Tableau 3. *Angles dièdres* (°) *des chaînes polyoxyéthyléniques*

	AA44(4CO)	AA66(4CO)
C(1)—O(30)—C(31)—C(32)	88	125
O(30)—C(31)—C(32)—O(33)	−16	−176
C(31)—C(32)—O(33)—C(34)	−175	170
C(32)—O(33)—C(34)—C(35)	−178	−103
O(33)—C(34)—C(35)—O(36)	−64	72
C(34)—C(35)—O(36)—C(37)	−164	−172
C(35)—O(36)—C(37)—C(38)	−176	−164
O(36)—C(37)—C(38)—O(39)	−117	−176
C(37)—C(38)—O(39)—C(40)	-	−161
C(38)—O(39)—C(40)—C(41)	-	−173
O(39)—C(40)—C(41)—O(42)	-	66
C(40)—C(41)—O(42)—C(43)	-	86
C(41)—O(42)—C(43)—C(44)	-	180
O(42)—C(43)—C(44)—O(45)	-	173
C(43)—C(44)—O(45)—C(22)	-	131
C(37)—C(38)—O(39)—C(22)	−159	-

tionnelle: à ce jour aucun complexe stable cristallisé n'a pu être obtenu (ion ou molécule non chargée) avec cette nouvelle série de composés.

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Structure of 5-(β-D-Erythrofuranosyl)-3-methyl-2(3*H*)-thiazolethione

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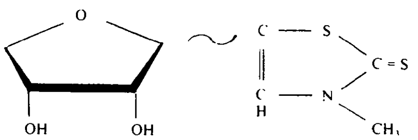
(*Received* 24 *October* 1988; *accepted* 13 *April* 1989)

Abstract. $C_8H_{11}NO_3S_2$, $M_r = 233{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}887\,(1)$, $b = 21{\cdot}412\,(3)$, $c = 9{\cdot}717\,(2)$ Å, $V = 2057{\cdot}1$ Å^3, $Z = 8$, $D_x = 1{\cdot}51$, D_m (by flotation) = $1{\cdot}50$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}7107$ Å, $\mu = 0{\cdot}048$ mm^{-1}, $F(000) = 976$, $T = 293$ K, $R = 0{\cdot}06$ for 2393 independent reflections. The conformations of the two sugar rings are described as $^{4}_{3}T$. The crystal structure is stabilized by van der Waals contacts with specific interactions between the O(12) and C(13) atoms of one molecule and the O(23) atom of another molecule.

Introduction. In recent years, the synthesis of *C*-nucleosides (James, 1979) has attracted considerable attention due to their antitumour and antiviral activities (Suhadolnik, 1979). However, little effort has been devoted to the synthesis of *C*-nucleosides analogous to 2(3*H*)-thiazolethiones. The synthesis of 5-(α- and β-D-erythrofuranosyl)-3-methyl-2(3*H*)-thiazolethiones was achieved by acid-catalyzed dehydration, with trifluoroacetic acid at room temperature, of 3-methyl-5-(D-*arabino*-tetritol-1-yl)-2(3*H*)-thiazolethiones (Blasco-López, 1988; Dalton, 1966). The two anomers were isolated by fractional crystallization. The X-ray analysis of the title compound, as well as of the α-compound (Bellver, Moreno, López-Castro & Márquez, 1988), was undertaken in order to elucidate structural details.



Experimental. Crystals appear as colourless orthorhombic prisms. Crystal size 0·20 × 0·09 × 0·19 mm. Enraf–Nonius CAD-4 diffractometer, graphite monochromator. Space group $P2_12_12_1$. 25 reflections ($4 < \theta < 14°$) for refining unit-cell dimensions, ω–2θ scan. 3359 reflections measured ($2 < \theta < 30°$), $\pm h, k, l$, $h_{\max} = 13$, $k_{\max} = 30$, $l_{\max} = 13$. Two standard reflections (311, $3\bar{1}\bar{1}$) monitored every 100 reflections showed only random variations within 3% intensity. 2393 reflections with $I \geq 2\sigma(I)$ observed. Lorentz and polarization corrections. No correction for absorption. Structure solved by direct methods with *MULTAN* (Main *et al.*, 1980). Anisotropic full-

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Table 1. *Final positional and equivalent isotropic thermal parameters* (Å^2 × 10^3) *of non-*H *atoms, with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*a_ia_j\cos(\mathbf{a}_i.\mathbf{a}_j).$$

	x	y	z	U_{eq}
Molecule 1				
S(11)	0·7901 (4)	0·1527 (1)	0·8302 (4)	48 (1)
S(12)	0·7544 (4)	0·2898 (1)	0·7622 (4)	58 (1)
O(11)	0·8894 (11)	0·0208 (4)	0·8925 (10)	58 (3)
O(12)	0·9295 (11)	0·0774 (3)	1·2370 (9)	56 (3)
O(13)	0·9707 (10)	−0·0424 (3)	1·1745 (11)	55 (3)
N(1)	0·9529 (11)	0·2350 (4)	0·9097 (11)	47 (3)
C(11)	0·8387 (14)	0·2298 (5)	0·8351 (14)	45 (4)
C(12)	1·0207 (17)	0·2950 (5)	0·9351 (18)	70 (6)
C(13)	1·0044 (14)	0·1800 (5)	0·9632 (14)	46 (4)
C(14)	0·9265 (14)	0·1312 (4)	0·9287 (13)	42 (4)
C(15)	0·9412 (13)	0·0666 (5)	0·9892 (14)	45 (4)
C(16)	0·8627 (13)	0·0558 (5)	1·1209 (14)	43 (4)
C(17)	0·8504 (13)	−0·0163 (5)	1·1194 (15)	46 (4)
C(18)	0·8379 (15)	−0·0325 (5)	0·9731 (15)	54 (4)
Molecule 2				
S(21)	0·5786 (4)	0·4017 (1)	1·4536 (4)	47 (1)
S(22)	0·5087 (4)	0·5385 (1)	1·4886 (4)	57 (1)
O(21)	0·6464 (9)	0·2707 (4)	1·3566 (12)	58 (3)
O(22)	0·9857 (8)	0·3275 (3)	1·3206 (12)	54 (3)
O(23)	0·9238 (10)	0·2073 (3)	1·2806 (10)	57 (3)
N(2)	0·6597 (10)	0·4846 (4)	1·2915 (11)	42 (3)
C(21)	0·5852 (13)	0·4801 (5)	1·4011 (15)	47 (4)
C(22)	0·6889 (17)	0·5434 (5)	1·2223 (17)	66 (5)
C(23)	0·7169 (13)	0·4292 (5)	1·2386 (15)	50 (4)
C(24)	0·6822 (12)	0·3802 (4)	1·3190 (14)	42 (4)
C(25)	0·7416 (13)	0·3151 (5)	1·3052 (14)	47 (4)
C(26)	0·8686 (13)	0·3059 (4)	1·3883 (14)	41 (4)
C(27)	0·8718 (14)	0·2346 (5)	1·4015 (15)	46 (4)
C(28)	0·7226 (14)	0·2183 (5)	0·4158 (16)	52 (4)

Table 2. *Molecular geometry* (Å *and* °) *with e.s.d.'s in parentheses*

Molecule 1		Molecule 2	
S(11)—C(11)	1·720 (11)	S(21)—C(21)	1·757 (12)
S(11)—C(14)	1·717 (14)	S(21)—C(24)	1·723 (13)
S(12)—C(11)	1·687 (13)	S(22)—C(21)	1·690 (13)
O(11)—C(15)	1·452 (16)	O(21)—C(25)	1·428 (15)
O(11)—C(18)	1·473 (16)	O(21)—C(28)	1·469 (15)
O(12)—C(16)	1·387 (16)	O(22)—C(26)	1·409 (15)
O(13)—C(17)	1·420 (16)	O(23)—C(27)	1·409 (17)
N(1)—C(12)	1·470 (16)	N(2)—C(22)	1·456 (15)
N(1)—C(11)	1·345 (18)	N(2)—C(21)	1·298 (18)
N(1)—C(13)	1·383 (15)	N(2)—C(23)	1·412 (15)
C(13)—C(14)	1·341 (16)	C(23)—C(24)	1·351 (17)
C(14)—C(15)	1·510 (16)	C(24)—C(25)	1·519 (15)
C(15)—C(16)	1·515 (19)	C(25)—C(26)	1·506 (18)
C(16)—C(17)	1·548 (15)	C(26)—C(27)	1·532 (14)
C(17)—C(18)	1·468 (20)	C(27)—C(28)	1·522 (19)
C(11)—S(11)—C(14)	91·3 (6)	C(21)—S(21)—C(24)	90·7 (6)
C(15)—O(11)—C(18)	107·5 (9)	C(25)—O(21)—C(28)	107·9 (9)
C(12)—N(1)—C(13)	120·8 (11)	C(22)—N(2)—C(23)	118·6 (11)
C(11)—N(1)—C(13)	116·2 (10)	C(21)—N(2)—C(23)	117·6 (10)
C(11)—N(1)—C(12)	123·0 (10)	C(21)—N(2)—C(22)	123·8 (10)
S(12)—C(11)—N(1)	125·3 (8)	S(22)—C(21)—N(2)	127·7 (9)
S(11)—C(11)—N(1)	109·1 (8)	S(21)—C(21)—N(2)	109·3 (8)
S(11)—C(11)—S(12)	125·5 (7)	S(21)—C(21)—S(22)	123·0 (8)
N(1)—C(13)—C(14)	111·0 (11)	N(2)—C(23)—C(24)	109·8 (11)
S(11)—C(14)—C(13)	112·4 (9)	S(21)—C(24)—C(23)	112·5 (9)
C(13)—C(14)—C(15)	124·2 (12)	C(23)—C(24)—C(25)	124·3 (11)
S(11)—C(14)—C(15)	122·6 (9)	S(21)—C(24)—C(25)	122·7 (9)
O(11)—C(15)—C(14)	109·5 (10)	O(21)—C(25)—C(24)	109·0 (10)
C(14)—C(15)—C(16)	114·8 (10)	C(24)—C(25)—C(26)	113·3 (9)
O(11)—C(15)—C(16)	105·2 (9)	O(21)—C(25)—C(26)	106·0 (9)
O(12)—C(16)—C(15)	113·1 (10)	O(22)—C(26)—C(25)	113·1 (10)
C(15)—C(16)—C(17)	100·6 (10)	C(25)—C(26)—C(27)	101·1 (10)
O(12)—C(16)—C(17)	112·3 (10)	O(22)—C(26)—C(27)	110·4 (10)
O(13)—C(17)—C(16)	108·8 (10)	O(23)—C(27)—C(26)	110·5 (10)
C(16)—C(17)—C(18)	104·6 (10)	C(26)—C(27)—C(28)	102·5 (9)
O(13)—C(17)—C(18)	110·0 (10)	O(23)—C(27)—C(28)	109·6 (10)
O(11)—C(18)—C(17)	107·6 (10)	O(21)—C(28)—C(27)	106·6 (9)

matrix least-squares refinement (on F) for non-H atoms, isotropic for H atoms, $U_{\rm iso}$ tied to those of carrier atoms, $w = 1/\sigma^2(F_o)$.

Refinement produced convergence with R = 0·06, wR = 0·06, max. Δ/σ = 0·017, $\Delta\rho$ = ±0·5 e Å^{-3}, S = 2·62. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Calculation performed with the *XRAY76* system of crystallographic programs (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) and *PARST* (Nardelli, 1983).

Discussion. The final positional and equivalent isotropic thermal parameters for the non-H atoms are reported in Table 1.* Geometric data are listed in Table 2. There are two independent molecules in the unit cell, they are shown in Fig. 1.

The methylthiazolethione group is practically planar and the C(15) and C(25) atoms are −0·22 (1) and −0·20 (1) Å from the least-squares plane of the thiazole rings. The exocyclic C—S bond lengths are C(11)—S(12) = 1·688 (13) and C(21)—S(22) = 1·690 (13) Å. The hybridization of C(11), N(1), C(13), C(14), C(21), N(2), C(23) and C(24) is all sp^2. The endocyclic C(11)—S(11)—C(14) and C(21)—S(21)—C(24) angles are 91·3 and 90·7° respectively.

The furanose rings are not planar, as expected. In terms of ring-puckering coordinates (Cremer & Pople, 1975), the amplitude phase magnitudes are q = 0·37 (1) Å and φ = 113 (2)° in molecule 1 and sequence O(11)—C(18)—C(17)—C(16)—C(15), and q = 0·39 (1) Å and φ = 109 (2)° in molecule 2 and sequence O(21)—C(28)—C(27)—C(26)—C(25). The resulting conformations are both twist ${}^4_3T$. The glycoside bond lengths are 1·510 (15) and 1·519 (15) Å and the most important torsion angles are: S(11)—C(14)—C(15)—O(11) = 37 (1), S(21)—C(24)—C(25)—O(21) = 34 (1), C(13)—C(14)—C(15)—C(16) = 87 (2) and C(23)—C(24)—C(25)—C(26) = 88 (1)°. O(12) and O(13), and O(22) and O(23) lie on different sides of the furanose mean plane to C(14) and C(24), which confirms the β configuration. O(12) and O(22) are quasi-equatorial and O(13) and O(32) are axial.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52148 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

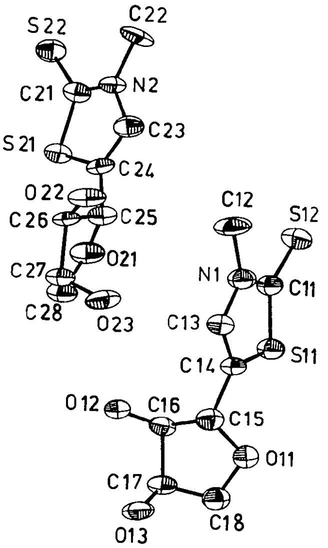

Fig. 1. View along **a** of the independent molecules in the asymmetric unit.

The endocyclic C—O bonds [C(15)—O(11) = 1·452 (15) and O(21)—C(28) = 1·469 (15) Å] are asymmetric, showing the anomeric effect (Jeffrey & French, 1978), a normal feature of this group. The average values of the C—C—C, C—C—O and C—O—C endocyclic angles are 102·3 (10), 106·4 (10) and 107·7 (9)° respectively.

The crystal structure is stabilized by van der Waals contacts with specific interactions between the O(12) and C(13) atoms of one molecule and the O(23) atom of another [O(12)···O(23) = 2·814 (10); O(23)···C(13) = 3·239 (16) Å].

We thank Professor Fernandez-Bolaños for supplying the crystals, and the Comision Asesora de Investigación Científica y Técnica for financial support.

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Acta Cryst. (1989). C**45**, 1979–1983

Structure of 7-Methyl-8-oxo-7,8-dihydroguanosine Monohydrate

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(*Received* 21 *December* 1988; *accepted* 6 *March* 1989)

Abstract. 2-Amino-7-methyl-9-(β-D-ribofuranosyl)-1*H*,9*H*-purine-6,8-dione monohydrate, $C_{11}H_{15}N_5O_6.H_2O$, $M_r = 331·29$, orthorhombic, $P2_12_12_1$, $a = 6·9811$ (6), $b = 9·808$ (2), $c = 20·61$ (2) Å, $V = 1411·1$ (13) Å^3, $Z = 4$, $D_x = 1·559$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1·54178$ Å, $\mu = 10·825$ cm^{-1}, $F(000) = 696$, $T = 295$ K, $R = 0·0296$ for 2472 reflections ($F \geq 4\sigma_F$). The sugar conformation and puckering parameters are ^2E (C2′-*endo*), $P = 161·8°$ and $\tau_m = 39·2°$. The side chain is *gauche–gauche*. The glycosidic torsion angle is 65·1 (2)° corresponding to the *syn* conformation which is stabilized by the O5′—H···N3 intramolecular hydrogen bond. The purine ring is nearly planar [r.m.s. deviation: 0·014 (2) Å]; the dihedral angle between the pyrimidine and imidazole rings is 1·14 (8)°.

Introduction. Certain ribonucleosides of guanine substituted at C8 have been shown to stimulate the immune system, and have been extensively studied as

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