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1,4-Bis(pyridin-3-ylmethoxy)benzene

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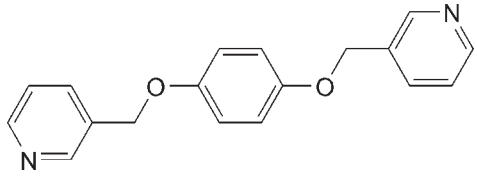
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 16.8.

The asymmetric unit of the centrosymmetric title compound, $C_{18}H_{16}N_2O_2$, contains one half-molecule. The central benzene ring forms a dihedral angle of 66.8 (1)° with two outer aromatic rings. In the crystal structure, weak intermolecular C—H···N hydrogen bonds link molecules into sheets parallel to (104).

Related literature

For general background to bridging molecules with pyridyl substituents at the terminal positions, see: McMorran & Steel (1998); Zaman *et al.* (2005). For details of the synthesis, see: Gao *et al.* (2004). For a related structure, see: Gao *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{16}N_2O_2$
M_r = 292.33
Monoclinic, $P2_1/c$
a = 6.852 (5) Å
b = 5.688 (3) Å
c = 18.861 (12) Å
β = 90.60 (3)°
V = 735.0 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 291 K
0.22 × 0.20 × 0.19 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.981, T_{max} = 0.984
6855 measured reflections
1684 independent reflections
1213 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.09
1684 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N1^{i}	0.93	2.57	3.437 (3)	155

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2613).

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supporting information

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1,4-Bis(pyridin-3-ylmethoxy)benzene

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S1. Comment

The bridging molecules with pyridyl substituents at the terminal positions are hoped to construct interesting supramolecular architectures by intermolecular hydrogen bonding and coordination with metals. McMorran′ group have reported the synthesis of a quadruply stranded helicate that encapsulates a hexafluorophosphate anion by the reaction of 1,4-bis(3-pyridylmethoxy)benzene with palladium chlorate (McMorran *et al.*, 1998). Zaman's group have designed a long rigid organic ligand, 1,4-bis[(3-pyridyl)ethynyl]benzene, which reacted with metal salts to form interpenetrating two-dimensional and three-dimensional cross-zigzag chains and metallocyclic chain structures (Zaman *et al.*, 2005). As an extension of our work about bipyridyl aromatic ligands, we report the crystal structure of the title compound here.

In the title compound (Fig. 1), all bond lengths and angles are normal and correpond to those observed in the related compound (Gao *et al.*, 2006). The 1,4-bis(3-pyridylmethoxy)benzene molecule is centrosymmetric. The planes of two terminal pyridyl groups rotate drastically and make dihedral angles of 66.8 (1) ° with the plane of the central benzene ring.

In the crystal structure, the adjacent 1,4-bis(3-pyridylmethoxy)benzene molecules are linked into two-dimensional supramolecular sheets by intermolecular C—H···N hydrogen bonds (Table 1, Figure 2).

S2. Experimental

The 1,4-bis(3-pyridylmethoxy)benzene was synthesized by the reaction of *p*-benzenediol and 3-chloromethylpyridine hydrochloride under nitrogen atmosphere and alkaline condition (Gao *et al.*, 2004; Gao *et al.*, 2006). Colourless block-shaped crystals of title compound were obtained by slow evaporation of an methanol solution after three days.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å (aromatic), C—H = 0.97 Å (methylene), and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

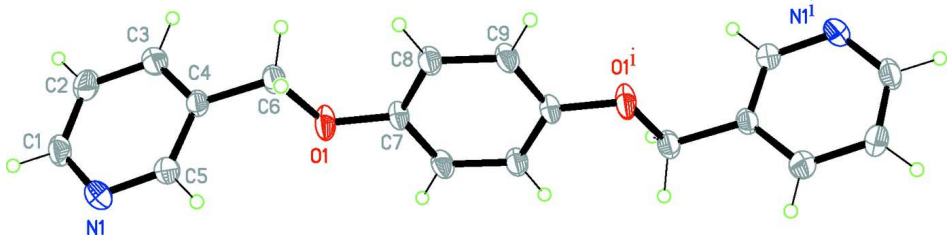

Figure 1

The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids at the 30% probability level [symmetry code: (i) -*x*, 1 - *y*, -*z*].

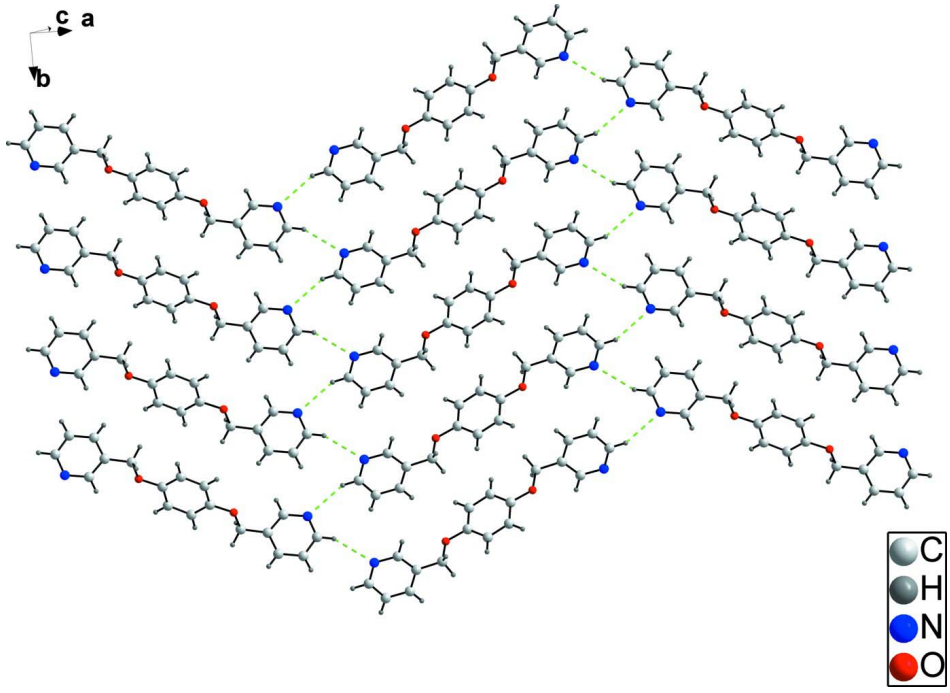

Figure 2

A portion of the crystal packing showing the two-dimensional hydrogen bonded (dashed lines) sheet.

1,4-Bis(pyridin-3-ylmethoxy)benzene

Crystal data

$C_{18}H_{16}N_2O_2$
$M_r = 292.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.852$ (5) Å
$b = 5.688$ (3) Å
$c = 18.861$ (12) Å
$\beta = 90.60$ (3)°
$V = 735.0$ (8) Å^3
$Z = 2$
$F(000) = 308$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4889 reflections
$\theta = 3.7$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 291$ K
Block, colourless
0.22 × 0.20 × 0.19 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.981$, $T_{max} = 0.984$
6855 measured reflections
1684 independent reflections
1213 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.7°$
$h = -8 \rightarrow 8$
$k = -6 \rightarrow 7$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.118$
$S = 1.09$
1684 reflections
100 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
$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 0.0635P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8460 (2)	−0.0288 (3)	0.20865 (8)	0.0485 (4)
H1	0.9650	−0.0611	0.2307	0.058*
C2	0.7721 (2)	−0.1906 (3)	0.16191 (8)	0.0530 (4)
H2	0.8404	−0.3281	0.1524	0.064*
C3	0.5951 (2)	−0.1469 (3)	0.12921 (8)	0.0484 (4)
H3	0.5422	−0.2545	0.0972	0.058*
C4	0.49744 (18)	0.0588 (2)	0.14460 (7)	0.0367 (3)
C5	0.5857 (2)	0.2119 (3)	0.19208 (7)	0.0428 (4)
H5	0.5213	0.3517	0.2022	0.051*
C6	0.30072 (19)	0.1158 (3)	0.11378 (7)	0.0433 (4)
H6A	0.2437	−0.0233	0.0922	0.052*
H6B	0.2144	0.1704	0.1507	0.052*
C7	0.15874 (17)	0.3913 (2)	0.03246 (7)	0.0368 (3)
C8	−0.02824 (18)	0.3034 (3)	0.04198 (7)	0.0408 (3)
H8	−0.0477	0.1710	0.0700	0.049*
C9	−0.18583 (18)	0.4142 (3)	0.00955 (7)	0.0408 (3)
H9	−0.3112	0.3563	0.0163	0.049*
N1	0.75686 (17)	0.1729 (2)	0.22431 (7)	0.0510 (4)
O1	0.32526 (13)	0.29466 (19)	0.06180 (5)	0.0509 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0308 (7)	0.0572 (9)	0.0571 (9)	0.0002 (6)	−0.0101 (6)	0.0171 (7)
C2	0.0439 (9)	0.0449 (8)	0.0700 (10)	0.0117 (7)	−0.0063 (7)	0.0064 (8)

C3	0.0487 (8)	0.0432 (8)	0.0532 (8)	0.0035 (7)	−0.0108 (6)	−0.0038 (7)
C4	0.0308 (6)	0.0395 (7)	0.0396 (7)	−0.0005 (5)	−0.0056 (5)	0.0083 (6)
C5	0.0371 (7)	0.0388 (7)	0.0525 (8)	0.0016 (6)	−0.0069 (6)	0.0008 (6)
C6	0.0334 (7)	0.0482 (8)	0.0482 (8)	−0.0010 (6)	−0.0093 (6)	0.0109 (6)
C7	0.0264 (6)	0.0465 (8)	0.0374 (6)	0.0056 (5)	−0.0046 (5)	0.0038 (6)
C8	0.0308 (7)	0.0475 (8)	0.0438 (7)	−0.0007 (6)	−0.0045 (5)	0.0111 (6)
C9	0.0250 (6)	0.0530 (8)	0.0444 (7)	−0.0016 (6)	−0.0030 (5)	0.0073 (6)
N1	0.0394 (7)	0.0538 (8)	0.0596 (8)	−0.0056 (6)	−0.0145 (6)	0.0004 (6)
O1	0.0269 (5)	0.0683 (7)	0.0573 (6)	0.0058 (4)	−0.0048 (4)	0.0267 (5)

Geometric parameters (Å, º)

C1—N1	1.334 (2)	C6—O1	1.4239 (17)
C1—C2	1.368 (2)	C6—H6A	0.9700
C1—H1	0.9300	C6—H6B	0.9700
C2—C3	1.378 (2)	C7—C9^{i}	1.374 (2)
C2—H2	0.9300	C7—O1	1.3773 (17)
C3—C4	1.380 (2)	C7—C8	1.389 (2)
C3—H3	0.9300	C8—C9	1.3869 (19)
C4—C5	1.3839 (19)	C8—H8	0.9300
C4—C6	1.4979 (19)	C9—C7^{i}	1.374 (2)
C5—N1	1.3336 (19)	C9—H9	0.9300
C5—H5	0.9300		
N1—C1—C2	123.64 (13)	O1—C6—H6A	110.1
N1—C1—H1	118.2	C4—C6—H6A	110.1
C2—C1—H1	118.2	O1—C6—H6B	110.1
C1—C2—C3	119.03 (14)	C4—C6—H6B	110.1
C1—C2—H2	120.5	H6A—C6—H6B	108.4
C3—C2—H2	120.5	C9^{i}—C7—O1	115.88 (11)
C2—C3—C4	119.04 (14)	C9^{i}—C7—C8	119.64 (12)
C2—C3—H3	120.5	O1—C7—C8	124.47 (13)
C4—C3—H3	120.5	C9—C8—C7	119.64 (14)
C3—C4—C5	117.37 (13)	C9—C8—H8	120.2
C3—C4—C6	122.56 (13)	C7—C8—H8	120.2
C5—C4—C6	120.04 (13)	C7^{i}—C9—C8	120.71 (12)
N1—C5—C4	124.50 (14)	C7^{i}—C9—H9	119.6
N1—C5—H5	117.7	C8—C9—H9	119.6
C4—C5—H5	117.7	C5—N1—C1	116.41 (13)
O1—C6—C4	108.04 (11)	C7—O1—C6	117.28 (10)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1^{ii}	0.93	2.57	3.437 (3)	155

Symmetry code: (ii) −*x*+2, *y*−1/2, −*z*+1/2.