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O-Methyl[2-(2-Ethyl-5-nitroimidazol-1-yl)ethyl]thiocarbamate (sulnidazole)

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Abstract. $C_9H_{14}N_4O_3S$, $M_r = 258{\cdot}3$, monoclinic, $P2_1/c$, $a = 7{\cdot}313$ (2), $b = 15{\cdot}907$ (2), $c = 10{\cdot}868$ (2) Å, $\beta = 108{\cdot}02$ (3)°, 25 °C, $Z = 4$. The molecules are held together by packing forces only.

Introduction. Sulnidazole is an antiprotozoal drug. Transparent pale-green crystals were obtained by cooling a solution in ethanol. Cell dimensions and intensities were measured on a Picker four-circle diffractometer with the experimental conditions given in Table 1. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971) and refined by block-diagonal anisotropic least squares (Ahmed, Hall, Pippy & Huber, 1966). The final $R = \Sigma\|F_o| - |F_c\|/\Sigma|F_o|$ is 0·10 for all observed reflexions. The final coordinates are given in Table 2. The scattering factors were those given in *International Tables for X-ray Crystallography* (1962).†

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Table 1. *Experimental conditions*

Source Cu $K\bar{\alpha}$; $\lambda = 1{\cdot}5418$ Å
ω–2θ scan; $\theta_{max} = 50°$
Confidence level: 2·5
Total number of independent reflexions: 1230
Total observed: 1131

† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32506 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. *Final positional parameters* (×10⁴), *with standard deviations in parentheses*

	x	*y*	*z*
C(1)	7668 (6)	11781 (3)	2489 (5)
C(2)	8019 (6)	10868 (2)	2433 (4)
C(3)	9716 (5)	10669 (2)	2019 (3)
N(4)	10691 (4)	11208 (1)	1550 (2)
C(5)	12068 (4)	10753 (2)	1235 (3)
C(6)	11902 (4)	9937 (2)	1541 (3)
N(7)	10385 (4)	9880 (1)	2005 (3)
C(8)	9341 (6)	9129 (3)	2205 (4)
C(9)	10177 (6)	8799 (3)	3554 (4)
N(10)	8959 (4)	8132 (2)	3823 (3)
C(11)	7651 (5)	8328 (2)	4402 (3)
S(12)	6843 (2)	9262 (0)	4604 (1)
O(13)	7117 (3)	7614 (1)	4839 (2)
C(14)	5806 (5)	7677 (2)	5592 (4)
N(15)	13008 (4)	9255 (1)	1336 (3)
O(16)	14296 (3)	9421 (1)	845 (2)
O(17)	12704 (4)	8556 (1)	1637 (3)

Table 3. *Bond distances* (Å) *and angles* (°), *with standard deviations in parentheses*

C(1)–C(2)	1·480 (5)	C(1)–C(2)–C(3)	113·2 (4)
C(2)–C(3)	1·479 (6)	C(2)–C(3)–N(4)	125·8 (3)
C(3)–N(4)	1·315 (4)	C(2)–C(3)–N(7)	122·9 (3)
C(3)–N(7)	1·349 (4)	N(4)–C(3)–N(7)	111·1 (3)
N(4)–C(5)	1·367 (4)	C(3)–N(4)–C(5)	106·3 (3)
C(5)–C(6)	1·355 (4)	N(4)–C(5)–C(6)	108·5 (3)
C(6)–N(7)	1·356 (4)	C(5)–C(6)–N(7)	107·5 (3)
C(6)–N(15)	1·411 (4)	C(5)–C(6)–N(15)	126·8 (3)
N(7)–C(8)	1·471 (5)	N(7)–C(6)–N(15)	125·6 (3)
C(8)–C(9)	1·498 (6)	C(3)–N(7)–C(6)	106·5 (3)
C(9)–N(10)	1·472 (6)	C(3)–N(7)–C(8)	123·2 (3)
N(10)–C(11)	1·335 (5)	C(6)–N(7)–C(8)	129·1 (3)
C(11)–S(12)	1·640 (3)	N(7)–C(8)–C(9)	110·8 (3)
C(11)–O(13)	1·334 (4)	C(8)–C(9)–N(10)	110·9 (4)
O(13)–C(14)	1·444 (5)	C(9)–N(10)–C(11)	119·4 (3)
N(15)–O(16)	1·246 (4)	N(10)–C(11)–S(12)	128·0 (3)
N(15)–C(17)	1·199 (4)	N(10)–C(11)–O(13)	107·5 (3)
		S(12)–C(11)–O(13)	124·5 (2)
		C(11)–O(13)–C(14)	117·5 (3)
		C(6)–N(15)–O(16)	116·7 (3)
		C(6)–N(15)–O(17)	120·4 (3)
		O(16)–N(15)–O(17)	122·9 (3)

Table 4. *Torsion angles in sulnidazole*

C(1)–C(2)–C(3)–N(4)	−10°
C(5)–C(6)–N(15)–O(16)	1
C(3)–N(7)–C(8)–C(9)	−102
N(7)–C(8)–C(9)–N(10)	171
C(8)–C(9)–N(10)–C(11)	−95
C(9)–N(10)–C(11)–S(12)	14
C(9)–N(10)–C(11)–O(13)	−164
N(10)–C(11)–O(13)–O(14)	175

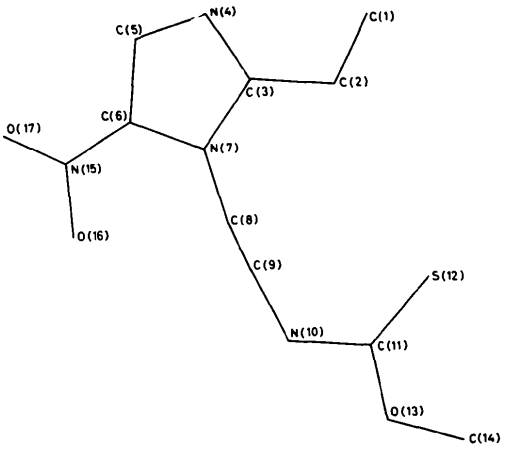

Fig. 1. The conformation and numbering scheme of $C_9H_{14}N_4O_3S$.

Discussion. The conformation of the molecule and the numbering scheme are shown in Fig. 1, and the bond distances and angles in Table 3. The torsion angles defining the conformation of the molecule are given in Table 4. All relevant structural information is given in the *Abstract*.

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Tellurure de Gallium

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Abstract. Ga_2Te_5, tetragonal, $I4/m$, $a = 7{\cdot}913$ (1), $c = 6{\cdot}848$ (3) Å, $Z = 2$, $D_c = 6{\cdot}02$, $D_m = 5{\cdot}85$ g cm^{-3}, μ(Mo $K\alpha$) = 231 cm^{-1}. The final R value is 0·069 for 475 independent reflexions. $GaTe_4$ tetrahedra involve Te atoms which form covalent Te–Te bonds.

Introduction. Au cours de l'étude du diagramme de phase GaTe (Alapini, Guittard, Julien-Pouzol & Flahaut, 1976) le composé de formule Ga_2Te_5 a été mis en évidence. Newman, Brice & Wright (1961) avaient déjà décrit cette phase et lui avaient attribué la composition $GaTe_3$, sans preuves définitives. Elle n'est stable que dans un étroit domaine de température entre 400 et 495 °C.

Le monocristal de Ga_2Te_5 présente une couleur noire, sa forme ne peut pas être approchée par un polyèdre convexe.

Les extinctions systématiques observées pour une tache hkl sont $h + k + l = 2n + 1$, ce qui conduit à trois groupes d'espace possibles: $I4$, $I\bar{4}$ et $I4/m$. C'est la