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6-Benzyl-6,10-dimethyl-11-oxatricyclo[5.3.1.0^{5,10}]undecan-1-ol, $C_{19}H_{26}O_2$

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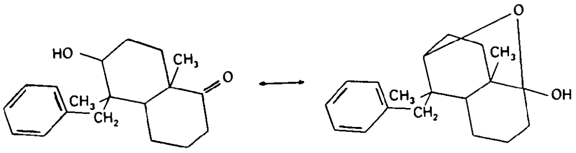
Abstract. $M_r = 286{\cdot}42$, monoclinic, $P2_1/n$, $a = 15{\cdot}181\,(1)$, $b = 11{\cdot}677\,(1)$, $c = 18{\cdot}296\,(1)$ Å, $\beta = 91{\cdot}37\,(1)°$, $V = 3242{\cdot}4\,(7)$ Å^3, $Z = 8$, $D_x = 1{\cdot}17$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}40$ cm^{-1}, $F(000) = 1248$, $T = 293$ K. Final $R = 0{\cdot}052$ for 3103 unique observed reflections. The asymmetric unit consists of two enantiomorphic molecules which form a pseudo-centrosymmetric dimer about $x = 0{\cdot}26$, $y = -0{\cdot}03$, $z = 0{\cdot}48$ by two hydrogen bonds, involving the hydroxyl groups both as donor and acceptor. The geometries of the two independent molecules correspond within 2σ. The tricycloundecane skeleton has four six-membered rings, three of which have a nearly ideal-boat conformation, whereas the remaining ring adopts a distorted-chair conformation.

Introduction. Studies on the intermediates in the syntheses of physiologically important diterpenoids are at present under way and one of the isolated products with molecular formula $C_{19}H_{26}O_2$ was tentatively proposed as 5-benzyl-6-hydroxy-5,9-dimethyl-l-oxodecalin:



PROPOSED STRUCTURE OBSERVED STRUCTURE

In order to prove its structure and elucidate its stereochemistry an X-ray analysis was undertaken.

Experimental. Crystals obtained from Dr A. Sharma, Department of Organic Chemistry, Indian Association for the Cultivation of Science, Calcutta; needle-shaped crystal, 0·3 × 0·05 × 0·04 mm. Nonius CAD-4 diffractometer, θ–2θ scan, Zr-filtered Mo $K\alpha$ radiation. Lattice parameters refined by a least-squares procedure utilizing 15 reflections. Systematic absences in $h0l$ plane for $h + l = 2n + 1$ and along $0k0$ for $k = 2n + 1$ indicated space group $P2_1/n$. In one quadrant of reflection sphere (h −19–19, k 0–14, l 0–23) a set of 7425 independent intensities were measured up to $2\theta_{\max} = 55°$ of which 3103 above $2{\cdot}5\sigma(I)$ level were considered observed. Two periodically measured standard reflections showed no significant change in intensity during data collection. No correction for absorption applied. Structure solved by direct methods using *MULTAN*80 (Main, 1980) and subsequent Fourier methods. Usual sequence of isotropic and anisotropic full-matrix least-squares refinements on F was followed, after which all H atoms could be located by difference syntheses; inclusion in the refinement of the positional parameters of the H atoms, except those of the methyl groups which were refined in the rigid-body constraint model with fixed C—H distances and H—C—H angles, with a constant isotropic thermal parameter of 0·05 Å^2 resulted in final $R = 0{\cdot}052$, $R_w = 0{\cdot}054$; $w = 2{\cdot}011/[\sigma^2(F_o) + 0{\cdot}000634\,F_o^2]$. Refinement of an isotropic extinction parameter in the last cycles gave $g = 4{\cdot}0 \times 10^{-8}$. Average and maximum shift/error ratios for non-H-atom parameters 0·03 and 0·18 respectively, for H 0·07 and 0·32 respectively. Maximum and minimum densities in final difference synthesis 0·20 and −0·23 e Å^{-3}. Scattering factors for non-H atoms taken from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965). All calculations performed with *SHELX* (Sheldrick, 1976).

Discussion. The atomic coordinates and equivalent isotropic temperature factors are listed in Table 1.*

The results of the analysis do not agree with the proposed formula. Evidently a ring closure has occurred under elimination of water between the hydrated oxo function and the hydroxyl group leading to the

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* Lists of structure factors, anisotropic thermal parameters, coordinates of methyl-group H atoms, and valence and torsion angles involving H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38515 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Positional and equivalent isotropic thermal parameters* (× 10^2) *for* $C_{19}H_{26}O_2$

Least-squares-derived standard deviations of the least significant figures are given in parentheses in all tables.

	Molecule (I)				Molecule (II)			
	x	y	z	U^{*}_{eq} (Å^2)	x	y	z	U^{*}_{eq} (Å^2)
C(1)	0·1882 (2)	0·1321 (4)	0·7435 (2)	6·3 (1)	0·3705 (2)	−0·1834 (3)	0·2328 (2)	6·1 (1)
C(2)	0·1480 (2)	0·0263 (4)	0·7335 (2)	6·6 (1)	0·4086 (3)	−0·0802 (4)	0·2528 (2)	7·0 (2)
C(3)	0·0801 (3)	−0·0090 (4)	0·7768 (2)	8·1 (2)	0·4905 (3)	−0·0482 (4)	0·2284 (3)	8·6 (2)
C(4)	0·0513 (3)	0·0609 (6)	0·8312 (2)	9·8 (2)	0·5352 (3)	−0·1191 (6)	0·1840 (3)	9·9 (2)
C(5)	0·0894 (3)	0·1611 (6)	0·8430 (2)	11·1 (2)	0·4995 (3)	−0·2199 (5)	0·1622 (2)	9·5 (2)
C(6)	0·1582 (3)	0·1987 (5)	0·8003 (2)	9·4 (2)	0·4173 (3)	−0·2525 (4)	0·1861 (2)	8·0 (2)
C(7)	0·2635 (2)	0·1694 (4)	0·6972 (2)	6·3 (1)	0·2807 (2)	−0·2170 (3)	0·2591 (2)	6·0 (1)
C(8)	0·3076 (2)	0·2547 (2)	0·5012 (2)	4·6 (1)	0·1793 (2)	−0·3086 (3)	0·4396 (2)	5·0 (1)
C(9)	0·3051 (2)	0·1256 (2)	0·4909 (2)	4·3 (1)	0·1824 (2)	−0·1799 (3)	0·4527 (2)	5·6 (1)
O(10)	0·2429 (1)	0·0779 (2)	0·5420 (1)	4·28 (6)	0·2575 (1)	−0·1343 (2)	0·4146 (1)	4·94 (7)
C(11)	0·1852 (2)	0·1627 (3)	0·5726 (2)	4·4 (1)	0·3208 (2)	−0·2205 (3)	0·3939 (2)	4·6 (1)
C(12)	0·2397 (2)	0·2365 (3)	0·6264 (2)	4·7 (1)	0·2799 (2)	−0·2888 (3)	0·3305 (2)	4·7 (1)
C(13)	0·3241 (2)	0·2730 (3)	0·5837 (2)	4·9 (1)	0·1852 (2)	−0·3225 (3)	0·3555 (2)	5·3 (1)
C(14)	0·4121 (2)	0·2174 (3)	0·6081 (2)	5·6 (1)	0·1070 (2)	−0·2607 (4)	0·3176 (2)	7·6 (2)
C(15)	0·4235 (2)	0·0932 (3)	0·5861 (2)	5·8 (1)	0·0929 (3)	−0·1375 (4)	0·3406 (3)	8·6 (2)
C(16)	0·3926 (2)	0·0671 (3)	0·5086 (2)	5·3 (1)	0·1034 (3)	−0·1174 (3)	0·4216 (3)	7·5 (2)
C(17)	0·2173 (2)	0·3023 (3)	0·4771 (2)	5·4 (1)	0·2603 (2)	−0·3609 (3)	0·4783 (2)	6·0 (1)
C(18)	0·1444 (2)	0·2325 (3)	0·5110 (2)	4·9 (1)	0·3424 (2)	−0·2936 (3)	0·4603 (2)	5·8 (1)
C(19)	0·3779 (2)	0·3121 (3)	0·4550 (2)	6·3 (1)	0·0974 (2)	−0·3664 (3)	0·4698 (2)	6·8 (1)
O(20)	0·2759 (1)	0·1011 (2)	0·4187 (1)	5·52 (8)	0·1934 (2)	−0·1592 (2)	0·5281 (1)	7·7 (1)
C(21)	0·1870 (2)	0·3433 (3)	0·6483 (2)	6·5 (1)	0·3324 (2)	−0·3989 (3)	0·3168 (2)	6·8 (1)
H(2)†	0·1697 (18)	−0·0223 (23)	0·6956 (15)		0·3792 (19)	−0·0330 (25)	0·2827 (15	
H(3)	0·0560 (18)	−0·0814 (26)	0·7682 (15)		0·5087 (19)	0·0221 (26)	0·2451 (16)	
H(4)	0·0065 (18)	0·0317 (23)	0·8616 (15)		0·5851 (19)	−0·0895 (24)	0·1661 (15)	
H(5)	0·0724 (18)	0·2126 (24)	0·8769 (16)		0·5209 (19)	−0·2729 (25)	0·1340 (16)	
H(6)	0·1789 (19)	0·2725 (25)	0·8039 (16)		0·3935 (19)	−0·3180 (25)	0·1719 (16)	
H(7*a*)	0·3037 (17)	0·2185 (24)	0·7266 (14)		0·2487 (17)	−0·2612 (23)	0·2205 (15)	
H(7*b*)	0·2934 (18)	0·0990 (24)	0·6834 (14)		0·2499 (17)	−0·1447 (25)	0·2698 (14)	
H(11)	0·1403 (17)	0·1190 (22)	0·5965 (14)		0·3738 (17)	−0·1771 (23)	0·3792 (14)	
H(13)	0·3273 (17)	0·3501 (24)	0·5902 (15)		0·1779 (17)	−0·4030 (25)	0·3467 (15)	
H(14*a*)	0·4217 (17)	0·2223 (23)	0·6618 (15)		0·1124 (18)	−0·2675 (24)	0·2663 (15)	
H(14*b*)	0·4554 (18)	0·2611 (23)	0·5879 (14)		0·0536 (18)	−0·3010 (23)	0·3320 (14)	
H(15*a*)	0·4849 (18)	0·0691 (23)	0·5954 (14)		0·1372 (18)	−0·0856 (24)	0·3185 (14)	
H(15*b*)	0·3920 (18)	0·0402 (24)	0·6190 (15)		0·0420 (19)	−0·1164 (24)	0·3264 (15)	
H(16*a*)	0·3852 (17)	−0·0155 (25)	0·5007 (14)		0·1124 (17)	−0·0336 (26)	0·4334 (15)	
H(16*b*)	0·4349 (18)	0·0914 (22)	0·4706 (15)		0·0520 (18)	−0·1418 (23)	0·4473 (15)	
H(17*a*)	0·2117 (17)	0·3076 (23)	0·4248 (15)		0·2478 (17)	−0·3595 (24)	0·5310 (16)	
H(17*b*)	0·2147 (17)	0·3788 (25)	0·4919 (15)		0·2670 (17)	−0·4390 (25)	0·4634 (15)	
H(18*a*)	0·1161 (17)	0·1806 (24)	0·4782 (15)		0·3599 (17)	−0·2400 (24)	0·5001 (15)	
H(18*b*)	0·0950 (17)	0·2839 (23)	0·5289 (14)		0·3925 (18)	−0·3371 (24)	0·4493 (14)	
H(20)	0·2749 (19)	0·0298 (25)	0·4161 (16)		0·2078 (19)	−0·0928 (26)	0·5338 (16)	

* $U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta)$.

† All H atoms were given fixed isotropic temperature factors $U = 0{\cdot}05$ Å^2. The H atoms of the methyl groups, H(19*a*)–H(19*c*) and H(21*a*)–H(21*c*), were refined in the rigid-body constraint model with C—H distances of 1·08 Å and H—C—H angles of 109·5°. Their coordinates have been deposited.

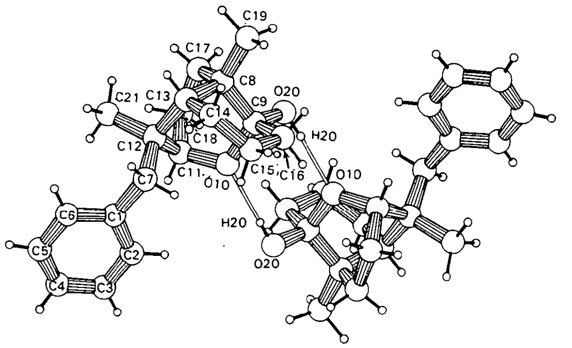

Fig. 1. The conformations of molecule (I) and molecule (II) in the hydrogen-bonded dimer. The atom numbering is given for molecule (I).

formation of a strained tricycloundecane derivative with the same molecular formula as that of the proposed structure.

In the asymmetric unit there are two independent molecules which are related by a pseudo-center of symmetry. By averaging the coordinates of corresponding non-H atoms of these two molecules the pseudo-center is calculated at $x = 0{\cdot}261$ (19), $y = -0{\cdot}027$ (13), $z = 0{\cdot}480$ (14), with a range of x, y and z values of 0·235 to 0·295, −0·022 to −0·031 and 0·454 to 0·508, respectively. The antipodal molecules are tightly bonded to form a pseudo-centrosymmetric dimer by two hydrogen bonds, in which the hydroxyl groups mutually act as donor and acceptor. The pseudosymmetry is clearly demonstrated by the presence of a large maximum in the Patterson map at $u = 0{\cdot}503$, $v = 0{\cdot}059$, $w = 0{\cdot}037$ with a height 23% that of the origin maximum. The atomic numbering and a view of the independent molecules are shown in Fig. 1.

The distances, angles and torsion angles (which are listed in Table 2) of the two independent molecules shown an excellent correspondence, the average deviation of these quantities being 0·006 Å, 0·4° and 0·7°, respectively. The phenyl rings in both molecules are planar and the angle between them is 16·2 (2)°. The conformation of the benzyl group relative to C(7)–C(12) is such that C(1)—C(7) is *trans* with respect to C(12)–C(13) and that the plane of the

Table 2. *Interatomic distances* (Å), *intramolecular angles* (°) *and torsion angles* (°)

	(I)	(II)		(I)	(II)		(I)	(II)		(I)	(II)
C(1)–C(2)	1·388 (6)	1·382 (6)	C(8)–C(19)	1·532 (5)	1·530 (5)	C(15)–C(16)	1·514 (5)	1·505 (8)	C(14)–H(14*a*)	0·99 (3)	0·95 (3)
C(1)–C(6)	1·384 (6)	1·384 (5)	C(9)–O(10)	1·455 (4)	1·452 (4)	C(17)–C(18)	1·519 (5)	1·516 (5)	C(14)–H(14*b*)	0·92 (3)	0·98 (3)
C(1)–C(7)	1·503 (5)	1·508 (4)	C(9)–C(16)	1·522 (4)	1·504 (6)	C(2)–H(2)	0·96 (3)	0·90 (3)	C(15)–H(15*a*)	0·99 (3)	1·00 (3)
C(2)–C(3)	1·378 (5)	1·382 (6)	C(9)–O(20)	1·413 (4)	1·407 (4)	C(3)–H(3)	0·93 (3)	0·92 (3)	C(15)–H(15*b*)	0·99 (3)	0·85 (3)
C(3)–C(4)	1·367 (7)	1·354 (8)	O(10)–C(11)	1·444 (4)	1·448 (4)	C(4)–H(4)	0·95 (3)	0·90 (3)	C(16)–H(16*a*)	0·98 (3)	1·01 (3)
C(4)–C(5)	1·321 (9)	1·352 (9)	C(11)–C(12)	1·535 (5)	1·527 (5)	C(5)–H(5)	0·91 (3)	0·87 (3)	C(16)–H(16*b*)	1·00 (3)	0·96 (3)
C(5)–C(6)	1·390 (6)	1·385 (6)	C(11)–C(18)	1·512 (5)	1·514 (5)	C(6)–H(6)	0·92 (3)	0·88 (3)	C(17)–H(17*a*)	0·96 (3)	0·99 (3)
C(7)–C(12)	1·549 (5)	1·553 (5)	C(12)–C(13)	1·575 (5)	1·569 (4)	C(7)–H(7*a*)	0·99 (3)	0·99 (3)	C(17)–H(17*b*)	0·94 (3)	0·96 (3)
C(8)–C(9)	1·520 (3)	1·522 (5)	C(12)–C(21)	1·540 (5)	1·536 (5)	C(7)–H(7*b*)	0·98 (3)	0·99 (3)	C(18)–H(18*a*)	0·95 (3)	0·99 (3)
C(8)–C(13)	1·539 (5)	1·552 (5)	C(13)–C(14)	1·542 (4)	1·540 (5)	C(11)–H(11)	0·97 (3)	0·99 (3)	C(18)–H(18*b*)	1·02 (3)	0·94 (3)
C(8)–C(17)	1·534 (4)	1·531 (5)	C(14)–C(15)	1·516 (5)	1·516 (7)	C(13)–H(13)	0·91 (3)	0·96 (3)	O(20)–H(20)	0·83 (3)	0·81 (3)

	(I)	(II)		(I)	(II)		(I)	(II)
C(2)–C(1)–C(6)	116·6 (4)	117·0 (3)	C(13)–C(8)–C(19)	112·4 (3)	112·3 (3)	C(7)–C(12)–C(13)	112·0 (3)	114·0 (3)
C(2)–C(1)–C(7)	121·4 (4)	121·2 (3)	C(17)–C(8)–C(19)	108·2 (3)	107·9 (3)	C(7)–C(12)–C(21)	107·7 (3)	107·5 (3)
C(6)–C(1)–C(7)	121·9 (4)	121·8 (3)	C(8)–C(9)–O(10)	108·3 (3)	108·0 (3)	C(11)–C(12)–C(13)	105·4 (3)	105·6 (3)
C(1)–C(2)–C(3)	121·5 (4)	121·6 (4)	C(8)–C(9)–C(16)	113·6 (3)	113·5 (3)	C(11)–C(12)–C(21)	110·2 (3)	111·0 (3)
C(2)–C(3)–C(4)	119·8 (5)	119·7 (5)	C(8)–C(9)–O(20)	108·9 (3)	109·2 (3)	C(13)–C(12)–C(21)	110·1 (3)	108·7 (3)
C(3)–C(4)–C(5)	120·1 (4)	120·4 (4)	O(10)–C(9)–C(16)	105·5 (2)	105·6 (3)	C(8)–C(13)–C(12)	109·5 (3)	109·7 (3)
C(4)–C(5)–C(6)	121·3 (5)	120·3 (4)	O(10)–C(9)–O(20)	109·2 (2)	109·4 (3)	C(8)–C(13)–C(14)	110·2 (3)	109·6 (3)
C(1)–C(6)–C(5)	120·6 (5)	120·9 (4)	C(16)–C(9)–O(20)	111·2 (3)	111·3 (3)	C(12)–C(13)–C(14)	116·9 (3)	116·9 (3)
C(1)–C(7)–C(12)	116·9 (3)	115·7 (3)	C(9)–O(10)–C(11)	113·3 (2)	113·8 (2)	C(13)–C(14)–C(15)	115·4 (3)	115·6 (3)
C(9)–C(8)–C(13)	105·2 (3)	104·9 (3)	O(10)–C(11)–C(12)	108·1 (2)	107·5 (2)	C(14)–C(15)–C(16)	114·0 (3)	114·1 (4)
C(9)–C(8)–C(17)	107·7 (2)	107·4 (3)	O(10)–C(11)–C(18)	108·8 (3)	108·3 (3)	C(9)–C(16)–C(15)	111·0 (3)	111·2 (4)
C(9)–C(8)–C(19)	112·4 (3)	113·6 (3)	C(12)–C(11)–C(18)	112·4 (3)	113·0 (3)	C(8)–C(17)–C(18)	110·1 (3)	110·4 (3)
C(13)–C(8)–C(17)	110·8 (3)	110·6 (3)	C(7)–C(12)–C(11)	111·3 (3)	110·2 (3)	C(11)–C(18)–C(17)	107·7 (3)	107·6 (3)

C(2)–C(1)–C(7)–C(12)	90·8 (5)	−92·6 (4)	C(19)–C(8)–C(13)–C(12)	167·4 (3)	−166·3 (3)	C(18)–C(11)–C(12)–C(7)	167·5 (3)	−166·1 (3)
C(1)–C(7)–C(12)–C(11)	−63·5 (4)	61·9 (4)	C(19)–C(8)–C(13)–C(14)	−62·7 (3)	64·0 (4)	C(18)–C(11)–C(12)–C(13)	−70·8 (3)	70·4 (3)
C(1)–C(7)–C(12)–C(13)	178·7 (3)	−179·6 (3)	C(9)–C(8)–C(17)–C(18)	47·7 (4)	−47·5 (4)	C(18)–C(11)–C(12)–C(21)	48·0 (4)	−47·2 (4)
C(1)–C(7)–C(12)–C(21)	57·5 (4)	−59·1 (4)	C(13)–C(8)–C(17)–C(18)	−66·9 (3)	66·4 (4)	O(10)–C(11)–C(18)–C(17)	−67·6 (3)	67·5 (3)
C(13)–C(8)–C(9)–O(10)	51·8 (3)	−50·8 (3)	C(19)–C(8)–C(17)–C(18)	169·5 (3)	−170·4 (3)	C(12)–C(11)–C(18)–C(17)	52·0 (4)	−51·5 (4)
C(13)–C(8)–C(9)–C(16)	−65·1 (3)	65·9 (4)	C(8)–C(9)–O(10)–C(11)	15·7 (3)	−16·6 (3)	C(7)–C(12)–C(13)–C(8)	138·4 (3)	−138·3 (3)
C(13)–C(8)–C(9)–O(20)	170·5 (2)	−169·5 (2)	C(16)–C(9)–O(10)–C(11)	137·7 (2)	−138·3 (3)	C(7)–C(12)–C(13)–C(14)	12·3 (4)	−12·7 (4)
C(17)–C(8)–C(9)–O(10)	−66·4 (3)	67·0 (3)	O(20)–C(9)–O(10)–C(11)	−102·8 (2)	101·9 (3)	C(11)–C(12)–C(13)–C(8)	17·2 (3)	−17·2 (4)
C(17)–C(8)–C(9)–C(16)	176·7 (3)	−176·4 (3)	C(8)–C(9)–C(16)–C(15)	57·0 (4)	−57·9 (4)	C(11)–C(12)–C(13)–C(14)	−108·9 (3)	108·4 (3)
C(17)–C(8)–C(9)–O(20)	52·2 (3)	−51·8 (3)	O(10)–C(9)–C(16)–C(15)	−61·5 (3)	60·2 (4)	C(21)–C(12)–C(13)–C(8)	−101·7 (3)	101·9 (3)
C(19)–C(8)–C(9)–O(10)	174·4 (2)	−173·7 (3)	O(20)–C(9)–C(16)–C(15)	−179·8 (2)	178·7 (3)	C(21)–C(12)–C(13)–C(14)	132·2 (3)	−132·5 (3)
C(19)–C(8)–C(9)–C(16)	57·5 (4)	−57·1 (4)	C(8)–C(9)–O(20)–H(20)	−179·1 (21)	165·3 (22)	C(8)–C(13)–C(14)–C(15)	−51·8 (4)	51·3 (4)
C(19)–C(8)–C(9)–O(20)	−66·9 (3)	67·5 (4)	C(9)–O(10)–C(11)–C(12)	−71·7 (3)	72·8 (3)	C(12)–C(13)–C(14)–C(15)	74·0 (4)	−74·4 (4)
C(9)–C(8)–C(13)–C(12)	−69·9 (3)	69·8 (3)	C(9)–O(10)–C(11)–C(18)	50·6 (3)	−49·7 (3)	C(13)–C(14)–C(15)–C(16)	42·5 (4)	−42·2 (5)
C(9)–C(8)–C(13)–C(14)	60·0 (3)	−59·8 (3)	O(10)–C(11)–C(12)–C(7)	−72·4 (3)	74·4 (3)	C(14)–C(15)–C(16)–C(9)	−43·1 (4)	43·2 (5)
C(17)–C(8)–C(13)–C(12)	46·2 (3)	−45·7 (4)	O(10)–C(11)–C(12)–C(13)	49·3 (3)	−49·1 (3)	C(8)–C(17)–C(18)–C(11)	15·7 (4)	−16·3 (4)
C(17)–C(8)–C(13)–C(14)	176·1 (3)	−175·4 (3)	O(10)–C(11)–C(12)–C(21)	168·1 (3)	−166·7 (3)			

phenyl ring is nearly perpendicular to C(7)–C(12) for both molecules.

The tricycloundecane ring system consists of four six-membered rings, three of which have almost ideal-boat conformations whereas the fourth ring has a distorted-chair conformation, as follows from the puckering parameters φ and θ of Cremer & Pople (1975). For molecules (I) and (II) the values of φ and θ are:

ring C(8)–C(9)–O(10)–C(11)–C(12)–C(13)
168°, 92° 167°, 92°
ring C(8)–C(9)–O(10)–C(11)–C(18)–C(17)
15°, 90° 15°, 90°
ring C(8)–C(13)–C(12)–C(11)–C(18)–C(17)
164°, 89° 164°, 89°
ring C(8)–C(9)–C(16)–C(15)–C(14)–C(13)
9°, 16° 9°, 17°.

The two methyl groups at C(19) and C(21) are in a nearly staggered conformation with respect to C(8)–C(9) and C(7)–C(12) respectively, the average deviation being 2 and 10°; for molecule (II) these deviations are 6 and 7° respectively.

The geometries of the hydrogen bonds (distance O···O, H···O, angle O–H···O) O(20)–H(20··· O′(10) and O′(20)–H′(20)···O(10) linking molecules (I) and (II) are 2·764 (3), 1·93 (3) Å, 173 (2)° and 2·879 (3), 2·07 (3) Å, 177 (2)°. The torsion angles of O(2)–H(20) relative to C(8)–C(9) differ for both molecules and are −179 (2) and 165 (2)° for molecules (I) and (II) respectively.

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