Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Naphthyl quinoxalin-2-yl ether

Noor Doha Hassan, Hairul Anuar Tajuddin, Zanariah Abdullah and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

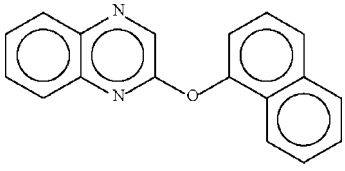
Received 2 March 2009; accepted 4 March 2009

Key indicators: single-crystal X-ray study; T = 118 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.087; data-to-parameter ratio = 8.6.

In the crystal structure of the title compound, $C_{18}H_{12}N_2O$, the dihedral angle between the two fused-ring systems is 84.3 (1) °; the C—O—C angle at the ether O atom is 117.31 (18)°.

Related literature

For the crystal structure of the two forms of quinoxalinyl 2-phenyl ether, see: Abdullah & Ng (2008); Hassan *et al.* (2008).



Experimental

Crystal data

$C_{18}H_{12}N_2O$
M_r = 272.30
Orthorhombic, *Aba*2
a = 18.2758 (6) Å
b = 18.5123 (6) Å
c = 7.7947 (3) Å
V = 2637.2 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 118 K
0.12 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
12370 measured reflections
1626 independent reflections
1316 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.087
S = 1.02
1626 reflections
190 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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).

We thank the University of Malaya for supporting this study (FS358/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2386).

References

Abdullah, Z. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o2165.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hassan, N. D., Tajuddin, H. A., Abdullah, Z. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o1820.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, o731 [doi:10.1107/S1600536809007867]

1-Naphthyl quinoxalin-2-yl ether

Noor Doha Hassan, Hairul Anuar Tajuddin, Zanariah Abdullah and Seik Weng Ng

S1. Experimental

1-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 a chloroform/ether mixture.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were averaged in the final refinement.

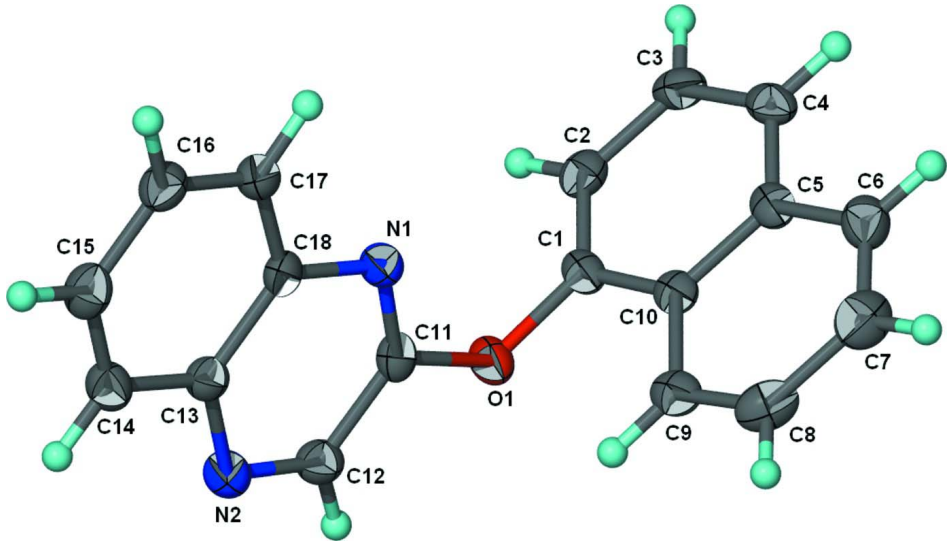


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the molecule of $C_{18}H_{12}N_2O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

1-Naphthyl quinoxalin-2-yl ether

Crystal data

$C_{18}H_{12}N_2O$
M_r = 272.30
Orthorhombic, *Aba*2
Hall symbol: A 2 -2ac

a = 18.2758 (6) Å
b = 18.5123 (6) Å
c = 7.7947 (3) Å
V = 2637.2 (2) Å^3

$Z = 8$
$F(000) = 1136$
$D_x = 1.372$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1495 reflections

$\theta = 2.2$–$21.2°$
$\mu = 0.09$ mm^{-1}
$T = 118$ K
Prism, colorless
0.12 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
12370 measured reflections
1626 independent reflections

1316 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -22 \rightarrow 23$
$k = -24 \rightarrow 23$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.087$
$S = 1.02$
1626 reflections
190 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.5804P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.19391 (9)	0.24366 (9)	0.5000 (2)	0.0217 (4)
N1	0.15328 (11)	0.34927 (11)	0.3713 (3)	0.0192 (5)
N2	0.30285 (11)	0.38838 (11)	0.3387 (3)	0.0218 (5)
C1	0.12235 (13)	0.21546 (12)	0.4887 (4)	0.0192 (5)
C2	0.07744 (14)	0.22066 (13)	0.6269 (4)	0.0222 (6)
H2	0.0930	0.2454	0.7273	0.027*
C3	0.00734 (14)	0.18873 (13)	0.6196 (3)	0.0234 (6)
H3	−0.0246	0.1922	0.7155	0.028*
C4	−0.01480 (14)	0.15306 (13)	0.4762 (3)	0.0231 (6)
H4	−0.0619	0.1314	0.4737	0.028*
C5	0.03121 (13)	0.14761 (12)	0.3301 (3)	0.0198 (5)
C6	0.00887 (15)	0.11230 (14)	0.1784 (4)	0.0269 (6)
H6	−0.0381	0.0903	0.1737	0.032*
C7	0.05358 (16)	0.10925 (15)	0.0388 (4)	0.0301 (7)
H7	0.0375	0.0857	−0.0627	0.036*
C8	0.12373 (16)	0.14110 (15)	0.0448 (4)	0.0278 (6)

H8	0.1546	0.1388	−0.0531	0.033*
C9	0.14764 (14)	0.17502 (13)	0.1890 (4)	0.0219 (6)
H9	0.1952	0.1957	0.1917	0.026*
C10	0.10190 (13)	0.17973 (13)	0.3355 (3)	0.0180 (5)
C11	0.20655 (14)	0.30943 (13)	0.4253 (3)	0.0189 (5)
C12	0.28187 (14)	0.32836 (13)	0.4113 (3)	0.0213 (6)
H12	0.3178	0.2964	0.4560	0.026*
C13	0.24804 (15)	0.43279 (12)	0.2773 (3)	0.0190 (5)
C14	0.26686 (14)	0.49812 (13)	0.1965 (4)	0.0232 (6)
H14	0.3168	0.5114	0.1841	0.028*
C15	0.21262 (15)	0.54275 (14)	0.1356 (4)	0.0247 (6)
H15	0.2253	0.5866	0.0798	0.030*
C16	0.13869 (15)	0.52397 (13)	0.1552 (4)	0.0231 (6)
H16	0.1017	0.5552	0.1123	0.028*
C17	0.11934 (14)	0.46108 (13)	0.2357 (3)	0.0212 (6)
H17	0.0691	0.4494	0.2501	0.025*
C18	0.17350 (13)	0.41378 (13)	0.2971 (3)	0.0190 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0185 (9)	0.0192 (9)	0.0275 (10)	−0.0015 (7)	−0.0032 (8)	0.0043 (8)
N1	0.0177 (11)	0.0189 (10)	0.0211 (12)	−0.0005 (8)	−0.0005 (8)	0.0002 (9)
N2	0.0202 (11)	0.0228 (11)	0.0223 (11)	−0.0011 (8)	−0.0006 (10)	−0.0001 (10)
C1	0.0154 (13)	0.0156 (11)	0.0266 (14)	0.0005 (9)	−0.0035 (12)	0.0063 (11)
C2	0.0246 (14)	0.0183 (12)	0.0237 (14)	0.0038 (10)	−0.0013 (12)	0.0002 (11)
C3	0.0228 (14)	0.0215 (13)	0.0259 (15)	0.0046 (10)	0.0077 (12)	0.0030 (12)
C4	0.0164 (13)	0.0212 (12)	0.0316 (16)	0.0026 (9)	0.0011 (12)	0.0054 (12)
C5	0.0179 (13)	0.0159 (12)	0.0255 (14)	0.0015 (10)	−0.0038 (11)	0.0057 (11)
C6	0.0244 (14)	0.0236 (13)	0.0326 (16)	−0.0003 (11)	−0.0065 (13)	−0.0009 (13)
C7	0.0321 (16)	0.0316 (15)	0.0266 (16)	0.0045 (12)	−0.0094 (13)	−0.0040 (13)
C8	0.0325 (15)	0.0312 (15)	0.0198 (14)	0.0087 (12)	0.0021 (12)	0.0017 (12)
C9	0.0206 (13)	0.0194 (12)	0.0257 (14)	0.0031 (10)	0.0009 (11)	0.0065 (12)
C10	0.0184 (12)	0.0152 (11)	0.0205 (13)	0.0019 (9)	−0.0007 (11)	0.0045 (10)
C11	0.0225 (14)	0.0169 (12)	0.0172 (12)	−0.0021 (10)	−0.0020 (11)	−0.0011 (10)
C12	0.0193 (14)	0.0229 (13)	0.0217 (13)	0.0016 (10)	−0.0012 (11)	−0.0018 (11)
C13	0.0191 (12)	0.0193 (11)	0.0184 (13)	0.0000 (10)	−0.0003 (10)	−0.0023 (10)
C14	0.0226 (14)	0.0226 (12)	0.0243 (14)	−0.0037 (10)	0.0031 (12)	−0.0002 (12)
C15	0.0312 (15)	0.0203 (12)	0.0225 (14)	−0.0016 (11)	0.0019 (12)	0.0017 (11)
C16	0.0243 (14)	0.0199 (12)	0.0252 (14)	0.0032 (10)	−0.0034 (12)	−0.0006 (11)
C17	0.0192 (13)	0.0199 (12)	0.0245 (14)	−0.0004 (10)	−0.0005 (11)	−0.0023 (11)
C18	0.0205 (13)	0.0160 (11)	0.0204 (13)	−0.0010 (10)	0.0000 (11)	−0.0043 (11)

Geometric parameters (Å, º)

O1—C11	1.369 (3)	C7—C8	1.412 (4)
O1—C1	1.411 (3)	C7—H7	0.9500
N1—C11	1.292 (3)	C8—C9	1.360 (4)

N1—C18	1.378 (3)	C8—H8	0.9500
N2—C12	1.304 (3)	C9—C10	1.418 (3)
N2—C13	1.382 (3)	C9—H9	0.9500
C1—C2	1.358 (4)	C11—C12	1.425 (3)
C1—C10	1.415 (3)	C12—H12	0.9500
C2—C3	1.412 (4)	C13—C14	1.406 (3)
C2—H2	0.9500	C13—C18	1.415 (4)
C3—C4	1.360 (4)	C14—C15	1.375 (4)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.419 (4)	C15—C16	1.404 (4)
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.411 (4)	C16—C17	1.369 (4)
C5—C10	1.423 (3)	C16—H16	0.9500
C6—C7	1.362 (4)	C17—C18	1.405 (3)
C6—H6	0.9500	C17—H17	0.9500

C11—O1—C1	117.31 (18)	C10—C9—H9	119.8
C11—N1—C18	115.4 (2)	C1—C10—C9	123.5 (2)
C12—N2—C13	116.4 (2)	C1—C10—C5	117.4 (2)
C2—C1—O1	119.0 (2)	C9—C10—C5	119.1 (2)
C2—C1—C10	122.9 (2)	N1—C11—O1	121.3 (2)
O1—C1—C10	118.1 (2)	N1—C11—C12	124.2 (2)
C1—C2—C3	119.1 (2)	O1—C11—C12	114.5 (2)
C1—C2—H2	120.5	N2—C12—C11	121.8 (2)
C3—C2—H2	120.5	N2—C12—H12	119.1
C4—C3—C2	120.4 (2)	C11—C12—H12	119.1
C4—C3—H3	119.8	N2—C13—C14	119.3 (2)
C2—C3—H3	119.8	N2—C13—C18	120.8 (2)
C3—C4—C5	121.2 (2)	C14—C13—C18	119.9 (2)
C3—C4—H4	119.4	C15—C14—C13	119.7 (2)
C5—C4—H4	119.4	C15—C14—H14	120.2
C6—C5—C4	122.3 (2)	C13—C14—H14	120.2
C6—C5—C10	118.8 (2)	C14—C15—C16	120.5 (2)
C4—C5—C10	119.0 (2)	C14—C15—H15	119.7
C7—C6—C5	121.0 (2)	C16—C15—H15	119.7
C7—C6—H6	119.5	C17—C16—C15	120.6 (2)
C5—C6—H6	119.5	C17—C16—H16	119.7
C6—C7—C8	120.0 (3)	C15—C16—H16	119.7
C6—C7—H7	120.0	C16—C17—C18	120.3 (2)
C8—C7—H7	120.0	C16—C17—H17	119.9
C9—C8—C7	120.8 (3)	C18—C17—H17	119.9
C9—C8—H8	119.6	N1—C18—C17	119.6 (2)
C7—C8—H8	119.6	N1—C18—C13	121.3 (2)
C8—C9—C10	120.3 (2)	C17—C18—C13	119.1 (2)
C8—C9—H9	119.8		

C11—O1—C1—C2	−101.4 (3)	C18—N1—C11—O1	−179.3 (2)
C11—O1—C1—C10	81.6 (3)	C18—N1—C11—C12	−0.3 (4)

O1—C1—C2—C3	−176.3 (2)	C1—O1—C11—N1	10.9 (3)
C10—C1—C2—C3	0.5 (3)	C1—O1—C11—C12	−168.2 (2)
C1—C2—C3—C4	0.2 (3)	C13—N2—C12—C11	0.4 (4)
C2—C3—C4—C5	−0.7 (4)	N1—C11—C12—N2	−1.0 (4)
C3—C4—C5—C6	−178.6 (2)	O1—C11—C12—N2	178.1 (2)
C3—C4—C5—C10	0.5 (3)	C12—N2—C13—C14	−179.6 (2)
C4—C5—C6—C7	178.6 (2)	C12—N2—C13—C18	1.4 (4)
C10—C5—C6—C7	−0.5 (4)	N2—C13—C14—C15	−179.7 (2)
C5—C6—C7—C8	0.6 (4)	C18—C13—C14—C15	−0.7 (4)
C6—C7—C8—C9	0.1 (4)	C13—C14—C15—C16	0.7 (4)
C7—C8—C9—C10	−0.8 (4)	C14—C15—C16—C17	0.2 (4)
C2—C1—C10—C9	178.8 (2)	C15—C16—C17—C18	−1.2 (4)
O1—C1—C10—C9	−4.4 (3)	C11—N1—C18—C17	−179.5 (2)
C2—C1—C10—C5	−0.7 (3)	C11—N1—C18—C13	2.1 (3)
O1—C1—C10—C5	176.1 (2)	C16—C17—C18—N1	−177.3 (2)
C8—C9—C10—C1	−178.6 (2)	C16—C17—C18—C13	1.2 (4)
C8—C9—C10—C5	0.9 (4)	N2—C13—C18—N1	−2.8 (4)
C6—C5—C10—C1	179.3 (2)	C14—C13—C18—N1	178.2 (2)
C4—C5—C10—C1	0.2 (3)	N2—C13—C18—C17	178.8 (2)
C6—C5—C10—C9	−0.2 (3)	C14—C13—C18—C17	−0.3 (4)
C4—C5—C10—C9	−179.3 (2)		