Related literature. For the structure of two closely related pentaazabicyclononanes formed by a condensation reaction from the title compound see George (1987) and George & Gilardi (1987).

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Structure of (–)-Savinin

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Abstract. 4-Piperonyl-3-piperonylidenetetrahydrofuran-2-one, $C_{20}H_{16}O_6$, $M_r = 352$, monoclinic, $C2/c$, $a = 14{\cdot}997\ (2)$, $b = 10{\cdot}875\ (3)$, $c = 20{\cdot}708\ (7)$ Å, $\beta = 108{\cdot}79\ (2)°$, $V = 3197\ (21)$ Å^3, $Z = 8$, $D_m = 1{\cdot}46$, $D_x = 1{\cdot}45$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 1{\cdot}0$ cm^{-1}, $F(000) = 1472$, $T = 298$ K, final $R = 0{\cdot}049$ for 1111 observed reflections. The structure contains three planar parts: two (3,4-methylenedioxy)benzyl(idene) moieties (*A* and *B*) and a tetrahydrofuran-2-one ring (*C*). The dihedral angles between the planes are *A*&*B*: 17·01 (1), *A*&*C*: 10·59 (2), *B*&*C*: 26·15 (2)°. The bond distances and angles are normal.

Table 1. *Atomic fractional coordinates and equivalent isotropic temperature factors* (Å^2)

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

	x	y	z	B_{eq}
C1	0·3679 (3)	0·8977 (4)	0·3044 (2)	3·2 (2)
C2	0·3379 (3)	0·8981 (3)	0·3624 (2)	3·6 (2)
C3	0·3214 (3)	0·7876 (4)	0·3867 (2)	3·5 (2)
C4	0·3330 (3)	0·6772 (3)	0·3570 (2)	3·7 (2)
C5	0·3621 (3)	0·6722 (4)	0·3014 (2)	4·2 (3)
C6	0·3796 (3)	0·7859 (3)	0·2756 (2)	3·6 (2)
C7	0·3831 (3)	1·0106 (3)	0·2710 (2)	3·5 (2)
C8	0·3822 (3)	1·1279 (3)	0·2890 (2)	3·1 (2)
C9	0·3924 (3)	1·2244 (4)	0·2409 (2)	3·7 (2)
O10	0·3831 (2)	1·3368 (2)	0·2673 (1)	4·6 (2)
C11	0·3620 (3)	1·3259 (4)	0·3307 (2)	4·4 (3)
C12	0·3719 (3)	1·1888 (3)	0·3519 (2)	3·1 (2)
C13	0·4547 (3)	1·1650 (4)	0·4177 (2)	3·5 (2)
C14	0·4305 (3)	1·2117 (4)	0·4794 (2)	3·4 (2)
C15	0·4534 (3)	1·3329 (4)	0·5015 (2)	3·7 (2)
C16	0·4251 (3)	1·3726 (4)	0·5542 (2)	3·4 (2)
C17	0·3770 (3)	1·3002 (4)	0·5855 (2)	3·9 (3)
C18	0·3553 (4)	1·1812 (4)	0·5661 (2)	6·1 (4)
C19	0·3822 (3)	1·1379 (4)	0·5116 (2)	4·8 (3)
O9	0·4031 (2)	1·2156 (3)	0·1863 (1)	4·9 (2)
O3	0·2932 (2)	0·7661 (2)	0·4426 (1)	5·0 (2)
O4	0·3108 (2)	0·5820 (2)	0·3929 (1)	5·2 (2)
O16	0·4400 (2)	1·4878 (2)	0·5851 (1)	5·1 (2)
O17	0·3569 (2)	1·3667 (3)	0·6364 (1)	5·8 (2)
C20	0·2740 (3)	0·6372 (4)	0·4429 (2)	5·1 (3)
C30	0·4010 (3)	1·4820 (4)	0·6392 (2)	4·9 (3)

Experimental. The compound was extracted from an acetone solution of *Calocedrus formosana* Florin.

Crystal 0·15 × 0·25 × 0·25 mm. CAD-4 diffractometer. Unit cell: 25 reflections, 2θ range 19·72 to 26·54°. D_m by flotation (*n*-hexane/CCl_4). $2\theta_{max} = 50°$.

Table 2. *Bond lengths* (Å) *and bond angles* (°) *of* $C_{20}H_{16}O_6$

C1	C2	1·411 (5)	C1	C6	1·390 (5)		
C1	C7	1·463 (5)	C2	C3	1·356 (5)		
C3	C4	1·386 (5)	C3	O3	1·374 (4)		
C4	C5	1·358 (5)	C4	O4	1·377 (4)		
C5	C6	1·404 (5)	C7	C8	1·331 (5)		
C8	C9	1·488 (5)	C8	C12	1·513 (4)		
C9	O10	1·365 (4)	C9	O9	1·195 (4)		
O10	C11	1·450 (4)	C11	C12	1·549 (5)		
C12	C13	1·541 (5)	C13	C14	1·524 (5)		
C14	C15	1·402 (5)	C14	C19	1·388 (5)		
C15	C16	1·362 (5)	C16	C17	1·364 (5)		
C16	O16	1·391 (4)	C17	C18	1·363 (5)		
C17	O17	1·389 (4)	C18	C19	1·396 (5)		
O3	C20	1·432 (4)	O4	C20	1·450 (4)		
O16	C30	1·423 (4)	O17	C30	1·410 (5)		
C2	C1	C6	119·1 (3)	C2	C1	C7	122·8 (3)
C6	C1	C7	118·0 (3)	C1	C2	C3	117·3 (3)
C2	C3	C4	122·6 (3)	C2	C3	O3	127·3 (3)
C4	C3	O3	110·1 (3)	C3	C4	C5	122·2 (3)
C3	C4	O4	108·9 (3)	C5	C4	O4	128·9 (3)
C4	C5	C6	115·9 (3)	C1	C6	C5	122·8 (3)
C1	C7	C8	130·9 (3)	C7	C8	C9	118·4 (3)
C7	C8	C12	132·3 (3)	C9	C8	C12	109·2 (3)
C8	C9	O10	108·5 (3)	C8	C9	O9	130·5 (3)
O10	C9	O9	120·9 (3)	C9	O10	C11	111·7 (2)
O10	C11	C12	107·8 (2)	C8	C12	C11	101·8 (2)
C8	C12	C13	114·2 (3)	C11	C12	C13	112·8 (3)
C12	C13	C14	110·1 (3)	C13	C14	C15	119·2 (3)
C13	C14	C19	120·9 (3)	C15	C14	C19	119·8 (3)
C14	C15	C16	116·9 (3)	C15	C16	C17	123·1 (3)
C15	C16	O16	127·4 (3)	C17	C16	O16	109·5 (3)
C16	C17	C18	121·4 (3)	C16	C17	O17	109·6 (3)
C18	C17	O17	129·0 (3)	C17	C18	C19	117·0 (3)
C14	C19	C18	121·7 (3)	C3	O3	C20	106·7 (2)
C4	O4	C20	106·8 (2)	C16	O16	C30	106·0 (2)
C17	O17	C30	106·3 (2)	O3	C20	O4	106·2 (2)
O16	C30	O17	108·3 (3)				

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Ranges of h, k, l: 0 to 17, 0 to 12, −24 to 24, respectively. Three standard reflections monitored every half an hour: variation on $I < 3\%$. No correction for absorption. 3617 unique reflections, 1111 observed with $I > 2\sigma(I)$. $R = 4{\cdot}86\%$, $wR = 2{\cdot}90\%$, $S = 1{\cdot}72$. Weighting scheme from counting statistics. The structure solution was attempted with direct methods both in $C2/c$ and Cc using the *MULTAN* program and solved in Cc with 339 highest E's, 93 smallest E's and 4486 $\sum_2$ relationships. The space group was then changed to $C2/c$ owing to the correlation of the two molecules in the asymmetric unit. $\sum w(\Delta F)^2$ minimized. H atoms found in difference Fourier map after isotropic refinement and then refined. $(\Delta/\sigma)_{max} = 0{\cdot}87$. Peaks in final difference Fourier map $< \pm 0{\cdot}18$ e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Computing programs: NRCC *SDP* PDP-11 package (Gabe & Lee, 1981), *MULTAN* and *ORTEP* from Enraf–Nonius (1979) *SDP*.

Atomic parameters are given in Table 1,* bond distances and angles in Table 2. A drawing of the molecule is shown in Fig. 1.

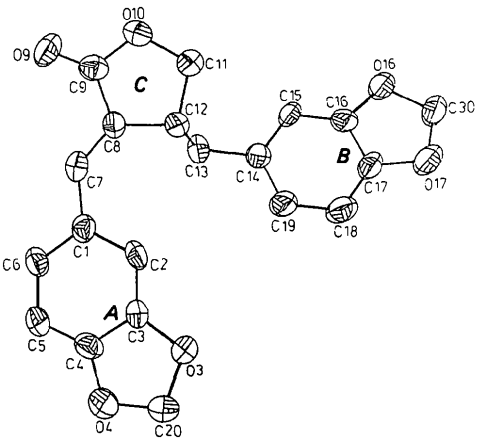

Fig. 1. *ORTEP* drawing of the molecule with 50% probability thermal ellipsoids.

Related literature. The bond distances and angles of the (3,4-methylenedioxy)benzyl(idene) moieties are quite similar to those of piperine (Grynpas & Lindley, 1975) and other derivatives (Herbstein, Schwotzer, Addae-Mensah, Torto & Woode, 1981; Begley, Crombie, Havard & Reynolds, 1977; Desiraju, Kamala, Kumari & Sarma, 1984).

* Lists of anisotropic thermal parameters, structure factors and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43679 (26 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 (+)-Calocedrin

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Abstract. 5-Hydroxy-4-piperonyl-3-piperonylidene-tetrahydrofuran-2-one, $C_{20}H_{16}O_7$, $M_r = 368$, monoclinic, $P2_1/c$, $a = 10{\cdot}974$ (2), $b = 21{\cdot}045$ (4), $c = 7{\cdot}325$ (2) Å, $\beta = 92{\cdot}03$ (2)°, $V = 1690$ (2) Å^3, $Z = 4$, $D_m = 1{\cdot}43$, $D_x = 1{\cdot}45$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1{\cdot}0$ cm^{-1}, $F(000) = 768$, $T = 298$ K, final $R = 0{\cdot}045$ for 1503 observed reflections. The structure contains three planar parts as in (–)-savinin [Wang, Cheng, Jan & Cheng (1987). *Acta Cryst.* C**43**, 1005–1006]: two (3,4-methylenedioxy)benzyl(idene) moieties (A and B) and a 5-hydroxytetrahydrofuran-2-one ring (C). The dihedral angles between them are $A\&B$: 8·00 (2), $A\&C$: 7·77 (2), $B\&C$: 13·88 (1)°. The compound can be reduced to (+)-savinin. There is intermolecular hydrogen bonding through the hydroxyl H atom and the ketone O atom, with an O···O distance of 2·721 (6) Å.

Experimental. This is a new compound isolated from the wood of *Calocedrus formosana*. It was charac-

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