Nova 4S computer and plots drawn on a Tektronix plotter with the *SHELXTL* system of programs.

Atomic coordinates are given in Table 1.* A perspective molecular drawing and the atom labelling are shown in Fig. 1. Bond distances, angles and selected torsion angles are listed in Table 2.

Related literature. The title compound was prepared as part of an investigation on the ultraviolet irradiation of *O*-methylmethoxyperezone (Barrera, Barrios & Walls, 1980). Its chemical structure was formulated from chemical and spectroscopic evidence (Barrios, Salazar, Diaz, Walls & Joseph-Nathan, 1986).

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* Lists of structure amplitudes, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51877 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 9,11-Dimethoxy-2,6,7-trimethyltetracyclo-[4.3.3.0^{1,5}.0^{7,11}]dodecane-8,10-dione*

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Abstract. $C_{17}H_{24}O_4$, $M_r = 292{\cdot}4$, orthorhombic, $P2_12_12_1$, $a = 7{\cdot}376$ (1), $b = 13{\cdot}612$ (6), $c = 15{\cdot}551$ (4) Å, $V = 1561$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}24$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}082$ mm^{-1}, $F(000) = 632$, $T = 293$ K, $R = 0{\cdot}061$ for 832 observed reflections. The stereochemistry of the title compound is C(5)—αH *trans* to C(6)—βCH$_3$, C(8)—βO(1) *trans* to C(9)—α(methoxy), C(10)—αO(3) *cis* to C(11)—α(methoxy) with a *cis, anti, anti* relationship of methyl groups at C(6), C(7); C(6), C(13); and C(7), C(13), respectively. The four- and five-membered rings adopt puckered [38·9 (5)°] and half-chair conformations, respectively. Both six-membered rings [C(1)—C(5)—C(6)—C(7)—C(8)—C(9) and C(1)—C(10)—C(11)—C(7)—C(8)—C(9)] exhibit a boat conformation. The four-membered ring has three long bonds [1·580 (11)–1·601 (10) Å] and one short bond at 1·532 (10) Å. A C—H···O intermolecular contact is present, C(16)···O(3)($-\frac{1}{2}+x, \frac{1}{2}-y, -z$) 3·25 (1) Å. The packing in the crystal is entirely due to van der Waals forces.

Experimental. The title compound was recrystallized from acetone–ethanol and gave colourless crystals, m.p. 427–428 K. Crystal size 0·15 × 0·32 × 0·32 mm. Nicolet *R*3 four-circle diffractometer. Unit-cell parameters by least-squares refinement from 25 machine-centred reflections with $4{\cdot}5 < 2\theta < 18{\cdot}5°$. 1204 unique reflections measured for an octant, $3 < 2\theta < 45°$, of which 832 with $I > 2{\cdot}5\sigma(I)$ were used in the analysis. Index range h 0→7, k 0→14, l 0→16, ω-scan mode and variable scan speed. Two standard reflections ($\bar{1}0\bar{3}$, $\bar{1}10$) monitored every 50 measurements; no significant variation. Lp correction, absorption ignored and $R_{int} = 0{\cdot}012$. Structure solved by direct methods using *SHELXTL5* (Sheldrick, 1985). Least-squares refinement of all non-H atoms with anisotropic thermal parameters; H atoms in calculated positions riding on the bonded C with a

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Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^3$)

$U_{eq} = (U_{11} \times U_{22} \times U_{33})^{1/3}$.

	x	y	z	U_{eq}
O(1)	6796 (7)	10722 (4)	−502 (3)	52 (2)
O(2)	8121 (7)	8744 (4)	71 (3)	49 (2)
O(3)	11308 (7)	8781 (4)	1395 (3)	56 (2)
O(4)	12437 (6)	10398 (4)	362 (3)	58 (2)
C(1)	8273 (9)	9451 (5)	1453 (4)	34 (2)
C(2)	7378 (10)	8717 (5)	2062 (5)	52 (3)
C(3)	5665 (12)	9278 (6)	2367 (5)	70 (4)
C(4)	5929 (10)	10369 (6)	2144 (4)	55 (3)
C(5)	7943 (9)	10427 (5)	1940 (4)	45 (3)
C(6)	8865 (11)	11298 (5)	1501 (4)	45 (3)
C(7)	9160 (10)	11044 (5)	509 (4)	40 (2)
C(8)	7644 (9)	10462 (5)	125 (4)	36 (2)
C(9)	7290 (9)	9505 (5)	575 (4)	38 (2)
C(10)	10255 (10)	9433 (5)	1231 (4)	37 (3)
C(11)	10866 (10)	10430 (6)	849 (4)	46 (3)
C(12)	10974 (10)	11138 (6)	1613 (4)	50 (3)
C(13)	6982 (12)	7702 (5)	1712 (5)	68 (3)
C(14)	8149 (12)	12284 (5)	1741 (5)	70 (4)
C(15)	9698 (11)	11910 (5)	−55 (5)	64 (3)
C(16)	7015 (14)	8410 (6)	−623 (5)	81 (4)
C(17)	12286 (11)	9798 (6)	−381 (5)	68 (3)

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

O(1)—C(8)	1·212 (8)	O(2)—C(9)	1·436 (8)
O(2)—C(16)	1·427 (10)	O(3)—C(10)	1·206 (9)
O(4)—C(11)	1·385 (9)	O(4)—C(17)	1·420 (9)
C(1)—C(2)	1·526 (19)	C(1)—C(5)	1·548 (10)
C(1)—C(9)	1·549 (9)	C(1)—C(10)	1·502 (10)
C(2)—C(3)	1·550 (12)	C(2)—C(13)	1·514 (11)
C(3)—C(4)	1·537 (11)	C(4)—C(5)	1·521 (10)
C(5)—C(6)	1·528 (10)	C(6)—C(7)	1·595 (9)
C(6)—C(12)	1·580 (11)	C(6)—C(14)	1·491 (11)
C(7)—C(8)	1·494 (10)	C(7)—C(11)	1·601 (10)
C(7)—C(15)	1·522 (10)	C(8)—C(9)	1·502 (19)
C(10)—C(11)	1·549 (11)	C(11)—C(12)	1·532 (10)

C(9)—O(2)—C(16)	113·5 (6)	C(11)—O(4)—C(17)	113·5 (6)
C(2)—C(1)—C(5)	101·0 (5)	C(2)—C(1)—C(9)	112·0 (6)
C(5)—C(1)—C(9)	108·5 (5)	C(2)—C(1)—C(10)	123·6 (6)
C(5)—C(1)—C(10)	106·2 (6)	C(9)—C(1)—C(10)	104·7 (5)
C(1)—C(2)—C(3)	102·7 (6)	C(1)—C(2)—C(13)	117·3 (6)
C(3)—C(2)—C(13)	113·7 (7)	C(2)—C(3)—C(4)	107·7 (6)
C(3)—C(4)—C(5)	102·7 (6)	C(1)—C(5)—C(4)	102·2 (6)
C(1)—C(5)—C(6)	112·2 (5)	C(4)—C(5)—C(6)	124·6 (6)
C(5)—C(6)—C(7)	109·0 (6)	C(5)—C(6)—C(12)	106·4 (6)
C(7)—C(6)—C(12)	86·8 (5)	C(5)—C(6)—C(14)	115·4 (6)
C(7)—C(6)—C(14)	119·0 (6)	C(12)—C(6)—C(14)	116·4 (6)
C(6)—C(7)—C(8)	113·5 (6)	C(6)—C(7)—C(11)	84·3 (5)
C(8)—C(7)—C(11)	116·3 (6)	C(6)—C(7)—C(15)	115·2 (6)
C(8)—C(7)—C(15)	112·0 (6)	C(11)—C(7)—C(15)	112·9 (6)
O(1)—C(8)—C(7)	123·6 (6)	O(1)—C(8)—C(9)	122·5 (6)
C(7)—C(8)—C(9)	113·9 (5)	O(2)—C(9)—C(1)	104·3 (5)
O(2)—C(9)—C(8)	107·3 (5)	C(1)—C(9)—C(8)	111·7 (5)
O(3)—C(10)—C(1)	126·1 (7)	O(3)—C(10)—C(11)	122·6 (7)
C(1)—C(10)—C(11)	110·9 (6)	O(4)—C(11)—C(7)	119·6 (6)
O(4)—C(11)—C(10)	115·2 (6)	C(7)—C(11)—C(10)	110·9 (6)
O(4)—C(11)—C(12)	113·6 (6)	C(7)—C(11)—C(12)	88·2 (5)
C(10)—C(11)—C(12)	105·6 (6)	C(6)—C(12)—C(11)	87·1 (5)

fixed isotropic temperature factor, $U = 0{\cdot}06$ Å^2. $\sum w(\Delta F)^2$ minimized, $w = [\sigma^2(F_o) + 0{\cdot}001(F_o)^2]^{-1}$, where σ is standard deviation of observed amplitudes, based on counting statistics; isotropic extinction parameter $X = 0{\cdot}0012$. In the last cycle $(\Delta/\sigma)_{max} = 0{\cdot}54$; $\Delta\rho$ from $-0{\cdot}24$ to $0{\cdot}22$ e Å^{-3}, $S = 1{\cdot}17$; final $R = 0{\cdot}061$, $R_w = 0{\cdot}058$ and $wR = 0{\cdot}063$. Scattering factors from *International Tables for X-ray Crystallography* (1974). All computations performed on a Nova 4S computer and plots drawn on a Tektronix plotter with the *SHELXTL* system of programs.

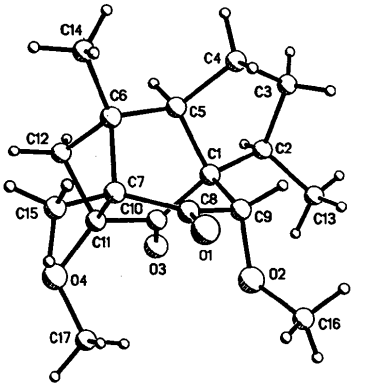

Fig. 1. The molecular structure of the title compound with atom numbering.

Atomic coordinates are given in Table 1.* A perspective molecular drawing and the atom labelling are shown in Fig. 1. Bond distances and angles are listed in Table 2.

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