The angle at O, 107·5 (2)°, is markedly smaller than that in $(Ph_3C)_2O$, 127·9 (1)°, which was ascribed to repulsive interactions between the two Ph_3C groups (Glidewell & Liles, 1978). A similar substantial reduction in interbond angle at O has been observed on going from $(Me_3Si)_2O$ (Csákvári, Wagner, Gömöry, Mijlhoff, Rozsondai & Hargittai, 1976) to $(Me_3Si)_2O_2$ (Käss, Oberhammer, Brandes & Blaschette, 1977): in this case also the wider angle in the oxo compound can be ascribed to steric factors.

The angle between the two COO planes is 180°; such a large dihedral angle occurs only rarely in peroxo compounds. In the simplest peroxide, H_2O_2, the dihedral angle in the solid state is 90·2 (6)° (Busing & Levy, 1965), but the barrier to rotation about the O—O bond is very small, being 4·62 kJ mol^{-1} towards the *trans* conformation and 29·4 kJ mol^{-1} towards the *cis* (Hunt, Leacock, Peters & Hecht, 1965). However, marked deviations from a dihedral angle of ca 90° usually occur only as a consequence of either hydrogen bonding or steric repulsion (Table 4), although the value of 180° in $M_2S_2O_8$ (M = NH_4 or Cs) (Zachariasen & Mooney, 1934) has no obvious interpretation.

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The *meso* Condensation Dimer from 2-(3-Bromopropyl)-6-hydroxy-2-methyl-1-indanone

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Abstract. $C_{26}H_{28}O_4$, M_r = 404·5, triclinic, $P\bar{1}$, a = 6·04 (1), b = 8·73 (2), c = 10·65 (4) Å, α = 99·90 (3), β = 95·28 (3), γ = 69·33 (3)° from diffractometer measurements (Mo $K\bar{\alpha}$ radiation). V = 516 Å^3, Z = 1, D_c = 1·296 Mg m^{-3}, $F(000)$ = 216, μ = 0·049 mm^{-1}. The molecule was shown to be the *meso* isomer.

Introduction. The title compound was recrystallized from chloroform.

Weissenberg and precession photographs indicated a triclinic space group. Data were collected for 0–6*kl*

with θ_{max} = 27·5° on a Stoe STADI-2 diffractometer (graphite-monochromated Mo $K\bar{\alpha}$ radiation). This gave 2175 data of which 1843 unique reflexions with $I > 3\sigma(I)$ were used in subsequent calculations. Lorentz and polarization corrections (but none for extinction or absorption) were applied, and the data were scaled by a Wilson plot. The structure was solved by direct methods with *SHELX* 76 (Sheldrick, 1976), which was used for all calculations. Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Weighted full-matrix least-

Table 1. *Fractional atomic coordinates* $\times 10^4$ *with e.s.d.'s in parentheses*

	x	y	z
C(1)	3546 (2)	7456 (1)	9389 (1)
C(2)	1387 (2)	7580 (2)	8718 (1)
C(3)	1218 (2)	6404 (2)	7711 (1)
C(4)	3229 (2)	5044 (2)	7348 (1)
C(5)	3476 (2)	3536 (2)	6356 (1)
C(6)	6114 (2)	2431 (2)	6450 (1)
C(7)	7188 (2)	3392 (1)	7538 (1)
C(8)	5343 (2)	4966 (1)	8006 (1)
C(9)	5574 (2)	6153 (2)	9013 (1)
C(10)	6614 (2)	651 (2)	6716 (1)
C(11)	4965 (2)	356 (2)	7584 (1)
C(12)	4406 (2)	1502 (2)	8836 (1)
C(13)	7411 (3)	2337 (2)	5250 (1)
O(1)	6556 (1)	1340 (1)	9586 (1)
O(2)	9237 (1)	2925 (1)	7917 (1)
H(1)	50 (24)	8524 (17)	9022 (14)
H(2)	−298 (25)	6485 (19)	7270 (14)
H(3)	2335 (27)	2966 (18)	6548 (15)
H(4)	3087 (24)	3837 (19)	5453 (14)
H(5)	7056 (22)	6039 (16)	9429 (13)
H(6)	8284 (24)	278 (17)	7031 (13)
H(7)	6616 (24)	−73 (18)	5891 (14)
H(8)	3445 (23)	431 (17)	7125 (13)
H(9)	5644 (26)	−789 (19)	7770 (14)
H(10)	3359 (22)	1212 (16)	9320 (13)
H(11)	3735 (21)	2655 (16)	8696 (12)
H(12)	6715 (28)	1840 (21)	4509 (16)
H(13)	9098 (29)	1659 (21)	5336 (17)
H(14)	7222 (29)	3479 (21)	5092 (16)

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

C(1)–C(2)	1·408 (2)	C(6)–C(10)	1·546 (2)
C(1)–C(9)	1·381 (1)	C(6)–C(13)	1·535 (2)
C(2)–C(3)	1·374 (2)	C(7)–C(8)	1·472 (1)
C(3)–C(4)	1·396 (2)	C(7)–O(2)	1·214 (1)
C(4)–C(5)	1·511 (2)	C(8)–C(9)	1·392 (2)
C(4)–C(8)	1·386 (2)	C(10)–C(11)	1·532 (2)
C(5)–C(6)	1·551 (2)	C(11)–C(12)	1·509 (2)
C(6)–C(7)	1·543 (2)	C(12)–O(1)	1·437 (1)

C(9)–C(1)–C(2)	119·8 (1)	C(13)–C(6)–C(10)	108·6 (1)
C(3)–C(2)–C(1)	121·7 (1)	C(8)–C(7)–C(6)	108·9 (1)
C(4)–C(3)–C(2)	119·4 (1)	O(2)–C(7)–C(6)	124·9 (1)
C(5)–C(4)–C(3)	129·7 (1)	O(2)–C(7)–C(8)	126·2 (1)
C(8)–C(4)–C(3)	117·9 (1)	C(7)–C(8)–C(4)	109·2 (1)
C(8)–C(4)–C(5)	112·3 (1)	C(9)–C(8)–C(4)	123·9 (1)
C(6)–C(5)–C(4)	105·1 (1)	C(9)–C(8)–C(7)	126·7 (1)
C(7)–C(6)–C(5)	104·4 (1)	C(8)–C(9)–C(1)	117·2 (1)
C(10)–C(6)–C(5)	116·3 (1)	C(11)–C(10)–C(6)	118·7 (1)
C(10)–C(6)–C(7)	110·3 (1)	C(12)–C(11)–C(10)	116·7 (1)
C(13)–C(6)–C(5)	111·2 (1)	O(1)–C(12)–C(11)	109·4 (1)
C(13)–C(6)–C(7)	105·5 (1)		

squares refinement (including isotropic H atoms) converged at $R = 0\cdot040$ for 1843 observed reflexions $(R = \sum \|F_o\| - |F_c\|/\sum |F_o|)$; $R_w = 0\cdot047$ $\{R_w = \sum (\|F_o\| - |F_c\| w^{1/2})/\sum (|F_o| w^{1/2})$, $w = 5\cdot025/[\sigma^2(F_o) + 0\cdot000316F_o^2]\}$. In the final cycle all shifts in parameters were less than their e.s.d.'s. Positional parameters

are given in Table 1, bond distances and angles in Table 2.*

Discussion. In the attempted synthesis of aconane alkaloids by cyclization of (I) (Chatterjee, Misra, Mukherjee & Dutta, 1975) an unexpected product was obtained, which was assigned structure (IIa) on the basis of NMR, mass spectral and analytical data. On treatment of this substance with Zn dust and subsequent work-up a second substance was obtained which had essentially identical spectral and analytical data but nevertheless was a different compound as shown by TLC (Chatterjee & Watt, 1976). Both substances were recrystallized and shown to be pure by TLC, and structure analyses of both were undertaken.

(I)
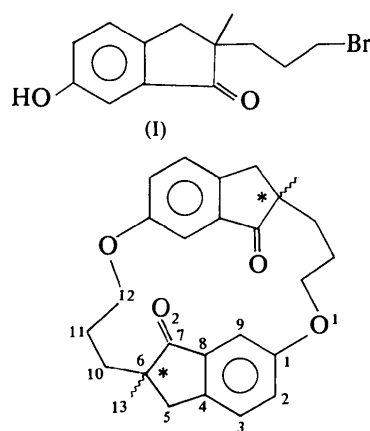
(II) (a) Indeterminate stereochemistry.
    (b) R,S centrosymmetric *meso* isomer.

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34041 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
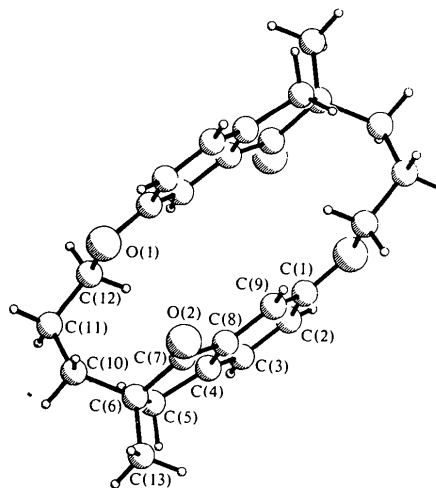

Fig. 1. General view of the molecule.

Table 3. *Torsion angles* (°)

C(2)–C(1)–O(1)–C(12')	176·0
C(9)–C(1)–O(1)–C(12')	−2·4
C(1')–O(1')–C(12)–C(11)	165·5
O(1')–C(12)–C(11)–C(10)	−61·0
C(12)–C(11)–C(10)–C(6)	−48·3
C(11)–C(10)–C(6)–C(5)	−34·9
C(11)–C(10)–C(6)–C(7)	83·6

The compound described in this paper was isolated from the reaction mixture after dimerization of (I). It is shown to be (IIb), *i.e.* the *meso* isomer, where the two quaternary C atoms have opposite chiralities. The conformation is centrosymmetric, and similar to *ansa* molecules since the anisolic group O(1)–C(12) is essentially planar with the benzene ring (Fig. 1). The

C(1)–O(1)–C(12)–C(11) torsion angle (Table 3) is nearly *trans*, so that the *ansa* bridging is effectively a three-carbon system C(6)–C(10)–C(11).

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The Racemic Condensation Dimer from 2-(3-Bromopropyl)-6-hydroxy-2-methyl-1-indanone

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Abstract. $C_{26}H_{28}O_4$, $M_r = 404·5$, monoclinic, $P2_1/c$, $a = 7·93$ (2), $b = 19·47$ (6), $c = 13·98$ (5) Å, $\beta = 101·55$ (3)° from diffractometer measurements (Mo $K\bar{a}$ radiation). $V = 2115$ Å^3, $Z = 4$, $D_c = 1·279$ Mg m^{-3}, $F(000) = 864$, $\mu = 0·048$ mm^{-1}. The substance was shown to be the racemic diastereoisomer.

Introduction. Systematic absences (from precession photographs) $h0l$, l odd and $0k0$, k odd indicated space group $P2_1/c$. Data were collected for 0–6kl with $\theta_{max} = 22·5°$ on a Stoe STADI-2 diffractometer (graphite-monochromated Mo $K\bar{a}$ radiation). This gave 2425 data of which 1493 unique reflexions with $I > 3\sigma(I)$ were used in subsequent calculations. Lorentz and polarization corrections (but none for extinction or absorption) were applied, and the data were scaled by a Wilson plot. The structure was solved by direct methods with *SHELX* 76 (Sheldrick, 1976), which was used for all calculations. Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Weighted full-matrix least-squares refinement (including isotropic H atoms) converged at $R = 0·048$ for 1493 observed reflexions $(R = \sum ||F_o| - |F_c||/\sum |F_o|)$; $R_w = 0·044$ $\{R_w = \sum (||F_o| - |F_c|| w^{1/2})/\sum (|F_o| w^{1/2})$, $w = 3·7157/[\sigma^2(F_o) + 0·0002F_o^2]\}$. In the final cycle all shifts in parameters

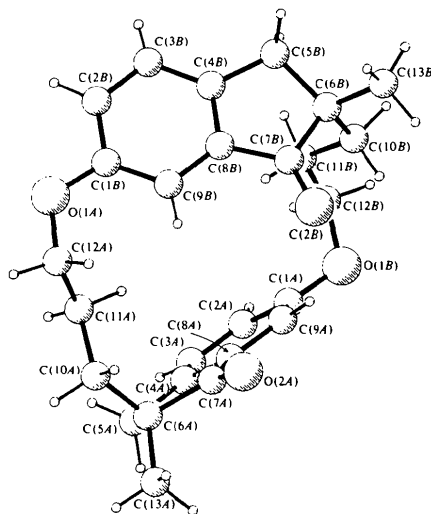were less than their e.s.d.'s. Positional parameters are given in Table 1, bond distances and angles in Table 2.*

Fig. 1. General view of the molecule.