

2-Amino-6-(hydroxymethyl)pyridine

Shyamaprosad Goswami,^a
Swapan Dey,^a Hoong-Kun Fun^{b*}
and Suchada Chantrapromma^{c‡}^aDepartment of Chemistry, Bengal Engineering and Science University, Shibpur, Howrah 711 103, India, ^bX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^cDepartment of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand

‡ Additional correspondence author, email: suchada.c@psu.ac.th

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
 $T = 297$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.042
 wR factor = 0.117
Data-to-parameter ratio = 14.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

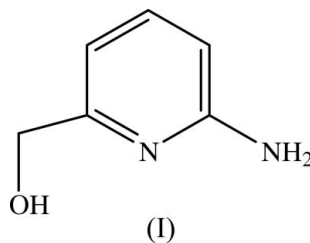
The molecule of the title compound, $\text{C}_6\text{H}_8\text{N}_2\text{O}$, is almost planar; the hydroxymethyl group deviates slightly from the plane of the ring. The molecules are linked into a chain running along the a -axis direction by an $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond. $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds connect the chains, forming a molecular layer parallel to the (001) plane. A $\text{C}-\text{H}\cdots\pi$ interaction is also observed in the layer.

Received 13 June 2006

Accepted 3 July 2006

Comment

The role of hydrogen bonds involving the NH group and a carbonyl O atom in the controlled assembly of biologically relevant architectures in nature has been reported; two- and three-dimensional molecular networks (Felix *et al.*, 1997), extended sheet structures (Zhao *et al.*, 1990), columnar networks (Kinbara *et al.*, 1996), molecular tapes (Zerowski *et al.*, 1990) and helical aggregates (Sanchez-Quesada *et al.*, 1996) exemplify the different architectures in crystal engineering. From these numerous reports dealing with the role of hydrogen bonding in the process of molecular recognition, self-assembled dimerization and self-assembled polymerization are useful tools for a supramolecular chemist. The title compound, (I), is an important hydrogen-bonding synthon as it is a very useful substrate for the synthesis of designed receptors in the fields of molecular recognition (Goswami, Dey, Maity & Jana, 2005; Goswami, Dey, Fun *et al.*, 2005) and supramolecular chemistry (Lehn, 1995; Steed & Atwood, 2001). The crystal structure of (I) has been determined as part of our crystal engineering research since it is a simple design for generating a supramolecular three-dimensional assembly in solid-state crystal engineering.



The bond lengths and angles of (I) are normal (Allen *et al.*, 1987). The hydroxymethyl group deviates slightly from the molecular ring plane, as indicated by the $\text{C}4-\text{C}5-\text{C}6-\text{O}1$ torsion angle of 10.67 (17)° (Fig. 1). The solid state structure of (I) has several interesting hydrogen bonds due to the fact that (I) contains one alcohol and one primary amino group attached to the pyridine ring. All the H atoms attached to O and N take part in the complementary dimerization as well as in the supramolecular array.

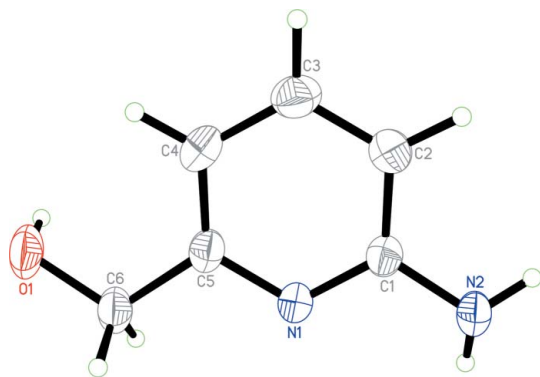


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids and the atomic numbering.

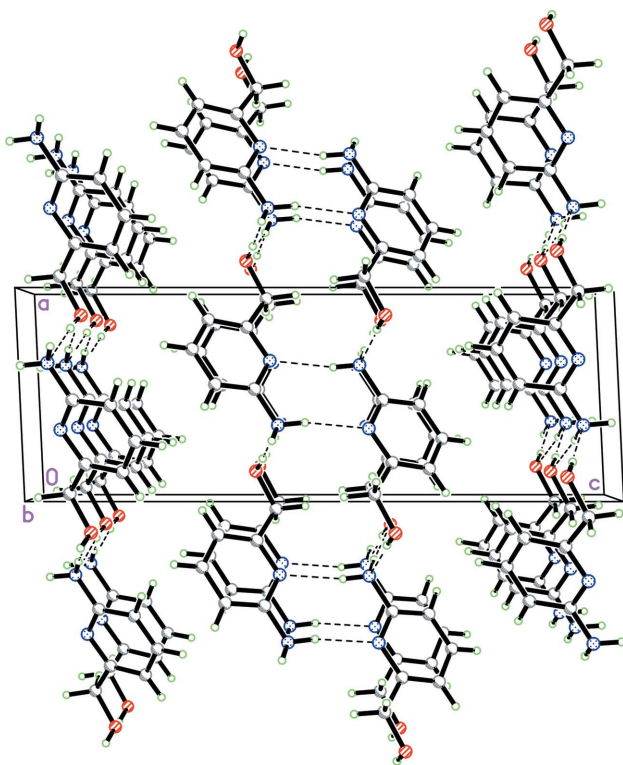


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

The crystal packing (Fig. 2) shows that the alcohol H atom is hydrogen-bonded to the amine N atom [O1—H1O1 \cdots N2ⁱ; symmetry code: (i) $-1 + x, y, z$], forming a chain along the *a* axis. The alcohol O atom forms a hydrogen bond with the amine H atom [N2—H2N2 \cdots O1ⁱⁱ; symmetry code: (ii) $1 + x, 1 + y, z$], which connects neighboring chains related by translation along the *b* axis. There are two complementary hydrogen-bonding units for dimerization; one of the amine H atoms (H1N2) and the ring N atom (N1) are complementarily hydrogen-bonded to the neighboring molecule in the same plane [N2—H1N2 \cdots N1ⁱⁱⁱ; symmetry code: (iii) $1 - x, 1 - y, -z$] (Table 2). Therefore dimerization as well as three-dimensional propagation are simultaneously observed in the

solid-state structure of (I). A C—H \cdots π interaction is also observed (Table 2).

Experimental

A mixture of 2-*N*-pivaloylamino-6-bromomethylpyridine (0.5 g, 1.84 mmol) and sodium acetate (0.38 g, 4.6 mmol) was refluxed in acetonitrile (10 ml) for 8 h. The intermediate compound, 6-(2,2-dimethyl-propionylamino)-pyridin-2-ylmethyl acetate was then refluxed with 10% NaOH (H₂O—EtOH 1:1) for 6 h to afford compound (I). Single crystals of (I) were grown by slow evaporation of a CH₃OH/CHCl₃ (*v/v* 1:5) solution.

Crystal data

C ₆ H ₈ N ₂ O	<i>Z</i> = 4
<i>M_r</i> = 124.14	<i>D_x</i> = 1.295 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 6.9279 (2) Å	μ = 0.09 mm ⁻¹
<i>b</i> = 4.7570 (1) Å	<i>T</i> = 297 (2) K
<i>c</i> = 19.3436 (5) Å	Block, colorless
β = 92.657 (2)°	0.44 × 0.36 × 0.23 mm
<i>V</i> = 636.80 (3) Å ³	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	8090 measured reflections
ω scans	1699 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	1373 reflections with $I > 2\sigma(I)$
<i>T</i> _{min} = 0.961, <i>T</i> _{max} = 0.979	<i>R</i> _{int} = 0.024
	θ _{max} = 29.0°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.0978P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.117$	$(\Delta/\sigma)_{\max} < 0.001$
<i>S</i> = 1.04	$\Delta\rho_{\max} = 0.17 \text{ e \AA}^{-3}$
1699 reflections	$\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$
114 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

O1—C6	1.4156 (14)	N1—C5	1.3460 (13)
N1—C1	1.3353 (14)	N2—C1	1.3850 (14)
C1—N1—C5	118.24 (9)	N2—C1—C2	120.48 (10)
N1—C1—N2	116.98 (10)	O1—C6—C5	114.14 (10)
C5—N1—C1—N2	176.38 (10)	N1—C5—C6—O1	-170.27 (10)
N2—C1—C2—C3	-176.45 (11)	C4—C5—C6—O1	10.67 (17)
C3—C4—C5—C6	179.40 (11)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1O1 \cdots N2 ⁱ	0.89 (2)	2.00 (2)	2.8837 (16)	175 (2)
N2—H2N2 \cdots O1 ⁱⁱ	0.889 (18)	2.113 (18)	2.9991 (16)	174.5 (15)
N2—H1N2 \cdots N1 ⁱⁱⁱ	0.883 (17)	2.209 (17)	3.0745 (15)	166.5 (13)
C6—H6A \cdots Cg1 ^{iv}	0.971 (16)	2.711 (17)	3.6257 (14)	156.8 (12)

Symmetry codes: (i) $x - 1, y, z$; (ii) $x + 1, y + 1, z$; (iii) $-x + 1, -y + 1, -z$; (iv) $x, y - 1, z$.

All H atoms were located in a difference map and refined isotropically. The O–H, N–H and C–H bond lengths are 0.89 (2), 0.883 (17)–0.889 (19) and 0.954 (15)–0.992 (17) Å, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The CSIR [project No. 01(1913)/04/EMR-II], Government of India, is acknowledged for financial support. The authors also thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version V7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Felix, O., Hosseini, M. W., De Cian, A. & Fischer, J. (1997). *Angew. Chem. Int. Ed. Engl.* **36**, 102–104.
- Goswami, S. P., Dey, S., Fun, H.-K., Anjum, S. & Atta-ur-Rahman (2005). *Tetrahedron Lett.* **46**, 7187–7191.
- Goswami, S. P., Dey, S., Maity, A. C. & Jana, S. (2005). *Tetrahedron Lett.* **46**, 1315–1318.
- Kinbara, K., Hashimoto, Y., Sukewaga, M., Nohira, H. & Saigo, K. (1996). *J. Am. Chem. Soc.* **118**, 3441–3449.
- Lehn, J. M. (1995). *Supramolecular Chemistry: Concepts and Perspectives*. Weinheim: VCH.
- Sanchez-Quesada, J., Seel, C., Prados, P. & De Mendoza, J. (1996). *J. Am. Chem. Soc.* **118**, 277–278.
- Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Steed, J. W. & Atwood, J. L. (2001). *Supramolecular Chemistry*. New York: Wiley.
- Zerowski, D. J. A., Seto, C., Wierda, D. A. & Whitesides, G. M. (1990). *J. Am. Chem. Soc.* **112**, 9025–9026.
- Zhao, X., Chang, Y.-L., Fowler, F. W. & Lauher, J. W. (1990). *J. Am. Chem. Soc.* **112**, 6627–6634.