Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-1-[(6-Chloropyridin-3-yl)methyl]-*N*-nitroimidazolidin-2-imine (imidachloprid)

Deepak Chopra,[a]* T. P. Mohan,[b] K. S. Rao[b] and T. N. Guru Row[a]

[a]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and [b]Rallis India Limited, Peenya Industrial Area, Bangalore 560 078, India

Correspondence e-mail: deepak@sscu.iisc.ernet.in

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.162
Data-to-parameter ratio = 12.2

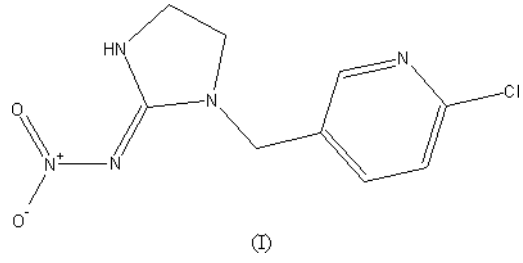
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 November 2004
Accepted 16 November 2004
Online 27 November 2004

The title compound (also known as imidachloprid), $C_9H_{10}ClN_5O_2$, is an active agrochemical possessing insecticidal activity. The dihedral angle between the mean planes passing through the pyridine ring and the imidazolidine ring is 76.9 (1)°. There are intramolecular and intermolecular N—H···O hydrogen bonds and C—H···O intermolecular interactions.

Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the levels of biological activity. Correlation of the results obtained from X-ray crystallography with biological activity has aided in the chemical design of few active agrochemicals. The activity of a series of triazolyl ketone herbicides (Anderson *et al.*, 1983) has been investigated along with the fungicidal activities of *N*-phenylsuccinamides (Zenei *et al.*, 1988). In this paper, we report the structure of the title compound, (I).



(I)

In (I), the five-membered ring N2/C7/C8/N3/C9 is approximately planar and the dihedral angle it makes with the pyridine ring (N1/C1–C5) is 76.9 (1)° (Fig. 1). An intramolecular N—H···O hydrogen bond (Table 2) forms a pseudo-

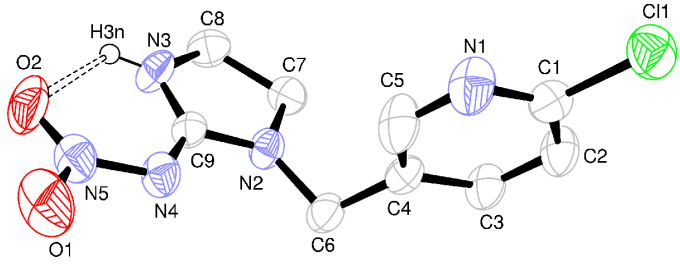


Figure 1
The molecular structure of (I), showing 50% probability ellipsoids. H atoms have been omitted for clarity, except for that involved in the N—H···O hydrogen bond (broken lines).

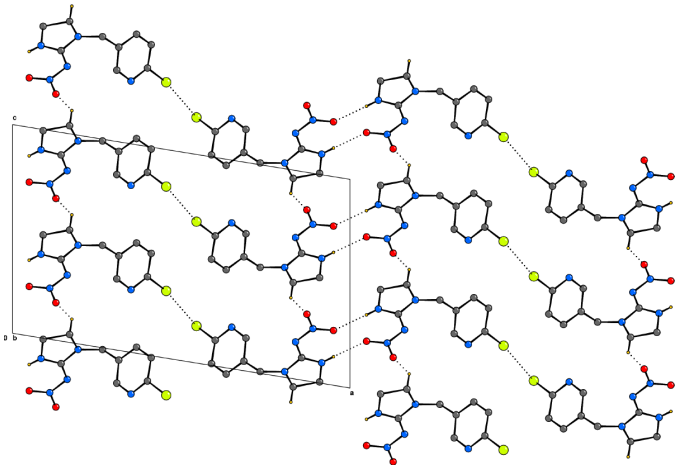


Figure 2
Packing diagram of (I), showing the N—H···O and C—H···O hydrogen bonds (dashed lines), forming molecular chains; Cl···Cl short contacts are also shown.

six-membered ring [Etter symbol $S(6)$; Bernstein *et al.*, 1995], which restricts the conformational freedom. Intermolecular N—H···O hydrogen bonds also further stabilize the packing of molecules [Etter symbol $C(6)$]. In addition, a C—H···O intermolecular interaction generates molecular chains [Etter symbol $C(7)$] parallel to the *c* axis, forming a sheet-like structure (Fig. 2), and further held together by a Cl···Cl intermolecular contact that links molecules, forming a zigzag chain along the *b* axis (Fig. 3).

Experimental

Compound (I) was obtained from Rallis India, Bangalore. Single crystals were grown by slow evaporation of a methanol/dichloromethane solution at 278 K.

Crystal data

$C_9H_{10}ClN_5O_2$
$M_r = 255.67$
Monoclinic, $P2_1/c$
$a = 19.290\ (8)$ Å
$b = 4.839\ (2)$ Å
$c = 11.784\ (5)$ Å
$\beta = 99.220\ (6)^\circ$
$V = 1085.8\ (8)$ Å^3
$Z = 4$
$D_x = 1.564$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 865 reflections
$\theta = 1.4$–25.7°
$\mu = 0.35$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
0.51 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.842$, $T_{max} = 0.953$
8430 measured reflections
2364 independent reflections
1822 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.8^\circ$
$h = -24 \rightarrow 24$
$k = -6 \rightarrow 6$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.162$
$S = 1.12$
2364 reflections
194 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0928P)^2 + 0.1346P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

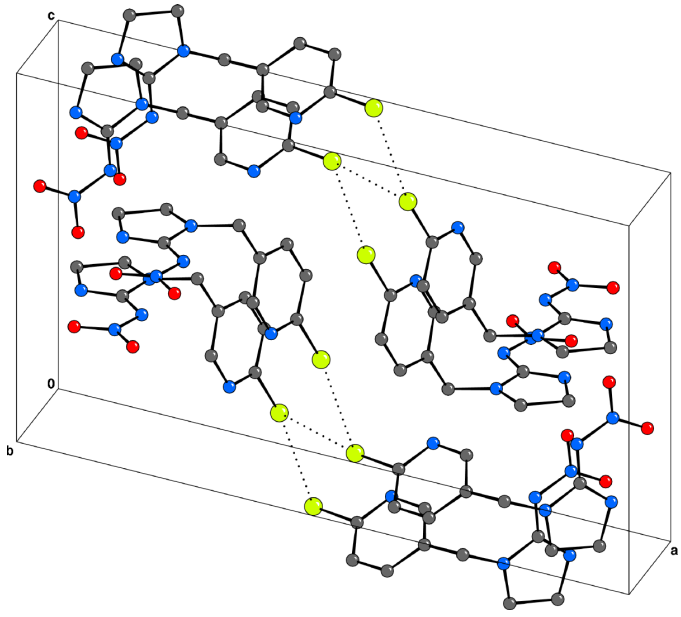


Figure 3
Intermolecular Cl···Cl contacts (dashed lines), forming a zigzag chain along the *b* axis.

Table 1
Selected geometric parameters (Å, °).

N2—C9	1.328 (3)	N4—C9	1.336 (3)
N3—C9	1.304 (3)		
N2—C6—C4	112.8 (2)		
C8—N3—C9—N2	0.8 (3)	C5—C4—C6—N2	63.0 (3)
C7—N2—C6—C4	69.6 (3)	C9—N2—C7—C8	−6.9 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O2	0.77 (3)	2.12 (3)	2.572 (3)	118 (3)
N3—H3N···O2^{i}	0.77 (3)	2.25 (3)	2.903 (4)	143 (2)
C7—H7*B*···O1^{ii}	0.90 (3)	2.42 (3)	3.015 (4)	123 (2)

Symmetry codes: (i) $2-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $x, \frac{3}{2}-y, z-\frac{1}{2}$.

All H atoms were located in difference Fourier maps and refined isotropically. The C—H bond lengths are in the range 0.91 (3)–1.00 (3) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

We thank the Department of Science and Technology, India, for data collection on the CCD facility set up under the

IRHPA–DST program. D. Chopra thanks the CSIR, India, for a Junior Research Fellowship.

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Anderson, N. H., Heritage, K. J. & Branch, S. K. (1983). *Quantitative Approaches to Drug Design*, edited by J. C. Dearden, p. 47. Amsterdam: Elsevier.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2000). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lewis, R. J., Camilleri, P., Kirby, A. J., Marby, C. A., Slawin, A. A. & Williams, D. J. (1991). *J. Chem. Soc. Perkin Trans.* 2, pp. 1625–1631.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst* **36**, 7–13.
Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON.* Chemical Crystallography Laboratory, University of Oxford, England.
Zenei, T., Takayami, C. & Terada, H. (1988). *J. Chem. Soc. Perkin Trans.* 2, pp. pp. 1439–1445.