Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A second monoclinic modification of phenyl quinoxalin-2-yl ether

Zanariah Abdullah and Seik Weng Ng*

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

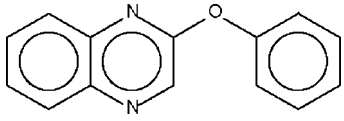
Received 10 September 2008; accepted 26 September 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.114; data-to-parameter ratio = 15.6.

The two aromatic systems in the title compound, $C_{14}H_{10}N_2O$, enclose a dihedral angle of 77.9 (1)°, and the C—O—C inter-ring bond angle is 117.6 (1)°.

Related literature

Another polymorph of this compound has recently been described in the *C*2/*c* space group; see Hassan *et al.* (2008).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Monoclinic, $P2_1/n$
a = 7.9447 (2) Å
b = 6.5169 (1) Å
c = 20.2992 (5) Å
β = 91.983 (1)°
V = 1050.36 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
7016 measured reflections
2398 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.114
S = 1.03
2398 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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).

The authors thank the University of Malaya for supporting this study (grant No. F2358/2008A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2084).

References

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. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o2165 [doi:10.1107/S1600536808031243]

A second monoclinic modification of phenyl quinoxalin-2-yl ether

Zanariah Abdullah and Seik Weng Ng

S1. Comment

The compound was recently described in the *C*2/*c* space group with the two aromatic substituents in $C_{14}H_{10}N_2O$ enclosing a dihedral angle of 63.8 (1)°. The bond angle at oxygen measures to 118.2 (1)° (Hassan *et al.*, 2008). In the $P2_1/n$ modification described herein (Scheme I, Fig. 1), the two aromatic systems show a dihedral angle of 77.9 (1)° and they subtend an angle of 117.6 (1)° at oxygen.

S2. Experimental

The monoclinic modification was obtained when the *C*2/*c* modification of quinoxalinyl phenyl ether was recrystallized from ethanol in the presence of a small quantity of manganese acetate. Slow evaporation of the solvent gave colorless crystals mixed with unchanged manganese acetate.

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 1.2*U*(C).

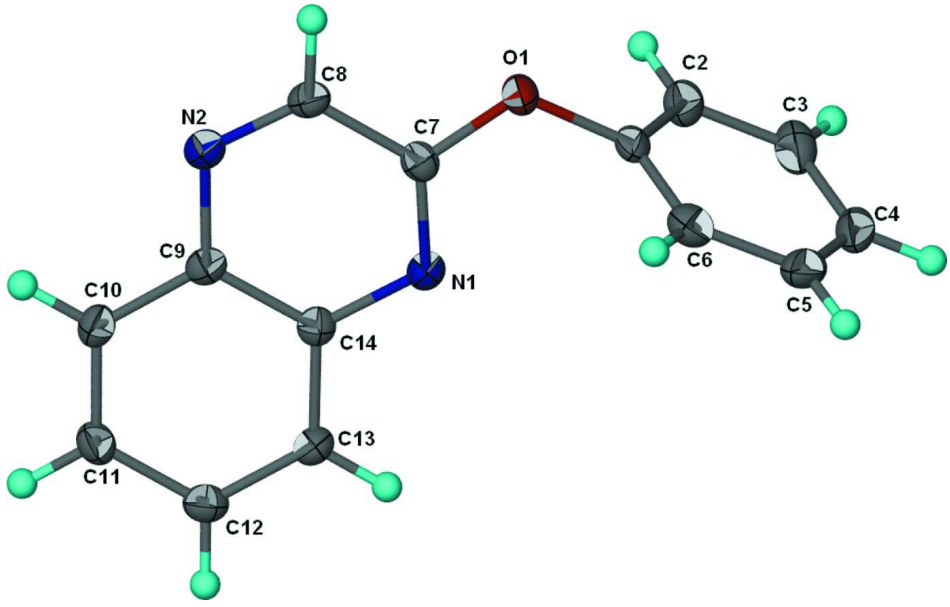


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{14}H_{10}N_2O$ 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, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9447$ (2) Å
$b = 6.5169$ (1) Å
$c = 20.2992$ (5) Å
$\beta = 91.983$ (1)°
$V = 1050.36$ (4) Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.405$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2712 reflections
$\theta = 2.7$–$28.4°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Block, colorless
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
7016 measured reflections
2398 independent reflections
1960 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.114$
$S = 1.03$
2398 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
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.2602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34884 (10)	0.24973 (13)	0.66577 (4)	0.0189 (2)
N1	0.58503 (12)	0.26591 (14)	0.60174 (5)	0.0150 (2)
N2	0.35723 (12)	0.23610 (14)	0.49088 (5)	0.0153 (2)
C1	0.45193 (13)	0.28653 (19)	0.72247 (5)	0.0170 (3)
C2	0.44960 (15)	0.48057 (19)	0.74939 (6)	0.0199 (3)
H2	0.3836	0.5863	0.7292	0.024*
C3	0.54551 (15)	0.5187 (2)	0.80653 (6)	0.0233 (3)
H3	0.5461	0.6519	0.8255	0.028*
C4	0.64037 (15)	0.3635 (2)	0.83596 (6)	0.0232 (3)
H4	0.7066	0.3906	0.8749	0.028*
C5	0.63876 (15)	0.1689 (2)	0.80870 (6)	0.0242 (3)
H5	0.7029	0.0622	0.8293	0.029*
C6	0.54360 (15)	0.1286 (2)	0.75122 (6)	0.0219 (3)
H6	0.5419	−0.0047	0.7323	0.026*

C7	0.42352 (15)	0.25028 (16)	0.60650 (5)	0.0148 (2)
C8	0.30741 (14)	0.23391 (17)	0.55103 (6)	0.0158 (3)
H8	0.1905	0.2211	0.5586	0.019*
C9	0.52855 (14)	0.25143 (16)	0.48299 (5)	0.0139 (2)
C10	0.59172 (15)	0.25296 (17)	0.41912 (5)	0.0160 (3)
H10	0.5161	0.2467	0.3819	0.019*
C11	0.76232 (15)	0.26345 (17)	0.41025 (6)	0.0174 (3)
H11	0.8043	0.2630	0.3670	0.021*
C12	0.87492 (15)	0.27483 (18)	0.46528 (6)	0.0179 (3)
H12	0.9927	0.2808	0.4589	0.021*
C13	0.81557 (14)	0.27741 (18)	0.52800 (6)	0.0167 (3)
H13	0.8925	0.2878	0.5647	0.020*
C14	0.64163 (14)	0.26477 (16)	0.53833 (5)	0.0141 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0148 (4)	0.0292 (5)	0.0127 (4)	−0.0019 (3)	0.0008 (3)	−0.0024 (3)
N1	0.0146 (5)	0.0160 (5)	0.0144 (5)	0.0003 (3)	−0.0008 (4)	−0.0002 (3)
N2	0.0155 (5)	0.0137 (5)	0.0166 (5)	0.0004 (3)	−0.0011 (4)	−0.0005 (4)
C1	0.0119 (5)	0.0277 (6)	0.0116 (5)	−0.0025 (4)	0.0025 (4)	0.0000 (4)
C2	0.0208 (6)	0.0237 (6)	0.0153 (5)	−0.0008 (5)	0.0014 (4)	0.0026 (4)
C3	0.0253 (6)	0.0276 (7)	0.0170 (6)	−0.0061 (5)	0.0017 (5)	−0.0019 (5)
C4	0.0160 (6)	0.0396 (8)	0.0140 (5)	−0.0056 (5)	0.0002 (4)	0.0014 (5)
C5	0.0164 (6)	0.0368 (7)	0.0195 (6)	0.0047 (5)	0.0025 (4)	0.0076 (5)
C6	0.0199 (6)	0.0262 (7)	0.0199 (6)	0.0018 (5)	0.0042 (4)	−0.0001 (5)
C7	0.0168 (5)	0.0137 (5)	0.0139 (5)	0.0000 (4)	0.0014 (4)	−0.0007 (4)
C8	0.0134 (5)	0.0162 (6)	0.0177 (6)	0.0003 (4)	−0.0005 (4)	−0.0009 (4)
C9	0.0146 (5)	0.0113 (5)	0.0158 (6)	0.0011 (4)	−0.0008 (4)	0.0001 (4)
C10	0.0188 (6)	0.0148 (6)	0.0142 (5)	0.0015 (4)	−0.0024 (4)	0.0002 (4)
C11	0.0200 (6)	0.0186 (6)	0.0138 (5)	0.0017 (4)	0.0030 (4)	0.0013 (4)
C12	0.0147 (5)	0.0195 (6)	0.0196 (6)	0.0009 (4)	0.0023 (4)	0.0011 (4)
C13	0.0145 (5)	0.0192 (6)	0.0161 (6)	0.0009 (4)	−0.0020 (4)	0.0007 (4)
C14	0.0158 (6)	0.0121 (5)	0.0142 (5)	0.0007 (4)	−0.0002 (4)	0.0005 (4)

Geometric parameters (Å, º)

O1—C7	1.3598 (14)	C5—H5	0.9500
O1—C1	1.4099 (13)	C6—H6	0.9500
N1—C7	1.2941 (15)	C7—C8	1.4346 (15)
N1—C14	1.3781 (14)	C8—H8	0.9500
N2—C8	1.2966 (15)	C9—C10	1.4066 (15)
N2—C9	1.3796 (15)	C9—C14	1.4165 (16)
C1—C2	1.3780 (17)	C10—C11	1.3751 (16)
C1—C6	1.3786 (17)	C10—H10	0.9500
C2—C3	1.3880 (16)	C11—C12	1.4086 (16)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.3847 (18)	C12—C13	1.3730 (15)

C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.383 (2)	C13—C14	1.4073 (16)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.3931 (17)		

C7—O1—C1	117.58 (9)	O1—C7—C8	113.94 (10)
C7—N1—C14	115.20 (10)	N2—C8—C7	121.96 (11)
C8—N2—C9	116.40 (10)	N2—C8—H8	119.0
C2—C1—C6	122.08 (11)	C7—C8—H8	119.0
C2—C1—O1	117.68 (10)	N2—C9—C10	119.51 (10)
C6—C1—O1	120.14 (11)	N2—C9—C14	120.90 (10)
C1—C2—C3	118.77 (11)	C10—C9—C14	119.59 (10)
C1—C2—H2	120.6	C11—C10—C9	120.38 (10)
C3—C2—H2	120.6	C11—C10—H10	119.8
C4—C3—C2	120.30 (12)	C9—C10—H10	119.8
C4—C3—H3	119.8	C10—C11—C12	120.04 (11)
C2—C3—H3	119.8	C10—C11—H11	120.0
C5—C4—C3	119.98 (11)	C12—C11—H11	120.0
C5—C4—H4	120.0	C13—C12—C11	120.46 (11)
C3—C4—H4	120.0	C13—C12—H12	119.8
C4—C5—C6	120.32 (12)	C11—C12—H12	119.8
C4—C5—H5	119.8	C12—C13—C14	120.53 (10)
C6—C5—H5	119.8	C12—C13—H13	119.7
C1—C6—C5	118.53 (12)	C14—C13—H13	119.7
C1—C6—H6	120.7	N1—C14—C13	119.52 (10)
C5—C6—H6	120.7	N1—C14—C9	121.50 (10)
N1—C7—O1	122.03 (10)	C13—C14—C9	118.98 (11)
N1—C7—C8	124.02 (11)		

C7—O1—C1—C2	100.70 (12)	O1—C7—C8—N2	178.65 (10)
C7—O1—C1—C6	−82.79 (13)	C8—N2—C9—C10	179.47 (10)
C6—C1—C2—C3	1.36 (17)	C8—N2—C9—C14	−0.26 (15)
O1—C1—C2—C3	177.79 (10)	N2—C9—C10—C11	−178.53 (10)
C1—C2—C3—C4	−0.52 (17)	C14—C9—C10—C11	1.21 (16)
C2—C3—C4—C5	−0.52 (18)	C9—C10—C11—C12	−0.64 (16)
C3—C4—C5—C6	0.77 (18)	C10—C11—C12—C13	−0.59 (17)
C2—C1—C6—C5	−1.11 (17)	C11—C12—C13—C14	1.22 (17)
O1—C1—C6—C5	−177.45 (10)	C7—N1—C14—C13	−178.90 (10)
C4—C5—C6—C1	0.02 (17)	C7—N1—C14—C9	1.19 (15)
C14—N1—C7—O1	−179.82 (10)	C12—C13—C14—N1	179.46 (10)
C14—N1—C7—C8	−0.37 (15)	C12—C13—C14—C9	−0.63 (16)
C1—O1—C7—N1	5.91 (15)	N2—C9—C14—N1	−0.94 (16)
C1—O1—C7—C8	−173.59 (10)	C10—C9—C14—N1	179.33 (10)
C9—N2—C8—C7	1.10 (15)	N2—C9—C14—C13	179.15 (10)
N1—C7—C8—N2	−0.84 (17)	C10—C9—C14—C13	−0.58 (15)