Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Bis(2-pyridylmethyl)amine–borane

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**Key indicators**

Single-crystal X-ray study
$T$ = 150 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.043
$wR$ factor = 0.116
Data-to-parameter ratio = 19.3

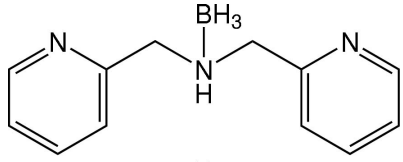
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{12}H_{12}N_3{\cdot}BH_3$ or $C_{12}H_{15}BN_3$, contains a $BH_3$ group and two picolyl groups attached to a central N atom. Both edge-to-face and face-to-face $\pi$-stacking interactions are found.

Received 22 December 2004
Accepted 18 January 2005
Online 5 February 2005

## Comment

The asymmetric unit of the title compound, (I), contains one molecule. The two planar pyridyl rings are twisted (Fig. 1) about the central N atom, with an interplanar angle of 110.9°. The amine N atom is not involved in any hydrogen bonding but pyridyl atom N1 interacts with atom C3 in an adjacent ring (Table 1).




(I)

An edge-to-face interaction is found between the H atom on C2 and the plane of the pyridine ring containing atom N3 (Fig. 2). This H atom is 2.806 Å from the mean plane of the pyridine ring at $(\frac{1}{2}+x,\ \frac{1}{2}-y,\ \frac{1}{2}+z)$. The pyridine ring containing atom N3 is $\pi$-stacked with its symmetry equivalent by inversion (symmetry code: $2-x,\ -y,\ 1-z$). The interplanar and the centroid-to-centroid distances are 3.496 (2) and 3.971 Å respectively (Fig. 2).

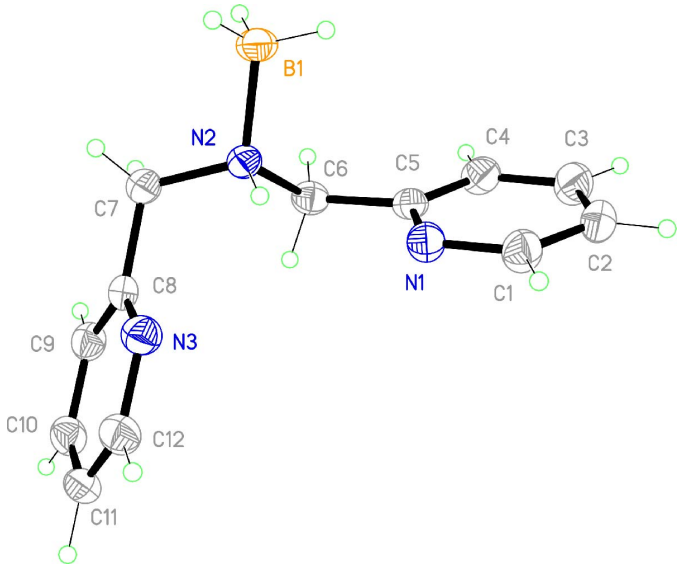



**Figure 1**
Perspective view of (I), showing 50% probability displacement ellipsoids.

## Experimental

2-(Aminomethyl)pyridine (4.95 g, 44.77 mmol) and pyridine-2-carboxaldehyde (4.96 g, 46.31 mmol) were dissolved in methanol (150 ml) (Lambert *et al.*, 1997). The solution was stirred for 2 h at room temperature (yellow–orange solution). After slow addition of an excess of sodium borohydride, stirring was continued for 1 h (pale-yellow solution). The solvent was removed by rotary evaporation to give bis(pyridin-2-ylmethyl)amine (6.43 g, 73%) as an orange oil. Colourless crystals of the borane adduct appeared as a minor product after the oil was stored in a freezer overnight.

### *Crystal data*

$C_{12}H_{15}BN_3$
$M_r$ = 213.09
Monoclinic, $P2_1/n$
$a$ = 5.3172 (4) Å
$b$ = 24.8494 (19) Å
$c$ = 9.3896 (7) Å
$\beta$ = 102.938 (1)°
$V$ = 1209.14 (16) Å$^3$
$Z$ = 4
$D_x$ = 1.171 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3633 reflections
$\theta$ = 2.4–27.5°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 150 (2) K
Needle, colourless
0.55 × 0.17 × 0.09 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.946, $T_{max}$ = 0.990
10293 measured reflections
2860 independent reflections
2156 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 28.8°
$h = -7 \rightarrow 6$
$k = -32 \rightarrow 32$
$l = -12 \rightarrow 12$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
$S$ = 1.02
2860 reflections
148 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.3966P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

**Table 1**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3···N1$^{i}$ | 0.95 | 2.66 | 3.5215 (19) | 150 |

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

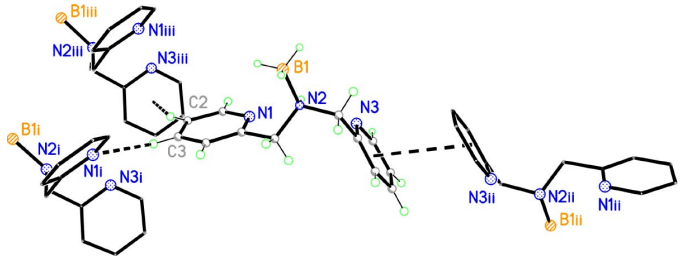



**Figure 2**
View showing the C—H···N bond (C3 and N1), the interaction between the H atom bonded to C2 and the pyridyl ring, and the $\pi$-stacking of the N3-containing pyridine rings [symmetry codes: (i) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$; (ii) $2-x, -y, 1-z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.]

H atoms bonded to C and B atoms were placed at calculated positions; the constrained C—H distances were 0.95, 0.98 and 0.99 Å for H atoms bonded to C$sp^2$, B$sp^3$ and methylene C atoms, respectively. They were refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(B,C). The H atom bonded to the amine N atom was located in a difference map and the coordinates freely refined with a fixed $U_{iso}$ value of 0.03 Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We are grateful to the Socrates Exchange Programme for support. JW thanks the Erskine fund at the University of Canterbury for support.

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