

2-(2-Methoxyphenoxy)pyrazine

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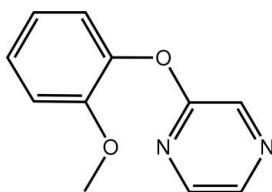
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.107; data-to-parameter ratio = 12.6.

A significant twist is observed in the title molecule, $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2$, 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 [$\text{C}-\text{O}-\text{C}$ torsion angle = 175.83 (15)°]. Centrosymmetric dimers are formed in the crystal structure which are held together by weak $\pi-\pi$ 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

$\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2$
 $M_r = 202.21$
 Monoclinic, $P2_1/n$
 $a = 7.7497$ (10) Å
 $b = 5.8826$ (8) Å
 $c = 21.845$ (3) Å
 $\beta = 92.459$ (2)°
 $V = 995.0$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ K
 $0.35 \times 0.3 \times 0.2$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

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).

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supplementary materials

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2-(2-Methoxyphenoxy)pyrazine

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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 \cdots centroidⁱ distance = 3.8534 (10) Å for *i*: 1 - *x*, -*y*, 1 - *z*]. The dimeric aggregates stack along the *b* axis, Fig. 2.

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.

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 $U(\text{H})$ set to 1.2–1.5 $U_{\text{eq}}(\text{C})$.

Figures

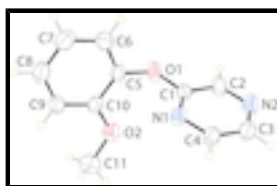


Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

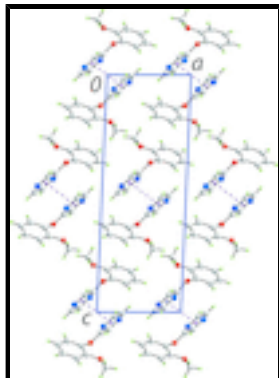


Fig. 2. Unit-cell contents for (I) shown in projection down the *b* axis. The π - π interactions are shown as purple dashed lines.

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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) Å³

$Z = 4$

$F(000) = 424$

$D_x = 1.350$ 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

$0.35 \times 0.3 \times 0.2$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube
graphite

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 1.9$ °

$h = -9 \rightarrow 8$

$k = -6 \rightarrow 6$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.107$

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 $P = (F_o^2 + 2F_c^2)/3$

$S = 1.03$	$(\Delta/\sigma)_{\max} = 0.001$
1743 reflections	$\Delta\rho_{\max} = 0.13 \text{ e } \text{\AA}^{-3}$
138 parameters	$\Delta\rho_{\min} = -0.13 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.105 (7)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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)

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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, °)

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)

supplementary materials

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)		

Fig. 1

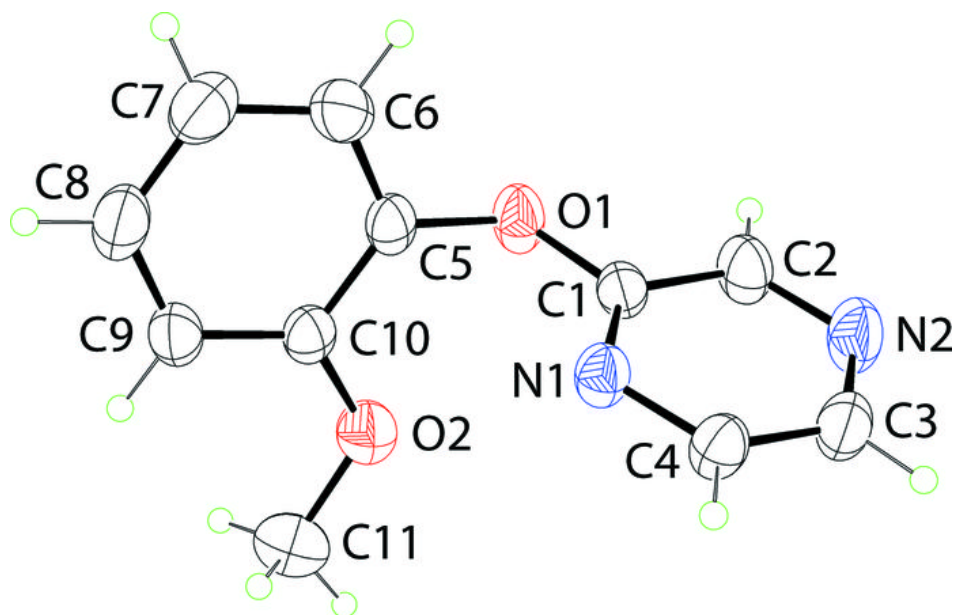


Fig. 2

