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N-(2-Hydroxybenzylideneamino)-1,8-naphthalimide

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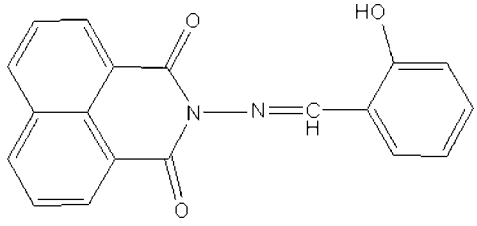
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.175; data-to-parameter ratio = 11.4.

The title compound, $C_{19}H_{12}N_2O_3$, was prepared by the reaction of hydrazine and salicylaldehyde with 1,8-naphthoic anhydride in refluxing dimethylformamide. The structure is stabilized by an intramolecular O—H···N hydrogen bond and the crystal packing exhibits C—H···O hydrogen bonds. The dihedral angle formed by the benzene and naphthalimide systems is 175.9°.

Related literature

For related literature, see: Niemz & Rotello (1997); Ofir (2006); Poteau *et al.* (2000); De Silva *et al.* (1996).



Experimental

Crystal data

$C_{19}H_{12}N_2O_3$
M_r = 316.31
Monoclinic, $P2_1/c$
a = 11.285 (2) Å
b = 18.310 (4) Å
c = 6.9540 (14) Å
β = 94.39 (3)°
V = 1432.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
7451 measured reflections
2526 independent reflections
1873 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.175
S = 1.19
2526 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···N2	0.91 (4)	1.88 (4)	2.612 (4)	134 (4)
C3—H3B···O1^{i}	0.93	2.55	3.341 (4)	143
C14—H14A···O2^{ii}	0.93	2.52	3.166 (4)	127

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2584).

References

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supplementary materials

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N-(2-Hydroxybenzylideneamino)-1,8-naphthalimide

F.-F. Jian, L. Du and W. Yi

Comment

1,8-Naphthlimide derivatives are an important class of compounds. 1,8-Naphthalimides exhibit hydrogen-bonding (Niemz *et al.*, 1997) and cation-dependent (Poteau *et al.*, 2000; De Silva *et al.*, 1996) fluorescence.

In the title compound, the bond lengths and angles are normal (Ofir *et al.*, 2006). The bond lengths of two C═O are little different, with 1.212 (4)Å for C19—O1 and 1.208 (4)Å for C8–02, respectively. The dihedral angle formed by the phenyl ring and naphthalimide moiety is 80.6 (3)°. The molecular conformation is stabilized by a O—H···N hydrogen bond and the crystal packing shows, CH···O hydrogen bonds (Table 2).

Experimental

The single crystals of the title compound were obtained by the reaction hydrazine (0.1 mmol), 1,8-naphthalic anhydride (0.1 mmol) with salicylaldehyde (0.1 mmol) in refluxing DMF. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from a DMF solution at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H=0.93 Å, and with U_{iso}=1.2U_{eq}. The hydroxyl H atom was freely refined.

Figures

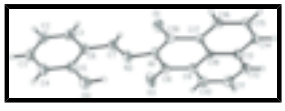


Fig. 1. The molecular structure and atom-labeling scheme for the title compound, with displacement ellipsoids drawn at the 30% probability level.

N-(2-Hydroxybenzylideneamino)-1,8-naphthalimide

Crystal data

$C_{19}H_{12}N_2O_3$	F_{000} = 656
M_r = 316.31	D_x = 1.466 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 220 K
Hall symbol: -P 2y bc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.285 (2) Å	θ = 0–25º
b = 18.310 (4) Å	μ = 0.10 mm^{-1}
c = 6.9540 (14) Å	T = 295 (2) K

β = 94.39 (3)º	Block, yellow
V = 1432.7 (5) Å^3	0.30 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1873 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.028
Monochromator: graphite	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 1.8º
phi and ω scans	h = −13→13
Absorption correction: none	k = −17→21
7451 measured reflections	l = −7→8
2526 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.175	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 1.5868P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.19	$(\Delta/\sigma)_{max} < 0.001$
2526 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
221 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.3228 (2)	0.20728 (13)	0.6655 (4)	0.0573 (7)
O2	0.0289 (2)	0.04509 (12)	0.7451 (4)	0.0676 (8)

O3	0.3368 (2)	−0.01677 (15)	0.4076 (4)	0.0571 (7)
N1	0.1751 (2)	0.12810 (13)	0.7147 (4)	0.0425 (7)
N2	0.2506 (3)	0.07138 (14)	0.6572 (4)	0.0485 (7)
C1	0.4126 (3)	−0.07501 (18)	0.9058 (6)	0.0518 (9)
H1A	0.3999	−0.0616	1.0316	0.062*
C2	0.4805 (3)	−0.1357 (2)	0.8730 (7)	0.0617 (11)
H2B	0.5136	−0.1633	0.9758	0.074*
C3	0.4986 (3)	−0.1551 (2)	0.6859 (7)	0.0597 (11)
H3B	0.5442	−0.1961	0.6635	0.072*
C4	0.4514 (3)	−0.11538 (19)	0.5336 (6)	0.0553 (10)
H4A	0.4651	−0.1294	0.4087	0.066*
C5	0.3827 (3)	−0.05398 (17)	0.5628 (6)	0.0447 (8)
C6	0.3629 (3)	−0.03349 (16)	0.7522 (5)	0.0430 (8)
C7	0.2908 (3)	0.02979 (17)	0.7936 (5)	0.0426 (8)
H7A	0.2743	0.0398	0.9199	0.051*
C8	0.0574 (3)	0.10867 (16)	0.7415 (5)	0.0423 (8)
C9	−0.0255 (3)	0.16947 (16)	0.7623 (4)	0.0372 (7)
C10	−0.1421 (3)	0.15537 (19)	0.7914 (5)	0.0476 (9)
H10A	−0.1687	0.1074	0.7969	0.057*
C11	−0.2206 (3)	0.2130 (2)	0.8128 (5)	0.0507 (9)
H11A	−0.2995	0.2030	0.8329	0.061*
C12	−0.1842 (3)	0.28320 (19)	0.8049 (5)	0.0451 (8)
H12A	−0.2383	0.3207	0.8196	0.054*
C13	−0.0651 (3)	0.30016 (16)	0.7746 (4)	0.0386 (7)
C14	−0.0231 (3)	0.37226 (17)	0.7648 (5)	0.0457 (8)
H14A	−0.0751	0.4109	0.7792	0.055*
C15	0.0915 (3)	0.38627 (17)	0.7348 (5)	0.0451 (8)
H15A	0.1174	0.4344	0.7297	0.054*
C16	0.1716 (3)	0.32912 (17)	0.7113 (5)	0.0416 (8)
H16A	0.2501	0.3395	0.6889	0.050*
C17	0.1350 (3)	0.25784 (16)	0.7212 (4)	0.0345 (7)
C18	0.0156 (3)	0.24226 (15)	0.7523 (4)	0.0323 (7)
C19	0.2195 (3)	0.19840 (16)	0.6968 (5)	0.0393 (7)
H3A	0.297 (5)	0.026 (3)	0.432 (8)	0.13 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0383 (13)	0.0475 (15)	0.087 (2)	0.0010 (11)	0.0099 (13)	−0.0127 (13)
O2	0.0728 (18)	0.0271 (13)	0.106 (2)	−0.0027 (12)	0.0247 (16)	−0.0003 (13)
O3	0.0655 (17)	0.0497 (16)	0.0564 (17)	0.0107 (13)	0.0056 (13)	−0.0027 (13)
N1	0.0478 (16)	0.0285 (14)	0.0520 (17)	0.0096 (12)	0.0091 (13)	−0.0012 (12)
N2	0.0565 (18)	0.0345 (15)	0.0550 (19)	0.0149 (13)	0.0073 (14)	−0.0033 (13)
C1	0.0470 (19)	0.045 (2)	0.062 (2)	0.0022 (16)	−0.0014 (17)	0.0040 (18)
C2	0.044 (2)	0.044 (2)	0.095 (3)	0.0043 (16)	−0.007 (2)	0.011 (2)
C3	0.0362 (18)	0.0365 (19)	0.106 (4)	0.0048 (15)	0.005 (2)	−0.008 (2)
C4	0.0396 (18)	0.041 (2)	0.086 (3)	−0.0004 (16)	0.0107 (19)	−0.015 (2)
C5	0.0326 (16)	0.0341 (17)	0.068 (2)	−0.0033 (13)	0.0059 (16)	−0.0062 (16)

C6	0.0329 (16)	0.0300 (16)	0.066 (2)	−0.0019 (13)	0.0051 (15)	−0.0032 (15)
C7	0.0415 (17)	0.0335 (17)	0.053 (2)	0.0023 (14)	0.0025 (15)	−0.0044 (15)
C8	0.053 (2)	0.0287 (17)	0.046 (2)	0.0023 (14)	0.0090 (15)	0.0006 (14)
C9	0.0418 (17)	0.0329 (16)	0.0372 (18)	0.0002 (13)	0.0043 (14)	−0.0016 (13)
C10	0.051 (2)	0.0408 (19)	0.052 (2)	−0.0077 (16)	0.0110 (16)	0.0007 (16)
C11	0.0382 (18)	0.060 (2)	0.054 (2)	0.0011 (16)	0.0090 (16)	0.0023 (18)
C12	0.0426 (18)	0.049 (2)	0.0438 (19)	0.0119 (15)	0.0052 (15)	0.0028 (16)
C13	0.0423 (17)	0.0360 (17)	0.0369 (18)	0.0100 (14)	−0.0007 (14)	−0.0019 (14)
C14	0.052 (2)	0.0311 (17)	0.053 (2)	0.0129 (15)	−0.0020 (16)	−0.0036 (15)
C15	0.055 (2)	0.0258 (16)	0.053 (2)	−0.0012 (14)	−0.0073 (16)	−0.0031 (14)
C16	0.0412 (17)	0.0376 (18)	0.0450 (19)	−0.0043 (14)	−0.0032 (14)	−0.0025 (14)
C17	0.0361 (16)	0.0308 (16)	0.0356 (17)	0.0012 (12)	−0.0037 (13)	−0.0045 (13)
C18	0.0389 (16)	0.0294 (15)	0.0283 (15)	0.0016 (12)	−0.0002 (12)	−0.0009 (12)
C19	0.0401 (18)	0.0353 (17)	0.0416 (19)	0.0025 (14)	−0.0015 (14)	−0.0065 (14)

Geometric parameters (Å, °)

O1—C19	1.212 (4)	C8—C9	1.469 (4)
O2—C8	1.208 (4)	C9—C10	1.370 (4)
O3—C5	1.346 (4)	C9—C18	1.414 (4)
O3—H3A	0.92 (6)	C10—C11	1.393 (5)
N1—C19	1.391 (4)	C10—H10A	0.9300
N1—C8	1.401 (4)	C11—C12	1.352 (5)
N1—N2	1.420 (3)	C11—H11A	0.9300
N2—C7	1.273 (4)	C12—C13	1.410 (5)
C1—C2	1.379 (5)	C12—H12A	0.9300
C1—C6	1.394 (5)	C13—C14	1.406 (4)
C1—H1A	0.9300	C13—C18	1.414 (4)
C2—C3	1.378 (6)	C14—C15	1.350 (5)
C2—H2B	0.9300	C14—H14A	0.9300
C3—C4	1.360 (6)	C15—C16	1.401 (4)
C3—H3B	0.9300	C15—H15A	0.9300
C4—C5	1.389 (5)	C16—C17	1.372 (4)
C4—H4A	0.9300	C16—H16A	0.9300
C5—C6	1.403 (5)	C17—C18	1.410 (4)
C6—C7	1.457 (4)	C17—C19	1.466 (4)
C7—H7A	0.9300		
C5—O3—H3A	117 (4)	C18—C9—C8	119.7 (3)
C19—N1—C8	126.8 (2)	C9—C10—C11	119.9 (3)
C19—N1—N2	115.1 (3)	C9—C10—H10A	120.0
C8—N1—N2	116.5 (2)	C11—C10—H10A	120.0
C7—N2—N1	114.5 (3)	C12—C11—C10	121.2 (3)
C2—C1—C6	120.6 (4)	C12—C11—H11A	119.4
C2—C1—H1A	119.7	C10—C11—H11A	119.4
C6—C1—H1A	119.7	C11—C12—C13	120.8 (3)
C3—C2—C1	119.2 (4)	C11—C12—H12A	119.6
C3—C2—H2B	120.4	C13—C12—H12A	119.6
C1—C2—H2B	120.4	C14—C13—C12	122.9 (3)
C4—C3—C2	121.4 (3)	C14—C13—C18	118.4 (3)

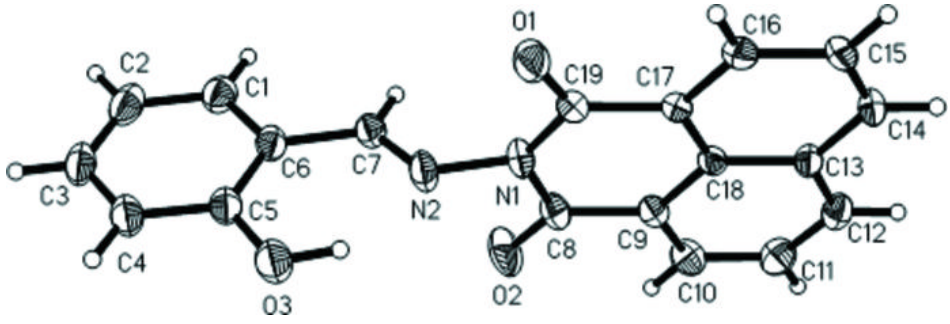
C4—C3—H3B	119.3	C12—C13—C18	118.7 (3)
C2—C3—H3B	119.3	C15—C14—C13	121.1 (3)
C3—C4—C5	120.5 (4)	C15—C14—H14A	119.5
C3—C4—H4A	119.7	C13—C14—H14A	119.5
C5—C4—H4A	119.7	C14—C15—C16	120.7 (3)
O3—C5—C4	118.5 (3)	C14—C15—H15A	119.6
O3—C5—C6	122.6 (3)	C16—C15—H15A	119.6
C4—C5—C6	119.0 (3)	C17—C16—C15	120.3 (3)
C1—C6—C5	119.3 (3)	C17—C16—H16A	119.8
C1—C6—C7	118.7 (3)	C15—C16—H16A	119.8
C5—C6—C7	122.0 (3)	C16—C17—C18	119.7 (3)
N2—C7—C6	120.1 (3)	C16—C17—C19	119.9 (3)
N2—C7—H7A	120.0	C18—C17—C19	120.4 (3)
C6—C7—H7A	120.0	C17—C18—C13	119.8 (3)
O2—C8—N1	120.3 (3)	C17—C18—C9	121.2 (3)
O2—C8—C9	123.7 (3)	C13—C18—C9	119.0 (3)
N1—C8—C9	116.0 (3)	O1—C19—N1	119.9 (3)
C10—C9—C18	120.4 (3)	O1—C19—C17	124.4 (3)
C10—C9—C8	119.9 (3)	N1—C19—C17	115.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···N2	0.91 (4)	1.88 (4)	2.612 (4)	134 (4)
C3—H3B···O1^{i}	0.93	2.55	3.341 (4)	143
C14—H14A···O2^{ii}	0.93	2.52	3.166 (4)	127

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

Fig. 1


O1
C16
C15
C2
C1
C19
C17
C14
C6
C7
C13
C3
N2
N1
C18
C5
C8
C9
C12
C4
O2
C11
O3
C10