Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2-Methoxyphenoxy)pyrazine

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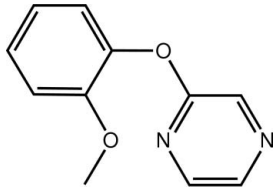
Received 24 October 2011; accepted 25 October 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.107; data-to-parameter ratio = 12.6.

A significant twist is observed in the title molecule, $C_{11}H_{10}N_2O_2$, as seen in the dihedral angle between the pyrazine and benzene rings of 72.79 (8)°. The methoxy group is almost coplanar with the benzene ring to which it is attached [C—O—C—C torsion angle = 175.83 (15)°]. Centrosymmetric dimers are formed in the crystal structure which are held together by weak π–π interactions between pyrazine rings [centroid–centroid distance = 3.8534 (10) Å].

Related literature

For the structure of a related pyrimidine derivative, see: Aznan Akhmad *et al.* (2010).



Experimental

Crystal data

$C_{11}H_{10}N_2O_2$
M_r = 202.21
Monoclinic, $P2_1/n$
a = 7.7497 (10) Å
b = 5.8826 (8) Å
c = 21.845 (3) Å
β = 92.459 (2)°
V = 995.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.35 × 0.3 × 0.2 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.789, T_{max} = 0.862
7364 measured reflections
1743 independent reflections
1262 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.03
1743 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank the University of Malaya (grant No. RG027/09AFR) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5121).

References

Aznan Akhmad, M. A., Abdullah, Z., Fairuz, Z. A., Ng, S. W. & Tiekink, E. R. T. (2010). *Acta Cryst.* E**66**, o2400.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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supporting information

Acta Cryst. (2011). E**67**, o3088 [doi:10.1107/S1600536811044321]

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S1. Comment

As a part of an on-going synthetic and structural study of *N*-heterocyclic derivatives (Aznan Akhmad *et al.*, 2010), the title compound, (I), was investigated. In (I), Fig. 1, the benzene ring is almost orthogonal to the pyrazine ring, forming a dihedral angle of 72.79 (8)°. The methoxy substituent is co-planar to the benzene ring to which it is connected: the C11—O2—C10—C5 torsion angle is 175.83 (15)°. In the crystal structure, centrosymmetrically related pyrazine rings associate *via* weak *π*–*π* interactions [centroid···centroid^{i} distance = 3.8534 (10) Å for *i*: 1 - *x*, -*y*, 1 - *z*]. The dimeric aggregates stack along the *b* axis, Fig. 2.

S2. Experimental

o-Methoxyphenol (2.50 g, 20 mmol) and sodium hydroxide (0.80 g, 20 mmol) were dissolved in water (50 ml) and to the solution was added 2-chloropyrazine (2.28 g, 20 mmol) dissolved in THF (50 ml). The mixture was heated for 6 h. Water was added and the organic phase extracted with chloroform. The chloroform solution was dried over sodium sulfate; slow evaporation led to the formation of colourless crystals.

S3. Refinement

Hydrogen atoms were placed at calculated positions (C—H 0.93–0.96 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2–1.5U_{eq}(C).

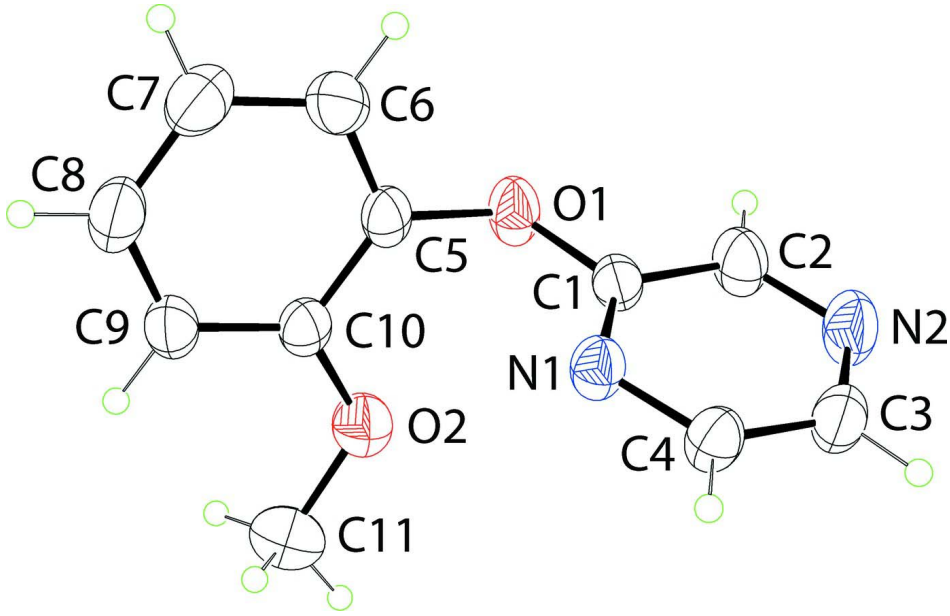

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

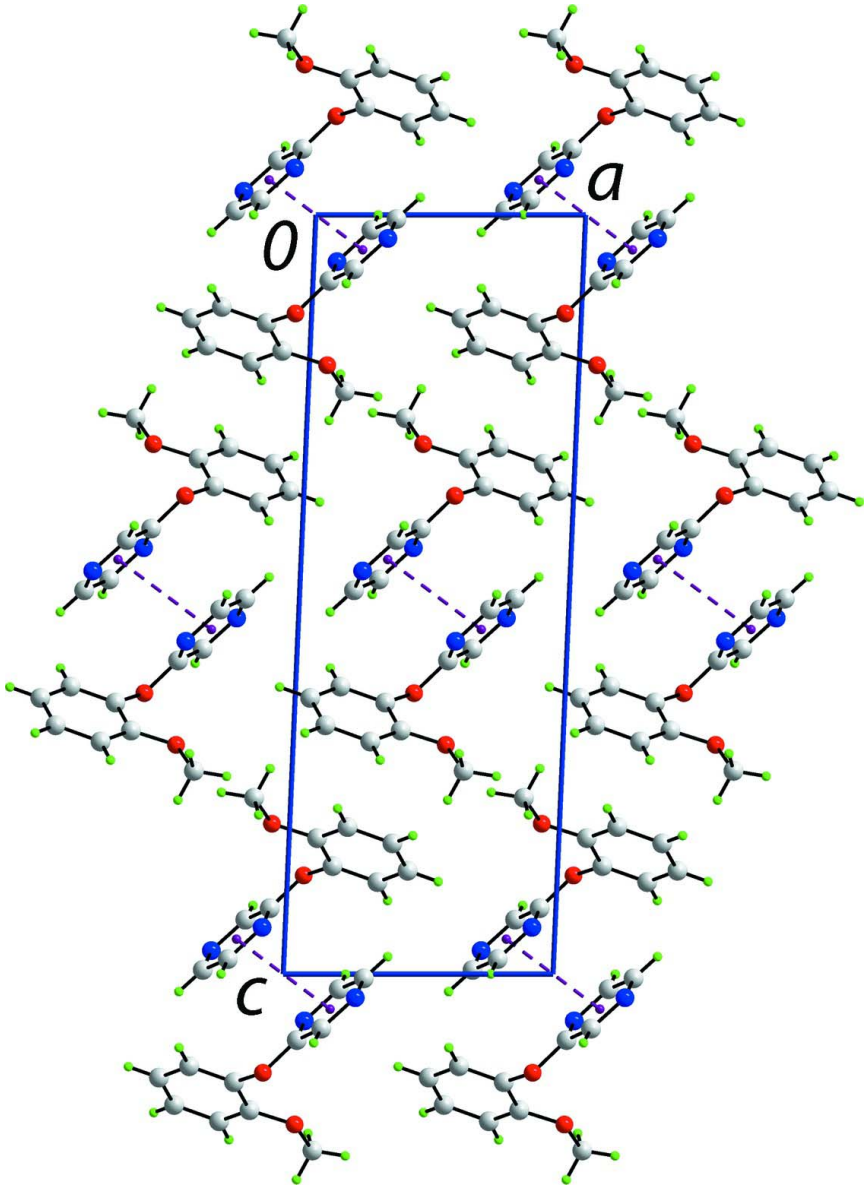

Figure 2

Unit-cell contents for (I) shown in projection down the *b* axis. The π–π interactions are shown as purple dashed lines.

2-(2-Methoxyphenoxy)pyrazine

Crystal data

$C_{11}H_{10}N_2O_2$
$M_r = 202.21$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.7497$ (10) Å
$b = 5.8826$ (8) Å
$c = 21.845$ (3) Å
$\beta = 92.459$ (2)°
$V = 995.0$ (2) Å^3
$Z = 4$

$F(000) = 424$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1739 reflections
$\theta = 2.8$–$27.3°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Block, colourless
0.35 × 0.3 × 0.2 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.789, T_{max} = 0.862
7364 measured reflections
1743 independent reflections
1262 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.0°, θ_{min} = 1.9°
$h = -9\rightarrow8$
$k = -6\rightarrow6$
$l = -25\rightarrow25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.03
1743 reflections
138 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
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.0981P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.105 (7)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.44004 (16)	0.13299 (17)	0.62993 (5)	0.0618 (4)
O2	0.56589 (16)	0.4818 (2)	0.69804 (6)	0.0658 (4)
N1	0.58582 (17)	0.3536 (2)	0.56159 (6)	0.0505 (4)
N2	0.7704 (2)	−0.0324 (2)	0.53106 (8)	0.0716 (5)
C1	0.5605 (2)	0.1567 (2)	0.58683 (7)	0.0455 (4)
C2	0.6494 (2)	−0.0375 (3)	0.57169 (8)	0.0626 (5)
H2	0.6235	−0.1744	0.5905	0.075*
C3	0.7991 (2)	0.1687 (3)	0.50551 (9)	0.0609 (5)
H3	0.8842	0.1806	0.4770	0.073*
C4	0.7080 (2)	0.3568 (3)	0.51984 (8)	0.0535 (5)
H4	0.7310	0.4928	0.5001	0.064*
C5	0.3345 (2)	0.3184 (3)	0.64234 (7)	0.0487 (4)
C6	0.1658 (3)	0.3139 (3)	0.62125 (8)	0.0637 (5)
H6	0.1254	0.1940	0.5969	0.076*
C7	0.0555 (2)	0.4879 (4)	0.63627 (9)	0.0711 (6)
H7	−0.0593	0.4862	0.6219	0.085*
C8	0.1162 (3)	0.6618 (3)	0.67224 (9)	0.0674 (6)
H8	0.0420	0.7789	0.6824	0.081*
C9	0.2854 (2)	0.6670 (3)	0.69370 (8)	0.0571 (5)
H9	0.3249	0.7873	0.7181	0.068*
C10	0.3965 (2)	0.4947 (3)	0.67918 (7)	0.0484 (4)
C11	0.6363 (3)	0.6667 (3)	0.73229 (10)	0.0794 (6)
H11A	0.7582	0.6441	0.7394	0.119*
H11B	0.5817	0.6761	0.7708	0.119*

H11C	0.6166	0.8052	0.7098	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0810 (9)	0.0387 (6)	0.0682 (8)	0.0039 (5)	0.0331 (7)	0.0021 (5)
O2	0.0604 (8)	0.0644 (8)	0.0725 (8)	0.0036 (6)	0.0023 (6)	−0.0089 (6)
N1	0.0558 (9)	0.0438 (8)	0.0529 (8)	0.0063 (6)	0.0124 (7)	0.0032 (6)
N2	0.0788 (12)	0.0533 (9)	0.0851 (11)	0.0142 (8)	0.0294 (9)	−0.0049 (8)
C1	0.0516 (10)	0.0403 (9)	0.0450 (9)	0.0003 (7)	0.0088 (7)	−0.0039 (7)
C2	0.0779 (13)	0.0399 (9)	0.0716 (12)	0.0082 (8)	0.0209 (10)	0.0004 (8)
C3	0.0575 (11)	0.0613 (11)	0.0655 (11)	0.0062 (9)	0.0200 (9)	−0.0036 (9)
C4	0.0531 (10)	0.0532 (10)	0.0551 (10)	0.0039 (8)	0.0130 (8)	0.0054 (8)
C5	0.0584 (11)	0.0415 (9)	0.0479 (9)	0.0004 (8)	0.0209 (8)	0.0017 (7)
C6	0.0681 (13)	0.0671 (12)	0.0569 (11)	−0.0133 (10)	0.0153 (9)	−0.0117 (9)
C7	0.0531 (12)	0.0906 (15)	0.0703 (12)	0.0018 (10)	0.0112 (9)	−0.0025 (12)
C8	0.0642 (13)	0.0642 (12)	0.0758 (13)	0.0118 (10)	0.0244 (10)	−0.0003 (10)
C9	0.0637 (12)	0.0478 (10)	0.0612 (11)	−0.0007 (8)	0.0204 (9)	−0.0056 (8)
C10	0.0539 (10)	0.0449 (9)	0.0476 (9)	−0.0006 (8)	0.0153 (7)	0.0024 (7)
C11	0.0816 (15)	0.0739 (14)	0.0819 (14)	−0.0131 (11)	−0.0062 (11)	−0.0045 (11)

Geometric parameters (Å, º)

O1—C1	1.3611 (18)	C5—C6	1.368 (2)
O1—C5	1.3969 (18)	C5—C10	1.386 (2)
O2—C10	1.361 (2)	C6—C7	1.382 (3)
O2—C11	1.416 (2)	C6—H6	0.9300
N1—C1	1.3013 (19)	C7—C8	1.362 (3)
N1—C4	1.343 (2)	C7—H7	0.9300
N2—C2	1.319 (2)	C8—C9	1.374 (3)
N2—C3	1.331 (2)	C8—H8	0.9300
C1—C2	1.382 (2)	C9—C10	1.376 (2)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.356 (2)	C11—H11A	0.9600
C3—H3	0.9300	C11—H11B	0.9600
C4—H4	0.9300	C11—H11C	0.9600
C1—O1—C5	118.61 (11)	C5—C6—H6	120.1
C10—O2—C11	117.50 (14)	C7—C6—H6	120.1
C1—N1—C4	115.09 (13)	C8—C7—C6	119.45 (19)
C2—N2—C3	116.06 (14)	C8—C7—H7	120.3
N1—C1—O1	120.31 (13)	C6—C7—H7	120.3
N1—C1—C2	123.27 (14)	C7—C8—C9	120.97 (17)
O1—C1—C2	116.42 (14)	C7—C8—H8	119.5
N2—C2—C1	121.24 (16)	C9—C8—H8	119.5
N2—C2—H2	119.4	C8—C9—C10	120.18 (17)
C1—C2—H2	119.4	C8—C9—H9	119.9
N2—C3—C4	122.03 (16)	C10—C9—H9	119.9

N2—C3—H3	119.0	O2—C10—C9	125.19 (16)
C4—C3—H3	119.0	O2—C10—C5	116.11 (14)
N1—C4—C3	122.29 (15)	C9—C10—C5	118.71 (17)
N1—C4—H4	118.9	O2—C11—H11A	109.5
C3—C4—H4	118.9	O2—C11—H11B	109.5
C6—C5—C10	120.86 (15)	H11A—C11—H11B	109.5
C6—C5—O1	118.58 (15)	O2—C11—H11C	109.5
C10—C5—O1	120.38 (16)	H11A—C11—H11C	109.5
C5—C6—C7	119.83 (17)	H11B—C11—H11C	109.5

C4—N1—C1—O1	179.84 (14)	O1—C5—C6—C7	175.72 (14)
C4—N1—C1—C2	−1.0 (2)	C5—C6—C7—C8	−0.3 (3)
C5—O1—C1—N1	5.6 (2)	C6—C7—C8—C9	0.1 (3)
C5—O1—C1—C2	−173.59 (15)	C7—C8—C9—C10	−0.2 (3)
C3—N2—C2—C1	−0.7 (3)	C11—O2—C10—C9	−4.0 (2)
N1—C1—C2—N2	1.7 (3)	C11—O2—C10—C5	175.83 (15)
O1—C1—C2—N2	−179.10 (16)	C8—C9—C10—O2	−179.69 (16)
C2—N2—C3—C4	−0.8 (3)	C8—C9—C10—C5	0.5 (2)
C1—N1—C4—C3	−0.5 (3)	C6—C5—C10—O2	179.48 (14)
N2—C3—C4—N1	1.5 (3)	O1—C5—C10—O2	4.4 (2)
C1—O1—C5—C6	106.12 (17)	C6—C5—C10—C9	−0.7 (2)
C1—O1—C5—C10	−78.74 (19)	O1—C5—C10—C9	−175.73 (13)
C10—C5—C6—C7	0.6 (3)		