Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Benzyl-2,3-dihydro-1*H*-naphtho-[1,2-e][1,3]oxazine

Xu-Hong Yang, Xiu-Ling Chen, Xiang-Ju Diao and Ming-Hu Wu*

Department of Chemistry and Life Sciences, Xianning College, Xianning 437005, People's Republic of China
Correspondence e-mail: minghuwu@hotmail.com

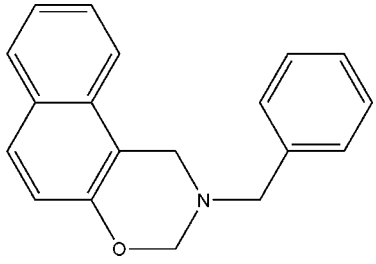
Received 14 June 2007; accepted 20 June 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.063; wR factor = 0.197; data-to-parameter ratio = 13.9.

In the title molecule, $C_{19}H_{17}NO$, the dihedral angle between the naphthyl fused-ring system and the phenyl ring is 17.4 (1)°. In the absence of hydrogen-bonding interactions and π–π stacking interactions, the crystal structure is stabilized by van der Waals interactions.

Related literature

For background information, see: Barker *et al.* (2006); Ren *et al.* (2001); Gentles *et al.* (1991); Petterson *et al.* (1990); Peglion *et al.* (1997).



Experimental

Crystal data

$C_{19}H_{17}NO$
M_r = 275.34
Monoclinic, $P2_1/n$
a = 9.8645 (11) Å
b = 5.2515 (6) Å
c = 27.811 (3) Å
β = 98.716 (1)°
V = 1424.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.04 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.977, T_{max} = 0.997
10025 measured reflections
2643 independent reflections
1556 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.197
S = 0.99
2643 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors gratefully acknowledge financial support of this work from the Plan of Group of Young Scientists Innovation Foundation of Hubei Province (grant No. 2004 T006).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2436).

References

Barker, M., Clackers, M., Copley, R., Demaine, D. A., Humphreys, D., Inglis, G. G. A., Johnston, M. J., Jones, H. T., Haase, M. V., House, D., Loiseau, R., Nisbet, L., Pacquet, F., Skone, P. A., Shanahan, S. E. *et al.* (2006). *J. Med. Chem.* **49**, 4216–4231.
Bruker (2001). *SMART* (Version 5.628) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Gentles, R. G., Middlemiss, D., Proctor, G. R. & Sneddon, A. H. (1991). *J. Chem. Soc. Perkin Trans. 1*, pp. 1423–1431.
Peglion, J. L., Vian, J., Gourment, B., Despaux, N., Audinot, V. & Millan, M. (1997). *Bioorg. Med. Chem. Lett.* **7**, 881–886.
Petterson, I., Liljefors, T. & Bodeso, K. (1990). *J. Med. Chem.* **33**, 2197–2204.
Ren, H. Y., Grady, S., Gamenara, D., Heinzen, H., Moyna, P., Croft, S. L., Kendrick, H., Yardley, V. & Moyna, G. (2001). *Bioorg. Med. Chem. Lett.* **11**, 1851–1854.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

  doi:10.1107/S1600536807030188

supplementary materials

Acta Cryst. (2007). E**63**, o3312 [**doi:10.1107/S1600536807030188**]

2-Benzyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

X.-H. Yang, X.-L. Chen, X.-J. Diao and M.-H. Wu

Comment

Contuning efforts have been made to synthesize oxazine compounds because of their wide applications in agonist triggers, antipsychotic agents (Barker *et al.*, 2006), antimalarial agents (Ren *et al.*, 2001) and serotonin, dopamine receptors (Gentles *et al.*, 1991; Petterson *et al.*, 1990; Peglion *et al.*, 1997). The title compound was prepared by reaction of 2-naphthol, formaldehyde and benzyl amine, The crystal structure of has been determined herein.

In the molecule (Fig. 1.), the dihedral angle between the C14—C19 phenyl ring and naphthyl system is 17.4 (1)°. The four atoms N1/C11/C13/C14 are essentially planar with a C14—C13—N1—C11 torsion angle of −176.5 (2)°.

Experimental

Formaldehyde (8 mL, 40%, 0.1 mol) was added slowly with stirring to a mixture of methanol (35 mL), benzylamine (10.7 g, 0.1 mol) and 2-naphthol (14.4 g, 0.1 mol) over 2 h. The mixture was stirred for additional 60 h at room temperature. The resulting bright yellow solid was filtered and washed with methanol. The solid residue was recrystallized from methanol to give colorless crystals of the title compound in a yield of 85%, which were suitable for X-ray analysis. ^{1}HNMR($CDCl_3$, 400 MHz), 7.79(m, 11H, aromatic), 4.95(s, 2H, N—CH_2—O), 4.33(s, 2H, N—CH_2-heterocyclic), 3.99 (s,2*H*, *N*—CH_2-benzyl).

Refinement

All H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and included in the riding model approximation, with U_{iso} (H) = 1.2U_{iso} (C).

Figures

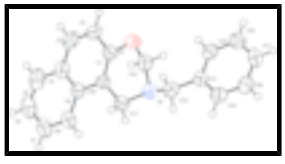


Fig. 1. View of the molecular structure with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-Benzyl-2,3-dihydro-1*H*-naphtho[1,2-e][1,3]oxazine

Crystal data

$C_{19}H_{17}NO$	F_{000} = 584
M_r = 275.34	D_x = 1.284 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 1051 reflections
a = 9.8645 (11) Å	θ = 2.3–20.8º
b = 5.2515 (6) Å	μ = 0.08 mm^{-1}
c = 27.811 (3) Å	T = 292 (2) K
β = 98.7160 (10)º	Block, colorless
V = 1424.1 (3) $Å^3$	0.30 × 0.20 × 0.04 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2643 independent reflections
Radiation source: fine-focus sealed tube	1556 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 292(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -11 \rightarrow 11$
T_{min} = 0.977, T_{max} = 0.997	$k = -6 \rightarrow 6$
10025 measured reflections	$l = -27 \rightarrow 33$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.197	$w = 1/[\sigma^2(F_o^2) + (0.1062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
2643 reflections	$\Delta\rho_{max}$ = 0.20 e $Å^{-3}$
190 parameters	$\Delta\rho_{min}$ = −0.17 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}
C1	0.5579 (3)	0.0173 (5)	0.15827 (10)	0.0455 (7)
C2	0.6084 (3)	−0.1653 (6)	0.12911 (12)	0.0591 (9)
H2	0.6904	−0.2484	0.1403	0.071*
C3	0.5382 (4)	−0.2223 (6)	0.08429 (12)	0.0674 (9)
H3	0.5714	−0.3472	0.0654	0.081*
C4	0.4149 (3)	−0.0924 (6)	0.06629 (11)	0.0546 (8)
C5	0.3421 (4)	−0.1401 (7)	0.01905 (12)	0.0749 (10)
H5	0.3744	−0.2625	−0.0006	0.090*
C6	0.2262 (4)	−0.0094 (8)	0.00225 (12)	0.0783 (11)
H6	0.1797	−0.0424	−0.0288	0.094*
C7	0.1763 (3)	0.1742 (7)	0.03115 (11)	0.0685 (10)
H7	0.0968	0.2634	0.0193	0.082*
C8	0.2435 (3)	0.2240 (6)	0.07684 (10)	0.0541 (8)
H8	0.2089	0.3472	0.0957	0.065*
C9	0.3647 (3)	0.0921 (5)	0.09599 (10)	0.0433 (7)
C10	0.4370 (2)	0.1433 (5)	0.14333 (9)	0.0415 (7)
C11	0.3827 (3)	0.3277 (5)	0.17737 (10)	0.0491 (7)
H11A	0.3955	0.5003	0.1665	0.059*
H11B	0.2851	0.2997	0.1763	0.059*
C12	0.5964 (3)	0.2834 (6)	0.22732 (11)	0.0526 (8)
H12A	0.6431	0.2825	0.2606	0.063*
H12B	0.6258	0.4342	0.2116	0.063*
C13	0.3999 (3)	0.0799 (5)	0.25237 (10)	0.0501 (7)
H13A	0.4184	−0.0749	0.2355	0.060*
H13B	0.3012	0.0954	0.2506	0.060*
C14	0.4638 (2)	0.0594 (5)	0.30480 (10)	0.0416 (7)
C15	0.5551 (3)	−0.1322 (5)	0.32051 (11)	0.0513 (8)
H15	0.5765	−0.2517	0.2982	0.062*
C16	0.6160 (3)	−0.1521 (6)	0.36869 (11)	0.0578 (8)
H16	0.6778	−0.2828	0.3783	0.069*
C17	0.5844 (3)	0.0220 (6)	0.40200 (11)	0.0568 (8)
H17	0.6248	0.0108	0.4344	0.068*
C18	0.4927 (3)	0.2132 (6)	0.38710 (11)	0.0582 (8)
H18	0.4704	0.3313	0.4096	0.070*
C19	0.4331 (3)	0.2312 (5)	0.33884 (11)	0.0530 (8)
H19	0.3713	0.3619	0.3293	0.064*
N1	0.4517 (2)	0.2993 (4)	0.22774 (8)	0.0462 (6)
O1	0.63734 (17)	0.0607 (4)	0.20267 (7)	0.0559 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0412 (14)	0.0474 (17)	0.0483 (18)	−0.0014 (13)	0.0081 (13)	0.0047 (14)
C2	0.0561 (17)	0.061 (2)	0.064 (2)	0.0178 (15)	0.0220 (16)	0.0074 (17)

C3	0.086 (2)	0.061 (2)	0.061 (2)	0.0145 (19)	0.0320 (19)	−0.0080 (17)
C4	0.0670 (19)	0.0519 (19)	0.0462 (19)	−0.0040 (15)	0.0128 (15)	−0.0013 (15)
C5	0.105 (3)	0.071 (2)	0.051 (2)	−0.004 (2)	0.019 (2)	−0.0146 (19)
C6	0.098 (3)	0.091 (3)	0.041 (2)	−0.012 (2)	−0.0062 (19)	−0.003 (2)
C7	0.068 (2)	0.083 (3)	0.050 (2)	−0.0060 (18)	−0.0037 (17)	0.0089 (19)
C8	0.0578 (17)	0.058 (2)	0.0448 (18)	−0.0015 (14)	0.0019 (15)	0.0035 (14)
C9	0.0466 (14)	0.0425 (16)	0.0416 (17)	−0.0062 (13)	0.0094 (13)	0.0005 (13)
C10	0.0418 (14)	0.0422 (16)	0.0413 (17)	−0.0004 (11)	0.0093 (12)	0.0013 (13)
C11	0.0512 (16)	0.0508 (18)	0.0435 (17)	0.0044 (13)	0.0021 (13)	−0.0063 (14)
C12	0.0436 (15)	0.064 (2)	0.0500 (19)	−0.0144 (14)	0.0058 (14)	0.0012 (15)
C13	0.0448 (14)	0.0532 (18)	0.0523 (19)	−0.0089 (14)	0.0074 (13)	−0.0071 (15)
C14	0.0445 (14)	0.0410 (16)	0.0393 (16)	−0.0093 (12)	0.0069 (12)	−0.0042 (13)
C15	0.0569 (17)	0.0454 (18)	0.0542 (19)	0.0016 (14)	0.0164 (15)	−0.0071 (15)
C16	0.0576 (18)	0.054 (2)	0.062 (2)	0.0038 (15)	0.0093 (16)	0.0069 (17)
C17	0.0672 (19)	0.060 (2)	0.0418 (18)	−0.0149 (17)	0.0024 (15)	0.0076 (16)
C18	0.0680 (19)	0.056 (2)	0.052 (2)	−0.0050 (16)	0.0118 (16)	−0.0121 (16)
C19	0.0540 (17)	0.0450 (17)	0.060 (2)	0.0016 (14)	0.0080 (16)	−0.0050 (15)
N1	0.0503 (13)	0.0430 (14)	0.0441 (14)	−0.0078 (10)	0.0034 (11)	−0.0029 (11)
O1	0.0383 (10)	0.0755 (15)	0.0523 (13)	0.0054 (10)	0.0019 (9)	0.0024 (11)

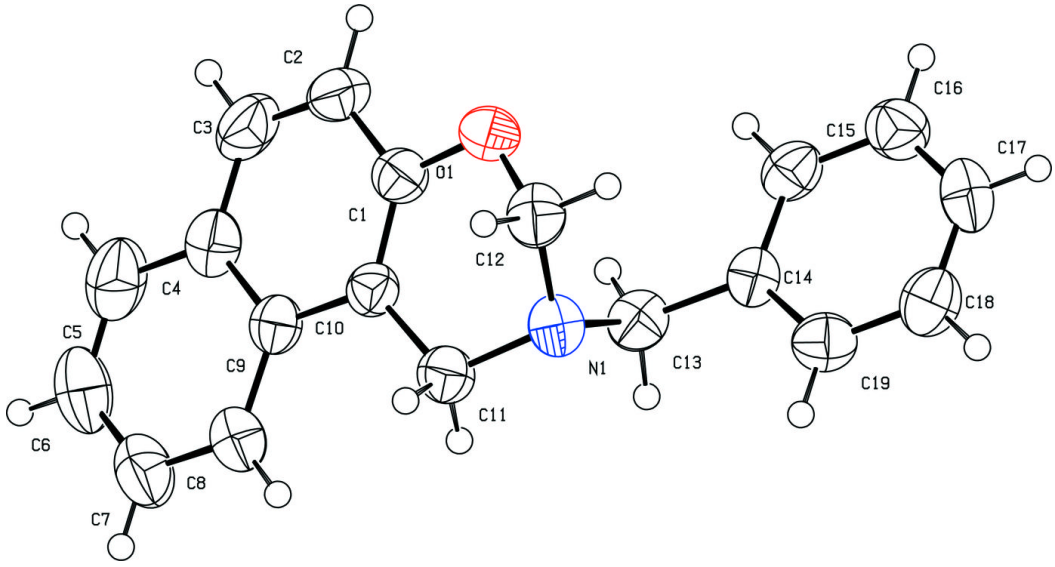
Geometric parameters (Å, °)

C1—C10	1.372 (3)	C11—H11B	0.9700
C1—O1	1.377 (3)	C12—N1	1.431 (3)
C1—C2	1.396 (4)	C12—O1	1.444 (3)
C2—C3	1.364 (4)	C12—H12A	0.9700
C2—H2	0.9300	C12—H12B	0.9700
C3—C4	1.418 (4)	C13—N1	1.471 (3)
C3—H3	0.9300	C13—C14	1.502 (3)
C4—C9	1.411 (4)	C13—H13A	0.9700
C4—C5	1.421 (4)	C13—H13B	0.9700
C5—C6	1.354 (5)	C14—C19	1.374 (4)
C5—H5	0.9300	C14—C15	1.376 (4)
C6—C7	1.392 (5)	C15—C16	1.387 (4)
C6—H6	0.9300	C15—H15	0.9300
C7—C8	1.367 (4)	C16—C17	1.371 (4)
C7—H7	0.9300	C16—H16	0.9300
C8—C9	1.414 (4)	C17—C18	1.373 (4)
C8—H8	0.9300	C17—H17	0.9300
C9—C10	1.425 (3)	C18—C19	1.384 (4)
C10—C11	1.508 (4)	C18—H18	0.9300
C11—N1	1.469 (3)	C19—H19	0.9300
C11—H11A	0.9700		
C10—C1—O1	122.8 (2)	H11A—C11—H11B	107.9
C10—C1—C2	121.7 (3)	N1—C12—O1	113.7 (2)
O1—C1—C2	115.5 (2)	N1—C12—H12A	108.8
C3—C2—C1	120.3 (3)	O1—C12—H12A	108.8
C3—C2—H2	119.8	N1—C12—H12B	108.8
C1—C2—H2	119.8	O1—C12—H12B	108.8

C2—C3—C4	120.4 (3)	H12A—C12—H12B	107.7
C2—C3—H3	119.8	N1—C13—C14	112.6 (2)
C4—C3—H3	119.8	N1—C13—H13A	109.1
C9—C4—C3	118.8 (3)	C14—C13—H13A	109.1
C9—C4—C5	119.3 (3)	N1—C13—H13B	109.1
C3—C4—C5	121.9 (3)	C14—C13—H13B	109.1
C6—C5—C4	120.8 (3)	H13A—C13—H13B	107.8
C6—C5—H5	119.6	C19—C14—C15	117.6 (3)
C4—C5—H5	119.6	C19—C14—C13	121.2 (3)
C5—C6—C7	120.4 (3)	C15—C14—C13	121.3 (3)
C5—C6—H6	119.8	C14—C15—C16	121.9 (3)
C7—C6—H6	119.8	C14—C15—H15	119.0
C8—C7—C6	120.3 (3)	C16—C15—H15	119.0
C8—C7—H7	119.8	C17—C16—C15	119.6 (3)
C6—C7—H7	119.8	C17—C16—H16	120.2
C7—C8—C9	121.3 (3)	C15—C16—H16	120.2
C7—C8—H8	119.3	C16—C17—C18	119.4 (3)
C9—C8—H8	119.3	C16—C17—H17	120.3
C4—C9—C8	117.9 (3)	C18—C17—H17	120.3
C4—C9—C10	119.9 (2)	C17—C18—C19	120.4 (3)
C8—C9—C10	122.1 (3)	C17—C18—H18	119.8
C1—C10—C9	118.6 (2)	C19—C18—H18	119.8
C1—C10—C11	119.7 (2)	C14—C19—C18	121.2 (3)
C9—C10—C11	121.7 (2)	C14—C19—H19	119.4
N1—C11—C10	112.1 (2)	C18—C19—H19	119.4
N1—C11—H11A	109.2	C12—N1—C11	108.5 (2)
C10—C11—H11A	109.2	C12—N1—C13	112.1 (2)
N1—C11—H11B	109.2	C11—N1—C13	112.3 (2)
C10—C11—H11B	109.2	C1—O1—C12	113.4 (2)
C10—C1—C2—C3	0.4 (4)	C8—C9—C10—C11	4.7 (4)
O1—C1—C2—C3	−179.7 (3)	C1—C10—C11—N1	−14.5 (4)
C1—C2—C3—C4	1.6 (5)	C9—C10—C11—N1	164.3 (2)
C2—C3—C4—C9	−1.5 (5)	N1—C13—C14—C19	70.5 (3)
C2—C3—C4—C5	177.5 (3)	N1—C13—C14—C15	−109.6 (3)
C9—C4—C5—C6	0.5 (5)	C19—C14—C15—C16	−0.7 (4)
C3—C4—C5—C6	−178.5 (3)	C13—C14—C15—C16	179.3 (2)
C4—C5—C6—C7	−0.1 (5)	C14—C15—C16—C17	0.4 (4)
C5—C6—C7—C8	−0.1 (5)	C15—C16—C17—C18	0.2 (4)
C6—C7—C8—C9	0.0 (5)	C16—C17—C18—C19	−0.4 (4)
C3—C4—C9—C8	178.4 (3)	C15—C14—C19—C18	0.5 (4)
C5—C4—C9—C8	−0.7 (4)	C13—C14—C19—C18	−179.6 (2)
C3—C4—C9—C10	−0.5 (4)	C17—C18—C19—C14	0.1 (4)
C5—C4—C9—C10	−179.6 (3)	O1—C12—N1—C11	−64.4 (3)
C7—C8—C9—C4	0.4 (4)	O1—C12—N1—C13	60.2 (3)
C7—C8—C9—C10	179.3 (3)	C10—C11—N1—C12	45.9 (3)
O1—C1—C10—C9	177.7 (2)	C10—C11—N1—C13	−78.4 (3)
C2—C1—C10—C9	−2.4 (4)	C14—C13—N1—C12	61.2 (3)
O1—C1—C10—C11	−3.5 (4)	C14—C13—N1—C11	−176.5 (2)
C2—C1—C10—C11	176.4 (2)	C10—C1—O1—C12	−11.7 (3)

C4—C9—C10—C1	2.5 (4)	C2—C1—O1—C12	168.4 (2)
C8—C9—C10—C1	−176.4 (2)	N1—C12—O1—C1	46.8 (3)
C4—C9—C10—C11	−176.4 (2)		

Fig. 1


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