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3,5-Dihydroxy-*N*′-[(2-hydroxy-1-naphthyl)methylene]benzohydrazide

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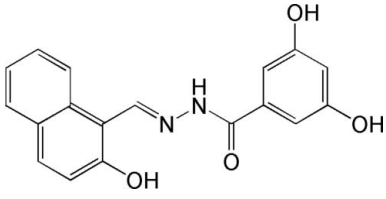
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.110; data-to-parameter ratio = 13.2.

In the title compound, $C_{18}H_{14}N_2O_4$, the dihedral angle between the benzene ring and the naphthyl ring system is 10.1 (2)°. The molecule is nearly planar, with a mean deviation from the plane of 0.141 (2) Å for 24 non-H atoms. An intramolecular O—H···N hydrogen bond forms a pseudo-6-membered ring and the molecules are linked into sheets by intermolecular N—H···O and O—H···O hydrogen bonds.

Related literature

For related structures, see: Brückner *et al.* (2000); Diao (2007); Diao *et al.* (2007); Harrop *et al.* (2003); Huang *et al.* (2007); Li *et al.* (2007); Ren *et al.* (2002).



Experimental

Crystal data

$C_{18}H_{14}N_2O_4$
M_r = 322.31
Orthorhombic, *Pbca*
a = 13.354 (3) Å
b = 14.133 (3) Å
c = 15.077 (3) Å
V = 2845.5 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.30 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.968, T_{max} = 0.971
15775 measured reflections
2949 independent reflections
2433 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
S = 1.03
2949 reflections
223 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4^{i}	0.82	1.96	2.7671 (15)	167
O2—H2···O3^{i}	0.82	1.91	2.7227 (15)	172
O4—H4···N2	0.82	1.78	2.5046 (16)	147
N1—H1*A*···O1^{ii}	0.903 (9)	2.141 (12)	2.9929 (16)	157.0 (19)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); 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: BI2266).

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3,5-Dihydroxy-*N*′-[(2-hydroxy-1-naphthyl)methylene]benzohydrazide

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S1. Comment

Schiff base compounds have received much attention in recent years. Some of the complexes have been found to have pharmacological and antitumor properties (Brückner *et al.*, 2000; Harrop *et al.*, 2003; Ren *et al.*, 2002). As part of our research programme on Schiff base compounds (Diao *et al.*, 2007; Diao, 2007; Li *et al.*, 2007; Huang *et al.*, 2007), we report here the structure of the title compound.

S2. Experimental

2-Hydroxy-1-naphthylaldehyde (1.0 mmol, 172.2 mg) and 3,5-dihydroxybenzoic acid hydrazide (1.0 mmol, 168.2 mg) were dissolved in a methanol solution (70 ml). The mixture was stirred at reflux for 1 h and cooled to room temperature. After keeping the solution in air for two days, yellow block-like crystals were formed.

S3. Refinement

H1A was located from a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. Other H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å, O—H distances of 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

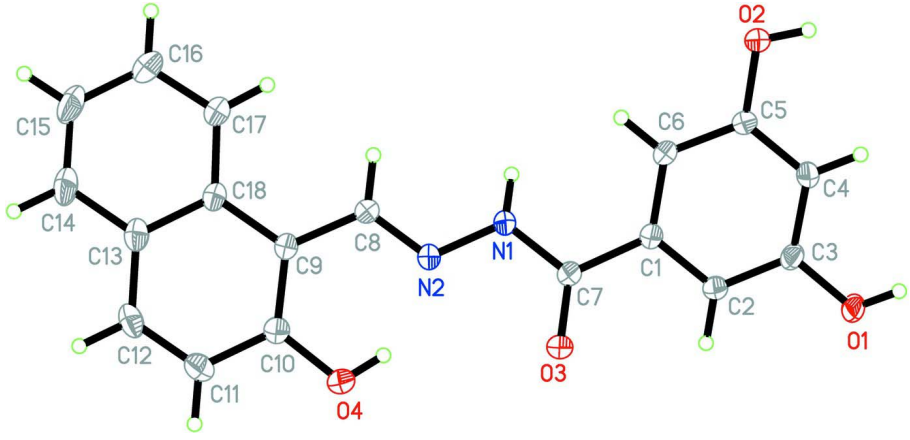

Figure 1

Molecular structure with displacement parameters drawn at the 30% probability level for non-H atoms.

3,5-Dihydroxy-*N*′-[(2-hydroxy-1-naphthyl)methylene]benzohydrazide

Crystal data

$C_{18}H_{14}N_2O_4$
M_r = 322.31

Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab

a = 13.354 (3) Å
b = 14.133 (3) Å
c = 15.077 (3) Å
V = 2845.5 (10) Å^3
Z = 8
F(000) = 1344
D_x = 1.505 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5426 reflections
θ = 2.4–27.8°
μ = 0.11 mm^{-1}
T = 298 K
Block, yellow
0.30 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.968, T_{max} = 0.971

15775 measured reflections
2949 independent reflections
2433 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.5°, θ_{min} = 2.5°
h = −16→15
k = −17→11
l = −18→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
S = 1.03
2949 reflections
223 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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.7945P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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}
O1	0.70957 (9)	−0.44067 (6)	0.65672 (7)	0.0446 (3)
H1	0.6882	−0.4716	0.6987	0.067*
O2	0.64726 (9)	−0.17869 (7)	0.84818 (6)	0.0425 (3)
H2	0.6418	−0.2214	0.8847	0.064*
O3	0.61626 (10)	−0.17124 (7)	0.45805 (7)	0.0468 (3)
O4	0.61263 (10)	0.02287 (7)	0.29946 (7)	0.0486 (3)
H4	0.6170	−0.0031	0.3480	0.073*
N1	0.64522 (10)	−0.04149 (8)	0.53870 (8)	0.0359 (3)
N2	0.62939 (10)	0.01212 (8)	0.46461 (8)	0.0363 (3)

C1	0.65842 (10)	−0.19422 (9)	0.60952 (9)	0.0308 (3)
C2	0.67691 (11)	−0.28981 (9)	0.59712 (9)	0.0336 (3)
H2A	0.6811	−0.3150	0.5402	0.040*
C3	0.68890 (11)	−0.34676 (9)	0.67002 (9)	0.0320 (3)
C4	0.68089 (11)	−0.31096 (9)	0.75469 (9)	0.0317 (3)
H4A	0.6893	−0.3504	0.8035	0.038*
C5	0.66031 (10)	−0.21629 (9)	0.76661 (9)	0.0308 (3)
C6	0.65109 (10)	−0.15717 (9)	0.69414 (9)	0.0317 (3)
H6	0.6400	−0.0928	0.7022	0.038*
C7	0.63939 (11)	−0.13645 (9)	0.52904 (9)	0.0330 (3)
C8	0.62525 (11)	0.10148 (9)	0.47179 (9)	0.0329 (3)
H8	0.6324	0.1299	0.5271	0.040*
C9	0.60931 (10)	0.15896 (9)	0.39384 (9)	0.0306 (3)
C10	0.60344 (11)	0.11717 (10)	0.31095 (9)	0.0350 (3)
C11	0.58622 (12)	0.17008 (11)	0.23410 (10)	0.0423 (4)
H11	0.5823	0.1401	0.1793	0.051*
C12	0.57537 (12)	0.26432 (11)	0.23968 (10)	0.0428 (4)
H12	0.5621	0.2988	0.1885	0.051*
C13	0.58356 (11)	0.31214 (10)	0.32116 (10)	0.0373 (3)
C14	0.57676 (13)	0.41122 (11)	0.32600 (12)	0.0503 (4)
H14	0.5644	0.4457	0.2746	0.060*
C15	0.58771 (15)	0.45740 (11)	0.40359 (14)	0.0577 (5)
H15	0.5848	0.5231	0.4053	0.069*
C16	0.60341 (14)	0.40619 (11)	0.48111 (13)	0.0540 (5)
H16	0.6103	0.4380	0.5347	0.065*
C17	0.60877 (12)	0.30993 (10)	0.47952 (11)	0.0433 (4)
H17	0.6182	0.2770	0.5323	0.052*
C18	0.60030 (10)	0.25964 (9)	0.39969 (10)	0.0325 (3)
H1A	0.6770 (14)	−0.0170 (14)	0.5862 (10)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0747 (8)	0.0223 (5)	0.0367 (6)	0.0096 (5)	0.0150 (5)	0.0020 (4)
O2	0.0740 (8)	0.0276 (5)	0.0261 (5)	0.0017 (5)	0.0004 (5)	−0.0018 (4)
O3	0.0836 (9)	0.0298 (5)	0.0271 (5)	−0.0008 (5)	−0.0043 (5)	−0.0024 (4)
O4	0.0827 (9)	0.0315 (6)	0.0316 (6)	0.0044 (5)	−0.0025 (6)	−0.0048 (4)
N1	0.0559 (8)	0.0243 (6)	0.0275 (6)	0.0007 (5)	−0.0070 (5)	0.0027 (5)
N2	0.0542 (8)	0.0258 (6)	0.0290 (6)	0.0012 (5)	−0.0034 (5)	0.0028 (5)
C1	0.0384 (7)	0.0249 (6)	0.0291 (7)	0.0001 (5)	0.0015 (5)	0.0017 (5)
C2	0.0453 (8)	0.0275 (7)	0.0280 (7)	0.0016 (6)	0.0047 (6)	−0.0022 (5)
C3	0.0388 (7)	0.0219 (6)	0.0352 (7)	0.0032 (5)	0.0054 (6)	−0.0003 (5)
C4	0.0396 (7)	0.0267 (6)	0.0288 (7)	0.0019 (5)	0.0017 (6)	0.0042 (5)
C5	0.0380 (7)	0.0269 (6)	0.0275 (7)	−0.0019 (5)	0.0007 (5)	−0.0027 (5)
C6	0.0413 (8)	0.0224 (6)	0.0315 (7)	0.0010 (5)	0.0006 (6)	−0.0010 (5)
C7	0.0445 (8)	0.0257 (6)	0.0288 (7)	0.0014 (6)	0.0020 (6)	−0.0011 (5)
C8	0.0434 (8)	0.0262 (6)	0.0292 (7)	0.0011 (5)	−0.0024 (6)	−0.0012 (5)
C9	0.0348 (7)	0.0255 (6)	0.0315 (7)	0.0011 (5)	−0.0005 (5)	0.0021 (5)

C10	0.0408 (8)	0.0318 (7)	0.0324 (7)	0.0021 (6)	0.0004 (6)	0.0007 (6)
C11	0.0500 (9)	0.0474 (9)	0.0296 (8)	0.0016 (7)	−0.0006 (6)	0.0010 (6)
C12	0.0463 (8)	0.0475 (9)	0.0346 (8)	0.0041 (7)	0.0014 (7)	0.0164 (7)
C13	0.0350 (7)	0.0335 (7)	0.0435 (8)	0.0025 (6)	0.0041 (6)	0.0101 (6)
C14	0.0563 (10)	0.0338 (8)	0.0607 (11)	0.0060 (7)	0.0075 (8)	0.0189 (7)
C15	0.0718 (12)	0.0246 (7)	0.0767 (13)	0.0041 (7)	0.0076 (10)	0.0062 (8)
C16	0.0724 (12)	0.0295 (8)	0.0602 (11)	0.0032 (7)	−0.0002 (9)	−0.0059 (7)
C17	0.0588 (10)	0.0289 (7)	0.0422 (9)	0.0034 (6)	−0.0019 (7)	−0.0004 (6)
C18	0.0337 (7)	0.0261 (7)	0.0378 (8)	0.0016 (5)	0.0015 (6)	0.0040 (6)

Geometric parameters (Å, º)

O1—C3	1.3704 (15)	C6—H6	0.930
O1—H1	0.820	C8—C9	1.4445 (18)
O2—C5	1.3511 (15)	C8—H8	0.930
O2—H2	0.820	C9—C10	1.3845 (19)
O3—C7	1.2177 (17)	C9—C18	1.4307 (18)
O4—C10	1.3496 (17)	C10—C11	1.398 (2)
O4—H4	0.820	C11—C12	1.342 (2)
N1—C7	1.3521 (17)	C11—H11	0.930
N1—N2	1.3661 (16)	C12—C13	1.406 (2)
N1—H1A	0.903 (9)	C12—H12	0.930
N2—C8	1.2688 (17)	C13—C14	1.405 (2)
C1—C6	1.3826 (19)	C13—C18	1.4150 (19)
C1—C2	1.3859 (18)	C14—C15	1.348 (3)
C1—C7	1.4845 (18)	C14—H14	0.930
C2—C3	1.3716 (19)	C15—C16	1.391 (3)
C2—H2A	0.930	C15—H15	0.930
C3—C4	1.3774 (19)	C16—C17	1.363 (2)
C4—C5	1.3776 (17)	C16—H16	0.930
C4—H4A	0.930	C17—C18	1.402 (2)
C5—C6	1.3810 (18)	C17—H17	0.930
C3—O1—H1	109.5	C10—C9—C18	118.36 (12)
C5—O2—H2	109.5	C10—C9—C8	120.20 (12)
C10—O4—H4	109.5	C18—C9—C8	121.44 (12)
C7—N1—N2	116.97 (11)	O4—C10—C9	122.13 (12)
C7—N1—H1A	119.6 (14)	O4—C10—C11	115.90 (13)
N2—N1—H1A	120.6 (14)	C9—C10—C11	121.96 (13)
C8—N2—N1	119.28 (12)	C12—C11—C10	119.77 (14)
C6—C1—C2	120.41 (12)	C12—C11—H11	120.1
C6—C1—C7	122.26 (12)	C10—C11—H11	120.1
C2—C1—C7	117.16 (12)	C11—C12—C13	121.54 (13)
C3—C2—C1	118.99 (12)	C11—C12—H12	119.2
C3—C2—H2A	120.5	C13—C12—H12	119.2
C1—C2—H2A	120.5	C14—C13—C12	121.28 (14)
O1—C3—C2	118.34 (12)	C14—C13—C18	119.30 (15)
O1—C3—C4	120.46 (12)	C12—C13—C18	119.42 (13)

C2—C3—C4	121.20 (12)	C15—C14—C13	121.38 (15)
C3—C4—C5	119.55 (12)	C15—C14—H14	119.3
C3—C4—H4A	120.2	C13—C14—H14	119.3
C5—C4—H4A	120.2	C14—C15—C16	119.60 (15)
O2—C5—C4	121.77 (12)	C14—C15—H15	120.2
O2—C5—C6	118.08 (12)	C16—C15—H15	120.2
C4—C5—C6	120.15 (12)	C17—C16—C15	120.85 (17)
C5—C6—C1	119.64 (12)	C17—C16—H16	119.6
C5—C6—H6	120.2	C15—C16—H16	119.6
C1—C6—H6	120.2	C16—C17—C18	121.13 (15)
O3—C7—N1	120.67 (12)	C16—C17—H17	119.4
O3—C7—C1	122.67 (12)	C18—C17—H17	119.4
N1—C7—C1	116.62 (12)	C17—C18—C13	117.72 (13)
N2—C8—C9	119.79 (13)	C17—C18—C9	123.38 (13)
N2—C8—H8	120.1	C13—C18—C9	118.90 (13)
C9—C8—H8	120.1		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4^{i}	0.82	1.96	2.7671 (15)	167
O2—H2···O3^{i}	0.82	1.91	2.7227 (15)	172
O4—H4···N2	0.82	1.78	2.5046 (16)	147
N1—H1*A*···O1^{ii}	0.90 (1)	2.14 (1)	2.9929 (16)	157 (2)

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