

(E)-N¹-[(6-Chloropyridin-3-yl)methyl]-N²-cyano-N¹-methylacetamide**Deepak Chopra,^{a*} T. P. Mohan,^b
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deepak@sscu.iisc.ernet.in**Key indicators**Single-crystal X-ray study
T = 293 K
Mean $\sigma(C-C)$ = 0.004 Å
R factor = 0.048
wR factor = 0.114
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, C₁₀H₁₁ClN₄, also known as acetamiprid, is a potent chemical found to exhibit insecticidal activity. The dihedral angle between the planes passing through the 6-chloropyridine ring and the *N*'-cyano-*N*-methylimidamide moiety is 76.7 (1) Å. The crystal structure is stabilized by C—H···N intermolecular interactions.

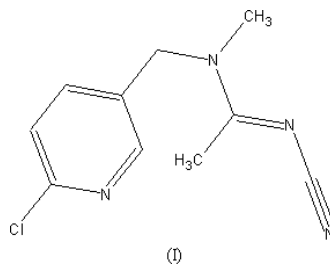
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Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformations of such molecules are found to influence their levels of biological activity. The correlation of results obtained from X-ray crystallography with biological activity has aided in the chemical design of a 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*-phenyl succinamides (Zenei *et al.*, 1988). Against this background, we present here the crystal structure of the title compound, (I).

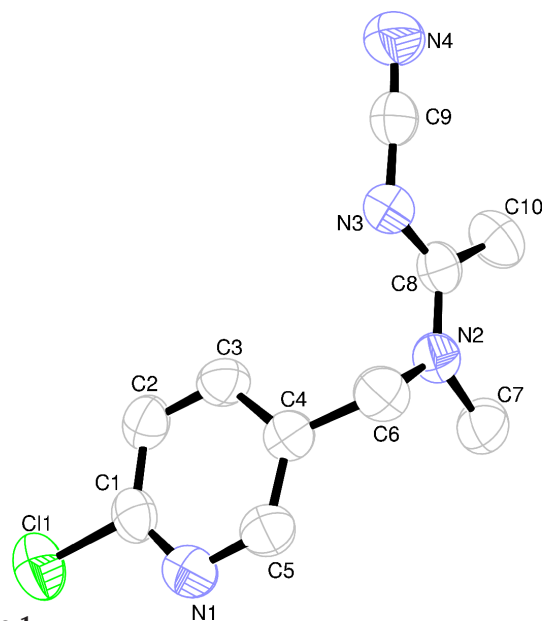


The molecular structure of (I) is shown in Fig. 1. The C8—N2, C9—N3 and C9—N4 bond lengths are 1.328 (3), 1.312 (4) and 1.149 (4) Å, respectively, highlighting the different electronic environment around each N atom. The C5—C4—C6—N2 and C4—C6—N2—C8 torsion angles are 117.3 (3) and 101.9 (3)°, respectively.

The crystal structure of (I) is stabilized by C—H···N intermolecular interactions, forming molecular chains related by a twofold screw [*C*(10) in the nomenclature of Etter (1990); Bernstein *et al.* (1995)] along the crystallographic *c* axis (Fig. 2).

Experimental

The title compound was obtained from Rallis India Limited, Bangalore. Single crystals of (I) were grown by slow evaporation of a methanol–ethylacetate mixture (1:1) at 278 K.

**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

Crystal dataC₁₀H₁₁ClN₄M_r = 222.68Orthorhombic, *Pca*2₁

a = 8.776 (3) Å

b = 11.780 (5) Å

c = 10.645 (4) Å

V = 1100.5 (7) Å³

Z = 4

D_x = 1.344 Mg m⁻³

Mo Kα radiation

Cell parameters from 875 reflections

θ = 1.6–25.4°

μ = 0.32 mm⁻¹

T = 293 (2) K

Prism, colourless

0.52 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.852, T_{max} = 0.970

8291 measured reflections

2336 independent reflections

1930 reflections with I > 2σ(I)

R_{int} = 0.023θ_{max} = 27.4°

h = -10 → 11

k = -14 → 15

l = -13 → 13

RefinementRefinement on F²R[F² > 2σ(F²)] = 0.048wR(F²) = 0.114

S = 1.17

2336 reflections

158 parameters

H atoms treated by a mixture of independent and constrained refinement

w = 1/[σ²(F_o²) + (0.0576P)² + 0.0103P]where P = (F_o² + 2F_c²)/3(Δ/σ)_{max} < 0.001Δρ_{max} = 0.20 e Å⁻³Δρ_{min} = -0.13 e Å⁻³

Absolute structure: Flack (1983),

1006 Friedel pairs

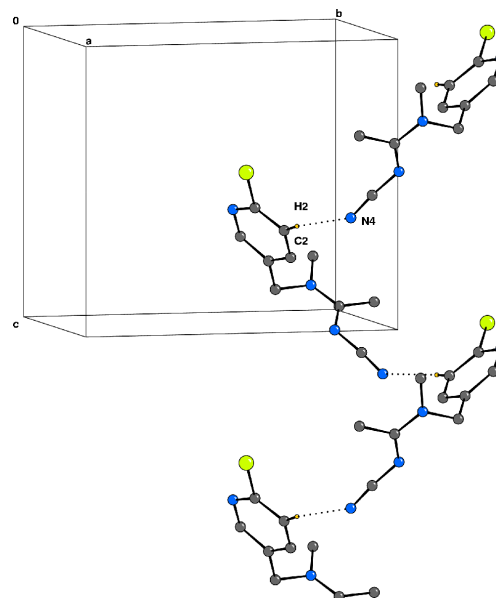
Flack parameter = -0.01 (8)

Table 1

Hydrogen-bonding geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C2—H2...N4 ⁱ	0.90 (3)	2.48 (2)	3.345 (4)	161 (2)

Symmetry code: (i) 1 - x, -y, z - ½.

**Figure 2**

A partial packing diagram for (I), highlighting the C—H...N intermolecular interactions (dotted lines) forming molecular chains along the c axis. The atom labelled N4 is in the symmetry-related molecule at position (1 - x, -y, z - ½).

Methyl H atoms were constrained to an ideal geometry, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C_{methyl}). The remaining H atoms were located in a difference Fourier map and refined isotropically. The refined C—H bond lengths are in the range 0.88 (3)–0.99 (4) Å.

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT (Bruker, 2000); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (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).

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