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3-(1,3-Benzodioxol-5-yl)-1-phenyl-2,3-dihydro-1*H*-naphtho[1,2-e][1,3]oxazine

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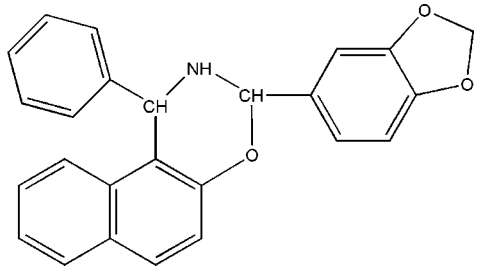
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.063; wR factor = 0.134; data-to-parameter ratio = 9.1.

In the title compound, $C_{25}H_{19}NO_3$, the oxazine ring displays a half-chair conformation. The fused benzene ring is nearly parallel to the naphthyl ring system, the dihedral angle between this benzene ring and the naphthyl system being 8.52 (11)°. The imino group is not involved in hydrogen bonding in the crystal structure.

Related literature

For general background, see: Katayama & Oshiyama (1997); Mahajan *et al.* (1991); Mishra *et al.* (1998).



Experimental

Crystal data

$C_{25}H_{19}NO_3$
M_r = 381.41
Monoclinic, $P2_1$
a = 9.180 (3) Å
b = 5.7585 (18) Å
c = 17.320 (5) Å
β = 97.707 (4)°
V = 907.3 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
5964 measured reflections
2412 independent reflections
1824 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.134
S = 1.18
2412 reflections
265 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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: XU2388).

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Mishra, P. D., Wahidullah, S. & Kamat, S. Y. (1998). *Indian J. Chem. Sect. B*, **37**, 199–200.

supporting information

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3-(1,3-Benzodioxol-5-yl)-1-phenyl-2,3-dihydro-1*H*-naphtho[1,2-e][1,3]oxazine

Yu-Feng Yang, Liang-Ru Yang, Zhi-Gang Yin and Heng-Yu Qian

S1. Comment

The oxazine derivatives display various applications and widespresd potential biological and pharmacological activities such as antimicrobial (Mahajan *et al.*, 1991), antitumor (Katayama & Oshiyama, 1997) and antihistaminic (Mishra *et al.*, 1998). In view of these important properties, we reported the crystal strucutre of the tilte compound.

The oxazine ring in the molecular is not planar. The 1,3-benzodioxole ring makes the dihedral angles of 68.24 (11)° and 8.52 (11)° with the benzene ring and the naphthyl ring, respectively, while the plane O1/C1/C10/C11 is co-planar with the naphthalene ring with the dihedral angle 1.43 (11)°. The dihedral angle between the benzene ring and the naphthalene ring is 71.48 (16)°.

S2. Experimental

1-(Amino(phenyl)methyl)naphthalen-2-ol (1 mmol, 0.249 g) was dissolved in anhydrous methanol, the mixture was stirred for several minitutes, 1,3-benzodioxole-5-carbaldehyde (1 mmol, 0.150 g) in methanol (6 ml) was added dropwise and the mixture was stirred at room temperature for 2 h. The product was isolated and recrystallized in dichloromethane. Colorless single crystals of (I) was obtained after 4 d.

S3. Refinement

Imino H atom was located in a difference Fourier map and positional parameters were refined, U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic) and 0.97 Å (methylene), and refined in riding mode with U_{iso}(H)=1.2U_{eq}(C). In absence of significant anomalous scattering, Friedel pairs were merged.

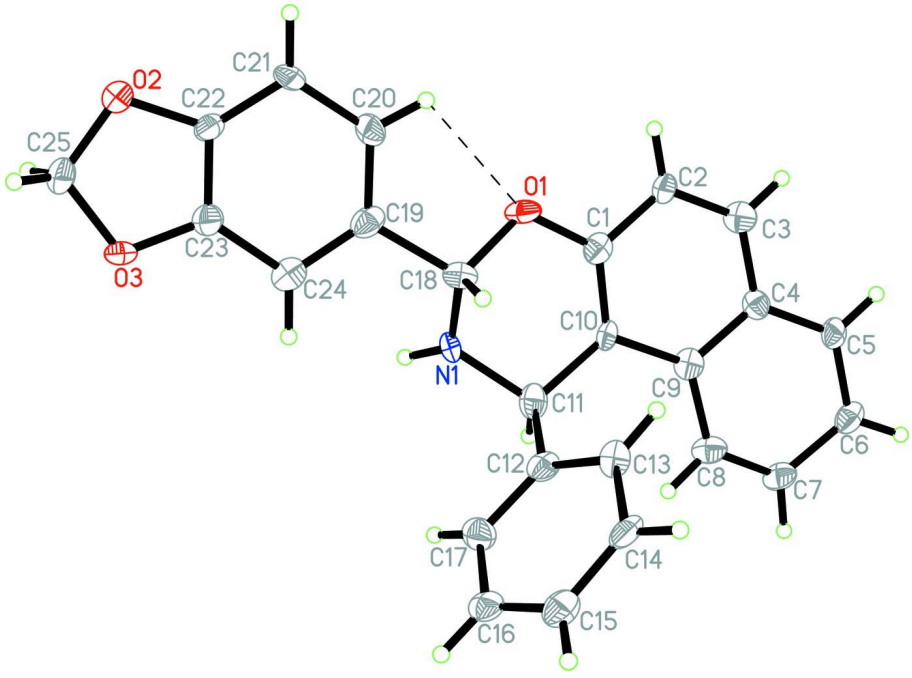

Figure 1

The *ORTEP* plot of (I). Displacement ellipsoids are drawn at the 30% probability level.

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Crystal data

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$c = 17.320\ (5)$ Å
$\beta = 97.707\ (4)°$
$V = 907.3\ (5)$ Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.396$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 912 reflections
$\theta = 2.1–25.1°$
$\mu = 0.09$ mm^{-1}
$T = 291$ K
Block, colorless
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.97$, $T_{max} = 0.98$
5964 measured reflections
2412 independent reflections
1824 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.2°$
$h = -12\rightarrow12$
$k = -7\rightarrow7$
$l = -15\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.134$
$S = 1.18$
2412 reflections
265 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
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.1645P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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}
C1	0.4757 (4)	1.2105 (7)	0.2026 (2)	0.0336 (8)
C2	0.5763 (4)	1.3803 (7)	0.1817 (2)	0.0357 (9)
H2	0.5449	1.4902	0.1438	0.043*
C3	0.7154 (4)	1.3826 (8)	0.2163 (2)	0.0394 (9)
H3	0.7794	1.4958	0.2026	0.047*
C4	0.7663 (4)	1.2181 (7)	0.2729 (2)	0.0333 (8)
C5	0.9118 (4)	1.2228 (7)	0.3104 (2)	0.0366 (9)
H5	0.9719	1.3457	0.2999	0.044*
C6	0.9709 (5)	1.0510 (8)	0.3631 (2)	0.0407 (10)
H6	1.0664	1.0603	0.3888	0.049*
C7	0.8740 (4)	0.8566 (8)	0.3752 (2)	0.0402 (9)
H7	0.9091	0.7295	0.4052	0.048*
C8	0.7357 (4)	0.8655 (8)	0.3425 (2)	0.0386 (9)
H8	0.6735	0.7503	0.3568	0.046*
C9	0.6719 (4)	1.0330 (7)	0.2877 (2)	0.0321 (8)
C10	0.5191 (4)	1.0343 (8)	0.2527 (2)	0.0376 (9)
C11	0.4128 (4)	0.8432 (8)	0.2724 (2)	0.0400 (9)
H11	0.4613	0.6936	0.2670	0.048*
C12	0.3653 (4)	0.8494 (7)	0.3526 (2)	0.0362 (8)
C13	0.4046 (4)	1.0273 (7)	0.4006 (2)	0.0328 (8)
H13	0.4569	1.1531	0.3849	0.039*
C14	0.3628 (4)	1.0156 (8)	0.4770 (2)	0.0421 (10)
H14	0.3893	1.1363	0.5118	0.051*
C15	0.2837 (5)	0.8292 (9)	0.5011 (3)	0.0461 (10)

H15	0.2581	0.8223	0.5512	0.055*
C16	0.2441 (4)	0.6531 (8)	0.4472 (2)	0.0395 (9)
H16	0.1881	0.5293	0.4613	0.047*
C17	0.2874 (4)	0.6570 (9)	0.3703 (3)	0.0441 (10)
H17	0.2642	0.5369	0.3349	0.053*
C18	0.2306 (4)	1.0885 (7)	0.2003 (2)	0.0378 (9)
H18	0.2162	1.1499	0.2515	0.045*
C19	0.0807 (5)	1.1079 (8)	0.1429 (2)	0.0411 (9)
C20	0.0568 (4)	1.2985 (8)	0.0972 (2)	0.0368 (9)
H20	0.1311	1.4084	0.0973	0.044*
C21	−0.0776 (4)	1.3335 (8)	0.0497 (2)	0.0360 (8)
H21	−0.0999	1.4701	0.0219	0.043*
C22	−0.1737 (4)	1.1502 (7)	0.0475 (2)	0.0326 (8)
C23	−0.1516 (5)	0.9640 (8)	0.0947 (2)	0.0427 (10)
C24	−0.0182 (4)	0.9259 (8)	0.1459 (2)	0.0360 (9)
H24	0.0002	0.7955	0.1773	0.043*
C25	−0.3700 (5)	0.9157 (8)	0.0285 (2)	0.0459 (11)
H25A	−0.4622	0.9372	0.0491	0.055*
H25B	−0.3875	0.8163	−0.0170	0.055*
N1	0.2826 (4)	0.8559 (7)	0.2088 (2)	0.0388 (8)
H1	0.246 (5)	0.740 (9)	0.182 (3)	0.047*
O1	0.3362 (3)	1.2333 (5)	0.16696 (15)	0.0380 (7)
O2	−0.3139 (3)	1.1315 (6)	0.00830 (16)	0.0414 (7)
O3	−0.2657 (3)	0.8142 (5)	0.08500 (15)	0.0392 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.039 (2)	0.030 (2)	0.0311 (18)	0.0063 (17)	0.0014 (15)	−0.0124 (15)
C2	0.0389 (19)	0.037 (2)	0.0284 (16)	−0.0056 (18)	−0.0063 (14)	−0.0042 (17)
C3	0.0299 (17)	0.043 (2)	0.047 (2)	0.0083 (18)	0.0127 (16)	0.0024 (19)
C4	0.0272 (17)	0.034 (2)	0.0397 (19)	0.0003 (16)	0.0071 (15)	−0.0007 (16)
C5	0.045 (2)	0.038 (2)	0.0265 (17)	−0.0072 (18)	0.0017 (16)	−0.0114 (16)
C6	0.040 (2)	0.041 (2)	0.038 (2)	0.0099 (19)	−0.0060 (17)	−0.0057 (18)
C7	0.0345 (19)	0.041 (2)	0.044 (2)	0.0158 (19)	0.0009 (16)	0.0089 (19)
C8	0.0339 (18)	0.043 (2)	0.041 (2)	0.0136 (18)	0.0123 (16)	0.0105 (19)
C9	0.0268 (17)	0.033 (2)	0.0381 (18)	0.0110 (16)	0.0101 (14)	−0.0079 (17)
C10	0.0371 (19)	0.043 (2)	0.0286 (17)	−0.0135 (19)	−0.0113 (15)	−0.0011 (17)
C11	0.0356 (18)	0.040 (2)	0.044 (2)	−0.001 (2)	0.0023 (16)	−0.0123 (19)
C12	0.0419 (19)	0.0265 (19)	0.0380 (19)	0.0106 (17)	−0.0025 (16)	−0.0006 (17)
C13	0.0241 (16)	0.034 (2)	0.0412 (19)	0.0112 (15)	0.0079 (14)	−0.0127 (16)
C14	0.046 (2)	0.045 (2)	0.0308 (18)	0.007 (2)	−0.0139 (16)	0.0014 (19)
C15	0.044 (2)	0.048 (3)	0.044 (2)	0.011 (2)	−0.0022 (18)	0.001 (2)
C16	0.0318 (18)	0.042 (2)	0.044 (2)	0.0108 (18)	0.0020 (16)	0.012 (2)
C17	0.037 (2)	0.044 (2)	0.052 (2)	0.0013 (19)	0.0081 (17)	0.007 (2)
C18	0.045 (2)	0.035 (2)	0.0345 (18)	0.0014 (19)	0.0093 (16)	0.0072 (17)
C19	0.046 (2)	0.035 (2)	0.040 (2)	0.0108 (19)	−0.0046 (17)	−0.0032 (18)
C20	0.0304 (17)	0.045 (2)	0.0375 (19)	−0.0078 (18)	0.0136 (15)	0.0042 (19)

C21	0.0363 (18)	0.037 (2)	0.0359 (18)	−0.0073 (18)	0.0113 (15)	0.0153 (17)
C22	0.0390 (19)	0.0253 (18)	0.0303 (16)	0.0039 (17)	−0.0076 (14)	−0.0012 (16)
C23	0.047 (2)	0.036 (2)	0.042 (2)	−0.0057 (19)	−0.0068 (18)	0.0018 (18)
C24	0.0367 (19)	0.039 (2)	0.0338 (18)	0.0135 (17)	0.0096 (15)	−0.0067 (17)
C25	0.039 (2)	0.049 (3)	0.045 (2)	−0.007 (2)	−0.0106 (18)	−0.001 (2)
N1	0.0329 (16)	0.0346 (19)	0.0460 (18)	−0.0174 (15)	−0.0059 (13)	0.0043 (16)
O1	0.0395 (14)	0.0368 (15)	0.0384 (14)	0.0117 (13)	0.0078 (11)	0.0163 (13)
O2	0.0378 (14)	0.0425 (17)	0.0416 (14)	−0.0021 (14)	−0.0035 (12)	0.0058 (14)
O3	0.0398 (14)	0.0368 (16)	0.0396 (13)	0.0003 (13)	−0.0003 (11)	0.0185 (13)

Geometric parameters (Å, º)

C1—O1	1.351 (4)	C14—H14	0.9300
C1—C10	1.359 (6)	C15—C16	1.393 (7)
C1—C2	1.425 (6)	C15—H15	0.9300
C2—C3	1.336 (5)	C16—C17	1.440 (6)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.398 (6)	C17—H17	0.9300
C3—H3	0.9300	C18—N1	1.424 (6)
C4—C5	1.405 (5)	C18—O1	1.456 (5)
C4—C9	1.419 (5)	C18—C19	1.589 (6)
C5—C6	1.405 (6)	C18—H18	0.9800
C5—H5	0.9300	C19—C20	1.354 (6)
C6—C7	1.462 (6)	C19—C24	1.392 (6)
C6—H6	0.9300	C20—C21	1.403 (5)
C7—C8	1.320 (5)	C20—H20	0.9300
C7—H7	0.9300	C21—C22	1.373 (5)
C8—C9	1.423 (5)	C21—H21	0.9300
C8—H8	0.9300	C22—C23	1.347 (6)
C9—C10	1.452 (5)	C22—O2	1.376 (4)
C10—C11	1.539 (6)	C23—O3	1.350 (5)
C11—C12	1.511 (5)	C23—C24	1.429 (5)
C11—N1	1.514 (5)	C24—H24	0.9300
C11—H11	0.9800	C25—O3	1.401 (5)
C12—C13	1.339 (5)	C25—O2	1.408 (6)
C12—C17	1.375 (6)	C25—H25A	0.9700
C13—C14	1.428 (5)	C25—H25B	0.9700
C13—H13	0.9300	N1—H1	0.86 (5)
C14—C15	1.391 (7)		

O1—C1—C10	122.9 (4)	C14—C15—C16	117.4 (4)
O1—C1—C2	115.1 (3)	C14—C15—H15	121.3
C10—C1—C2	122.0 (3)	C16—C15—H15	121.3
C3—C2—C1	120.4 (4)	C15—C16—C17	121.9 (4)
C3—C2—H2	119.8	C15—C16—H16	119.0
C1—C2—H2	119.8	C17—C16—H16	119.0
C2—C3—C4	121.2 (4)	C12—C17—C16	115.8 (4)
C2—C3—H3	119.4	C12—C17—H17	122.1

C4—C3—H3	119.4	C16—C17—H17	122.1
C3—C4—C5	121.3 (4)	N1—C18—O1	110.3 (3)
C3—C4—C9	118.7 (3)	N1—C18—C19	112.4 (3)
C5—C4—C9	119.8 (4)	O1—C18—C19	106.2 (3)
C4—C5—C6	123.2 (4)	N1—C18—H18	109.3
C4—C5—H5	118.4	O1—C18—H18	109.3
C6—C5—H5	118.4	C19—C18—H18	109.3
C5—C6—C7	116.3 (3)	C20—C19—C24	125.2 (4)
C5—C6—H6	121.9	C20—C19—C18	118.8 (4)
C7—C6—H6	121.9	C24—C19—C18	116.0 (4)
C8—C7—C6	118.5 (4)	C19—C20—C21	121.3 (4)
C8—C7—H7	120.7	C19—C20—H20	119.3
C6—C7—H7	120.7	C21—C20—H20	119.3
C7—C8—C9	126.8 (4)	C22—C21—C20	114.6 (4)
C7—C8—H8	116.6	C22—C21—H21	122.7
C9—C8—H8	116.6	C20—C21—H21	122.7
C4—C9—C8	115.0 (3)	C23—C22—C21	123.5 (3)
C4—C9—C10	120.0 (3)	C23—C22—O2	107.0 (3)
C8—C9—C10	124.8 (4)	C21—C22—O2	128.9 (3)
C1—C10—C9	117.0 (4)	C22—C23—O3	112.5 (3)
C1—C10—C11	122.3 (3)	C22—C23—C24	123.0 (4)
C9—C10—C11	120.6 (3)	O3—C23—C24	124.4 (4)
C12—C11—N1	111.8 (3)	C19—C24—C23	111.7 (4)
C12—C11—C10	117.1 (3)	C19—C24—H24	124.1
N1—C11—C10	105.4 (3)	C23—C24—H24	124.1
C12—C11—H11	107.3	O3—C25—O2	107.7 (3)
N1—C11—H11	107.3	O3—C25—H25A	110.2
C10—C11—H11	107.3	O2—C25—H25A	110.2
C13—C12—C17	125.6 (4)	O3—C25—H25B	110.2
C13—C12—C11	120.2 (4)	O2—C25—H25B	110.2
C17—C12—C11	114.2 (4)	H25A—C25—H25B	108.5
C12—C13—C14	117.2 (4)	C18—N1—C11	110.0 (3)
C12—C13—H13	121.4	C18—N1—H1	125 (3)
C14—C13—H13	121.4	C11—N1—H1	125 (3)
C15—C14—C13	122.0 (4)	C1—O1—C18	113.8 (3)
C15—C14—H14	119.0	C22—O2—C25	107.2 (3)
C13—C14—H14	119.0	C23—O3—C25	105.4 (3)