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1,4-Bis(pyrazin-2-yloxy)benzene

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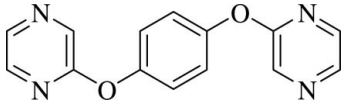
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.101; data-to-parameter ratio = 11.5.

The title compound, $C_{14}H_{10}N_4O_2$, was synthesized by the reaction of hydroquinone with 2-chloropyrazine in dimethyl sulfoxide. The molecules possesses crystallographic inversion symmetry with one half-molecule in the asymmetric unit. Weak face-to-face π–π stacking interactions are observed between the pyrazinyl rings [centroid-to-centroid distance 3.611 (2) Å], linking the molecules into a three-dimensional structure.

Related literature

For related literature, see: Hartshorn & Steel (1996, 1998).



Experimental

Crystal data

$C_{14}H_{10}N_4O_2$
M_r = 266.26
Triclinic, $P\overline{1}$
a = 5.8927 (18) Å
b = 6.720 (2) Å
c = 8.212 (3) Å
α = 70.136 (4)°
β = 89.296 (5)°
γ = 82.674 (5)°
V = 303.19 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.984
1581 measured reflections
1056 independent reflections
889 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.101
S = 1.04
1056 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2604).

References

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Hartshorn, C. M. & Steel, P. J. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3927–3933.
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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*, University of Göttingen, Germany.

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supplementary materials

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1,4-Bis(pyrazin-2-yloxy)benzene

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Comment

Pyridyloxybenzenes have been reported (Hartshorn & Steel, 1996; Hartshorn & Steel, 1998) as useful ligands to form numerous metallosupramolecular species with novel topological structures (Hartshorn & Steel, 1998). Pyrazinyl ring contain two N atoms coordinated to metal ions and it may be used to construct specific molecular architectures. As a continuous work of our group, we here report the crystal structure of 1,4-bis(2-pyrazinyloxy)benzene (I).

The title compound is composed of two pyrazinyl rings and one phenyl ring (Fig. 1). The two pyrazinyl rings enclose a dihedral angle of 74.67 (12) ° with the phenyl ring. There are weak face-to-face π–π stacking interactions between two neighboring molecules, with the centroids of the two pyrazinyl rings separated by 3.730 (2)Å (symmetry operator: −*x*, −*y*, −*z*) and 3.611 (2)Å (symmetry operator: −*x*, 1 − *y*, −*z*) (Fig. 2).

Experimental

For the synthesis of 1,4-bis(2-pyrazinyloxy)benzene, (I), a mixture of 2-chloropyrazine (0.01 mol, 1.14 g), hydroquinone (0.005 mol, 0.55 g) and potassium carbonate (0.01 mol, 1.38 g) in DMSO was refluxed for 6 h under nitrogen atmosphere. The solid product obtained on cooling was filtered, washed with water, dried and crystallized from acetonitrile (yield 75%). The resulting product (1.0 mmol, 0.266 g) was dissolved in acetonitrile (15 ml) and kept at room temperature for one week, after which colorless block shaped single crystals formed, were collected and washed with acetonitrile.

Refinement

All H atoms were initially located in a difference Fourier map. They were constrained to an ideal geometry, *C*(phenyl)—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

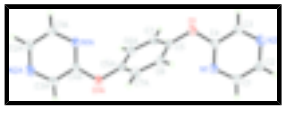

Fig. 1. The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

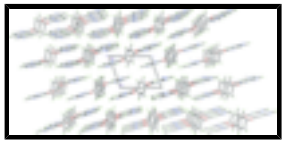

Fig. 2. Packing of the molecules, viewed down the *a* axis.

1,4-Bis(pyrazin-2-yloxy)benzene

Crystal data

$C_{14}H_{10}N_4O_2$	$Z = 1$
$M_r = 266.26$	$F_{000} = 138$
Triclinic, $P\overline{1}$	$D_x = 1.458$ Mg m^{-3}
$a = 5.8927$ (18) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 6.720$ (2) Å	Cell parameters from 965 reflections
$c = 8.212$ (3) Å	$\theta = 2.6$–$26.3°$
$\alpha = 70.136$ (4)°	$\mu = 0.10$ mm^{-1}
$\beta = 89.296$ (5)°	$T = 294$ (2) K
$\gamma = 82.674$ (5)°	Block, colorless
$V = 303.19$ (16) Å^3	0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1056 independent reflections
Radiation source: fine-focus sealed tube	889 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 294$(2) K	$\theta_{max} = 25.0°$
phi and ω scans	$\theta_{min} = 2.6°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -4\rightarrow7$
$T_{min} = 0.978$, $T_{max} = 0.984$	$k = -7\rightarrow7$
1581 measured reflections	$l = -9\rightarrow9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.0426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.101$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
1056 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
92 parameters	Extinction correction: SHELXL
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.37 (4)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.10275 (16)	0.12708 (18)	0.29608 (12)	0.0511 (4)
N1	0.31332 (19)	0.19754 (18)	0.04800 (15)	0.0419 (4)
N2	−0.0998 (2)	0.30881 (19)	−0.14276 (16)	0.0476 (4)
C1	0.3052 (3)	0.2596 (2)	−0.12524 (18)	0.0467 (4)
H1	0.4416	0.2658	−0.1839	0.056*
C2	0.1027 (3)	0.3140 (2)	−0.21823 (19)	0.0499 (4)
H2	0.1057	0.3561	−0.3384	0.060*
C3	−0.0938 (2)	0.2474 (2)	0.02777 (18)	0.0413 (4)
H3	−0.2300	0.2410	0.0866	0.050*
C4	0.1147 (2)	0.1920 (2)	0.12088 (17)	0.0367 (4)
C5	0.3092 (2)	0.0643 (2)	0.39486 (16)	0.0414 (4)
C6	0.4373 (3)	0.2142 (2)	0.40865 (19)	0.0487 (4)
H6	0.3941	0.3582	0.3470	0.058*
C7	0.3681 (3)	−0.1486 (2)	0.48455 (18)	0.0476 (4)
H7	0.2784	−0.2480	0.4738	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0320 (6)	0.0801 (8)	0.0358 (6)	−0.0028 (5)	−0.0028 (4)	−0.0145 (5)
N1	0.0339 (7)	0.0502 (7)	0.0390 (7)	−0.0028 (5)	−0.0025 (5)	−0.0128 (5)
N2	0.0432 (7)	0.0498 (7)	0.0460 (8)	−0.0033 (5)	−0.0121 (6)	−0.0118 (5)
C1	0.0429 (8)	0.0544 (9)	0.0398 (8)	−0.0069 (6)	0.0012 (6)	−0.0121 (6)
C2	0.0525 (9)	0.0562 (9)	0.0359 (8)	−0.0086 (7)	−0.0062 (7)	−0.0085 (6)
C3	0.0332 (7)	0.0434 (8)	0.0466 (8)	−0.0029 (6)	−0.0045 (6)	−0.0148 (6)
C4	0.0346 (7)	0.0384 (7)	0.0361 (7)	−0.0031 (5)	−0.0033 (5)	−0.0117 (5)
C5	0.0312 (7)	0.0617 (9)	0.0296 (7)	−0.0028 (6)	−0.0002 (5)	−0.0146 (6)
C6	0.0476 (9)	0.0498 (8)	0.0428 (8)	−0.0028 (7)	−0.0035 (7)	−0.0096 (6)
C7	0.0440 (8)	0.0555 (9)	0.0444 (9)	−0.0117 (7)	−0.0027 (6)	−0.0162 (7)

Geometric parameters (Å, °)

O1—C4	1.3580 (16)	C3—C4	1.3949 (19)

O1—C5	1.4060 (16)	C3—H3	0.9300
N1—C4	1.3068 (18)	C5—C6	1.368 (2)
N1—C1	1.3393 (18)	C5—C7	1.369 (2)
N2—C3	1.3181 (18)	C6—C7^{i}	1.382 (2)
N2—C2	1.337 (2)	C6—H6	0.9300
C1—C2	1.365 (2)	C7—C6^{i}	1.382 (2)
C1—H1	0.9300	C7—H7	0.9300
C2—H2	0.9300		
C4—O1—C5	117.97 (10)	N1—C4—O1	120.38 (12)
C4—N1—C1	115.39 (12)	N1—C4—C3	123.42 (13)
C3—N2—C2	116.24 (12)	O1—C4—C3	116.20 (12)
N1—C1—C2	121.93 (14)	C6—C5—C7	121.73 (13)
N1—C1—H1	119.0	C6—C5—O1	120.35 (13)
C2—C1—H1	119.0	C7—C5—O1	117.79 (13)
N2—C2—C1	122.33 (14)	C5—C6—C7^{i}	119.08 (14)
N2—C2—H2	118.8	C5—C6—H6	120.5
C1—C2—H2	118.8	C7^{i}—C6—H6	120.5
N2—C3—C4	120.70 (13)	C5—C7—C6^{i}	119.20 (14)
N2—C3—H3	119.7	C5—C7—H7	120.4
C4—C3—H3	119.7	C6^{i}—C7—H7	120.4
C4—N1—C1—C2	0.3 (2)	N2—C3—C4—N1	0.3 (2)
C3—N2—C2—C1	−0.2 (2)	N2—C3—C4—O1	−178.79 (11)
N1—C1—C2—N2	0.0 (2)	C4—O1—C5—C6	76.42 (17)
C2—N2—C3—C4	0.0 (2)	C4—O1—C5—C7	−107.78 (14)
C1—N1—C4—O1	178.61 (11)	C7—C5—C6—C7^{i}	0.3 (2)
C1—N1—C4—C3	−0.40 (19)	O1—C5—C6—C7^{i}	175.91 (12)
C5—O1—C4—N1	−0.76 (19)	C6—C5—C7—C6^{i}	−0.3 (2)
C5—O1—C4—C3	178.32 (12)	O1—C5—C7—C6^{i}	−176.02 (12)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Fig. 1

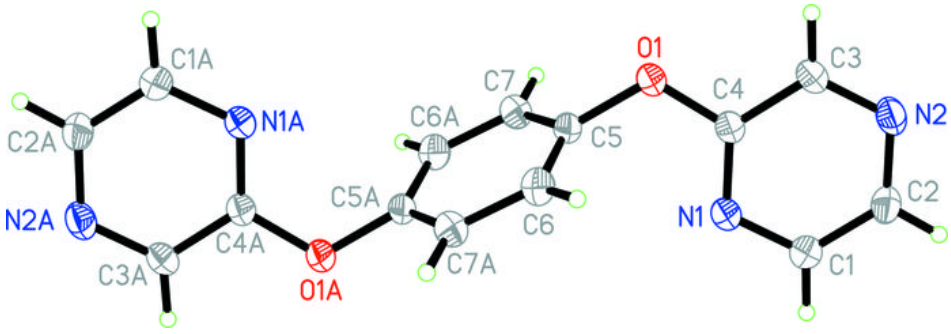
C1A
N1A
C2A
N2A
C3A
C4A
O1A
C5A
C6A
C7
C7A
C6
O1
C5
C4
C3
N2
C2
N1
C1

Fig. 2