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Phenyl quinoxalin-2-yl ether

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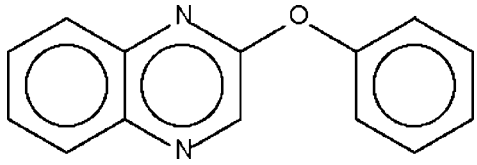
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 16.1.

The aromatic ring systems in the title compound, $C_{14}H_{10}N_2O$, form a dihedral angle of 63.8 (1)°, resulting in an opening up of the ether-O atom angle to 118.2 (1)°.

Related literature

The title compound exhibits fluorescence; see: Abdullah (2005); Kawai *et al.* (2001); Mohd Salleh *et al.* (2007). For the only previously reported structural example of a quinoxalin-oxy compound, see: Csikós *et al.* (1999).



Experimental

Crystal data

$C_{14}H_{10}N_2O$ M_r = 222.24
Monoclinic, $C2/c$
a = 18.175 (2) Å
b = 6.6589 (8) Å
c = 19.488 (2) Å
β = 112.937 (2)°
V = 2172.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
6018 measured reflections
2478 independent reflections
1909 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
S = 1.07
2478 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2297).

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supporting information

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S1. Comment

The title compound (I) belongs to a class of compounds that exhibits fluorescence (Abdullah, 2005; Kawai *et al.*, 2001; Mohd Salleh *et al.*, 2007). In the crystal structure, the two aromatic systems aligned at 63.8 (1) °; these open up the angle at the oxygen atom to 118.2 (1) ° (Fig. 1).

In the structural literature, there is only one example of a quinoxalinoxy compound, 2(1*H*-quinoxalone *O*-(2′-quinoxalinyl)hydroxylamine, which exists in two colored forms (Csikós *et al.*, 1999).

S2. Experimental

Phenol (0.47 g, 5 mmol) was dissolved in a small volume of water containing potassium hydroxide (0.20 g, 5 mmol). The mixture was heated to remove the water to give a brown compound. The compound and 2-chloroquinoxaline (0.82 g, 5 mmol) were heated in THF (15 ml) for 8 h. The mixture was in 1 N sodium hydroxide; the aqueous solution was extracted with dichloromethane. The organic phase was dried over sodium sulfate. Evaporation of the solvent gave a yellow product, which was was washed with chloroform to remove impurities. Crystals were obtained upon recrystallization from an ethyl acetate/hexane mixture of (I).

S3. 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) fixed at 1.2U(C).

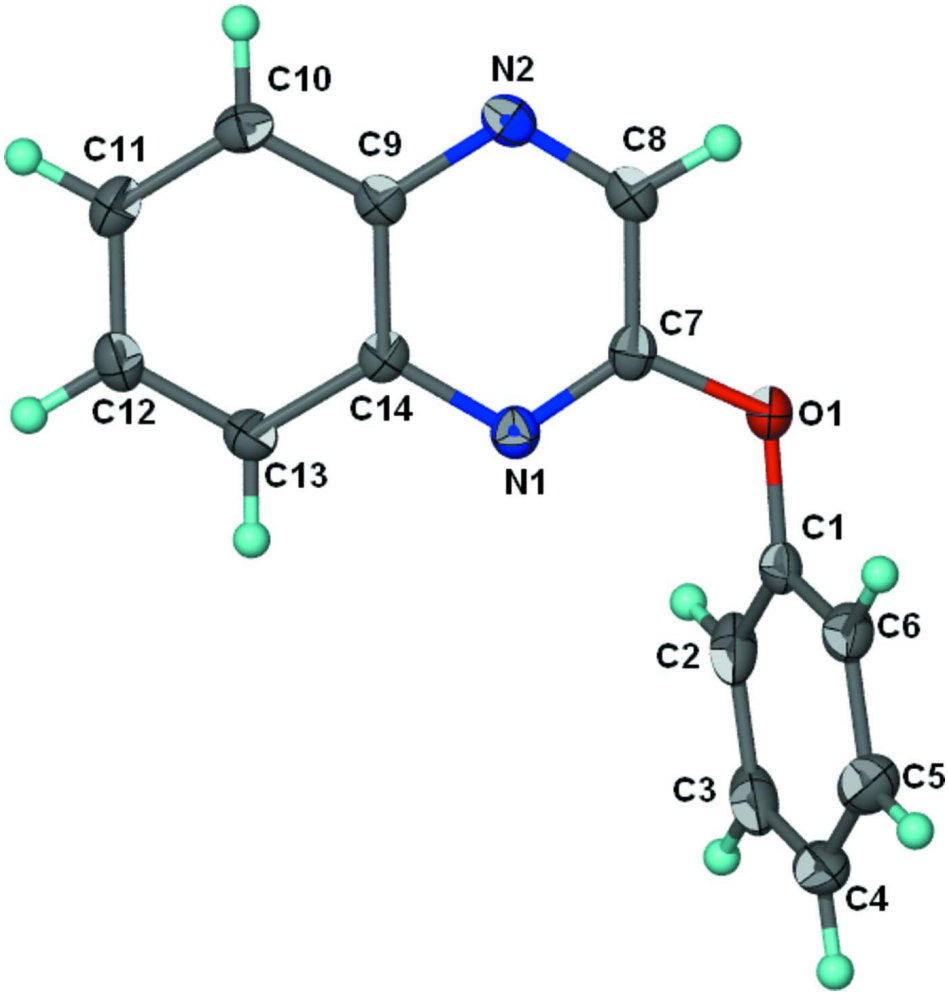

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of (I) drawn at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Phenyl quinoxalin-2-yl ether

Crystal data

$C_{14}H_{10}N_2O$
$M_r = 222.24$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 18.175\ (2)$ Å
$b = 6.6589\ (8)$ Å
$c = 19.488\ (2)$ Å
$\beta = 112.937\ (2)°$
$V = 2172.1\ (5)$ Å^3
$Z = 8$

$F(000) = 928$
$D_x = 1.359$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1614 reflections
$\theta = 2.4–28.2°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Prism, colorless
0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6018 measured reflections
2478 independent reflections
1909 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -23 \rightarrow 16$
$k = -8 \rightarrow 8$
$l = -23 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.104$
$S = 1.07$
2478 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.7132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.68658 (5)	0.68613 (14)	0.55215 (5)	0.0196 (2)
N1	0.59181 (6)	0.76551 (15)	0.59977 (6)	0.0166 (2)
N2	0.47638 (6)	0.72591 (16)	0.45219 (6)	0.0176 (2)
C1	0.74734 (7)	0.7128 (2)	0.62327 (7)	0.0178 (3)
C2	0.75301 (8)	0.5866 (2)	0.68141 (8)	0.0242 (3)
H2	0.7143	0.4846	0.6749	0.029*
C3	0.81628 (9)	0.6118 (2)	0.74933 (8)	0.0291 (4)
H3	0.8209	0.5269	0.7900	0.035*
C4	0.87301 (9)	0.7599 (2)	0.75850 (8)	0.0293 (4)
H4	0.9163	0.7763	0.8053	0.035*
C5	0.86637 (8)	0.8838 (2)	0.69930 (8)	0.0267 (3)
H5	0.9053	0.9849	0.7055	0.032*
C6	0.80290 (8)	0.8608 (2)	0.63088 (7)	0.0208 (3)
H6	0.7980	0.9456	0.5901	0.025*
C7	0.60973 (7)	0.71759 (18)	0.54400 (7)	0.0167 (3)
C8	0.55218 (8)	0.69640 (19)	0.46909 (7)	0.0180 (3)
H8	0.5698	0.6599	0.4309	0.022*
C9	0.45400 (7)	0.77709 (18)	0.50983 (7)	0.0156 (3)
C10	0.37309 (8)	0.81243 (19)	0.49536 (7)	0.0184 (3)
H10	0.3341	0.8006	0.4460	0.022*
C11	0.35029 (8)	0.86377 (19)	0.55218 (7)	0.0202 (3)
H11	0.2955	0.8882	0.5420	0.024*
C12	0.40760 (8)	0.8806 (2)	0.62563 (7)	0.0204 (3)
H12	0.3912	0.9162	0.6647	0.025*
C13	0.48681 (8)	0.8460 (2)	0.64120 (7)	0.0189 (3)
H13	0.5249	0.8564	0.6910	0.023*

C14	0.51180 (7)	0.79510 (18)	0.58369 (7)	0.0157 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0157 (5)	0.0261 (5)	0.0182 (5)	0.0021 (4)	0.0079 (4)	−0.0013 (4)
N1	0.0167 (6)	0.0160 (5)	0.0179 (5)	−0.0007 (4)	0.0077 (4)	−0.0009 (4)
N2	0.0214 (6)	0.0154 (5)	0.0166 (5)	−0.0008 (4)	0.0079 (4)	−0.0009 (4)
C1	0.0158 (6)	0.0218 (6)	0.0172 (6)	0.0052 (5)	0.0079 (5)	−0.0004 (5)
C2	0.0238 (7)	0.0257 (7)	0.0295 (7)	0.0071 (6)	0.0174 (6)	0.0064 (6)
C3	0.0297 (8)	0.0404 (9)	0.0233 (7)	0.0181 (7)	0.0169 (6)	0.0118 (6)
C4	0.0222 (7)	0.0439 (9)	0.0184 (7)	0.0127 (7)	0.0045 (6)	−0.0019 (6)
C5	0.0208 (7)	0.0291 (7)	0.0277 (7)	0.0011 (6)	0.0067 (6)	−0.0045 (6)
C6	0.0196 (7)	0.0228 (7)	0.0215 (7)	0.0036 (5)	0.0097 (6)	0.0029 (5)
C7	0.0161 (6)	0.0148 (6)	0.0208 (6)	−0.0003 (5)	0.0090 (5)	0.0005 (5)
C8	0.0221 (7)	0.0164 (6)	0.0176 (6)	−0.0006 (5)	0.0102 (5)	−0.0007 (5)
C9	0.0182 (6)	0.0120 (6)	0.0170 (6)	−0.0008 (5)	0.0074 (5)	−0.0006 (5)
C10	0.0177 (7)	0.0159 (6)	0.0185 (6)	−0.0008 (5)	0.0037 (5)	0.0000 (5)
C11	0.0149 (6)	0.0189 (6)	0.0270 (7)	0.0001 (5)	0.0084 (5)	0.0006 (5)
C12	0.0220 (7)	0.0213 (6)	0.0215 (6)	−0.0001 (5)	0.0123 (6)	−0.0019 (5)
C13	0.0196 (7)	0.0205 (6)	0.0168 (6)	−0.0005 (5)	0.0072 (5)	−0.0009 (5)
C14	0.0152 (6)	0.0133 (6)	0.0184 (6)	−0.0006 (5)	0.0062 (5)	0.0003 (5)

Geometric parameters (Å, º)

O1—C7	1.3591 (15)	C5—H5	0.9500
O1—C1	1.4068 (15)	C6—H6	0.9500
N1—C7	1.2904 (17)	C7—C8	1.4335 (17)
N1—C14	1.3771 (16)	C8—H8	0.9500
N2—C8	1.3006 (17)	C9—C10	1.4051 (18)
N2—C9	1.3782 (17)	C9—C14	1.4182 (17)
C1—C6	1.3769 (19)	C10—C11	1.3685 (19)
C1—C2	1.3821 (18)	C10—H10	0.9500
C2—C3	1.384 (2)	C11—C12	1.4086 (18)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.387 (2)	C12—C13	1.3703 (18)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.385 (2)	C13—C14	1.4048 (18)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.3903 (18)		
C7—O1—C1	118.16 (10)	O1—C7—C8	114.37 (11)
C7—N1—C14	115.75 (11)	N2—C8—C7	121.57 (12)
C8—N2—C9	116.80 (11)	N2—C8—H8	119.2
C6—C1—C2	121.99 (12)	C7—C8—H8	119.2
C6—C1—O1	117.24 (11)	N2—C9—C10	119.73 (11)
C2—C1—O1	120.65 (12)	N2—C9—C14	120.73 (12)
C1—C2—C3	118.61 (14)	C10—C9—C14	119.54 (12)

C1—C2—H2	120.7	C11—C10—C9	120.18 (12)
C3—C2—H2	120.7	C11—C10—H10	119.9
C2—C3—C4	120.54 (13)	C9—C10—H10	119.9
C2—C3—H3	119.7	C10—C11—C12	120.33 (12)
C4—C3—H3	119.7	C10—C11—H11	119.8
C5—C4—C3	119.82 (13)	C12—C11—H11	119.8
C5—C4—H4	120.1	C13—C12—C11	120.57 (12)
C3—C4—H4	120.1	C13—C12—H12	119.7
C4—C5—C6	120.25 (14)	C11—C12—H12	119.7
C4—C5—H5	119.9	C12—C13—C14	120.16 (12)
C6—C5—H5	119.9	C12—C13—H13	119.9
C1—C6—C5	118.80 (13)	C14—C13—H13	119.9
C1—C6—H6	120.6	N1—C14—C13	119.60 (11)
C5—C6—H6	120.6	N1—C14—C9	121.18 (12)
N1—C7—O1	121.67 (11)	C13—C14—C9	119.22 (12)
N1—C7—C8	123.96 (12)		

C7—O1—C1—C6	−117.62 (13)	O1—C7—C8—N2	−178.58 (11)
C7—O1—C1—C2	66.18 (16)	C8—N2—C9—C10	179.57 (11)
C6—C1—C2—C3	0.5 (2)	C8—N2—C9—C14	−0.26 (17)
O1—C1—C2—C3	176.56 (12)	N2—C9—C10—C11	−179.85 (12)
C1—C2—C3—C4	−0.4 (2)	C14—C9—C10—C11	−0.03 (19)
C2—C3—C4—C5	0.0 (2)	C9—C10—C11—C12	−0.3 (2)
C3—C4—C5—C6	0.3 (2)	C10—C11—C12—C13	0.0 (2)
C2—C1—C6—C5	−0.2 (2)	C11—C12—C13—C14	0.6 (2)
O1—C1—C6—C5	−176.37 (11)	C7—N1—C14—C13	179.44 (12)
C4—C5—C6—C1	−0.2 (2)	C7—N1—C14—C9	−1.19 (17)
C14—N1—C7—O1	179.35 (11)	C12—C13—C14—N1	178.41 (11)
C14—N1—C7—C8	0.49 (18)	C12—C13—C14—C9	−0.98 (19)
C1—O1—C7—N1	−1.81 (18)	N2—C9—C14—N1	1.12 (18)
C1—O1—C7—C8	177.15 (10)	C10—C9—C14—N1	−178.70 (11)
C9—N2—C8—C7	−0.45 (18)	N2—C9—C14—C13	−179.50 (12)
N1—C7—C8—N2	0.3 (2)	C10—C9—C14—C13	0.68 (18)