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N,*N*-Bis[2-(2-pyridyl)ethyl]hydroxylamine

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.089
Data-to-parameter ratio = 11.7

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

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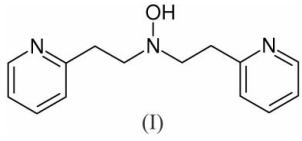
The crystal structure of the title compound, $C_{14}H_{17}N_3O$, at 180 K contains intermolecular hydrogen bonds between the hydroxyl group and the N atom of one pyridyl ring.

Comment

The title compound, (I) (Fig. 1), has recently appeared in the literature as a convenient source of the bis(2-pyridylethyl)-amino skeleton, commonly incorporated in ligands employed for biomimetic coordination chemistry (Leaver *et al.*, 2003). In its crystal structure at 180 K, both pyridyl rings adopt anti-clinal conformations with respect to the hydroxyl group so that the C_5H_4N and OH groups form angles of 120° with respect to each other in a Newman-type projection along the $(CH_2)_2N(CH_2)_2$ core of the molecule (Fig. 2). A dihedral angle of 67.5 (1)° exists between the least-squares planes of the two pyridyl rings. Intermolecular hydrogen bonds are formed between the hydroxyl group and the N atom of one pyridyl ring [$H1\cdots N3^{i}$ = 1.94 (3) Å, $O1-H1\cdots N3^{i}$ = 164 (2)°; symmetry code (i): 1 + *x*, *y*, *z*].



(I)

Experimental

The title compound was prepared according to the synthetic procedure of Leaver *et al.* (2003).

Crystal data

$C_{14}H_{17}N_3O$
M_r = 243.31
Orthorhombic, $P2_12_12_1$
a = 5.8501 (4) Å
b = 14.7210 (9) Å
c = 15.2578 (10) Å
V = 1313.99 (15) Å^3
Z = 4
D_x = 1.230 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3638 reflections
θ = 2.7–28.4°
μ = 0.08 mm^{-1}
T = 180 (2) K
Block, colourless
0.40 × 0.30 × 0.10 mm

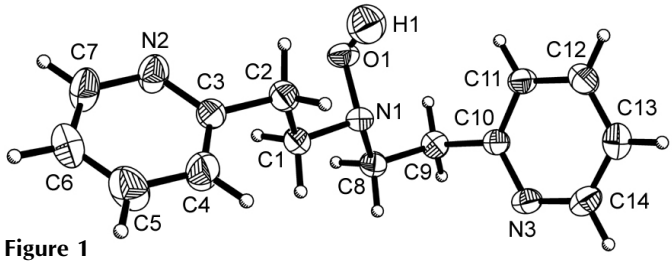


Figure 1
The molecular structure, showing displacement ellipsoids at the 50% probability level. H atoms bound to C are shown as spheres of arbitrary radius.

Data collection

Bruker–Nonius X8APEX-II CCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.885, T_{max} = 0.992
9849 measured reflections
1958 independent reflections
1681 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 28.7°
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 19$
$l = -20 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.06
1958 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.1214P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3^{i}	0.90 (3)	1.94 (3)	2.8174 (18)	164 (2)

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

H atoms bound to C were positioned geometrically and allowed to ride during subsequent refinement [C—H = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C) for H atoms bound to the pyridyl rings; C—H = 0.99 Å, U_{iso}(H) = 1.2U_{eq}(C) for H atoms of the methylene groups]. H1, associated with the hydroxyl group, was located in a difference Fourier map and refined freely with an isotropic displacement parameter. The absolute structure could not be determined and 1286 Friedel opposites were merged for the final cycles of refinement.

Data collection: *APEX*2 (Bruker–Nonius, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

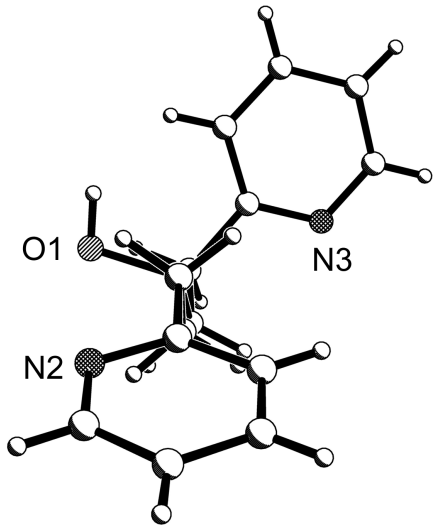


Figure 2
Newman-type projection along the $(CH_2)_2N(CH_2)_2$ core of the molecule, showing the anticlinal conformations of the pyridyl rings with respect to the hydroxyl group.

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References

Bruker–Nonius (2003). *APEX*2. Version 1.0-8. Bruker Nonius BV, Delft, The Netherlands.
Bruker (2003). *SAINT*. Version 7.06a. Bruker AXS Inc., Madison, Wisconsin, USA.
Leaver, S. A., Palaniandavar, M., Kilner, C. A. & Halcrow, M. A. (2003). *Dalton Trans.* pp. 4224–4225.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.