to be *S*,*S*. This result agrees with the absolute stereochemistry of ethambutol dihydrochloride by unambiguous synthesis. (B. Blessington, personal communication).

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Structure of (+)-(*S*)-1,3-Dimethyl-6-oxiranyl-2,4-pyrimidinedione Showing Anti-ASFV Activity

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Abstract. $C_8H_{10}N_2O_3$, $M_r = 182{\cdot}18$, monoclinic, $P2_1$, $a = 6{\cdot}6405\ (7)$, $b = 7{\cdot}9493\ (9)$, $c = 8{\cdot}3662\ (9)$ Å, $\beta = 103{\cdot}07\ (1)^\circ$, $V = 430{\cdot}18\ (8)$ Å^3, $Z = 2$, $D_x = 1{\cdot}41$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}54184$ Å, $\mu = 0{\cdot}879$ mm^{-1}, $F(000) = 192$, $T = 298$ K, $R = 0{\cdot}037$ for 1247 reflections with $F_o \geq 4\sigma(F_o)$. The configuration at C7 is *S*. The pyrimidine-2,4-dione ring is nearly planar [r.m.s. deviation: 0·010 (8) Å] and is antiperiplanar with respect to the epoxide ring. This arrangement is stabilized by intermolecular C—H···O interactions.

Introduction. The group of analogues of nucleic acids, the 5- and 6-substituted uracils, have recently aroused considerable interest with regard to antiviral activity (Chu & Cutler, 1986; Mijasaka, Tanaka, Baba, Hayakawa, Walker, Balzarini & De Clercq, 1989). African Swine Fever Virus (ASFV) is the agent of an important disease of wild and domestic pigs; no effective means of eradication have been found and the control of the disease is still confined to recognition, quarantine, slaughter and decontamination procedures. Here we report on the crystal and molecular structure of the title compound, which shows remarkable anti-ASFV activity (Botta, Saladino, Gambacorta & Nicoletti, 1990; Botta, Nicoletti, Saladino, La Colla, Lamba & Fabrizi, 1991).

Experimental. Transparent prismatic crystals of the title compound were grown by slow concentration of an ethyl acetate solution with the addition of few

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Table 1. *Atomic coordinates of the non*-H *atoms and equivalent isotropic displacement coefficients* (Å^2)

$U_{\rm eq}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	$U_{\rm eq}$
O2	−0·6049 (3)	0·0335 (4)	−0·5974 (3)	0·0875 (8)
O3	0·1982 (2)	−0·2542 (3)	−0·2510 (2)	0·0742 (7)
O4	−0·1579 (4)	−0·2333 (4)	−0·8510 (2)	0·0967 (9)
N1	−0·3009 (3)	−0·0592	−0·4407 (2)	0·0519 (5)
N3	−0·3836 (3)	−0·1011 (3)	−0·7250 (2)	0·0602 (6)
C1	−0·3695 (4)	−0·0098 (5)	−0·2930 (2)	0·0750 (10)
C2	−0·4398 (3)	−0·0368 (4)	−0·5891 (3)	0·0578 (7)
C3	−0·5313 (6)	−0·0753 (5)	−0·8817 (4)	0·0878 (12)
C4	−0·1961 (4)	−0·1809 (4)	−0·7233 (3)	0·0650 (9)
C5	−0·0586 (4)	−0·1933 (3)	−0·5659 (3)	0·0596 (8)
C6	−0·1114 (3)	−0·1345 (3)	−0·4306 (3)	0·0507 (6)
C7	−0·0264 (3)	−0·1453 (4)	−0·2649 (3)	0·0605 (8)
C8	0·0364 (4)	−0·3002 (4)	−0·1723 (3)	0·0693 (9)

Table 2. *Bond lengths* (Å), *valence angles* (°) *and geometrical parameters of selected intermolecular interactions* (Å, °)

O2—C2	1·218 (3)	N3—C2	1·373 (3)
O3—C7	1·416 (3)	N3—C3	1·463 (4)
O3—C8	1·429 (3)	N3—C4	1·394 (4)
O4—C4	1·225 (4)	C4—C5	1·426 (3)
N1—C1	1·464 (4)	C5—C6	1·342 (4)
N1—C2	1·381 (3)	C6—C7	1·481 (3)
N1—C6	1·379 (3)	C7—C8	1·448 (4)

C7—O3—C8	61·2 (2)	N3—C4—C5	115·1 (2)
C2—N1—C6	121·7 (2)	O4—C4—C5	124·5 (3)
C1—N1—C6	121·3 (2)	C4—C5—C6	121·4 (2)
C1—N1—C2	116·9 (2)	N1—C6—C5	120·6 (2)
C3—N3—C4	119·2 (2)	C5—C6—C7	123·1 (2)
C2—N3—C4	124·8 (2)	N1—C6—C7	116·4 (2)
C2—N3—C3	115·9 (2)	O3—C7—C6	115·3 (2)
N1—C2—N3	116·5 (2)	C6—C7—C8	119·6 (2)
O2—C2—N3	122·2 (2)	O3—C7—O8	59·8 (2)
O2—C2—N1	121·3 (2)	O3—C8—C7	59·0 (2)
O4—C4—N3	120·4 (2)		

D—H···*A*	*D*···*A*	*D*—H	H···*A*	*D*—H···*A*
C7—H7*A*···O4$^{\rm i}$	3·471 (4)	0·96 (4)	2·59 (3)	153 (3)
C8—H8*A*···O2$^{\rm ii}$	3·343 (3)	1·01 (3)	2·51 (3)	140 (3)
C8—H8*B*···O4$^{\rm iii}$	3·278 (4)	0·98 (3)	2·58 (3)	129 (2)

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

drops of chloroform. Preliminary oscillation and Weissenberg photographs showed the space group to be $P2_1$. A crystal of dimensions 0·05 × 0·07 × 0·10 mm was used for the data collection on a Siemens *R3m/V* diffractometer, graphite-monochromated Cu $K\alpha$ radiation; $2\theta_{\rm max}$ = 140°, *hkl* range *h* −8/8, *k* −8/8, *l* −10/10, ω–2θ scan mode, scan width $(2 + 0{\cdot}15\tan\theta)$°, scan rate 1·22–14·65° min^{-1}, background count time half of the total scan time. Accurate unit-cell parameters determined by least-squares fit of the setting angle of 25 reflections with $81 \leq 2\theta \leq 90$°. No significant intensity variation for three check reflections (200, 002 and 021) monitored every hundred reflections. Data were corrected for Lorentz–polarization effects and absorption (φ scan, transmission coefficients min. 0·77, max. 0·94), no extinction correction. Merging equivalents gave 1320 unique reflections, $R_{\rm int}$ = 0·014, of which 1247 with $F_o \geq 4\sigma(F_o)$ were used for the structural analysis. The structure was solved by direct methods using *SHELXTL-Plus* (Sheldrick, 1989) and refined on F_o by full-matrix least-squares methods.

Subsequent difference Fourier syntheses showed all H atoms. These were included in the later refinement with $U_{\rm iso}$ values fixed equal to the $U_{\rm eq}$ values of their bearing atoms. Hamilton's (1965) *R*-value test (the ratio of the *wR* values is 1·002) and the refinement of the chiralty parameter η, defined by Rogers (1981) [η = 1·1 (6)], were used to establish the absolute configuration at a very high level of confidence. The final R = 0·037, wR = 0·051, S = 1·45 and max. shift/e.s.d. = 0·567. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = [\sigma(F_o) + 0{\cdot}0009F_o^2]^{-1}$. Final Fourier synthesis was featureless with $-0{\cdot}26 \leq \Delta\rho \leq 0{\cdot}22$ e Å^{-3}. The atomic scattering factors were from *International Tables for X-ray Crystallography* (1974, Vol. IV). *PARST* (Nardelli, 1983) was used for molecular-geometry calculations. Final fractional coordinates and equivalent *U* values of the non-H atoms are listed in Table 1.* Bond lengths, valence angles and

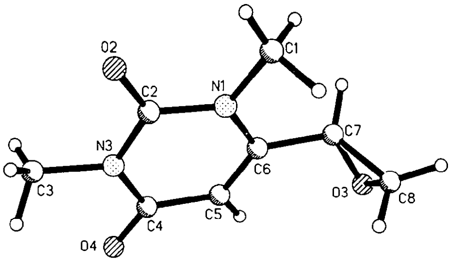

Fig. 1. Structure and conformation of the title compound with numbering of the atoms.

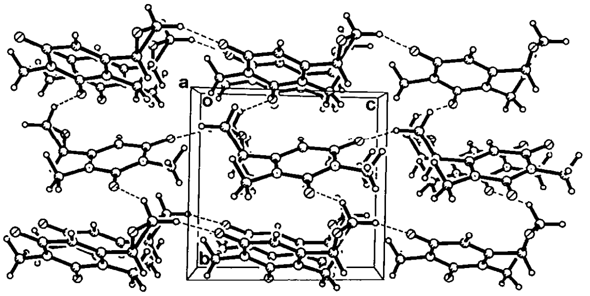

Fig. 2. The crystal packing of the molecules, projected along the *a* axis.

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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 54286 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

geometrical parameters of selected intermolecular interactions are given in Table 2. A perspective view of the title compound with the atom numbering is given in Fig. 1. The arrangement of the molecules in the crystal, viewed along the *a* axis, is shown in Fig. 2.

Discussion. Bond lengths and valence angles of the pyrimidine-2,4-dione moiety conform to those found for 6-[cinnamoyl(2-morpholinoethyl)amino]-1,3-dimethyluracil (Warin, Lobry, Bernier & Henichart, 1984) and for 1,3-dimethyluracil (Banerjee, Dattagupta, Saenger & Rabczenko, 1977). In the epoxide ring, the C7—O3 and C8—O3 bond lengths of 1·416 (3) and 1·429 (3) Å, respectively, are significantly shorter than the accepted value of 1·446 (14) Å for C_{sp^3}—O bonds in epoxides with any substitution (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The least-squares planes of the rings form a dihedral angle of 63·4 (1)°, showing an antiperiplanar arrangement, the N1—C6—C7—O3 torsion angle being 166·6 (2)°, which is stabilized by intermolecular C—H···O interactions (Taylor & Kennard, 1982) as listed in Table 2. The group of atoms defining the pyrimidine-2,4-dione ring deviate significantly from planarity, $\sum(d/\sigma)^2 = 141{\cdot}3$, and the value of χ^2 at 95% for three degrees of freedom is 7·81. The molecular arrangement, shown in Fig. 2, is governed by van der Waals interactions.

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Absolute Configuration of Seiricuprolide, a New Phytotoxin from *Seiridium cupressi*

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Abstract. $C_{14}H_{20}O_5$, $M_r = 268{\cdot}31$, monoclinic, $P2_1$, $a = 5{\cdot}0680\,(5)$, $b = 19{\cdot}519\,(2)$, $c = 7{\cdot}3968\,(8)$ Å, $\beta = 106{\cdot}03\,(1)°$, $V = 703{\cdot}3\,(1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}27$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}54184$ Å, $\mu = 7{\cdot}55$ cm^{-1}, $F(000) = 288$, $T = 298$ K, $R = 0{\cdot}029$ for 1286 reflections with $F_o \geq 4\sigma(F_o)$. The absolute configurations of C4, C5, C6, C7 and C13 are *R*, *S*, *R*, *S* and *S* respectively. The C1—C2 and C8—C9 double bonds have *E* and *Z* configurations respectively. The determination of the absolute configuration of the title compound also allows that of its *trans*-bromohydrin derivative to be established.

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