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# 1,3-Bis(2-pyridylaminomethyl)benzene

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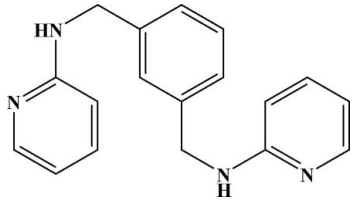
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.044; $wR$ factor = 0.116; data-to-parameter ratio = 17.5.

The complete molecule of the title compound, $C_{18}H_{18}N_4$, is generated by crystallographic twofold rotation symmetry, with two C atoms lying on the rotation axis. The pair of pyridyl rings form a dihedral angle of 78.4 (2)° and the dihedral angle between the pyridyl ring and the central benzene ring is 110.4 (2)°. The molecules are linked into a one-dimensional chain by N—H···N hydrogen bonds.

## Related literature

For a related structure, see: Zou *et al.* (2003). For background, see: Tao *et al.* (2000); Johnson (1976).




## Experimental

### Crystal data

$C_{18}H_{18}N_4$
$M_r$ = 290.36
Orthorhombic, *Pbcn*
$a$ = 23.844 (5) Å
$b$ = 7.0493 (14) Å
$c$ = 9.2504 (19) Å
$V$ = 1554.8 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 (2) K
0.38 × 0.24 × 0.20 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.972, $T_{max}$ = 0.979
13887 measured reflections
1764 independent reflections
982 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
$S$ = 1.06
1764 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 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···$A$ |
|---|---|---|---|---|
| N2—H1···N1$^{i}$ | 0.86 | 2.24 | 3.0625 (19) | 160 |

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

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: HB2587).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4399 [ **doi:10.1107/S1600536807051069** ]

# 1,3-Bis(2-pyridylaminomethyl)benzene

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## Comment

Recently, N-heterocyclic complexes have attracted much attention in the area of coordination and supramolecular chemistry. Many one-dimensional, two-dimensional, and three-dimensional frameworks can be assembled through the metal coordination of pyridine-based bridging complexes (Tao *et al.*, 2000). Accordingly, we have designed and synthesized the title molecule, (I). The corresponding molecule (Zou *et al.*, 2003), with terephthalaldehyde instead of isophthalaldehyde, has a related structure.

The molecule of (I) (Fig. 1) is symmetrical with twofold rotation symmetry. The pair of pyridyl rings form a dihedral angle of 78.4 °. And the dihedral angle between the pyridyl ring and the central benzene ring is 110.4 °. The crystal structure is stabilized by the presence of intermolecular N—H···N hydrogen-bonding interactions (Table 1) resulting in a one-dimensional chain structure.

## Experimental

To a solution of isophthalaldehyde in toluene was added a solution of 2-aminopyridine in toluene. The mixture was refluxed for 10 h, and a yellow precipitate was obtained. The solid product was reduced in absolute methanol by sodium borohydride. Colourless prisms of (I) were obtained by recrystallization from methanol with a yield of 80%.

## Refinement

The H atoms were placed in calculated positions (C—H = 0.95–0.97 Å, N—H = 0.86 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C, N).

## Figures

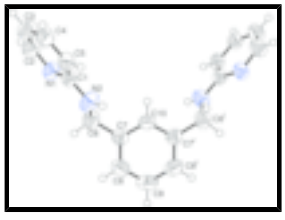

Fig. 1. A view of the molecular structure of (I). Displacement ellipsoids for the non-hydrogen atoms are drawn at the 50% probability level. Symmetry code: (i) −*x*, *y*, 1/2 − *z*.

## 1,3-Bis(2-pyridylaminomethyl)benzene

*Crystal data*

$C_{18}H_{18}N_4$ $F_{000} = 616$

| | |
|---|---|
| $M_r$ = 290.36 | $D_x$ = 1.240 Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2n 2ab | Cell parameters from 6970 reflections |
| *a* = 23.844 (5) Å | θ = 3.0–27.4º |
| *b* = 7.0493 (14) Å | μ = 0.08 mm$^{-1}$ |
| *c* = 9.2504 (19) Å | *T* = 295 (2) K |
| *V* = 1554.8 (6) Å$^3$ | Prism, colourless |
| *Z* = 4 | 0.38 × 0.24 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 1764 independent reflections |
| Radiation source: fine-focus sealed tube | 982 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.056 |
| Detector resolution: 10.000 pixels mm$^{-1}$ | $\theta_{max}$ = 27.4º |
| *T* = 295(2) K | $\theta_{min}$ = 3.0º |
| ω scans | *h* = −30→30 |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | *k* = −9→9 |
| $T_{min}$ = 0.972, $T_{max}$ = 0.979 | *l* = −11→10 |
| 13887 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | H-atom parameters constrained |
| $wR(F^2)$ = 0.116 | $w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.1871P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.06 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1764 reflections | $\Delta\rho_{max}$ = 0.12 e Å$^{-3}$ |
| 101 parameters | $\Delta\rho_{min}$ = −0.14 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.14189 (6) | 0.6534 (2) | 0.52951 (13) | 0.0539 (4) |
| N2 | 0.11264 (6) | 0.4662 (2) | 0.33872 (15) | 0.0634 (4) |
| H1 | 0.1127 | 0.4449 | 0.2472 | 0.076* |
| C1 | 0.14448 (6) | 0.6112 (2) | 0.38823 (16) | 0.0475 (4) |
| C2 | 0.17287 (8) | 0.8016 (3) | 0.57373 (18) | 0.0671 (5) |
| H2 | 0.1702 | 0.8362 | 0.6705 | 0.081* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.20785 (9) | 0.9053 (3) | 0.48820 (19) | 0.0683 (5) |
| H3 | 0.2287 | 1.0056 | 0.5255 | 0.082* |
| C4 | 0.21115 (7) | 0.8558 (3) | 0.34387 (18) | 0.0612 (5) |
| H4 | 0.2351 | 0.9212 | 0.2822 | 0.073* |
| C5 | 0.17922 (7) | 0.7112 (3) | 0.29261 (17) | 0.0535 (5) |
| H5 | 0.1804 | 0.6788 | 0.1952 | 0.064* |
| C6 | 0.07853 (7) | 0.3446 (3) | 0.42870 (18) | 0.0655 (5) |
| H6 | 0.0579 | 0.4210 | 0.4979 | 0.079* |
| H7 | 0.1024 | 0.2580 | 0.4821 | 0.079* |
| C7 | 0.03805 (7) | 0.2334 (2) | 0.33701 (17) | 0.0508 (4) |
| C8 | 0.03766 (8) | 0.0384 (3) | 0.3357 (2) | 0.0702 (5) |
| H8 | 0.0629 | −0.0285 | 0.3929 | 0.084* |
| C9 | 0.0000 | −0.0582 (4) | 0.2500 | 0.0870 (10) |
| H9 | 0.0000 | −0.1901 | 0.2500 | 0.104* |
| C10 | 0.0000 | 0.3274 (3) | 0.2500 | 0.0521 (6) |
| H10 | 0.0000 | 0.4593 | 0.2500 | 0.063* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0647 (9) | 0.0594 (9) | 0.0375 (7) | −0.0036 (8) | −0.0005 (6) | −0.0021 (7) |
| N2 | 0.0714 (9) | 0.0758 (11) | 0.0429 (7) | −0.0207 (8) | 0.0084 (7) | −0.0091 (8) |
| C1 | 0.0497 (9) | 0.0526 (10) | 0.0403 (8) | 0.0039 (8) | −0.0027 (7) | −0.0012 (8) |
| C2 | 0.0911 (13) | 0.0693 (13) | 0.0410 (9) | −0.0153 (11) | −0.0001 (10) | −0.0067 (9) |
| C3 | 0.0903 (13) | 0.0644 (12) | 0.0501 (10) | −0.0194 (11) | −0.0062 (10) | −0.0014 (9) |
| C4 | 0.0708 (11) | 0.0641 (12) | 0.0486 (9) | −0.0100 (10) | −0.0030 (9) | 0.0111 (9) |
| C5 | 0.0607 (10) | 0.0633 (11) | 0.0365 (8) | −0.0007 (9) | −0.0002 (8) | 0.0010 (8) |
| C6 | 0.0687 (11) | 0.0769 (14) | 0.0509 (10) | −0.0132 (10) | −0.0037 (9) | 0.0077 (9) |
| C7 | 0.0550 (9) | 0.0503 (10) | 0.0471 (9) | −0.0008 (8) | 0.0030 (8) | 0.0039 (8) |
| C8 | 0.0798 (12) | 0.0558 (12) | 0.0751 (13) | 0.0114 (10) | −0.0052 (11) | 0.0086 (10) |
| C9 | 0.116 (2) | 0.0406 (16) | 0.105 (2) | 0.000 | −0.014 (2) | 0.000 |
| C10 | 0.0662 (15) | 0.0389 (13) | 0.0512 (13) | 0.000 | 0.0022 (12) | 0.000 |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.3416 (19) | C5—H5 | 0.9300 |
| N1—C2 | 1.344 (2) | C6—C7 | 1.505 (2) |
| N2—C1 | 1.353 (2) | C6—H6 | 0.9700 |
| N2—C6 | 1.445 (2) | C6—H7 | 0.9700 |
| N2—H1 | 0.8600 | C7—C8 | 1.375 (3) |
| C1—C5 | 1.402 (2) | C7—C10 | 1.3819 (19) |
| C2—C3 | 1.362 (2) | C8—C9 | 1.378 (2) |
| C2—H2 | 0.9300 | C8—H8 | 0.9300 |
| C3—C4 | 1.382 (2) | C9—H9 | 0.9300 |
| C3—H3 | 0.9300 | C10—C7$^{i}$ | 1.3819 (19) |
| C4—C5 | 1.358 (2) | C10—H10 | 0.9300 |
| C4—H4 | 0.9300 | | |
| C1—N1—C2 | 116.33 (14) | N2—C6—C7 | 110.19 (14) |

| | | | |
|---|---|---|---|
| C1—N2—C6 | 124.67 (14) | N2—C6—H6 | 109.6 |
| C1—N2—H1 | 117.7 | C7—C6—H6 | 109.6 |
| C6—N2—H1 | 117.7 | N2—C6—H7 | 109.6 |
| N1—C1—N2 | 118.11 (14) | C7—C6—H7 | 109.6 |
| N1—C1—C5 | 122.04 (15) | H6—C6—H7 | 108.1 |
| N2—C1—C5 | 119.84 (14) | C8—C7—C10 | 118.02 (18) |
| N1—C2—C3 | 125.25 (16) | C8—C7—C6 | 122.00 (17) |
| N1—C2—H2 | 117.4 | C10—C7—C6 | 119.98 (16) |
| C3—C2—H2 | 117.4 | C7—C8—C9 | 120.2 (2) |
| C2—C3—C4 | 117.39 (18) | C7—C8—H8 | 119.9 |
| C2—C3—H3 | 121.3 | C9—C8—H8 | 119.9 |
| C4—C3—H3 | 121.3 | C8—C9—C8$^{i}$ | 120.7 (3) |
| C5—C4—C3 | 119.68 (17) | C8—C9—H9 | 119.6 |
| C5—C4—H4 | 120.2 | C8$^{i}$—C9—H9 | 119.6 |
| C3—C4—H4 | 120.2 | C7$^{i}$—C10—C7 | 122.7 (2) |
| C4—C5—C1 | 119.23 (15) | C7$^{i}$—C10—H10 | 118.6 |
| C4—C5—H5 | 120.4 | C7—C10—H10 | 118.6 |
| C1—C5—H5 | 120.4 | | |
| C2—N1—C1—N2 | −178.17 (15) | N2—C1—C5—C4 | −179.68 (15) |
| C2—N1—C1—C5 | 2.4 (2) | C1—N2—C6—C7 | 165.56 (15) |
| C6—N2—C1—N1 | −4.2 (2) | N2—C6—C7—C8 | 120.92 (19) |
| C6—N2—C1—C5 | 175.23 (16) | N2—C6—C7—C10 | −58.67 (19) |
| C1—N1—C2—C3 | −2.8 (3) | C10—C7—C8—C9 | −0.3 (2) |
| N1—C2—C3—C4 | 1.0 (3) | C6—C7—C8—C9 | −179.86 (13) |
| C2—C3—C4—C5 | 1.4 (3) | C7—C8—C9—C8$^{i}$ | 0.14 (12) |
| C3—C4—C5—C1 | −1.7 (3) | C8—C7—C10—C7$^{i}$ | 0.13 (12) |
| N1—C1—C5—C4 | −0.3 (2) | C6—C7—C10—C7$^{i}$ | 179.74 (16) |

Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H1···N1$^{ii}$ | 0.86 | 2.24 | 3.0625 (19) | 160 |

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

**Fig. 1**