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(*E*)-4-Hydroxy-*N*′-[(2-hydroxynaphthalen-1-yl)methylene]benzohydrazide

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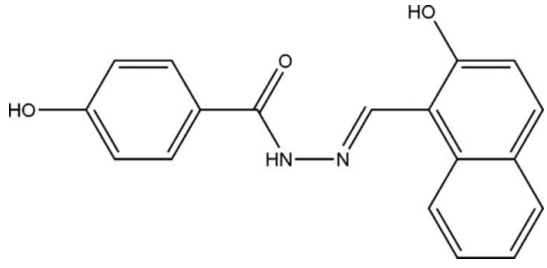
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.073; data-to-parameter ratio = 12.2.

The title molecule, $C_{18}H_{14}N_2O_3$, adopts a *trans* configuration with respect to the C=N double bond. The naphthalene system and the benzene ring make a dihedral angle of 30.3 (3)°. In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds result in the formation of two-dimensional layers parallel to the *bc* plane.

Related literature

Recently, we have reported some organotin(IV) complexes with the Schiff base *o*-vanillin-2-thiophenoylhydrazone (Yin & Chen, 2006).



Experimental

Crystal data

$C_{18}H_{14}N_2O_3$
M_r = 306.31
Monoclinic, $P2_1/c$
a = 14.702 (8) Å
b = 9.793 (5) Å
c = 10.505 (6) Å
β = 104.936 (8)°
V = 1461.4 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.33 × 0.15 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.988
6669 measured reflections
2533 independent reflections
1429 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.073
S = 1.00
2533 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 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
O2—H2···O1^{i}	0.82	1.87	2.681 (2)	169
N1—H1···O3^{ii}	0.86	2.22	3.020 (3)	155

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: CV2232).

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Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Yin, H. D. & Chen, S. W. (2006). *J. Organomet. Chem.* **691**, 3103–3108.

supplementary materials

Acta Cryst. (2007). E**63**, o2633 [**doi:10.1107/S1600536807019101**]

(*E*)-4-Hydroxy-*N*'-[(2-hydroxynaphthalen-1-yl)methylene]benzohydrazide

J.-C. Cui, Q.-X. Pan, H.-D. Yin and Y.-L. Qiao

Comment

Recently, we have reported some organotin(IV) complexes with Schiff base of *o*-vanillin-2-thiophenoylhydrazone (Yin, Chen, 2006). As an extension of our work on the structural characterization of Schiff base compounds, the title compound, (I), is reported here (Fig. 1).

In the title compound, (I), the C8=N2 bond length of 1.280 (2) Å conforms to the value for a double bond, while the C1—N1 bond [1.367 (2) Å] and N1—N2 bond [1.366 (2) Å] (Table 1) are greater than the value for a double bond and less than the value for a single bond because of conjugation effects in the molecule. The dihedral angle between the benzene ring and bicycle is 30.3 (3) Å.

The occurrence of O—H···O hydrogen bonds results in the formation of infinite chains which are linked by N—H···O hydrogen bonds, forming two-dimensional layers parallel to the bc plane (Table 2 and Fig. 2).

Experimental

The title compound was synthesized by the reaction of 2-hydroxynaphthaldehyde (5 mmol) with 4-hydroxybenzoylhydrazide (5 mmol). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

All H atoms were placed in geometrically idealized positions (N—H, O—H and C—H of 0.86, 0.82 and 0.93 Å, respectively) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Figures

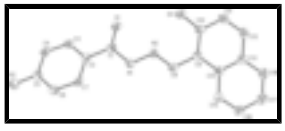

Fig. 1. The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

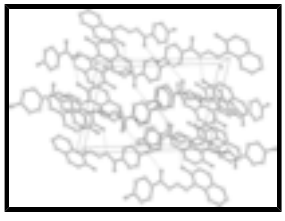

Fig. 2. Crystal packing of the title complex.

(*E*)-4-Hydroxy-*N*'-[(2-hydroxynaphthalen-1-yl)methylene]benzohydrazide

Crystal data

$C_{18}H_{14}N_2O_3$	F_{000} = 640
M_r = 306.31	D_x = 1.392 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.702 (8) Å	Cell parameters from 1267 reflections
b = 9.793 (5) Å	θ = 2.5–25.1º
c = 10.505 (6) Å	μ = 0.10 mm^{-1}
β = 104.936 (8)º	T = 293 (2) K
V = 1461.4 (14) Å^3	Block, colourless
Z = 4	0.33 × 0.15 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2533 independent reflections
Radiation source: fine-focus sealed tube	1429 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→17
T_{min} = 0.969, T_{max} = 0.988	k = −11→10
6669 measured reflections	l = −12→12

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0083P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.073	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
2533 reflections	Extinction correction: none
208 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.78273 (11)	0.63202 (17)	0.93917 (17)	0.0416 (5)
H1	0.7969	0.5977	1.0172	0.050*
N2	0.84010 (12)	0.72366 (17)	0.89997 (17)	0.0397 (5)
O1	0.68675 (9)	0.64966 (15)	0.73723 (15)	0.0510 (4)
O2	0.45522 (10)	0.21350 (15)	0.97122 (14)	0.0605 (5)
H2	0.4170	0.1872	0.9043	0.091*
O3	0.85922 (9)	0.90098 (14)	0.73316 (13)	0.0495 (4)
H3	0.8315	0.8434	0.7657	0.074*
C1	0.70159 (14)	0.5978 (2)	0.8476 (2)	0.0392 (6)
C2	0.63889 (13)	0.4983 (2)	0.8849 (2)	0.0368 (5)
C3	0.56692 (14)	0.4444 (2)	0.7848 (2)	0.0434 (6)
H3A	0.5605	0.4730	0.6985	0.052*
C4	0.50499 (14)	0.3497 (2)	0.8104 (2)	0.0469 (6)
H4	0.4573	0.3152	0.7419	0.056*
C5	0.51353 (14)	0.3055 (2)	0.9387 (2)	0.0428 (6)
C6	0.58525 (14)	0.3580 (2)	1.0384 (2)	0.0495 (6)
H6	0.5922	0.3287	1.1245	0.059*
C7	0.64653 (14)	0.4531 (2)	1.0119 (2)	0.0455 (6)
H7	0.6941	0.4876	1.0807	0.055*
C8	0.92587 (14)	0.7381 (2)	0.9656 (2)	0.0382 (6)
H8	0.9492	0.6893	1.0431	0.046*
C9	0.98642 (14)	0.8313 (2)	0.9178 (2)	0.0348 (5)
C10	0.95021 (14)	0.9103 (2)	0.8059 (2)	0.0375 (6)
C11	1.00636 (16)	1.0041 (2)	0.7607 (2)	0.0453 (6)
H11	0.9806	1.0571	0.6868	0.054*
C12	1.09888 (15)	1.0176 (2)	0.8251 (2)	0.0462 (6)
H12	1.1354	1.0811	0.7948	0.055*
C13	1.14085 (15)	0.9381 (2)	0.9367 (2)	0.0406 (6)
C14	1.08425 (14)	0.8449 (2)	0.9857 (2)	0.0360 (5)
C15	1.12880 (14)	0.7691 (2)	1.0987 (2)	0.0460 (6)
H15	1.0939	0.7062	1.1326	0.055*
C16	1.22179 (15)	0.7860 (2)	1.1592 (2)	0.0544 (7)
H16	1.2489	0.7350	1.2340	0.065*

C17	1.27718 (16)	0.8783 (3)	1.1110 (2)	0.0593 (7)
H17	1.3407	0.8887	1.1531	0.071*
C18	1.23707 (15)	0.9526 (2)	1.0020 (2)	0.0528 (7)
H18	1.2737	1.0143	0.9696	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0396 (11)	0.0534 (12)	0.0293 (11)	−0.0086 (10)	0.0044 (9)	0.0055 (9)
N2	0.0376 (11)	0.0443 (12)	0.0355 (11)	−0.0053 (9)	0.0067 (9)	−0.0028 (9)
O1	0.0445 (9)	0.0691 (12)	0.0359 (10)	−0.0018 (8)	0.0040 (8)	0.0075 (9)
O2	0.0614 (11)	0.0722 (12)	0.0414 (10)	−0.0287 (9)	0.0014 (8)	0.0013 (9)
O3	0.0477 (10)	0.0600 (11)	0.0369 (9)	0.0007 (8)	0.0038 (8)	0.0072 (8)
C1	0.0366 (13)	0.0455 (15)	0.0346 (14)	0.0088 (12)	0.0075 (11)	−0.0031 (12)
C2	0.0311 (12)	0.0431 (14)	0.0342 (13)	0.0024 (11)	0.0048 (10)	−0.0034 (11)
C3	0.0410 (13)	0.0569 (16)	0.0305 (13)	−0.0004 (12)	0.0063 (11)	0.0040 (12)
C4	0.0415 (14)	0.0603 (17)	0.0332 (15)	−0.0044 (12)	−0.0011 (11)	−0.0051 (12)
C5	0.0388 (14)	0.0477 (16)	0.0385 (15)	−0.0047 (12)	0.0036 (11)	−0.0011 (13)
C6	0.0494 (15)	0.0635 (17)	0.0313 (14)	−0.0106 (13)	0.0024 (11)	0.0022 (12)
C7	0.0379 (14)	0.0604 (17)	0.0320 (14)	−0.0071 (12)	−0.0020 (11)	−0.0054 (12)
C8	0.0428 (14)	0.0428 (14)	0.0268 (13)	0.0028 (11)	0.0048 (10)	0.0012 (11)
C9	0.0409 (13)	0.0326 (13)	0.0309 (13)	−0.0014 (11)	0.0091 (11)	−0.0054 (10)
C10	0.0435 (14)	0.0407 (15)	0.0283 (13)	0.0037 (12)	0.0091 (11)	−0.0037 (11)
C11	0.0604 (16)	0.0457 (15)	0.0300 (13)	−0.0003 (13)	0.0122 (12)	0.0044 (11)
C12	0.0542 (15)	0.0456 (16)	0.0426 (15)	−0.0083 (12)	0.0190 (13)	−0.0017 (12)
C13	0.0442 (14)	0.0418 (15)	0.0375 (14)	0.0016 (12)	0.0139 (11)	−0.0031 (12)
C14	0.0405 (13)	0.0368 (14)	0.0302 (13)	0.0005 (11)	0.0084 (11)	−0.0041 (11)
C15	0.0436 (15)	0.0493 (15)	0.0429 (15)	−0.0014 (12)	0.0070 (11)	0.0017 (12)
C16	0.0439 (15)	0.0637 (18)	0.0494 (16)	0.0061 (13)	0.0006 (12)	0.0051 (14)
C17	0.0385 (15)	0.078 (2)	0.0580 (19)	−0.0011 (14)	0.0072 (13)	−0.0002 (15)
C18	0.0450 (15)	0.0649 (18)	0.0502 (17)	−0.0114 (13)	0.0154 (13)	−0.0030 (14)

Geometric parameters (Å, °)

N1—C1	1.367 (2)	C8—C9	1.452 (3)
N1—N2	1.366 (2)	C8—H8	0.9300
N1—H1	0.8600	C9—C10	1.393 (3)
N2—C8	1.280 (2)	C9—C14	1.438 (3)
O1—C1	1.233 (2)	C10—C11	1.397 (3)
O2—C5	1.347 (2)	C11—C12	1.361 (3)
O2—H2	0.8200	C11—H11	0.9300
O3—C10	1.362 (2)	C12—C13	1.411 (3)
O3—H3	0.8200	C12—H12	0.9300
C1—C2	1.462 (3)	C13—C18	1.411 (3)
C2—C7	1.383 (3)	C13—C14	1.417 (3)
C2—C3	1.390 (3)	C14—C15	1.410 (3)
C3—C4	1.374 (3)	C15—C16	1.361 (3)
C3—H3A	0.9300	C15—H15	0.9300
C4—C5	1.390 (3)	C16—C17	1.396 (3)

C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.380 (3)	C17—C18	1.357 (3)
C6—C7	1.372 (3)	C17—H17	0.9300
C6—H6	0.9300	C18—H18	0.9300
C7—H7	0.9300		
C1—N1—N2	116.33 (18)	C10—C9—C14	118.9 (2)
C1—N1—H1	121.8	C10—C9—C8	120.39 (19)
N2—N1—H1	121.8	C14—C9—C8	120.7 (2)
C8—N2—N1	120.63 (18)	O3—C10—C9	122.9 (2)
C5—O2—H2	109.5	O3—C10—C11	115.8 (2)
C10—O3—H3	109.5	C9—C10—C11	121.4 (2)
O1—C1—N1	118.1 (2)	C12—C11—C10	119.9 (2)
O1—C1—C2	123.7 (2)	C12—C11—H11	120.1
N1—C1—C2	118.1 (2)	C10—C11—H11	120.1
C7—C2—C3	117.7 (2)	C11—C12—C13	121.8 (2)
C7—C2—C1	124.9 (2)	C11—C12—H12	119.1
C3—C2—C1	117.4 (2)	C13—C12—H12	119.1
C4—C3—C2	121.4 (2)	C12—C13—C18	121.1 (2)
C4—C3—H3A	119.3	C12—C13—C14	119.0 (2)
C2—C3—H3A	119.3	C18—C13—C14	119.8 (2)
C3—C4—C5	120.1 (2)	C15—C14—C13	117.10 (19)
C3—C4—H4	119.9	C15—C14—C9	123.9 (2)
C5—C4—H4	119.9	C13—C14—C9	119.0 (2)
O2—C5—C6	118.0 (2)	C16—C15—C14	121.5 (2)
O2—C5—C4	123.4 (2)	C16—C15—H15	119.3
C6—C5—C4	118.7 (2)	C14—C15—H15	119.3
C7—C6—C5	120.8 (2)	C15—C16—C17	121.3 (2)
C7—C6—H6	119.6	C15—C16—H16	119.4
C5—C6—H6	119.6	C17—C16—H16	119.4
C6—C7—C2	121.2 (2)	C18—C17—C16	119.1 (2)
C6—C7—H7	119.4	C18—C17—H17	120.5
C2—C7—H7	119.4	C16—C17—H17	120.5
N2—C8—C9	119.3 (2)	C17—C18—C13	121.2 (2)
N2—C8—H8	120.3	C17—C18—H18	119.4
C9—C8—H8	120.3	C13—C18—H18	119.4

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.87	2.681 (2)	169
N1—H1···O3^{ii}	0.86	2.22	3.020 (3)	155

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

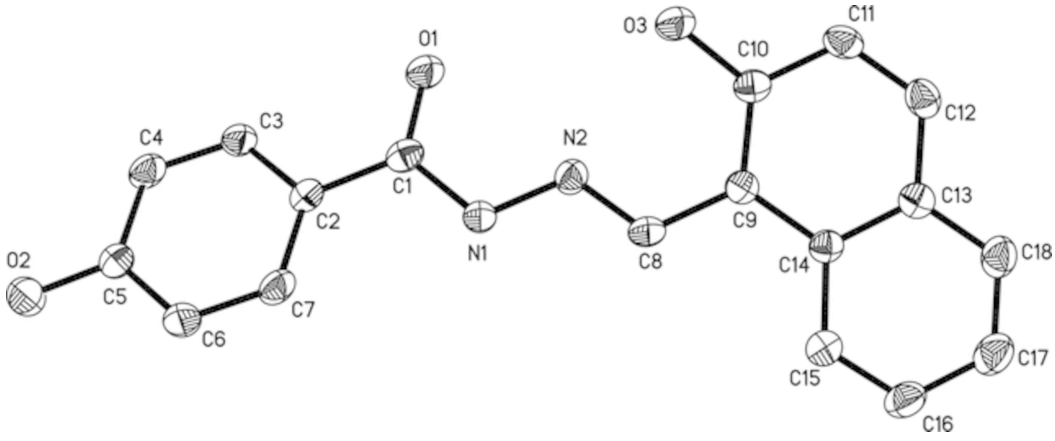
O1
O3
C11
C10
C12
C4
C3
N2
C1
C13
C2
C9
O2
N1
C8
C14
C18
C5
C7
C6
C17
C15
C16

Fig. 2