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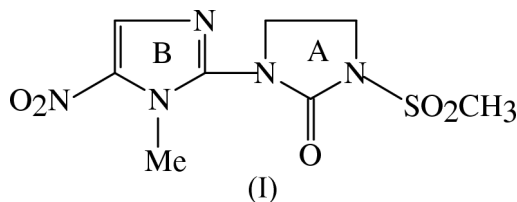
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$
 R factor = 0.060
 wR factor = 0.176
Data-to-parameter ratio = 10.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-(1-Methyl-5-nitroimidazol-2-yl)-1-(methyl-
sulfonyl)imidazolidin-2-one

In the title compound (satranidazole), $\text{C}_8\text{H}_{11}\text{N}_5\text{O}_5\text{S}$, the dihedral angle between the mean plane of the imidazolidine and imidazole rings is $49.0(2)^\circ$. In the solid state, the imidazole rings of the glide-related molecules are stacked along the a axis, with significant π - π interactions. The crystal structure is further stabilized by weak $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds.

Comment

1-Substituted 5-nitroimidazoles exhibit antiprotozoal activity, while the 4-nitroimidazole derivatives do not. There are at least five 5-nitroimidazole antiprotozoal drugs on the market, namely metronidazole, secnidazole, ornidazole, nimorazole and dimetridazole. The title compound, (I), synthesized by Nagarajan *et al.* (1982), is reported to have antiamebic activity (Nagarajan *et al.*, 1982) and has been launched as a drug by Alkem Laboratories. Crystals of (I) were obtained from three different solvents, *viz.*, boiling acetone (sample 1), DMF (sample 2) and H_2SO_4 (sample 3), in order to verify whether they yield any polymorphic substances, which have commercial value. Crystal structure determination and powder diffraction experiments showed that the three sample preparations led to the same structure. Hence, the crystal structure of sample 2 alone is described below.



A perspective view of the molecule of (I), including the atomic numbering, is shown in Fig. 1. The molecule contains an imidazolidine ring (A) and an imidazole ring (B) linked through a C-N bond. Ring A is twisted about the C4-C5 bond and the mean plane through this ring forms a dihedral angle of $49.0(2)^\circ$ with ring B. The methylsulfonyl group attached to ring A has a distorted tetrahedral geometry, as indicated by the widening of the O13-S11-O12 angle [$118.5(3)^\circ$]. This is caused by the repulsion between the lone pair orbitals of the two O atoms (McKenna *et al.*, 1989). The nitro group attached to the B ring is nearly coplanar with that ring, as is evident from the torsion angles C9-C8-N17-O19 [$4.0(9)^\circ$] and N7-C8-N17-O18 [$-1.5(9)^\circ$]. Weak $\text{C}-\text{H}\cdots\text{O}$ -type intramolecular hydrogen bonds are observed and they are shown in Fig. 1.

In the crystal structure, face-to-face stacking ($\alpha = 5.3^\circ$; α is the dihedral angle between stacking planes, in this case, the

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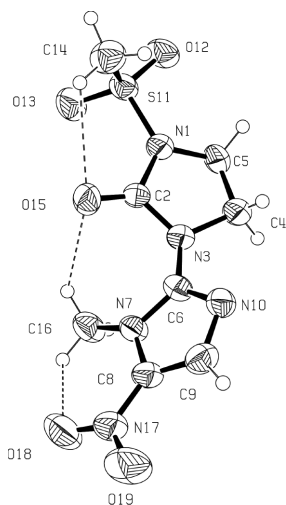


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Weak C—H...O intramolecular hydrogen bonds are also shown.

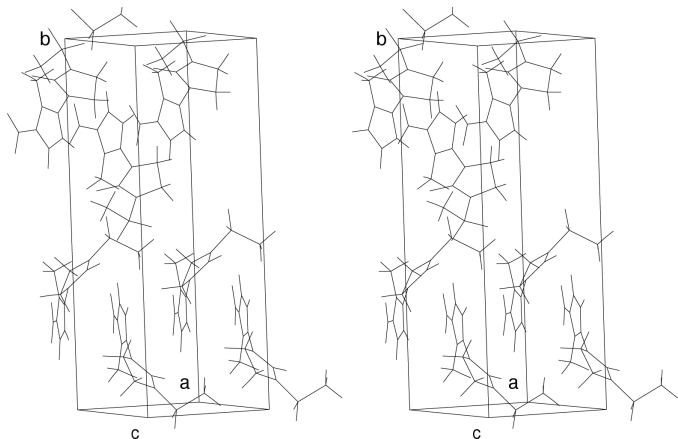


Figure 2
Stereoview showing the stacking interactions along the *a* axis.

angle between ring *B* and the glide-related ring *B*) of the *B* ring and the *B* rings of glide-related molecules at $(\frac{1}{2} + x, \frac{3}{2} - y, z)$ and $(-\frac{1}{2} + x, \frac{3}{2} - y, z)$ are observed. These rings are stacked along the *a* axis, with their centroids separated by a distance of 3.564 (3) Å, indicating significant π - π interactions. The crystal structure is stabilized by these stacking interactions (Fig. 2) and also by several weak C—H...O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized according to the procedure developed by Nagarajan *et al.* (1982). Expecting polymorphism, three crystalline samples of (I) were obtained from three different solvents, as follows. The title compound was dissolved in a large volume of boiling acetone and the solution was concentrated, to obtain a crystalline product with melting point 458–459 K (sample 1). The second sample was obtained by dissolving 0.5 g of (I) in 1 ml of DMF on a water bath and leaving the solution at room temperature for several hours; the melting point of this sample was found to be the same as that of sample 1. To prepare the third sample, 0.5 g of (I) was

dissolved in 1 ml of concentrated H₂SO₄ and 5 ml water, and the solution was set aside overnight. This sample was found to melt partially around 458 K, re-solidified at about 483 K and the melting was complete at about 493 K.

Crystal data

C₈H₁₁N₅O₅S
M_r = 289.28
 Orthorhombic, *Pna*2₁
a = 7.046 (2) Å
b = 19.566 (6) Å
c = 8.743 (2) Å
V = 1205.3 (6) Å³
Z = 4
D_x = 1.594 Mg m⁻³

Cu *K*α radiation
 Cell parameters from 25 reflections
 θ = 13.8–29.6°
 μ = 2.68 mm⁻¹
T = 293 (2) K
 Bipyramidal, pale yellow
 0.20 × 0.13 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω -2 θ scans
 Absorption correction: ψ scan (XRAYACS; Chandrasekaran, 1998)
T_{min} = 0.616, *T_{max}* = 0.775
 1851 measured reflections
 1195 independent reflections
 1035 reflections with *I* > 2 σ (*I*)

R_{int} = 0.047
 θ_{\max} = 71.7°
h = -6 → 8
k = -24 → 19
l = 0 → 10
 3 standard reflections every 200 reflections
 frequency: 120 min
 intensity decay: none

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.060
wR(*F*²) = 0.176
S = 1.11
 1851 reflections
 174 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1053P)^2 + 1.7101P]$
 where $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)_{max} < 0.001
 $\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.70 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.039 (4)
 Absolute structure: Flack (1983), 656 Friedel pairs
 Flack parameter = -0.01 (5)

Table 1

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>
C14—H14A...O15	0.96	2.67	3.221 (9)	117
C16—H16A...O18	0.96	2.16	2.853 (8)	128
C16—H16B...O15	0.96	2.28	3.017 (8)	133
C14—H14B...O18 ⁱ	0.96	2.53	3.443 (9)	158
C5—H5B...O19 ⁱⁱ	0.97	2.58	3.265 (8)	128
C9—H9...O13 ⁱⁱⁱ	0.93	2.50	3.412 (7)	168
C14—H14C...O15 ^{iv}	0.96	2.48	3.336 (8)	148
C14—H14C...O13 ^{iv}	0.96	2.60	3.342 (9)	134

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

All the H atoms were positioned geometrically and were allowed to ride on their parent atoms with SHELXL97 (Sheldrick, 1997) defaults for bond lengths and displacement parameters.

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1994); cell refinement: CAD-4 EXPRESS; data reduction: XCAD4 (Harms & Wocadlo, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PARST (Nardelli, 1983, 1995).

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