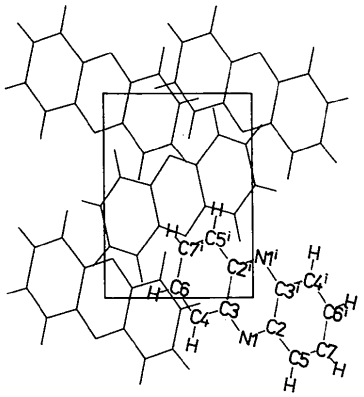

Fig. 1. A projection of the unit-cell content on the *ab* plane with the labelling of atoms.

largest residual electron density maximum is midway between C2 and C3^{i}. The second largest residual electron density maximum is less than 0·3 e Å^{-3}. Final fractional coordinates and equivalent isotropic temperature coefficients for non-H atoms are given in Table 1.* The atomic scattering factors used were those given in *SHELX*76. The molecular geometry is given in Table 2 with atom labelling shown in Fig. 1. The packing of the molecules in the unit cell is also given in Fig. 1. The figure was drawn with *PLUTO* (Motherwell & Clegg, 1978).

Related literature. The structure of phenazine was previously determined from photographic data (Glazer, 1970) with rather low accuracy ($R = 0{\cdot}10$) and not very precisely refined. Some of its TCNQ (7,7′,8,8′-tetracyano-*p*-quinodimethanide) derivatives are organic semiconductors (Fritchie, 1966; Morosin, 1975; Morosin, Plastas, Coleman & Stewart, 1978; Gundel, Sixl, Metzger, Heimer, Harms, Keller, Nöthe & Wehe, 1983; Endres, Keller, Moroni & Nöthe, 1980).

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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 53678 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of a 7,6-Lactone*

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Abstract. 9-Ethynyl-8,8-dimethyl-10-oxatricyclo-[7.2.2.0^{1,7}]tridec-6-en-11-one, $C_{16}H_{20}O_2$, $M_r = 244{\cdot}34$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}207$ (2), $b = 13{\cdot}199$ (1), $c = 16{\cdot}865$ (3) Å, $V = 1381{\cdot}9$ (7) Å^3, $Z = 4$, $D_m = 1{\cdot}16$ (3), $D_x = 1{\cdot}174$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}563$ mm^{-1}, $F(000) = 528$, $T = 298$ K, final $R = 0{\cdot}052$, $wR = 0{\cdot}057$ for 1134 reflections with $I > 2\sigma(I)$. All the three fused ring systems are in the boat conformation and the packing of the molecules is stabilized by van der Waals interactions.

Experimental. Needle shaped crystals from benzene, 0·30 × 0·40 × 0·20 mm, D_m measured by flotation. Enraf–Nonius CAD-4 single-crystal diffractometer, graphite monochromator, $\omega/2\theta$ scan, cell dimensions from 20 centred reflections, $30 \le 2\theta \le 60°$. Three check reflections for every 100 reflections, no significant change in the intensity of standard reflections. $0 \le h \le 6$, $0 \le k \le 14$, $0 \le l \le 18$, 1134 reflections

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Table 1. *Positional parameters of non-H atoms with e.s.d.'s*

	x	y	z	B(Å^2)
C1	0·6834 (6)	0·0709 (3)	0·7153 (2)	4·1 (1)
C2	0·7692 (8)	0·0664 (3)	0·6301 (2)	6·1 (1)
C3	0·6730 (10)	0·1388 (3)	0·5723 (2)	8·0 (1)
C4	0·7200 (10)	0·2455 (4)	0·5792 (3)	9·5 (2)
C5	0·8670 (1)	0·2775 (4)	0·6455 (2)	8·4 (1)
C6	0·7757 (8)	0·2578 (3)	0·7265 (2)	6·3 (1)
C7	0·6916 (7)	0·1727 (3)	0·7560 (2)	4·5 (1)
C8	0·5937 (7)	0·1719 (3)	0·8397 (2)	4·8 (1)
C9	0·5263 (6)	0·0614 (3)	0·8559 (2)	4·2 (1)
O10	0·3707 (4)	0·0320 (2)	0·7945 (1)	4·5 (1)
C11	0·4546 (6)	0·0339 (2)	0·7201 (2)	4·1 (1)
O12	0·3416 (5)	0·0038 (2)	0·6667 (1)	5·9 (1)
C13	0·8152 (6)	−0·0043 (3)	0·7685 (2)	5·0 (1)
C14	0·7130 (7)	−0·0133 (3)	0·8499 (2)	5·0 (1)
C15	0·4044 (7)	0·0495 (3)	0·9310 (2)	5·1 (1)
C16	0·3180 (9)	0·0373 (3)	0·9921 (2)	6·6 (1)
C17	0·3948 (9)	0·2398 (3)	0·8430 (2)	7·5 (1)
C18	0·7612 (9)	0·2063 (4)	0·9023 (2)	8·4 (1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(4/3)[a^{*2}B(1,1)+b^{*2}B(2,2)+c^{*2}B(3,3)]$.

Table 2. *Bond distances* (Å) *and bond angles* (°) *of non-H atoms with e.s.d.'s*

C1	C2	1·533 (4)		C8	C18	1·550 (6)	
C1	C13	1·568 (5)		C9	C8	1·542 (5)	
C2	C3	1·490 (6)		C9	C14	1·525 (5)	
C3	C4	1·443 (6)		O10	C9	1·469 (4)	
C5	C4	1·502 (7)		O10	C11	1·359 (3)	
C6	C5	1·503 (6)		C11	O12	1·209 (4)	
C7	C6	1·335 (5)		C11	C1	1·504 (5)	
C7	C8	1·538 (5)		C14	C13	1·517 (5)	
C7	C1	1·509 (5)		C15	C9	1·484 (4)	
C8	C17	1·527 (7)		C15	C16	1·173 (5)	
C11	C1	C13	104·9 (3)	C8	C9	C14	113·2 (3)
C11	C1	C7	107·2 (3)	C7	C8	C17	110·4 (3)
C11	C1	C2	111·5 (3)	C7	C8	C18	111·0 (3)
C7	C1	C13	106·6 (3)	C17	C8	C18	110·2 (3)
C7	C1	C2	116·6 (3)	C15	C9	C14	112·1 (3)
C13	C1	C2	109·3 (3)	O10	C9	C15	103·8 (3)
C1	C2	C3	116·6 (4)	O10	C9	C8	107·7 (2)
C2	C3	C4	119·4 (4)	O10	C9	C14	106·4 (2)
C5	C4	C3	117·3 (4)	C15	C9	C8	113·0 (3)
C6	C5	C4	113·5 (5)	C11	O10	C9	113·2 (3)
C7	C6	C5	129·2 (3)	O10	C11	O12	117·4 (3)
C8	C7	C1	113·5 (3)	O10	C11	C1	114·7 (3)
C8	C7	C6	120·1 (3)	O12	C11	C1	127·9 (3)
C1	C7	C6	126·4 (3)	C14	C13	C1	110·5 (3)
C9	C8	C7	106·1 (3)	C9	C14	C13	109·1 (3)
C9	C8	C17	109·2 (3)	C9	C15	C16	176·2 (4)
C9	C8	C18	109·7 (3)				

measured with $I > 2\sigma(I)$ used in the least-squares refinement, $2\theta_{max} = 120°$. Data corrected for Lorentz and polarization effects but not for absorption. Structure solved by direct methods, all H-atom positions from ΔF map, full-matrix least-squares refinement on F_o, anisotropic temperature factors for all non-H atoms, isotropic for H atoms. Final $R = 0{\cdot}052$, $wR = 0{\cdot}057$, $w = 1/[\sigma^2(F_o) + 0{\cdot}04F_o^2]$, $S = 1{\cdot}66$, final ΔF map featureless, $(\Delta/\sigma)_{max} = 0{\cdot}15$, final $\Delta\rho$ excursions $\pm 0{\cdot}40$ e Å^{-3}. Scattering factors from *SDP* package. All calculations performed using *SDP* (Frenz, 1978) on VAX 11/730 computer. Atomic positional parameters of non-H atoms are given in Table 1* and interatomic distances and angles in Table 2. A stereo diagram of the molecule (*PLUTO*, Motherwell & Clegg, 1978) is given in Fig. 1 and unit-cell packing down the *a* axis is shown in Fig. 2.

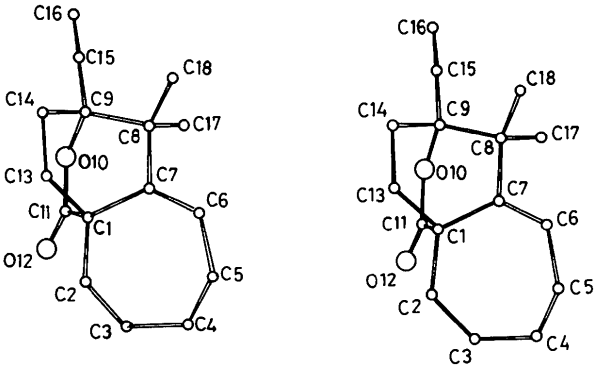

Fig. 1. Stereo diagram of the molecule.

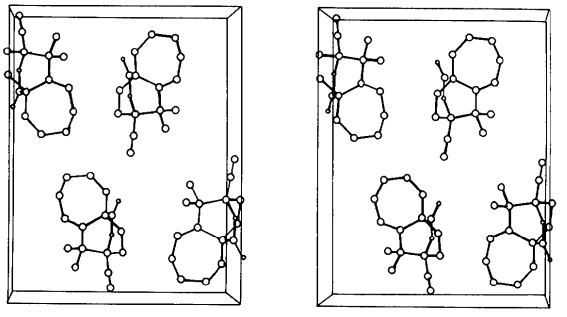

Fig. 2. Stereo packing diagram of the contents of the unit cell down **a**.

Related literature. The structural properties of 6,6-dimethyl-7-vinyl-8-oxatricyclo[5.2.2.0^{1,5}]undec-4-en-9-one have already been discussed (Geetha & Rajan, 1990).

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