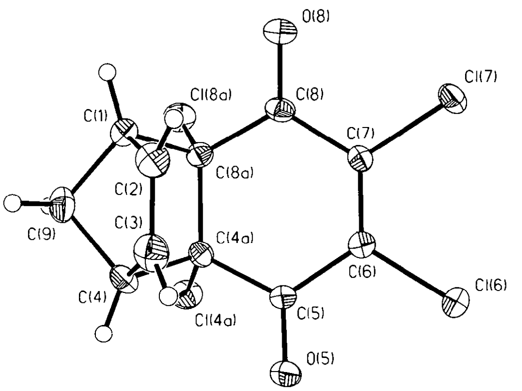

Fig. 1. Drawing of the title compound. Thermal ellipsoids are drawn at the 25% probability level. H atoms are represented by spheres of arbitrary size.

Crystallography (1974). Table 1 lists atomic positional parameters and U_{eq} values, while Table 2 gives bond lengths and bond angles. Fig. 1 is a drawing of the title compound.*

Related literature. The reaction between cyclopentadienes and 1,4-benzoquinones has been used extensively to prepare methanonaphthalenes (Cookson, Crundwell, Hill & Hudec, 1964), which are photochemically converted into precursors for the preparation of cage compounds and related species (Marchand, LaRoe, Sharma, Suri & Reddy, 1986; Goverdhan, Srikrishna, Reddy & Nair, 1981). The crystal structure of 4a,7-dibromo-1,4,4a,8a-tetrahydro-1,4-methanonaphthalene-5,8-dione has been reported (Syed, Umrigar, Griffin & Stevens, 1984).

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* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51049 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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6,7-Dimethoxy-2,2-dimethyl-4-chromanone

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Abstract. $C_{13}H_{16}O_4$, $M_r = 236{\cdot}27$, orthorhombic, *Pccn*, $a = 18{\cdot}230\,(4)$, $b = 15{\cdot}950\,(3)$, $c = 8{\cdot}410\,(2)$ Å, $V = 2445{\cdot}3\,(3)$ Å^3, $Z = 8$, $D_x = 1{\cdot}28$ g cm^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $\mu = 7{\cdot}9$ cm^{-1}, $F(000) = 1008$, $T = 293$ K, final $R = 0{\cdot}046$ for 997 observed reflections. The methoxy groups are coplanar with the aromatic ring. The dihydropyronic ring shows a distorted sofa conformation.

Experimental. The title compound (Fig. 1) was purchased from the Aldrich Chemical Company. Crystals grown from acetone. Data collected on an Enraf–Nonius CAD-4 diffractometer, graphite monochromator. The crystal had dimensions 0·1 × 0·2 × 0·2 mm. Cell parameters measured on the diffractometer using 25 reflections in the 2θ range 20–40°. Range of indices $0 \le h \le 20$, $0 \le k \le 17$, $0 \le l \le 9$ ($\theta < 60°$). Three standards 151, 333, 325, measured after every 200 reflections, showed a variation of 0·9%. No absorption corrections. Lorentz and polarization corrections. 1405 unique reflections measured. 997 observed reflections with $I > 3{\cdot}0\sigma(I)$. Direct methods (*MULTAN*11/82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) used for structure determination. H atoms located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement (on *F*) for non-H atoms, isotropic for H atoms. $\sum w(F_o - F_c)^2$ minimized. $wR = 0{\cdot}046$, max. $\Delta/\sigma = 0{\cdot}92$. Max. peak height in the final difference Fourier map $0{\cdot}49$ e Å^{-3}, $S = 1{\cdot}5$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius *SDP* (Frenz, 1984).

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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*

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

	x	y	z	B_{eq}(Å^2)
O(1)	0·4562 (2)	0·0756 (2)	0·1810 (4)	4·0 (1)
O(2)	0·3297 (2)	0·0931 (3)	0·5823 (4)	5·3 (1)
O(3)	0·6714 (2)	0·1432 (2)	0·4769 (4)	4·3 (1)
O(4)	0·5984 (2)	0·1600 (2)	0·7382 (4)	4·1 (1)
C(2)	0·3777 (2)	0·0925 (3)	0·1642 (6)	3·6 (1)
C(3)	0·3369 (2)	0·0561 (3)	0·3068 (6)	3·6 (1)
C(4)	0·3683 (2)	0·0866 (3)	0·4645 (6)	3·5 (1)
C(5)	0·4837 (2)	0·1248 (3)	0·6048 (5)	3·1 (1)
C(6)	0·5576 (2)	0·1376 (3)	0·6074 (5)	3·2 (1)
C(7)	0·5988 (2)	0·1282 (3)	0·4640 (6)	3·4 (1)
C(8)	0·5627 (2)	0·1071 (3)	0·3259 (6)	3·4 (1)
C(9)	0·4873 (2)	0·0962 (3)	0·3256 (5)	3·2 (1)
C(10)	0·4462 (2)	0·1038 (3)	0·4629 (5)	3·1 (1)
C(11)	0·3564 (3)	0·0440 (4)	0·0131 (6)	5·1 (1)
C(12)	0·3642 (3)	0·1849 (3)	0·1479 (7)	5·3 (1)
C(13)	0·7140 (3)	0·1349 (4)	0·3343 (7)	5·6 (1)
C(14)	0·5580 (3)	0·1674 (3)	0·8839 (6)	4·5 (1)

Table 2. *Bond distances* (Å), *bond angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

O(1)–C(2)	1·461 (5)	C(2)–C(12)	1·501 (7)
O(1)–C(9)	1·380 (5)	C(3)–C(4)	1·523 (7)
O(2)–C(4)	1·218 (6)	C(4)–C(10)	1·447 (6)
O(3)–C(7)	1·349 (5)	C(5)–C(6)	1·361 (6)
O(3)–C(13)	1·433 (6)	C(5)–C(10)	1·414 (6)
O(4)–C(6)	1·374 (5)	C(6)–C(7)	1·428 (6)
O(4)–C(14)	1·434 (6)	C(7)–C(8)	1·375 (6)
C(2)–C(3)	1·524 (7)	C(8)–C(9)	1·384 (6)
C(2)–C(11)	1·536 (7)	C(9)–C(10)	1·381 (6)
C(2)–O(1)–C(9)	116·3 (3)	O(4)–C(6)–C(5)	126·0 (4)
C(7)–O(3)–C(13)	116·6 (4)	O(4)–C(6)–C(7)	114·6 (3)
C(6)–O(4)–C(14)	115·2 (3)	C(5)–C(6)–C(7)	119·4 (4)
O(1)–C(2)–C(3)	109·3 (4)	O(3)–C(7)–C(6)	115·5 (4)
O(1)–C(2)–C(11)	103·5 (4)	O(3)–C(7)–C(8)	125·5 (4)
O(1)–C(2)–C(12)	110·5 (4)	C(6)–C(7)–C(8)	119·1 (4)
C(3)–C(2)–C(11)	109·5 (4)	C(7)–C(8)–C(9)	120·5 (4)
C(3)–C(2)–C(12)	111·5 (4)	O(1)–C(9)–C(8)	116·1 (4)
C(11)–C(2)–C(12)	112·2 (4)	O(1)–C(9)–C(10)	122·2 (3)
C(2)–C(3)–C(4)	112·3 (4)	C(8)–C(9)–C(10)	121·7 (4)
O(2)–C(4)–C(3)	121·2 (4)	C(4)–C(10)–C(5)	120·8 (4)
O(2)–C(4)–C(10)	123·9 (4)	C(4)–C(10)–C(9)	121·6 (4)
C(3)–C(4)–C(10)	114·9 (4)	C(5)–C(10)–C(9)	117·6 (4)
C(6)–C(5)–C(10)	121·8 (4)		
C(2)–O(1)–C(9)–C(10)	22·1 (6)	C(13)–O(3)–C(7)–C(8)	−1·1 (7)
C(14)–O(4)–C(6)–C(5)	2·0 (6)	O(1)–C(2)–C(3)–C(4)	53·7 (5)
C(2)–C(3)–C(4)–O(2)	150·7 (4)	C(2)–C(3)–C(4)–C(10)	−31·2 (5)
O(2)–C(4)–C(10)–C(9)	−179·3 (5)	C(3)–C(4)–C(10)–C(9)	2·7 (6)
O(1)–C(9)–C(10)–C(4)	3·1 (7)		

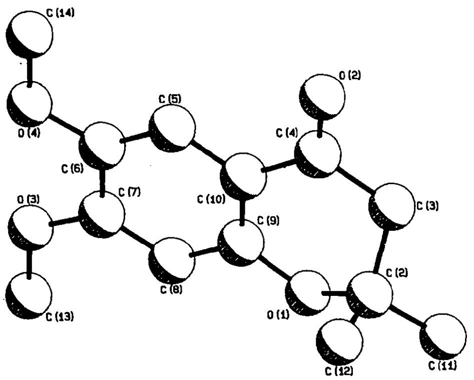

Fig. 1. Numbering of atoms and conformation of the molecule.

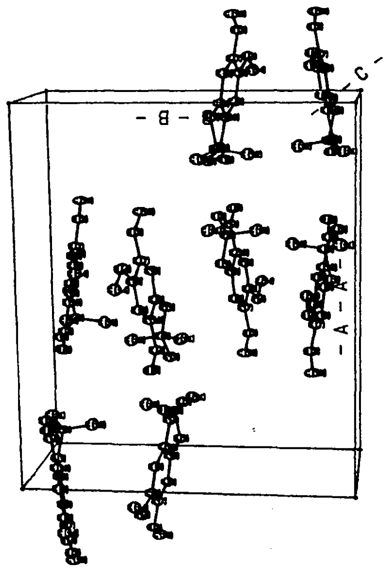

Fig. 2. Molecular packing diagram.

Atomic parameters are given in Table 1;* bond distances, bond angles and relevant torsion angles are presented in Table 2. The atomic numbering is shown in Fig. 1 and the packing diagram in Fig. 2.

Related literature. The distorted sofa conformation of the dihydropyronic ring in the title compound is more pronounced than in a related structure (Dolmazon & Gelin, 1985). The coplanar conformation of the *O*-dimethoxy groups occurs most frequently in solution (Schaefer & Laatikainen, 1983) and in the crystalline state (Caillet, 1982).

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