

(4E)-3-[(2-Chloro-4,5-dihydro-1,3-thiazol-5-yl)-methyl]-5-methyl-N-nitro-1,3,5-oxadiazinan-4-imine (thiamethaxam)**Deepak Chopra,^{a*} T. P. Mohan,^b K. S. Rao^b and T. N. Guru Row^a**^aSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and ^bRallis India Limited, Peenya Industrial Area, Bangalore 560 078, India

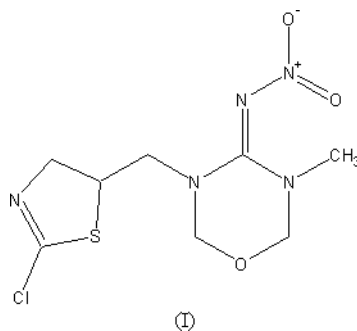
Correspondence e-mail: deepak@sscu.iisc.ernet.in

Key indicatorsSingle-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.065
wR factor = 0.176
Data-to-parameter ratio = 11.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound (also known as thiamethaxam), $\text{C}_8\text{H}_{10}\text{ClN}_5\text{O}_3\text{S}$, is a potent agrochemical exhibiting insecticidal activity. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ 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 [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*-phenylsuccinamides (Zenei *et al.*, 1988). In this paper, we report the structure of the title compound, (I).

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In (I), the 1,3,5-oxadiazinane ring shows a twist-boat conformation (Fig. 1). The displacements of the atoms O1 and

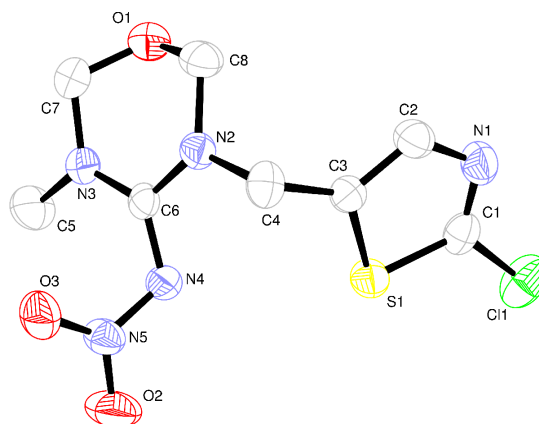


Figure 1
The molecular structure of (I), showing 50% probability ellipsoids. H atoms have been omitted for clarity.

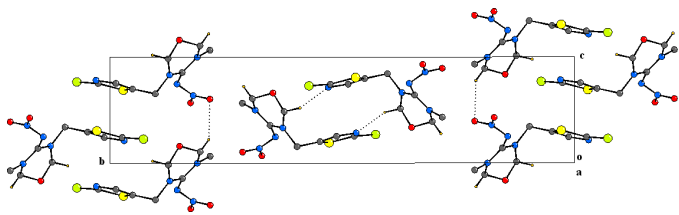


Figure 2
Packing diagram of (I), showing the C—H...N dimers and C—H...O interactions forming molecular chains.

C8 from the plane defined by atoms N2/C6/N3/C7 are 0.871 (3) and 0.400 (5) Å, respectively. The N-nitro group is twisted away from the methyl group (C5) to minimize steric interactions.

C—H...N intermolecular interactions (Table 2) generate dimers in the *bc* plane and C—H...O interactions form molecular chains along the *c* axis (Fig. 2). Packing motifs in accordance with Etter's analysis (Bernstein *et al.*, 1995) are $R_2^2(14)$, corresponding to C—H...N dimers, and $C(7)$ molecular chains, which correspond to C—H...O intermolecular interactions. There is a short contact C5...O3ⁱ of 3.003 (7) Å (see Table 2 for symmetry code), which is a forced contact and not a well defined C—H...O intermolecular interaction.

Experimental

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

Crystal data

C ₈ H ₁₀ ClN ₅ O ₃ S	$D_x = 1.582 \text{ Mg m}^{-3}$
$M_r = 291.73$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 564 reflections
$a = 6.493 (5) \text{ \AA}$	$\theta = 1.5\text{--}26.4^\circ$
$b = 28.74 (2) \text{ \AA}$	$\mu = 0.49 \text{ mm}^{-1}$
$c = 6.812 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 105.486 (12)^\circ$	Block, yellow
$V = 1225.0 (16) \text{ \AA}^3$	$0.31 \times 0.27 \times 0.20 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2370 independent reflections
φ and ω scans	1970 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.049$
$T_{\text{min}} = 0.863$, $T_{\text{max}} = 0.908$	$\theta_{\text{max}} = 26.4^\circ$
7937 measured reflections	$h = -7 \rightarrow 7$
	$k = -34 \rightarrow 35$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0829P)^2 + 1.5246P]$
$R[F^2 > 2\sigma(F^2)] = 0.176$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2370 reflections	$\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
203 parameters	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.280 (5)	N3—C6	1.327 (5)
N1—C2	1.375 (5)	N4—C6	1.362 (4)
N2—C6	1.337 (4)	N5—N4	1.330 (4)
N2—C4—C3	112.4 (3)		
C8—N2—C6—N3	−14.7 (5)	N5—N4—C6—N3	−60.0 (5)
C7—N3—C6—N2	−5.5 (5)	O3—N5—N4—C6	−15.9 (5)
C6—N3—C7—O1	45.9 (5)		

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H5B...O3 ⁱ	1.02 (8)	2.60 (8)	3.003 (7)	106 (6)
C7—H7B...O3 ⁱⁱ	0.93 (5)	2.54 (5)	3.354 (7)	146 (4)
C8—H8B...N1 ⁱⁱⁱ	1.01 (5)	2.48 (5)	3.396 (6)	150 (4)

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

All H atoms were located in difference Fourier maps and refined isotropically. C—H bond lengths are in the range 0.87 (8)–1.05 (5) Å.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; 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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