.8
C10—C5—C6	119.5 (3)	C15—C16—C17	122.0 (2)
C7—C6—C5	121.2 (3)	C15—C16—N3	118.9 (3)
C7—C6—H6	119.4	C17—C16—N3	119.0 (3)
C5—C6—H6	119.4	C16—C17—C18	119.1 (3)
C6—C7—C8	119.9 (3)	C16—C17—H17	120.5
C6—C7—H7	120.1	C18—C17—H17	120.5
C8—C7—H7	120.1	C17—C18—C13	120.0 (2)
C9—C8—C7	120.9 (3)	C17—C18—H18	120.0
C9—C8—H8	119.5	C13—C18—H18	120.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.86 (1)	1.85 (2)	2.599 (3)	144 (3)
N2—H2···O2^{i}	0.90 (1)	2.06 (1)	2.923 (3)	160 (3)

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

Fig. 1

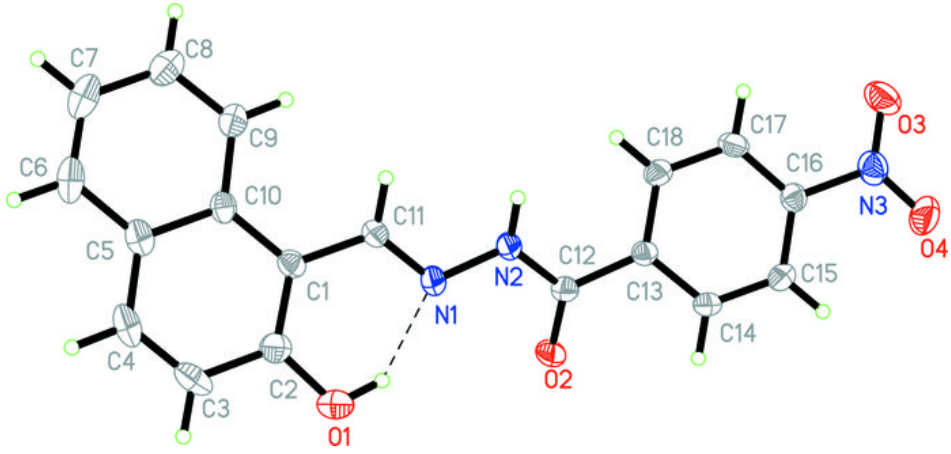

C7
C8
C9
C6
C10
C11
C5
C1
N1
N2
C12
C18
C17
O3
C16
N3
O4
C15
C13
C14
C4
C2
O2
C3
O1

Fig. 2