

## 1,4-Bis(4-pyridylmethoxy)benzene

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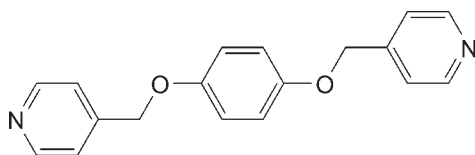
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Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.123; data-to-parameter ratio = 16.9.

The molecule of the title compound,  $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$ , lies about a center of inversion. The central phenylene ring is aligned at  $62.7$  (1)° with respect to the pyridyl ring. In the crystal, weak intermolecular  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds link molecules into sheets parallel to (104).  $\text{C}-\text{H}\cdots\text{O}$  interactions are also present.

### Related literature

For general background to metal-organic complexes with flexible pyridyl-based ligands, see: Hou *et al.* (2001). For details of the synthesis, see Gao *et al.* (2004). For related structures, see: Gao *et al.* (2006, 2009a,b).



### Experimental

#### Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$

$M_r = 292.33$

Monoclinic,  $P2_1/c$

$a = 6.7825$  (14) Å

$b = 5.8694$  (12) Å

$c = 18.542$  (4) Å

$\beta = 90.99$  (3)°

$V = 738.0$  (3) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 0.09$  mm<sup>-1</sup>

$T = 291$  K

$0.22 \times 0.17 \times 0.15$  mm

#### Data collection

Rigaku R-Axis RAPID diffractometer

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

$T_{\min} = 0.981$ ,  $T_{\max} = 0.987$

6972 measured reflections

1692 independent reflections

1381 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.123$

$S = 1.09$

1692 reflections

100 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.25$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C5}-\text{H5}\cdots\text{N1}^{\text{i}}$	0.93	2.62	3.4499 (18)	149
$\text{C9}-\text{H9}\cdots\text{O1}^{\text{ii}}$	0.93	2.63	3.5156 (17)	160

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 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: NG2651).

### References

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**supplementary materials**

*Acta Cryst.* (2009). E65, o2570 [ doi:10.1107/S1600536809038707 ]

## 1,4-Bis(4-pyridylmethoxy)benzene

P. Zou, Y. Liu, S. Zhang, X. Wang and J.-S. Gao

### Comment

The metal-organic complexes with flexible pyridyl-based ligands have been rapidly developed in the past few years owing to their abundant topology structures and potential applications. Hou's group (2001) has reported the synthesis of 1,4-bis(4-pyridylmethoxy)benzene ligand, which reacted with  $\text{Cd}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and  $\text{Co}(\text{NCS})_2$  to assemble into one-dimensional chain and two-dimensional plane network structures, respectively. It is worthy to note that the former cadmium complex consists of two kinds of chains: double zigzag linear chain and ladder-like one-dimensional chain. Our group has report three kinds of flexible pyridyl-based ligands in the previous report (Gao *et al.* 2006; Gao *et al.* 2009a; Gao *et al.* 2009b). As an extension of our work about bipyridyl aromatic ligands, we have synthesized and report the crystal structure of the title compound here.

In the title compound, the 1,4-bis(4-pyridylmethoxy)benzene ligand is centrosymmetric. The planes of two terminal pyridyl groups distort drastically and have dihedral angles of  $62.7(1)62.7(1)^\circ$  with the plane of the central benzene ring (Figure 1).

Within the packing structure, the adjacent 1,4-bis(4-pyridylmethoxy)benzene molecules are linked into two-dimensional wavy structure in (104) direction by intermolecular C—H $\cdots$ N hydrogen bonds interactions existing in the terminal pyridine rings (Figure 2, Table 1).

### Experimental

The 1,4-bis(4-pyridylmethoxy)benzene was synthesized by the reaction of *p*-benzenediol and 4-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 several days.

### Refinement

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

### Figures

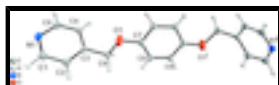


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms. [Symmetry codes: (i)  $-x, -y, 1 - z$ ]

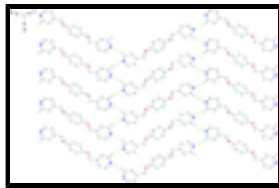


Fig. 2. A partial packing view, showing the two-dimensional hydrogen bonding sheet. Dashed lines indicate the hydrogen-bonding interactions.

## 1,4-Bis(4-pyridylmethoxy)benzene

### Crystal data

$C_{18}H_{16}N_2O_2$

$M_r = 292.33$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.7825$  (14) Å

$b = 5.8694$  (12) Å

$c = 18.542$  (4) Å

$\beta = 90.99$  (3)°

$V = 738.0$  (3) Å<sup>3</sup>

$Z = 2$

$F_{000} = 308$

$D_x = 1.315$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5914 reflections

$\theta = 3.0$ – $27.5$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 291$  K

Block, colorless

$0.22 \times 0.17 \times 0.15$  mm

### Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291$  K

$\omega$  scans

Absorption correction: Multi-scan  
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.981$ ,  $T_{\max} = 0.987$

6972 measured reflections

1692 independent reflections

1381 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 3.0$ °

$h = -8 \rightarrow 8$

$k = -7 \rightarrow 7$

$l = -24 \rightarrow 23$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.123$

$S = 1.09$

1692 reflections

100 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.0696P]$

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

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.25$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

Primary atom site location: structure-invariant direct methods Extinction correction: none

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7686 (2)	0.6857 (2)	0.33856 (8)	0.0480 (4)
H1	0.8310	0.8236	0.3485	0.058*
C2	0.5902 (2)	0.6432 (2)	0.37093 (7)	0.0432 (3)
H2	0.5355	0.7500	0.4018	0.052*
C3	0.49406 (16)	0.43997 (19)	0.35690 (6)	0.0328 (3)
C4	0.58453 (18)	0.2877 (2)	0.31094 (6)	0.0382 (3)
H4	0.5253	0.1487	0.3002	0.046*
C5	0.76321 (19)	0.3441 (2)	0.28130 (7)	0.0438 (3)
H5	0.8221	0.2394	0.2508	0.053*
C6	0.29658 (18)	0.3853 (2)	0.38841 (7)	0.0416 (3)
H6A	0.2471	0.5155	0.4148	0.050*
H6B	0.2023	0.3475	0.3503	0.050*
C7	0.15772 (16)	0.1050 (2)	0.46653 (6)	0.0336 (3)
C8	-0.03138 (17)	0.1943 (2)	0.45833 (6)	0.0367 (3)
H8	-0.0528	0.3245	0.4307	0.044*
C9	-0.18785 (16)	0.0872 (2)	0.49178 (7)	0.0372 (3)
H9	-0.3146	0.1457	0.4860	0.045*
N1	0.85625 (16)	0.5413 (2)	0.29416 (6)	0.0466 (3)
O1	0.32347 (12)	0.19635 (16)	0.43566 (5)	0.0472 (3)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0399 (7)	0.0388 (7)	0.0657 (9)	-0.0104 (5)	0.0077 (6)	0.0038 (6)
C2	0.0412 (7)	0.0387 (6)	0.0501 (7)	-0.0021 (5)	0.0115 (5)	-0.0033 (5)
C3	0.0271 (6)	0.0359 (6)	0.0357 (6)	-0.0002 (4)	0.0062 (4)	0.0068 (5)
C4	0.0342 (6)	0.0350 (6)	0.0455 (7)	-0.0027 (5)	0.0060 (5)	0.0000 (5)
C5	0.0362 (7)	0.0479 (7)	0.0476 (7)	0.0044 (5)	0.0127 (5)	-0.0008 (6)
C6	0.0304 (6)	0.0433 (7)	0.0515 (7)	0.0007 (5)	0.0128 (5)	0.0121 (6)
C7	0.0233 (5)	0.0431 (6)	0.0344 (6)	-0.0040 (4)	0.0052 (4)	0.0048 (5)
C8	0.0282 (6)	0.0422 (6)	0.0400 (6)	0.0007 (5)	0.0048 (5)	0.0111 (5)

## supplementary materials

C9	0.0214 (5)	0.0483 (7)	0.0421 (6)	0.0020 (4)	0.0045 (4)	0.0091 (5)
N1	0.0320 (6)	0.0504 (7)	0.0578 (7)	-0.0028 (4)	0.0127 (5)	0.0106 (5)
O1	0.0229 (4)	0.0619 (6)	0.0572 (6)	-0.0021 (4)	0.0080 (4)	0.0273 (5)

### Geometric parameters (Å, °)

C1—N1	1.3293 (18)	C6—O1	1.4231 (15)
C1—C2	1.3829 (19)	C6—H6A	0.9700
C1—H1	0.9300	C6—H6B	0.9700
C2—C3	1.3818 (17)	C7—O1	1.3789 (13)
C2—H2	0.9300	C7—C9 <sup>i</sup>	1.3806 (17)
C3—C4	1.3854 (16)	C7—C8	1.3914 (16)
C3—C6	1.5051 (15)	C8—C9	1.3888 (16)
C4—C5	1.3795 (17)	C8—H8	0.9300
C4—H4	0.9300	C9—C7 <sup>i</sup>	1.3806 (17)
C5—N1	1.3379 (18)	C9—H9	0.9300
C5—H5	0.9300		
N1—C1—C2	123.89 (12)	O1—C6—H6A	110.2
N1—C1—H1	118.1	C3—C6—H6A	110.2
C2—C1—H1	118.1	O1—C6—H6B	110.2
C3—C2—C1	119.20 (12)	C3—C6—H6B	110.2
C3—C2—H2	120.4	H6A—C6—H6B	108.5
C1—C2—H2	120.4	O1—C7—C9 <sup>i</sup>	115.87 (10)
C2—C3—C4	117.39 (11)	O1—C7—C8	124.38 (11)
C2—C3—C6	122.08 (11)	C9 <sup>i</sup> —C7—C8	119.75 (10)
C4—C3—C6	120.52 (11)	C9—C8—C7	119.39 (11)
C5—C4—C3	119.47 (11)	C9—C8—H8	120.3
C5—C4—H4	120.3	C7—C8—H8	120.3
C3—C4—H4	120.3	C7 <sup>i</sup> —C9—C8	120.86 (11)
N1—C5—C4	123.45 (12)	C7 <sup>i</sup> —C9—H9	119.6
N1—C5—H5	118.3	C8—C9—H9	119.6
C4—C5—H5	118.3	C1—N1—C5	116.60 (11)
O1—C6—C3	107.44 (10)	C7—O1—C6	117.51 (9)

Symmetry codes: (i)  $-x, -y, -z+1$ .

### Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C5—H5 $\cdots$ N1 <sup>ii</sup>	0.93	2.62	3.4499 (18)	149
C9—H9 $\cdots$ O1 <sup>iii</sup>	0.93	2.63	3.5156 (17)	160

Symmetry codes: (ii)  $-x+2, y-1/2, -z+1/2$ ; (iii)  $x-1, y, z$ .

Fig. 1

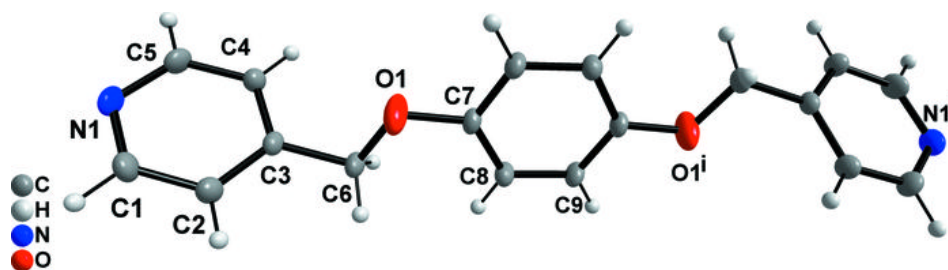


Fig. 2

