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1,4-Bis(3-pyridylaminomethyl)benzene

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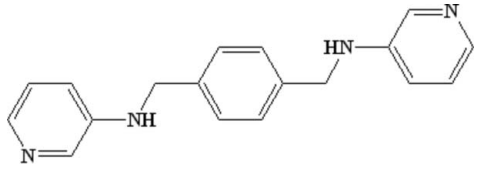
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.142; data-to-parameter ratio = 17.2.

A new flexible bis(pyridyl) complex, $C_{18}H_{18}N_4$, was prepared by the reaction of terephthalaldehyde with 3-aminopyridine. The molecule is centrosymmetric. Mononuclear units are linked into a one-dimensional chain by intermolecular N—H···N hydrogen bonds. The dihedral angle bentween the pyridyl ring and the central benzene ring is 63.6 (2)°.

Related literature

The corresponding complex (Zou *et al.*, 2003) with 2-aminopyridine instead of 3-aminopyridine has a similar structure. For related literature, see: Munno *et al.* (1999); Park *et al.* (1998).



Experimental

Crystal data

$C_{18}H_{18}N_4$
M_r = 290.36
Monoclinic, $P2_1/n$
a = 5.7064 (11) Å
b = 22.174 (4) Å
c = 6.1717 (12) Å
β = 105.29 (3)°
V = 753.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.32 × 0.26 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.971, T_{max} = 0.979
7359 measured reflections
1724 independent reflections
1173 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.142
S = 1.11
1724 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1^{i}	0.86	2.36	3.112 (2)	146

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); 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: AT2434).

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supplementary materials

Acta Cryst. (2007). E**63**, o4459 [**doi:10.1107/S1600536807052476**]

1,4-Bis(3-pyridylaminomethyl)benzene

L.-N. Zhu, S. Gao and L.-H. Huo

Comment

In recent years, extensive studies have been carried out to give many new one-dimensional, two-dimensional, and three-dimensional frameworks through the coordination of metal atoms with pyridine-based bridge ligands for example 4,4'-bipyridine and its derivatives like 1,2-bis(4-pyridyl)ethane (Park *et al.*, 1998), 1,2-bis(4-pyridyl)ethene (Munno *et al.*, 1999), and 1,3-bis(4-pyridyl)propane. Accordingly, we have designed and synthesized a new bis(pyridyl) complex, *viz*. 1,4-bis(pyridine-3-aminomethyl)benzene. The corresponding complex (Ru—Yi Zou *et al.*, 2003), with 2-aminopyridine instead of 3-aminopyridine, has the similar structure.

The molecule of the title complex, (I) (Fig. 1), is centrosymmetric. The pair of pyridyl rings is parallel in a *trans* arrangement. The dihedral angle bentween the pyridyl ring and the central benzene ring is 63.6 °. The pyridyl-N form intermolecular N—H···N hydrogen bonds with the amino-H atom of adjacent molecules. The N···N distance and N—H···N angle are 3.112 (2) Å and 145.9 °, respectively. These intermolecular hydrogen-bonding interactions give rise to a chain structure.

Experimental

A solution of terephthalaldehyde and 3-aminopyridine in toluene was heated under reflux. After 10 h, the solvent was removed under vacuum, and the remains were reduced in absolute methanol by sodium borohydride. Colourless crystals were obtained by recrystallization of the material from methanol with a yield of 83%.

Refinement

H atoms were placed in calculated positions, with phenyl C—H = 0.95 Å, methylene C—H = 0.97 Å and amine N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,*N*), which were included in the refinement in the riding-model approximation.

Figures

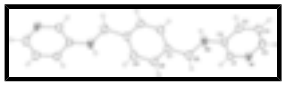

Fig. 1. A view of complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

1,4-Bis(3-pyridylaminomethyl)benzene

Crystal data

$C_{18}H_{18}N_4$	F_{000} = 308
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Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn
a = 5.7064 (11) Å
b = 22.174 (4) Å
c = 6.1717 (12) Å
β = 105.29 (3)º
V = 753.3 (3) Å^3
Z = 2

Cell parameters from 5126 reflections
θ = 3.4–27.5º
μ = 0.08 mm^{-1}
T = 295 (2) K
Prism, colourless
0.32 × 0.26 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 10.000 pixels mm^{-1}
T = 295(2) K
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.971, T_{max} = 0.979
7359 measured reflections

1724 independent reflections
1173 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5º
θ_{min} = 3.5º
h = −7→7
k = −28→28
l = −7→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.142
S = 1.11
1724 reflections
100 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.1768P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
N1	0.4126 (3)	0.16827 (7)	1.0083 (2)	0.0494 (4)
N2	0.3042 (3)	0.11085 (7)	0.4316 (2)	0.0515 (4)
H2	0.3734	0.1129	0.3238	0.062*
C1	0.3133 (3)	0.13915 (7)	0.8165 (3)	0.0421 (4)
H1	0.1770	0.1154	0.8090	0.050*
C2	0.4026 (3)	0.14236 (7)	0.6264 (2)	0.0378 (4)
C3	0.6056 (3)	0.17862 (7)	0.6430 (3)	0.0446 (4)
H3	0.6732	0.1820	0.5219	0.054*

C4	0.7054 (4)	0.20925 (8)	0.8379 (3)	0.0529 (5)
H4	0.8399	0.2340	0.8497	0.064*
C5	0.6044 (4)	0.20306 (9)	1.0172 (3)	0.0535 (5)
H5	0.6734	0.2241	1.1490	0.064*
C6	0.0894 (3)	0.07458 (9)	0.4027 (3)	0.0531 (5)
H7	−0.0495	0.1006	0.3935	0.064*
H6	0.1071	0.0485	0.5323	0.064*
C7	0.0442 (3)	0.03638 (7)	0.1924 (3)	0.0412 (4)
C8	−0.1740 (3)	0.03908 (8)	0.0311 (3)	0.0508 (5)
H8	−0.2939	0.0654	0.0501	0.061*
C9	−0.2180 (3)	0.00311 (9)	−0.1597 (3)	0.0526 (5)
H9	−0.3668	0.0057	−0.2668	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0630 (10)	0.0548 (9)	0.0345 (7)	−0.0082 (7)	0.0200 (7)	−0.0066 (6)
N2	0.0693 (11)	0.0566 (9)	0.0312 (7)	−0.0222 (7)	0.0181 (7)	−0.0080 (6)
C1	0.0495 (10)	0.0448 (9)	0.0337 (8)	−0.0051 (7)	0.0141 (7)	−0.0009 (6)
C2	0.0488 (9)	0.0344 (7)	0.0300 (7)	−0.0004 (6)	0.0101 (7)	0.0003 (6)
C3	0.0563 (10)	0.0469 (9)	0.0355 (8)	−0.0065 (8)	0.0208 (7)	−0.0017 (7)
C4	0.0607 (12)	0.0561 (10)	0.0446 (9)	−0.0185 (9)	0.0184 (8)	−0.0076 (8)
C5	0.0701 (13)	0.0556 (10)	0.0366 (9)	−0.0157 (9)	0.0175 (8)	−0.0114 (8)
C6	0.0595 (11)	0.0592 (11)	0.0433 (9)	−0.0144 (9)	0.0185 (8)	−0.0127 (8)
C7	0.0470 (9)	0.0410 (8)	0.0358 (8)	−0.0083 (7)	0.0111 (7)	−0.0031 (6)
C8	0.0469 (10)	0.0530 (10)	0.0508 (10)	0.0065 (8)	0.0098 (8)	−0.0079 (8)
C9	0.0443 (10)	0.0633 (11)	0.0433 (10)	0.0034 (8)	−0.0006 (8)	−0.0083 (8)

Geometric parameters (Å, °)

N1—C5	1.328 (2)	C4—H4	0.9300
N1—C1	1.336 (2)	C5—H5	0.9300
N2—C2	1.376 (2)	C6—C7	1.514 (2)
N2—C6	1.437 (2)	C6—H7	0.9700
N2—H2	0.8600	C6—H6	0.9700
C1—C2	1.399 (2)	C7—C8	1.375 (2)
C1—H1	0.9300	C7—C9^{i}	1.377 (2)
C2—C3	1.392 (2)	C8—C9	1.390 (2)
C3—C4	1.368 (2)	C8—H8	0.9300
C3—H3	0.9300	C9—C7^{i}	1.377 (2)
C4—C5	1.383 (3)	C9—H9	0.9300
C5—N1—C1	118.02 (14)	N1—C5—H5	118.7
C2—N2—C6	122.06 (14)	C4—C5—H5	118.7
C2—N2—H2	119.0	N2—C6—C7	111.49 (14)
C6—N2—H2	119.0	N2—C6—H7	109.3
N1—C1—C2	123.72 (16)	C7—C6—H7	109.3
N1—C1—H1	118.1	N2—C6—H6	109.3
C2—C1—H1	118.1	C7—C6—H6	109.3

N2—C2—C3	119.83 (14)	H7—C6—H6	108.0
N2—C2—C1	123.52 (15)	C8—C7—C9^{i}	118.11 (15)
C3—C2—C1	116.63 (14)	C8—C7—C6	120.87 (16)
C4—C3—C2	119.78 (14)	C9^{i}—C7—C6	121.00 (16)
C4—C3—H3	120.1	C7—C8—C9	121.03 (17)
C2—C3—H3	120.1	C7—C8—H8	119.5
C3—C4—C5	119.32 (16)	C9—C8—H8	119.5
C3—C4—H4	120.3	C7^{i}—C9—C8	120.86 (16)
C5—C4—H4	120.3	C7^{i}—C9—H9	119.6
N1—C5—C4	122.51 (16)	C8—C9—H9	119.6
C5—N1—C1—C2	1.3 (3)	C1—N1—C5—C4	−1.0 (3)
C6—N2—C2—C3	−177.61 (16)	C3—C4—C5—N1	0.0 (3)
C6—N2—C2—C1	4.1 (3)	C2—N2—C6—C7	−170.10 (15)
N1—C1—C2—N2	177.94 (16)	N2—C6—C7—C8	−124.94 (18)
N1—C1—C2—C3	−0.4 (3)	N2—C6—C7—C9^{i}	56.7 (2)
N2—C2—C3—C4	−179.05 (16)	C9^{i}—C7—C8—C9	−0.2 (3)
C1—C2—C3—C4	−0.6 (2)	C6—C7—C8—C9	−178.57 (17)
C2—C3—C4—C5	0.8 (3)	C7—C8—C9—C7^{i}	0.2 (3)

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1^{ii}	0.86	2.36	3.112 (2)	146

Symmetry codes: (ii) *x*, *y*, *z*−1.

Fig. 1