Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2-[(2-Chloro-5-phenyl-3-pyridinyl)(hydroxy)-methyl]acrylonitrile

G. Y. S. K. Swamy,[a]* K. Ravikumar,[a] P. Narender[b] and V. Jayathirtha Rao[b]

[a]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [b]Organic Chemistry Division II, Indian Institute of Chemical Technology, Hyderabad 500 007, India

Correspondence e-mail: swamy@ins.iictnet.com

Received 19 January 2005
Accepted 9 February 2005
Online 19 February 2005

Key indicators

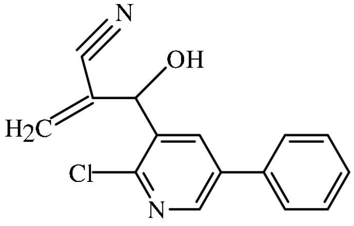
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.119
Data-to-parameter ratio = 18.6

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

In the title compound, $C_{15}H_{11}ClN_2O$, the dihedral angle between the pyridyl and phenyl rings is 38.7 (4)°. The molecules are linked *via* O—H···N and C—H···N interactions, forming infinite chains running along the *b* axis. The structure is further stabilized by weak C—H···π interactions.

Comment

The Baylis–Hillman reaction (Baylis & Hillman, 1972) is a well known method for the coupling of aldehydes and activated alkenes and is catalysed by tertiary amines or phosphines, affording a valuable C—C bond-forming reaction. The adducts formed have applications in biology (Kabat *et al.*, 1996; Kim *et al.*, 2002; Shi *et al.*, 2002). Keeping in mind the importance of such adducts, we report here the crystal and molecular structures of the title compound, (I).



(I)

The molecular configuration of (I) is shown in Fig. 1. Although the compound belongs to a centrosymmetric space group, it contains a chiral atom (C12) and is thus a racemate. The dihedral angle between the pyridyl (N1/C1–C5) and phenyl (C6–C11) rings is 38.7 (4)°. The hydroxy O atom is tilted away from the acrylonitrile group as the C13—C12—O1 bond angle is distinctly larger than that of C2—C12—O1 (Table 1).

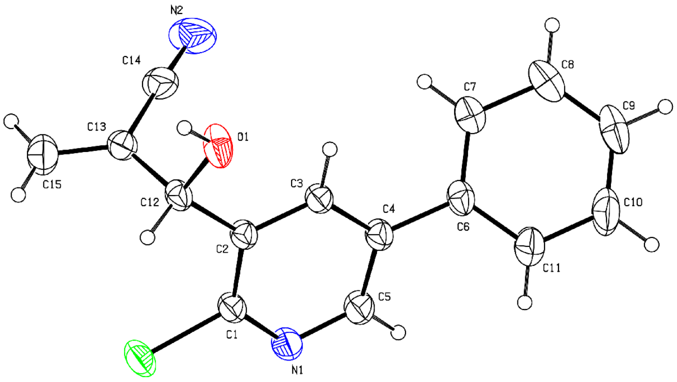


Figure 1
A view of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

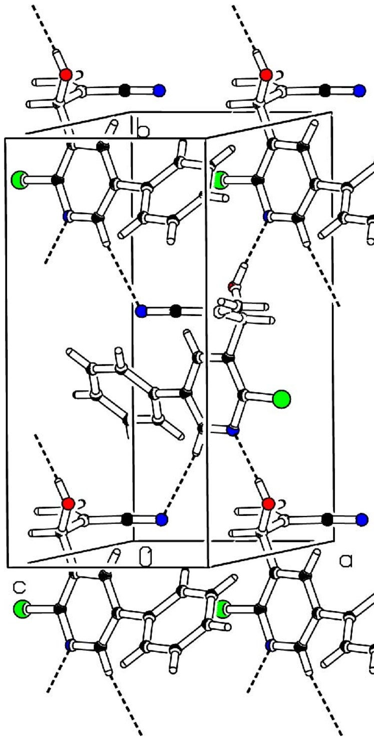


Figure 2
A partial packing diagram of (I), showing the O—H···N and C—H···N hydrogen-bonded (dashed lines) molecules forming chains along the *b* axis.

In the crystal structure, the molecules are linked by O—H···N and C—H···N interactions (Table 2). Atom O1 in the molecule at (*x*, *y*, *z*) acts as a donor to pyridine atom N1 in the molecule at ($\frac{1}{2} - x$, $-\frac{1}{2} + y$, $\frac{3}{2} - z$), forming molecular chains [*C*(6) in the nomenclature of Etter (1990) and Bernstein *et al.* (1995)] running along the *b* axis (Fig. 2). These chains are further linked into sheets by C—H···N [*C*(9) type] hydrogen bonds. Atom C5 at (*x*, *y*, *z*) acts as donor to atom N2 of the acrylonitrile group at ($\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{3}{2} - z$). The packing is further stabilized by weak C—H···Cl (intramolecular) and C—H···π [pyridyl ring with centroid *Cg* (Spek, 2003)] interactions (Table 2).

Experimental

Compound (I) was prepared by the coupling of 2-chloro-5-phenylpyridine-3-carbaldehyde (5 mmol) and acrylonitrile (5 mmol) in methanol, the reaction mixture being stirred at room temperature in the presence of 1,4-diazabicyclo[2.2.2]octane (5 mmol) for 15 min. This mixture was washed with water, extracted with chloroform and recrystallized from acetonitrile (yield 96%).

Crystal data

$C_{15}H_{11}ClN_2O$
$M_r = 270.71$
Monoclinic, $P2_1/n$
$a = 6.6461$ (5) Å
$b = 14.2172$ (10) Å
$c = 14.9057$ (10) Å
$\beta = 100.261$ (1)°
$V = 1385.90$ (17) Å^3
$Z = 4$

$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6876 reflections
$\theta = 5.6$–$55.8°$
$\mu = 0.27$ mm^{-1}
$T = 273$ (2) K
Block, colourless
0.21 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
11637 measured reflections
3226 independent reflections

2772 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\rm max} = 28.0°$
$h = -8 \rightarrow 8$
$k = -18 \rightarrow 17$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.119$
$S = 1.06$
3226 reflections
173 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.603P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.3201 (16)	C12—O1	1.4074 (14)
C1—Cl	1.7376 (13)	C14—N2	1.136 (2)
C5—N1	1.3398 (18)		
O1—C12—C13	110.62 (10)	O1—C12—C2	107.52 (9)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1$^{\rm i}$	0.82	2.04	2.8577 (14)	175
C5—H5···N2$^{\rm ii}$	0.93	2.55	3.453 (2)	165
C12—H12···Cl	0.98	2.72	3.0909 (12)	103
C8—H8···*Cg*$^{\rm iii}$	0.93	3.19	3.520 (4)	103

Symmetry codes: (i) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$; (ii) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$; (iii) $x - 1, y, z$.
Note: *Cg* is the centroid of the pyridyl ring.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms [C—H = 0.93–0.98 Å and O—H = 0.82 Å, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}$(C,O) for methyl and hydroxy H atoms and $1.2U_{\rm eq}$(C) for all other H atoms].

Data collection: *SMART* (Bruker, 2001); cell refinement and data reduction: *SAINT* (Bruker, 2001); structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

The authors thank Dr J. S. Yadav, Director, IICT, Hyderabad, for his kind encouragement.

References

Baylis, A. D. & Hillman, M. E. D. (1972). German Patent No. 2 155 113.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2001). *SAINT* (Version 6.28a) and *SMART* (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kabat, M. M., Kiegel, J., Cohen, N., Toth, K., Wovkulich, P. M. & Uskokovic, M. R. (1996). *J. Org. Chem.* **61**, 118–124.
Kim. J. N., Lee, H. J. & Gong, J. H. (2002). *Tetrahedron Lett.* **43**, 9141–9146.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shi, M., Zhao, G. L. & Wu, X. F. (2002). *Eur. J. Org. Chem.* pp. 3666–3679.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Acta Cryst. (2005). E**61**, o706–o707 G. Y. S. K. Swamy *et al.* • $C_{15}H_{11}ClN_2O$ **o707**