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Phenyl pyrazin-2-yl ether

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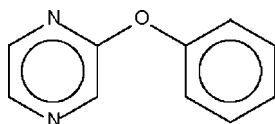
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.046; wR factor = 0.119; data-to-parameter ratio = 16.5.

 In the title compound, $\text{C}_{10}\text{H}_8\text{N}_2\text{O}$, the dihedral angle between the aromatic rings is $64.2(1)^\circ$ and the bridging $\text{C}-\text{O}-\text{C}$ angle is $119.1(1)^\circ$.

Related literature

 For the structure of quinoxaliny phenyl ether, see: Hassan *et al.* (2008). For the structure of *N*-(pyrazin-2-yl)aniline, see: Wan Saffiee *et al.* (2008).


Experimental

Crystal data

 $\text{C}_{10}\text{H}_8\text{N}_2\text{O}$
 $M_r = 172.18$
 Monoclinic, $P2_1/c$
 $a = 5.704(1)$ Å
 $b = 8.557(2)$ Å
 $c = 17.595(4)$ Å
 $\beta = 94.382(3)^\circ$
 $V = 856.4(3)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 100(2)$ K
 $0.20 \times 0.15 \times 0.10$ mm

Data collection

 Bruker SMART APEX
 diffractometer
 Absorption correction: none
 4641 measured reflections

 1950 independent reflections
 1207 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.119$
 $S = 0.97$
 1950 reflections

 118 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ 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: HB2867).

References

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supplementary materials

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Phenyl pyrazin-2-yl ether

A. Idris, A. Afiffin, Z. Abdullah and S. W. Ng

Experimental

Phenol (0.94 g, 0.01 mol) was dissolved in a small volume of water containing sodium hydroxide (0.40 g, 0.01 mol). The mixture was heated to remove most of the water. This and 2-chloropyrazine (1.15 g, 0.01 mol) were heated for 5 h. The material was extracted with chloroform and the organic phase then dried over sodium sulfate. Evaporation of the solvent gave the crude product, which was recrystallized from chloroform.

Refinement

The H atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

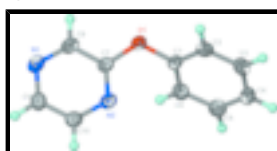


Fig. 1. The molecular structure of (I) at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Phenyl pyrazin-2-yl ether

Crystal data

$\text{C}_{10}\text{H}_8\text{N}_2\text{O}$

$M_r = 172.18$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.704$ (1) Å

$b = 8.557$ (2) Å

$c = 17.595$ (4) Å

$\beta = 94.382$ (3)°

$V = 856.4$ (3) Å³

$Z = 4$

$F_{000} = 360$

$D_x = 1.335$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 739 reflections

$\theta = 3.3$ – 26.1 °

$\mu = 0.09$ mm⁻¹

$T = 100$ (2) K

Irregular block, colorless

$0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

1207 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

supplementary materials

Monochromator: graphite $\theta_{\max} = 27.5^\circ$
 $T = 100(2)$ K $\theta_{\min} = 2.3^\circ$
 ω scans $h = -6 \rightarrow 7$
Absorption correction: None $k = -11 \rightarrow 10$
4641 measured reflections $l = -22 \rightarrow 21$
1950 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.046$ H-atom parameters constrained
 $wR(F^2) = 0.119$ $w = 1/[\sigma^2(F_o^2) + (0.0572P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $S = 0.97$ $(\Delta/\sigma)_{\max} = 0.001$
1950 reflections $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
118 parameters $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods Extinction correction: none

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.0900 (2)	0.70888 (14)	0.45704 (7)	0.0301 (3)
N1	0.4770 (3)	0.56153 (17)	0.60955 (8)	0.0281 (4)
N2	0.4352 (3)	0.81790 (16)	0.51088 (8)	0.0252 (4)
C1	0.0879 (3)	0.8138 (2)	0.39557 (9)	0.0244 (4)
C2	-0.1015 (3)	0.9128 (2)	0.38509 (10)	0.0288 (4)
H2	-0.2208	0.9130	0.4199	0.035*
C3	-0.1150 (3)	1.0127 (2)	0.32238 (10)	0.0320 (5)
H3	-0.2447	1.0819	0.3140	0.038*
C4	0.0604 (3)	1.0112 (2)	0.27248 (10)	0.0309 (5)
H4	0.0520	1.0803	0.2301	0.037*
C5	0.2481 (3)	0.9097 (2)	0.28386 (10)	0.0298 (5)
H5	0.3672	0.9086	0.2489	0.036*
C6	0.2641 (3)	0.8093 (2)	0.34580 (9)	0.0266 (4)
H6	0.3927	0.7393	0.3539	0.032*
C7	0.2816 (3)	0.70451 (19)	0.50838 (9)	0.0225 (4)
C8	0.2987 (3)	0.5762 (2)	0.55764 (10)	0.0279 (4)
H8	0.1799	0.4981	0.5537	0.033*
C9	0.6367 (3)	0.6767 (2)	0.61232 (10)	0.0275 (4)
H9	0.7686	0.6707	0.6486	0.033*
C10	0.6149 (3)	0.8027 (2)	0.56430 (9)	0.0274 (4)
H10	0.7311	0.8823	0.5690	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0285 (7)	0.0309 (8)	0.0299 (7)	-0.0092 (6)	-0.0033 (5)	0.0105 (6)
N1	0.0356 (9)	0.0253 (8)	0.0237 (8)	-0.0023 (7)	0.0037 (7)	0.0021 (7)
N2	0.0304 (9)	0.0229 (8)	0.0222 (8)	-0.0055 (6)	0.0020 (6)	0.0000 (7)
C1	0.0279 (10)	0.0230 (10)	0.0215 (9)	-0.0088 (8)	-0.0028 (7)	0.0039 (8)
C2	0.0233 (10)	0.0323 (11)	0.0307 (10)	-0.0049 (8)	0.0021 (7)	0.0031 (9)
C3	0.0267 (11)	0.0321 (11)	0.0362 (10)	-0.0007 (8)	-0.0041 (8)	0.0044 (9)
C4	0.0338 (11)	0.0344 (11)	0.0237 (9)	-0.0062 (9)	-0.0037 (8)	0.0068 (9)
C5	0.0316 (11)	0.0368 (11)	0.0209 (9)	-0.0056 (9)	0.0011 (8)	-0.0027 (9)
C6	0.0280 (10)	0.0256 (10)	0.0255 (9)	-0.0014 (8)	-0.0020 (8)	-0.0032 (8)
C7	0.0253 (10)	0.0224 (10)	0.0203 (8)	-0.0029 (7)	0.0043 (7)	-0.0007 (8)
C8	0.0319 (11)	0.0246 (10)	0.0274 (10)	-0.0060 (8)	0.0048 (8)	0.0015 (8)
C9	0.0315 (11)	0.0287 (10)	0.0219 (9)	-0.0001 (8)	-0.0011 (7)	0.0005 (8)
C10	0.0295 (10)	0.0287 (11)	0.0238 (9)	-0.0076 (8)	0.0003 (7)	-0.0011 (9)

Geometric parameters (\AA , $^\circ$)

O1—C7	1.364 (2)	C3—H3	0.9500
O1—C1	1.4050 (19)	C4—C5	1.382 (3)
N1—C8	1.320 (2)	C4—H4	0.9500
N1—C9	1.340 (2)	C5—C6	1.385 (2)
N2—C7	1.306 (2)	C5—H5	0.9500
N2—C10	1.343 (2)	C6—H6	0.9500
C1—C2	1.374 (3)	C7—C8	1.398 (2)
C1—C6	1.383 (2)	C8—H8	0.9500
C2—C3	1.394 (2)	C9—C10	1.370 (2)
C2—H2	0.9500	C9—H9	0.9500
C3—C4	1.381 (3)	C10—H10	0.9500
C7—O1—C1	119.11 (13)	C6—C5—H5	119.8
C8—N1—C9	116.18 (15)	C1—C6—C5	118.29 (17)
C7—N2—C10	115.21 (15)	C1—C6—H6	120.9
C2—C1—C6	122.28 (16)	C5—C6—H6	120.9
C2—C1—O1	117.23 (15)	N2—C7—O1	120.23 (15)
C6—C1—O1	120.38 (16)	N2—C7—C8	123.24 (16)
C1—C2—C3	118.68 (17)	O1—C7—C8	116.52 (15)
C1—C2—H2	120.7	N1—C8—C7	121.13 (16)
C3—C2—H2	120.7	N1—C8—H8	119.4
C4—C3—C2	119.90 (18)	C7—C8—H8	119.4
C4—C3—H3	120.0	N1—C9—C10	121.80 (16)
C2—C3—H3	120.0	N1—C9—H9	119.1
C3—C4—C5	120.36 (17)	C10—C9—H9	119.1
C3—C4—H4	119.8	N2—C10—C9	122.43 (17)
C5—C4—H4	119.8	N2—C10—H10	118.8
C4—C5—C6	120.49 (17)	C9—C10—H10	118.8
C4—C5—H5	119.8		

supplementary materials

C7—O1—C1—C2	-126.78 (17)	C10—N2—C7—O1	179.05 (14)
C7—O1—C1—C6	56.9 (2)	C10—N2—C7—C8	0.5 (2)
C6—C1—C2—C3	-0.5 (3)	C1—O1—C7—N2	15.5 (2)
O1—C1—C2—C3	-176.75 (15)	C1—O1—C7—C8	-165.92 (14)
C1—C2—C3—C4	-0.2 (3)	C9—N1—C8—C7	0.6 (2)
C2—C3—C4—C5	0.8 (3)	N2—C7—C8—N1	-1.1 (3)
C3—C4—C5—C6	-0.7 (3)	O1—C7—C8—N1	-179.72 (15)
C2—C1—C6—C5	0.6 (3)	C8—N1—C9—C10	0.4 (3)
O1—C1—C6—C5	176.75 (14)	C7—N2—C10—C9	0.5 (2)
C4—C5—C6—C1	0.0 (3)	N1—C9—C10—N2	-1.0 (3)

Fig. 1

