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1,4-Bis(pyridine-2-aminomethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.111
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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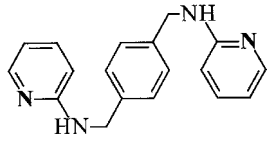
A novel, potentially tetradentate, ligand, $C_{18}H_{18}N_4$, was synthesized by the reaction of terephthalaldehyde with 2-aminopyridine. The molecule is centrosymmetric and the presence of hydrogen-bonding interactions results in a chain structure.

Comment

Studies of the molecular self-assembly of flexible *N*-heterocyclic ligands with metal ions have attracted much attention. This is mainly attributed to their applications in many fields, as well as the versatile structures and properties their molecular assemblies display (Clayden & Pink, 1998; Hong *et al.*, 2000; Kang *et al.*, 2002). There is growing interest in finding alternative approaches for building new, inexpensive and easy-to-prepare supramolecular systems. Accordingly, we designed and synthesized a new, flexible, potentially tetradentate, ligand, *viz*. 1,4-bis(pyridine-2-aminomethyl)benzene, (I), which may provide a new and versatile ligand for metal ions.



(I)

The molecule of (I) (Fig. 1) is centrosymmetric, with the two parallel pyridyl terminal groups in a *trans* arrangement. The dihedral angle between the pyridyl ring and the central benzene ring is 87.2 (2)°. The crystal structure is stabilized by the presence of intermolecular hydrogen-bonding interactions between pyridyl-N and the amino-H atom of a symmetry-related molecule: N1—H···N2^{i} is 2.198 (19) Å, N1···N2^{i} is 3.076 (3) Å and the angle subtended at H is 168.8 (17)° [symmetry code: (i) $\frac{1}{2}-x$, $\frac{3}{2}-y$, $1-z$]. These interactions give rise to a chain structure.

Experimental

A solution of terephthalaldehyde and 2-aminopyridine in toluene was heated under reflux with stirring in a Dean–Stark apparatus. After 12 h, the solvent was removed under vacuum, and the remains, without further purification, were reduced in absolute methanol by sodium borohydride, as described in the literature (Ashton *et al.*, 1997). Colorless crystals were obtained by recrystallization of the material from methanol. Yield: 87%, m.p.: 465–467 K. Analysis calculated for $C_{18}H_{18}N_4$: C 74.46, H 6.25, N 19.29%; found: C 74.08, H 6.58, N 19.34%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.50 (*s*, 4H), 6.37 (*d*, 2H), 6.59 (*m*, 2H), 7.33 (*s*, 4H), 7.40 (*m*, 2H), 8.10 (*m*, 2H).

Crystal data

$C_{18}H_{18}N_4$
M_r = 290.36
Monoclinic, $C2/c$
a = 18.547 (11) Å
b = 5.539 (3) Å
c = 15.303 (9) Å
β = 105.328 (8)°
V = 1516.3 (15) Å^3
Z = 4
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 548 reflections
θ = 4.6–25.4°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colorless
0.42 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.797, T_{max} = 0.990
3292 measured reflections
1534 independent reflections
1093 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°
$h = -22 \rightarrow 17$
$k = -6 \rightarrow 5$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.02
1534 reflections
104 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.3246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

H atoms on C atoms were included in the riding-model approximation, with phenyl C—H = 0.95 Å and methylene C—H = 0.97 Å and displacement parameters equal to 1.2 times U_{eq} of the atom to which they are bonded. The H atom on the N atom was allowed to refine freely.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

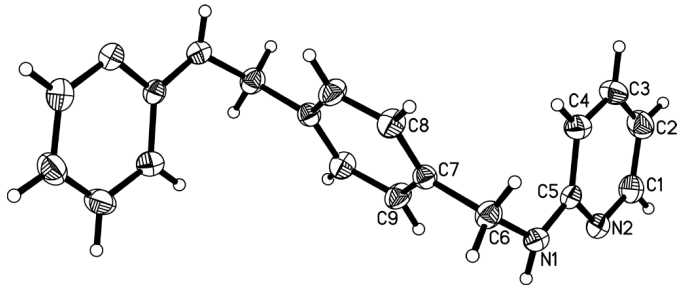


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

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