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2-Naphthyl quinoxalin-2-yl ether

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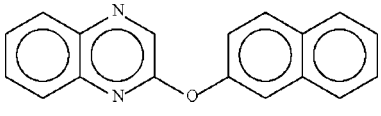
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.127; data-to-parameter ratio = 16.3.

In the crystal structure of the title compound, $C_{18}H_{12}N_2O$, the two fused rings are aligned at 64.2 (1)°; the C—O—C angle is 118.73 (12)°.

Related literature

For the crystal structure of 1-naphthyl quinoxalinyl ether, see: Hassan *et al.* (2009).



Experimental

Crystal data

$C_{18}H_{12}N_2O$ M_r = 272.30
Monoclinic, $P2_1/c$
a = 6.808 (1) Å
b = 7.609 (1) Å
c = 26.234 (3) Å
β = 92.522 (2)°
V = 1357.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.45 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
7510 measured reflections
3094 independent reflections
1950 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.127
S = 1.04
3094 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2387).

References

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supporting information

Acta Cryst. (2009). E**65**, o732 [doi:10.1107/S1600536809007855]

2-Naphthyl quinoxalin-2-yl ether

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S1. Experimental

2-Naphthol (2.88 g, 20 mmol) was mixed with sodium hydroxide (0.08 g, 20 mmol) in several drops of water. The water was then evaporated. The paste was heated with 2-chloroquinoxaline (3.29 g, 20 mmol) at 423–433 K for 6 h. The product was dissolved in water and the solution extracted with chloroform. The chloroform phase was dried over sodium sulfate; the evaporation of the solvent gave a product that was recrystallized from an ethyl acetate/hexane.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

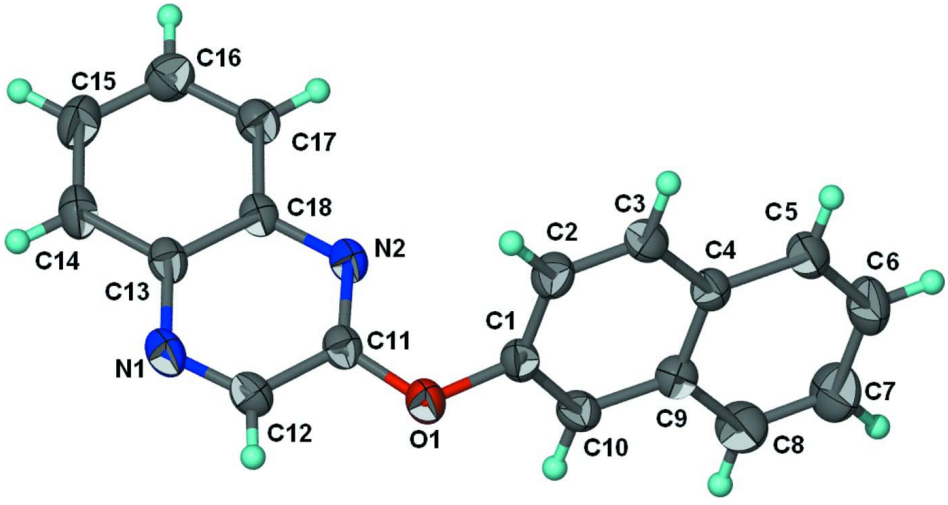

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the molecule of $C_{18}H_{12}N_2O$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

2-Naphthyl quinoxalin-2-yl ether

Crystal data

$C_{18}H_{12}N_2O$
M_r = 272.30
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.808 (1) Å
b = 7.609 (1) Å
c = 26.234 (3) Å
β = 92.522 (2)°
V = 1357.5 (3) Å^3
Z = 4
F(000) = 568
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1541 reflections

θ = 2.7–28.2°
μ = 0.08 mm^{-1}
T = 295 K

Block, colorless
0.45 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
7510 measured reflections
3094 independent reflections

1950 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −6→8
k = −9→8
l = −28→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.127
S = 1.04
3094 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.1253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.11303 (15)	0.36756 (17)	0.59259 (4)	0.0477 (3)
N1	−0.13352 (19)	0.2389 (2)	0.47654 (5)	0.0459 (4)
N2	0.25074 (18)	0.24104 (18)	0.52218 (5)	0.0379 (3)
C1	0.2995 (2)	0.3759 (2)	0.61786 (6)	0.0392 (4)
C2	0.4441 (2)	0.4866 (2)	0.59948 (6)	0.0447 (4)
H2	0.4210	0.5499	0.5695	0.054*
C3	0.6192 (2)	0.5003 (2)	0.62616 (6)	0.0435 (4)
H3	0.7168	0.5723	0.6138	0.052*
C4	0.6559 (2)	0.4077 (2)	0.67216 (6)	0.0371 (4)
C5	0.5053 (2)	0.3003 (2)	0.69082 (6)	0.0394 (4)
C6	0.3253 (2)	0.2858 (2)	0.66207 (6)	0.0412 (4)
H6	0.2253	0.2147	0.6735	0.049*
C7	0.8364 (2)	0.4201 (3)	0.70077 (6)	0.0483 (5)
H7	0.9372	0.4892	0.6888	0.058*
C8	0.8642 (3)	0.3322 (3)	0.74553 (7)	0.0618 (6)
H8	0.9839	0.3414	0.7638	0.074*
C9	0.7154 (3)	0.2285 (3)	0.76428 (7)	0.0694 (6)
H9	0.7355	0.1704	0.7953	0.083*
C10	0.5402 (3)	0.2116 (3)	0.73751 (7)	0.0593 (5)
H10	0.4424	0.1406	0.7502	0.071*
C11	0.0985 (2)	0.3003 (2)	0.54445 (6)	0.0375 (4)
C12	−0.0954 (2)	0.2999 (2)	0.52209 (6)	0.0439 (4)
H12	−0.1976	0.3445	0.5406	0.053*

C13	0.0233 (2)	0.1738 (2)	0.45104 (6)	0.0389 (4)
C14	−0.0076 (3)	0.1015 (3)	0.40208 (6)	0.0520 (5)
H14	−0.1333	0.1008	0.3867	0.062*
C15	0.1453 (3)	0.0325 (3)	0.37707 (7)	0.0561 (5)
H15	0.1237	−0.0157	0.3447	0.067*
C16	0.3351 (3)	0.0340 (2)	0.39983 (7)	0.0524 (5)
H16	0.4385	−0.0139	0.3824	0.063*
C17	0.3705 (2)	0.1044 (2)	0.44705 (6)	0.0430 (4)
H17	0.4977	0.1063	0.4615	0.052*
C18	0.2149 (2)	0.1739 (2)	0.47388 (5)	0.0348 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0342 (6)	0.0636 (9)	0.0449 (6)	0.0032 (5)	−0.0035 (5)	−0.0096 (6)
N1	0.0344 (8)	0.0508 (10)	0.0517 (8)	−0.0015 (6)	−0.0080 (6)	0.0037 (7)
N2	0.0336 (7)	0.0387 (8)	0.0409 (7)	−0.0003 (6)	−0.0048 (5)	0.0016 (6)
C1	0.0348 (9)	0.0424 (11)	0.0402 (9)	0.0010 (7)	−0.0013 (7)	−0.0076 (7)
C2	0.0497 (10)	0.0453 (11)	0.0389 (9)	−0.0025 (8)	−0.0017 (7)	0.0046 (8)
C3	0.0441 (9)	0.0424 (11)	0.0441 (9)	−0.0095 (8)	0.0033 (7)	0.0009 (8)
C4	0.0376 (8)	0.0339 (10)	0.0398 (8)	0.0010 (7)	0.0004 (6)	−0.0055 (7)
C5	0.0420 (9)	0.0356 (10)	0.0404 (9)	0.0010 (7)	0.0010 (7)	0.0008 (7)
C6	0.0392 (9)	0.0390 (11)	0.0457 (9)	−0.0056 (7)	0.0052 (7)	−0.0005 (8)
C7	0.0382 (9)	0.0534 (13)	0.0529 (10)	−0.0002 (8)	−0.0015 (7)	−0.0099 (9)
C8	0.0510 (12)	0.0723 (16)	0.0603 (12)	0.0077 (10)	−0.0177 (9)	−0.0017 (10)
C9	0.0681 (15)	0.0816 (17)	0.0571 (12)	0.0052 (12)	−0.0130 (10)	0.0210 (11)
C10	0.0594 (12)	0.0617 (15)	0.0566 (11)	−0.0039 (10)	−0.0004 (9)	0.0194 (10)
C11	0.0366 (9)	0.0351 (10)	0.0404 (8)	−0.0013 (7)	−0.0033 (7)	0.0026 (7)
C12	0.0332 (8)	0.0476 (11)	0.0506 (10)	0.0030 (8)	−0.0019 (7)	0.0007 (8)
C13	0.0387 (9)	0.0341 (10)	0.0431 (9)	−0.0050 (7)	−0.0058 (7)	0.0045 (7)
C14	0.0502 (11)	0.0557 (13)	0.0486 (10)	−0.0079 (9)	−0.0138 (8)	−0.0009 (9)
C15	0.0689 (13)	0.0558 (14)	0.0431 (10)	−0.0075 (10)	−0.0046 (9)	−0.0087 (9)
C16	0.0559 (11)	0.0509 (13)	0.0507 (10)	0.0038 (9)	0.0047 (8)	−0.0040 (9)
C17	0.0401 (9)	0.0415 (11)	0.0473 (9)	0.0018 (7)	−0.0013 (7)	0.0025 (8)
C18	0.0360 (8)	0.0295 (9)	0.0386 (8)	−0.0029 (7)	−0.0036 (6)	0.0060 (7)

Geometric parameters (Å, º)

O1—C11	1.3622 (18)	C7—H7	0.9300
O1—C1	1.4073 (18)	C8—C9	1.391 (3)
N1—C12	1.297 (2)	C8—H8	0.9300
N1—C13	1.377 (2)	C9—C10	1.363 (3)
N2—C11	1.2928 (19)	C9—H9	0.9300
N2—C18	1.3778 (19)	C10—H10	0.9300
C1—C6	1.352 (2)	C11—C12	1.421 (2)
C1—C2	1.398 (2)	C12—H12	0.9300
C2—C3	1.359 (2)	C13—C14	1.405 (2)
C2—H2	0.9300	C13—C18	1.411 (2)

C3—C4	1.410 (2)	C14—C15	1.360 (3)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.415 (2)	C15—C16	1.399 (2)
C4—C7	1.415 (2)	C15—H15	0.9300
C5—C10	1.410 (2)	C16—C17	1.361 (2)
C5—C6	1.414 (2)	C16—H16	0.9300
C6—H6	0.9300	C17—C18	1.401 (2)
C7—C8	1.357 (2)	C17—H17	0.9300

C11—O1—C1	118.73 (12)	C8—C9—H9	119.8
C12—N1—C13	116.62 (13)	C9—C10—C5	120.83 (19)
C11—N2—C18	115.58 (13)	C9—C10—H10	119.6
C6—C1—C2	122.30 (15)	C5—C10—H10	119.6
C6—C1—O1	117.50 (15)	N2—C11—O1	121.55 (13)
C2—C1—O1	119.95 (14)	N2—C11—C12	124.14 (15)
C3—C2—C1	118.92 (15)	O1—C11—C12	114.31 (14)
C3—C2—H2	120.5	N1—C12—C11	121.72 (15)
C1—C2—H2	120.5	N1—C12—H12	119.1
C2—C3—C4	121.39 (16)	C11—C12—H12	119.1
C2—C3—H3	119.3	N1—C13—C14	119.82 (15)
C4—C3—H3	119.3	N1—C13—C18	121.02 (14)
C3—C4—C5	118.72 (14)	C14—C13—C18	119.14 (15)
C3—C4—C7	122.55 (16)	C15—C14—C13	120.36 (16)
C5—C4—C7	118.72 (15)	C15—C14—H14	119.8
C10—C5—C4	118.70 (15)	C13—C14—H14	119.8
C10—C5—C6	122.33 (16)	C14—C15—C16	120.19 (16)
C4—C5—C6	118.97 (14)	C14—C15—H15	119.9
C1—C6—C5	119.65 (15)	C16—C15—H15	119.9
C1—C6—H6	120.2	C17—C16—C15	120.98 (17)
C5—C6—H6	120.2	C17—C16—H16	119.5
C8—C7—C4	120.72 (17)	C15—C16—H16	119.5
C8—C7—H7	119.6	C16—C17—C18	119.89 (16)
C4—C7—H7	119.6	C16—C17—H17	120.1
C7—C8—C9	120.65 (17)	C18—C17—H17	120.1
C7—C8—H8	119.7	N2—C18—C17	119.67 (14)
C9—C8—H8	119.7	N2—C18—C13	120.91 (14)
C10—C9—C8	120.38 (18)	C17—C18—C13	119.43 (14)
C10—C9—H9	119.8		

C11—O1—C1—C6	−119.60 (16)	C18—N2—C11—O1	178.93 (14)
C11—O1—C1—C2	65.9 (2)	C18—N2—C11—C12	−0.3 (2)
C6—C1—C2—C3	2.0 (3)	C1—O1—C11—N2	1.5 (2)
O1—C1—C2—C3	176.20 (15)	C1—O1—C11—C12	−179.20 (15)
C1—C2—C3—C4	−1.1 (3)	C13—N1—C12—C11	0.3 (2)
C2—C3—C4—C5	−0.7 (2)	N2—C11—C12—N1	−0.2 (3)
C2—C3—C4—C7	−179.77 (16)	O1—C11—C12—N1	−179.53 (15)
C3—C4—C5—C10	−178.29 (16)	C12—N1—C13—C14	178.37 (16)
C7—C4—C5—C10	0.8 (2)	C12—N1—C13—C18	0.1 (2)

C3—C4—C5—C6	1.7 (2)	N1—C13—C14—C15	−178.25 (17)
C7—C4—C5—C6	−179.25 (15)	C18—C13—C14—C15	0.0 (3)
C2—C1—C6—C5	−1.1 (3)	C13—C14—C15—C16	−0.4 (3)
O1—C1—C6—C5	−175.37 (14)	C14—C15—C16—C17	−0.2 (3)
C10—C5—C6—C1	179.15 (16)	C15—C16—C17—C18	1.1 (3)
C4—C5—C6—C1	−0.8 (2)	C11—N2—C18—C17	−179.07 (14)
C3—C4—C7—C8	178.35 (17)	C11—N2—C18—C13	0.8 (2)
C5—C4—C7—C8	−0.7 (3)	C16—C17—C18—N2	178.38 (15)
C4—C7—C8—C9	−0.2 (3)	C16—C17—C18—C13	−1.5 (2)
C7—C8—C9—C10	1.0 (3)	N1—C13—C18—N2	−0.7 (2)
C8—C9—C10—C5	−0.9 (3)	C14—C13—C18—N2	−178.94 (15)
C4—C5—C10—C9	0.0 (3)	N1—C13—C18—C17	179.13 (15)
C6—C5—C10—C9	−179.97 (18)	C14—C13—C18—C17	0.9 (2)