Related literature. The 4a,9,9a,10-tetrahydro-9,10-*o*-benzenoanthracene-1,4-diones are intermediates in the synthesis of triptycenes (Bartlett, Cohen, Cotman, Kornblum, Landry & Lewis, 1950). The above compounds and the corresponding triptycenes have been the subjects of EPR investigations (Quast & Fuchsbauer, 1986; Bertsch & Reinhardt, 1986).

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Structure of 4-*O*-Ethylascofuranone

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Abstract. [*S*-(*E*,*E*)]-5-Chloro-4-ethoxy-2-hydroxy-6-methyl-3-[3-methyl-7-(tetrahydro-5,5-dimethyl-4-oxo-2-furanyl)-2,6-octadienyl]benzaldehyde, $C_{25}H_{33}ClO_5$, $M_r = 448{\cdot}99$, orthorhombic, $P2_12_12_1$, $a = 11{\cdot}724\ (1)$, $b = 34{\cdot}626\ (2)$, $c = 6{\cdot}122\ (1)$ Å, $V = 2485{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}200$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 16{\cdot}13$ cm^{-1}, $F(000) = 960$, $T = 298$ K, final $R = 0{\cdot}050$ for 2423 unique reflections [$F_o^2 > 2\sigma(F_o^2)$]. The title compound has a 'round' molecular conformation, turning at the middle of the sesquiterpenoid moiety. The intramolecular van der Waals contacts, observed at the center of the molecule, stabilize the conformation.

Experimental. Colorless prisms of 4-*O*-ethylascofuranone from *n*-hexane–acetone [1:1 (*v*/*v*)]. Crystal size 0·40 × 0·35 × 0·20 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 0·87–4·12° min^{-1} in θ, scan width $(0{\cdot}40 + 0{\cdot}14\tan\theta)°$. Range of indices, $0 \le h \le 14$, $0 \le k \le 43$, $0 \le l \le 7$ ($2\theta < 150°$). Lattice constants determined based on 25 2θ values ($26 < 2\theta < 55°$). Variation of standard <0·6%; 2958 unique reflections measured; 2423 observed reflections with $F_o^2 > 2\sigma(F_o^2)$. Systematic absences $h00$, h odd; $0k0$, k odd; $00l$, l odd. No corrections for absorption. Structure solved by direct methods with *MULTAN* (Main, Woolfson & Germain, 1971). Refined by full-matrix least squares. The locations of all H atoms were found from a difference Fourier map. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters ($B = 5{\cdot}0$ Å^2: fixed). $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 1011{\cdot}59$, $w = (1011{\cdot}59/F_o)^2$ for $F_o \ge 1011{\cdot}59$. Final $R = 0{\cdot}050$, $wR = 0{\cdot}049$, $S = 7{\cdot}23$ for 413 variables, secondary-extinction factor $g = 2{\cdot}50\ (4) \times 10^{-6}$ [$|F_o| = |F_c|/(1 + gIc)$]; $\Delta/\sigma < 0{\cdot}47$, largest peak in final ΔF map + 0·21 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of the title

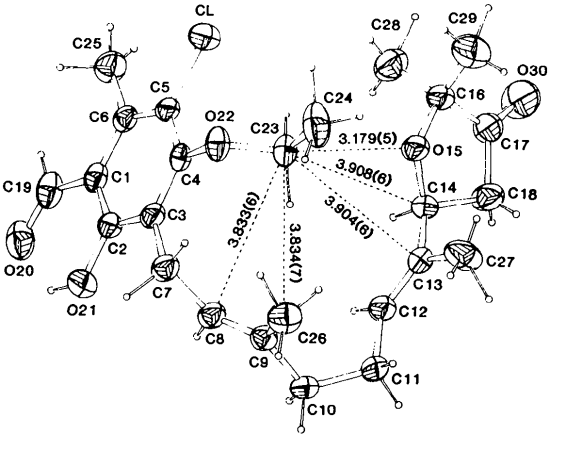

Fig. 1. A perspective view of the molecule with the numbering scheme.

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Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq}(Å²)
C(1)	0·7198 (3)	0·1045 (1)	−0·0425 (7)	4·32 (9)
C(2)	0·7068 (3)	0·1401 (1)	0·0617 (8)	4·46 (9)
C(3)	0·6463 (3)	0·1431 (1)	0·2587 (8)	4·23 (9)
C(4)	0·6007 (3)	0·1097 (1)	0·3425 (7)	3·93 (8)
C(5)	0·6118 (3)	0·0743 (1)	0·2397 (8)	4·06 (8)
C(6)	0·6715 (3)	0·0707 (1)	0·0430 (8)	4·29 (9)
C(7)	0·6360 (4)	0·1817 (1)	0·3735 (9)	5·1 (1)
C(8)	0·5423 (4)	0·2059 (1)	0·2756 (8)	4·60 (9)
C(9)	0·4582 (4)	0·2243 (1)	0·3808 (8)	4·37 (9)
C(10)	0·3735 (4)	0·2486 (1)	0·2550 (9)	4·9 (1)
C(11)	0·2468 (4)	0·2367 (1)	0·2811 (9)	5·2 (1)
C(12)	0·2237 (4)	0·1955 (1)	0·2184 (8)	4·7 (1)
C(13)	0·1616 (3)	0·1699 (1)	0·3254 (8)	4·50 (9)
C(14)	0·1418 (4)	0·1311 (1)	0·2279 (8)	4·6 (1)
O(15)	0·1715 (2)	0·10173 (7)	0·3841 (6)	5·21 (7)
C(16)	0·1183 (4)	0·0664 (1)	0·3317 (9)	5·2 (1)
C(17)	0·0185 (4)	0·0778 (1)	0·189 (1)	6·5 (1)
C(18)	0·0200 (4)	0·1206 (1)	0·164 (1)	6·4 (1)
C(19)	0·7857 (4)	0·1030 (2)	−0·2467 (9)	6·1 (1)
O(20)	0·8341 (3)	0·1316 (1)	−0·3234 (6)	7·32 (9)
O(21)	0·7518 (3)	0·17302 (8)	−0·0178 (6)	6·30 (8)
O(22)	0·5507 (2)	0·11069 (9)	0·5453 (5)	5·18 (7)
C(23)	0·4269 (4)	0·1139 (1)	0·5441 (9)	5·4 (1)
C(24)	0·3900 (5)	0·1084 (2)	0·775 (1)	8·8 (2)
C(25)	0·6859 (4)	0·0325 (1)	−0·070 (1)	6·4 (1)
C(26)	0·4422 (5)	0·2236 (1)	0·6221 (9)	6·3 (1)
C(27)	0·1035 (6)	0·1771 (1)	0·541 (1)	8·1 (2)
C(28)	0·1951 (5)	0·0399 (1)	0·201 (1)	7·6 (2)
C(29)	0·0797 (6)	0·0471 (2)	0·540 (1)	9·0 (2)
O(30)	−0·0496 (3)	0·0553 (1)	0·111 (1)	11·5 (1)
Cl	0·5527 (1)	0·03363 (3)	0·3619 (2)	6·08 (3)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)	1·396 (6)	C(10)–C(11)	1·550 (6)
C(1)–C(6)	1·400 (6)	C(11)–C(12)	1·502 (6)
C(1)–C(19)	1·470 (7)	C(12)–C(13)	1·321 (6)
C(2)–C(3)	1·403 (7)	C(13)–C(14)	1·490 (6)
C(2)–O(21)	1·349 (5)	C(13)–C(27)	1·504 (8)
C(3)–C(4)	1·374 (5)	C(14)–O(15)	1·438 (5)
C(3)–C(7)	1·514 (6)	C(14)–C(18)	1·525 (7)
C(4)–C(5)	1·387 (6)	O(15)–C(16)	1·410 (5)
C(4)–O(22)	1·373 (5)	C(16)–C(17)	1·512 (7)
C(5)–C(6)	1·398 (6)	C(16)–C(28)	1·511 (7)
C(5)–Cl	1·738 (4)	C(16)–C(29)	1·511 (9)
C(6)–C(25)	1·503 (6)	C(17)–C(18)	1·493 (6)
C(7)–C(8)	1·506 (6)	C(17)–O(30)	1·212 (6)
C(8)–C(9)	1·339 (6)	C(19)–O(20)	1·235 (6)
C(9)–C(10)	1·512 (6)	O(22)–C(23)	1·456 (5)
C(9)–C(26)	1·489 (7)	C(23)–C(24)	1·492 (8)
C(2)–C(1)–C(6)	121·4 (4)	C(9)–C(10)–C(11)	115·5 (4)
C(2)–C(1)–C(19)	118·4 (4)	C(10)–C(11)–C(12)	113·4 (4)
C(6)–C(1)–C(19)	120·1 (4)	C(11)–C(12)–C(13)	127·5 (5)
C(1)–C(2)–C(3)	121·0 (4)	C(12)–C(13)–C(14)	119·5 (4)
C(1)–C(2)–O(21)	122·7 (4)	C(12)–C(13)–C(27)	125·1 (4)
C(3)–C(2)–O(21)	116·3 (4)	C(14)–C(13)–C(27)	115·4 (4)
C(2)–C(3)–C(4)	117·0 (4)	C(13)–C(14)–O(15)	109·5 (4)
C(2)–C(3)–C(7)	120·4 (4)	C(13)–C(14)–C(18)	117·5 (4)
C(4)–C(3)–C(7)	122·5 (4)	O(15)–C(14)–C(18)	103·2 (3)
C(3)–C(4)–C(5)	122·6 (4)	C(14)–O(15)–C(16)	110·8 (4)
C(3)–C(4)–O(22)	119·0 (4)	O(15)–C(16)–C(17)	104·3 (3)
C(5)–C(4)–O(22)	118·1 (4)	O(15)–C(16)–C(28)	112·5 (4)
C(4)–C(5)–C(6)	121·1 (4)	O(15)–C(16)–C(29)	108·9 (5)
C(4)–C(5)–Cl	118·9 (3)	C(17)–C(16)–C(28)	108·4 (5)
C(6)–C(5)–Cl	120·0 (3)	C(17)–C(16)–C(29)	111·7 (4)
C(1)–C(6)–C(5)	116·8 (4)	C(28)–C(16)–C(29)	110·9 (4)
C(1)–C(6)–C(25)	121·2 (4)	C(16)–C(17)–C(18)	108·0 (4)
C(5)–C(6)–C(25)	122·0 (4)	C(16)–C(17)–O(30)	124·8 (4)
C(3)–C(7)–C(8)	111·3 (4)	C(18)–C(17)–O(30)	127·1 (5)
C(7)–C(8)–C(9)	127·6 (5)	C(14)–C(18)–C(17)	102·7 (4)
C(8)–C(9)–C(10)	120·2 (4)	C(1)–C(19)–O(20)	122·5 (5)
C(8)–C(9)–C(26)	124·2 (4)	C(4)–O(22)–C(23)	115·0 (3)
C(10)–C(9)–C(26)	115·6 (4)	O(22)–C(23)–C(24)	105·9 (4)

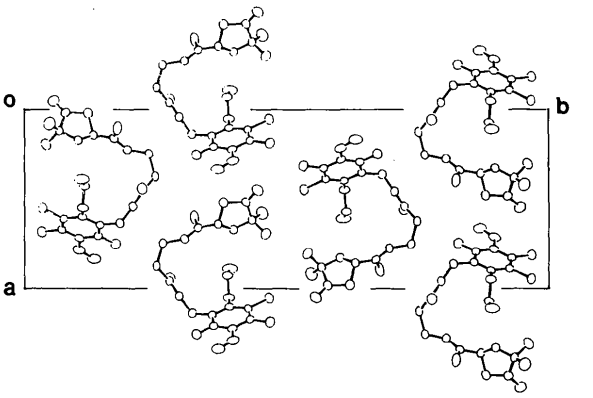

Fig. 2. Crystal structure projected along the *c* axis.

compound is shown in Fig. 1, and a projection of the crystal structure in Fig. 2. Positional parameters and equivalent values of the anisotropic temperature factors are given in Table 1, bond distances and angles are listed in Table 2.*

Related literature. Ascofuranone is an antibiotic (Sasaki, Okutomi, Hosokawa, Nawata & Ando, 1972) which possesses hypolipidemic (Sawada, Hosokawa, Okutomi & Ando, 1973) and antitumor activities (Magae, Hosokawa, Ando, Nagai & Tamura, 1982). (±)-Ascofuranone was successfully synthesized by Mori & Fujioka (1984). For the preparation of 4-*O*-ethylascofuranone and a preliminary report on the molecular structure see Ando, Sasaki, Hosokawa, Nawata & Iitaka (1975).

* Lists of anisotropic thermal parameters, H-atom coordinates, torsional angles, least-squares planes and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44473 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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