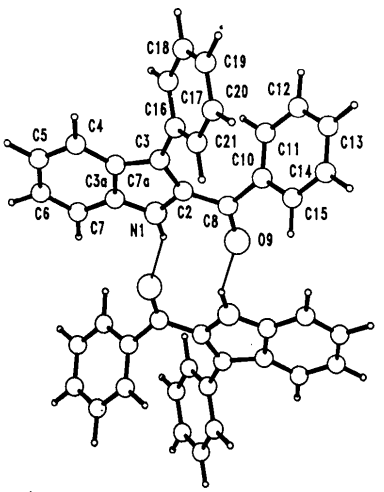

Fig. 1. View of the molecule, with atomic numbering, hydrogen-bonded to its centrosymmetric equivalent.

Table 2 lists bond lengths and angles for selected atoms and hydrogen-bond data. Fig. 1 shows the centrosymmetric arrangement of two hydrogen-bonded molecules, with atomic numbering of the unique molecule. Drawing by *PLUTO* (Motherwell & Clegg, 1978), geometrical calculations by *PARST* (Nardelli, 1983).

Related literature. The structure agrees very well with the X-ray structure of ethyl 3-phenyl-4,5,6,7-tetrahydroindole-2-carboxylate (Law, Lai, Sammes, Katritzky & Mak, 1984) regarding bond lengths and angles as well as hydrogen-bonding properties.

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The Structure of an Intermediate in the Synthesis of Avermectin B_{1a}

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Abstract. (±)-(2a*R**,4a*R**,5a*S**,6a*R**,6b*R**,6c*R**)-Octahydro-2a-methoxy-5a-methyl-4*H*-furo[2,3,4-*cd*]-oxireno[*g*]benzofuran-4-one, $C_{11}H_{14}O_5$, $M_r = 226{\cdot}23$, orthorhombic, $P2_12_12_1$ (spontaneous resolution), $a = 12{\cdot}705$ (2), $b = 5{\cdot}725$ (1), $c = 14{\cdot}617$ (2) Å, $V = 1063{\cdot}2$ (5) Å^3, $Z = 4$, $D_m = 1{\cdot}43$, $D_x = 1{\cdot}41$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}120$ mm^{-1}, $F(000) = 480$, $T = 293$ K, $R = 0{\cdot}043$ for 1690 observed unique reflections. The absolute configuration is not assigned. The C5—O1—C6 epoxide angle is 60·4 (1)° and the closest intermolecular contact (O1—C11) is 3·142 (3) Å. There are no unusual structural features.

Experimental. Colorless crystal of dimensions 0·2 × 0·5 × 0·6 mm. D_m by flotation in hexane/carbon tetrachloride. Syntex $P\bar{1}$ diffractometer with incident-beam monochromator, 15 centered reflections within $35 \le 2\theta \le 52°$ used for determining lattice parameters. Absorption ignored. $(\sin\theta/\lambda)_{max} = 1{\cdot}275$ Å^{-1}, range of *hkl*: $0 \le h \le 19$, $0 \le k \le 8$, $0 \le l \le 19$. Five standard reflections monitored every 200 reflections with random variation of 4·0% over data collection, θ–2θ scans of 2° min^{-1} in 2θ, 2256 independent reflections collected, 1690 observed [$F_o > 3\sigma(F_o)$]. Structure solved by direct methods with *MITHRIL* (Gilmore, 1983), *DIRDIF* (Beurskens, 1984), and Fourier procedures. All H atoms except H11*B* located in difference maps; constrained to idealized positions with isotropic $B = 1{\cdot}2 \times B$ of bonded atom. $\sum w(F_o - F_c)^2$ minimized where $w = 1/\sigma^2(F_o)$. 145 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, $\Delta/\sigma = 0{\cdot}00$, $R = 0{\cdot}043$, $wR = 0{\cdot}053$, $S = 1{\cdot}64$. Final difference electron density excursions between −0·15 and 0·24 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974) and programs used were those from the Texray Crystallographic Software Package (Molecular Structure Corporation, 1985). Atom num-

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Table 1. *Positional parameters and equivalent isotropic temperature factors (Hamilton, 1959)*

$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
O1	0·0766 (1)	0·1952 (2)	0·9793 (1)	3·08 (6)
O2	0·0676 (2)	0·2078 (3)	1·1776 (1)	4·19 (7)
O3	0·2875 (1)	−0·1327 (4)	0·9662 (1)	4·46 (8)
O4	0·2093 (1)	−0·3075 (3)	1·2345 (1)	3·53 (6)
O5	0·2554 (1)	−0·0663 (3)	1·1135 (1)	3·26 (6)
C1	0·0779 (1)	−0·1902 (3)	1·1260 (1)	2·48 (6)
C2	0·1221 (1)	−0·2673 (3)	1·0337 (1)	2·65 (7)
C3	0·1752 (1)	−0·1224 (4)	1·1815 (1)	2·73 (7)
C4	0·0518 (2)	−0·2257 (4)	0·9509 (1)	3·22 (8)
C5	−0·0143 (2)	0·1388 (4)	1·0352 (2)	3·07 (7)
C6	0·0040 (2)	0·0155 (4)	0·9492 (1)	2·94 (7)
C7	0·0104 (2)	0·0330 (4)	1·1268 (1)	3·09 (8)
C8	0·2287 (1)	−0·1484 (4)	1·0296 (1)	2·92 (7)
C9	−0·0610 (2)	0·0763 (5)	0·8667 (2)	4·2 (1)
C10	0·1453 (2)	0·0990 (5)	1·2322 (2)	3·8 (1)
C11	0·2892 (2)	−0·2541 (6)	1·3001 (2)	5·2 (1)

Table 2. *Bond lengths* (Å) *and bond angles* (°)

O1–C6	1·450 (2)	C1–C3	1·529 (3)
O1–C5	1·452 (3)	C1–C7	1·539 (3)
O2–C10	1·415 (3)	C2–C8	1·517 (3)
O2–C7	1·442 (3)	C2–C4	1·524 (3)
O3–C8	1·193 (2)	C3–C10	1·516 (3)
O4–C3	1·382 (3)	C4–C6	1·509 (3)
O4–C11	1·431 (3)	C5–C6	1·460 (3)
O5–C8	1·357 (3)	C5–C7	1·503 (3)
O5–C3	1·461 (2)	C6–C9	1·503 (3)
C1–C2	1·526 (3)		
C6–O1–C5	60·4 (1)	O1–C5–C6	59·7 (1)
C10–O2–C7	109·7 (2)	O1–C5–C7	115·2 (2)
C3–O4–C11	115·7 (2)	C6–C5–C7	122·6 (2)
C8–O5–C3	111·4 (1)	O1–C6–C5	59·8 (1)
C2–C1–C3	104·2 (1)	O1–C6–C9	115·4 (2)
C2–C1–C7	116·9 (2)	O1–C6–C4	112·9 (2)
C3–C1–C7	103·6 (2)	C5–C6–C9	119·4 (2)
C8–C2–C4	114·9 (2)	C5–C6–C4	119·5 (2)
C8–C2–C1	103·6 (1)	C9–C6–C4	116·5 (2)
C4–C2–C1	116·2 (2)	O2–C7–C5	106·5 (2)
O4–C3–O5	109·3 (2)	O2–C7–C1	107·4 (2)
O4–C3–C10	116·5 (2)	C5–C7–C1	116·4 (2)
O4–C3–C1	110·9 (2)	O3–C8–O5	121·2 (2)
O5–C3–C10	108·9 (2)	O3–C8–C2	128·6 (2)
O5–C3–C1	105·0 (1)	O5–C8–C2	110·1 (2)
C10–C3–C1	105·6 (2)	O2–C10–C3	105·5 (2)
C6–C4–C2	113·1 (2)		

bering for Tables 1 and 2, atom coordinates and bond distances and bond angles, follows that shown in Fig. 1.*

Related literature. The title compound (Figs. 1 and 2) spontaneously resolves during crystallization; it is an unexpected intermediate in the synthesis of the hexahydrobenzofuran segment of avermectin B_{1a} (Dantanarayana, 1987), an antihelminthic, antiparasitic agent that is isolated *via* solvent extraction of *Streptomyces avermitilis* (Albers-Schönberg *et al.*, 1981). For a structure of avermectin B_{1a} see Springer, Arison, Hirshfield & Hoogsteen (1981).

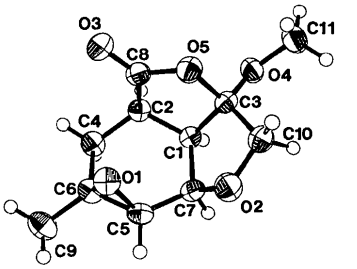

Fig. 1. A drawing of the molecule with thermal ellipsoids scaled at the 50% probability level.

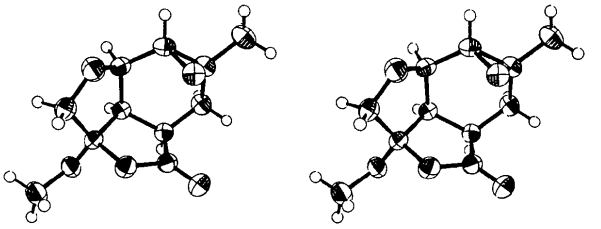

Fig. 2. A stereodrawing of the molecule.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and intermolecular distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44213 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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