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Phenyl pyrazin-2-yl ether

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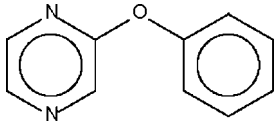
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.119; data-to-parameter ratio = 16.5.

In the title compound, $C_{10}H_8N_2O$, the dihedral angle between the aromatic rings is 64.2 (1)° and the bridging C—O—C angle is 119.1 (1)°.

Related literature

For the structure of quinoxalinyl 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

$C_{10}H_8N_2O$
M_r = 172.18
Monoclinic, $P2_1/c$
a = 5.704 (1) Å
b = 8.557 (2) Å
c = 17.595 (4) Å
β = 94.382 (3)°
V = 856.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.20 × 0.15 × 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_{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
$\Delta\rho_{max}$ = 0.20 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: HB2867).

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supporting information

Acta Cryst. (2009). E**65**, o7 [doi:10.1107/S1600536808040099]

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S1. 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.

S2. Refinement

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

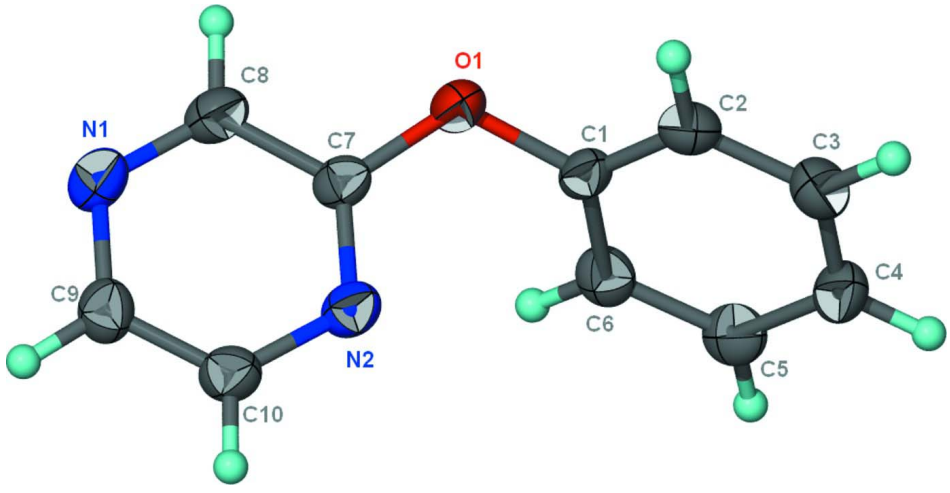

Figure 1

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

$C_{10}H_8N_2O$
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
β = 94.382 (3)°
V = 856.4 (3) Å^3
Z = 4
F(000) = 360
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 739 reflections
θ = 3.3–26.1°
μ = 0.09 mm^{-1}
T = 100 K
Irregular block, colorless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
4641 measured reflections
1950 independent reflections
1207 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 7$
$k = -11 \rightarrow 10$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.119$
$S = 0.97$
1950 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ 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	0.0900 (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 (Å²)

	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 (Å, º)

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		
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)