The mean plane of the isoprenyl side chain attached to ring *A* makes an angle of 111·5 (1)° with the mean plane of the xanthone ring system. The corresponding angle in other xanthones is 95·4° in epishamixanthone and 102° in morellin (Kartha & Ambady, 1982).

The molecular arrangement projected along the *bc* plane is shown in Fig. 3. The xanthone rings are stacked on one another. Packing of the molecules in the crystal is essentially by hydrogen bonds between the water molecule and the carbonyl hydroxyl groups. The carbonyl and the adjacent hydroxyl are also involved in an intramolecular hydrogen bond.* The $O \cdots O$ (donor→acceptor) hydrogen-bond distances vary from 2·503 (6) to 2·949 (5) Å.

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* See deposition footnote.

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Structure of a Dioxabicyclic Fluoro Octane Derivative

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Abstract. 2,2,3,3,4,4-Hexafluoro-1,7-dihydroxy-7-phenyl-6,8-dioxabicyclo[3.2.1]oct-5-yl phenyl ketone, $C_{19}H_{12}F_6O_5$, $M_r = 434·3$, monoclinic, $P2_1/n$, $a = 6·789$ (1), $b = 23·554$ (3), $c = 11·486$ (2) Å, $\beta = 99·03°$ (1), $V = 1813·98$ Å^3, $Z = 4$, $D_x = 1·590$ g cm^{-3}, λ(Mo $K\alpha_1$) = 0·70926 Å (cell constants), λ(Mo $K\alpha$) = 0·7107 Å (intensity data), $\mu = 1·46$ cm^{-1}, $F(000) = 880$, $T = 293$ K, $R = 0·074$ for all 5325 independent reflections. Full-matrix least-squares refinement included isotropic H atoms and gave bond distances and angles with e.s.d.'s of 0·002 Å and 0·1° respectively. Comparison with published *exo*-7-phenyl-5,7-dimethyl-6,8-dioxabicyclo[3.2.1]octane parameters shows that the conformation of the bicyclic framework is similar, but in the six-membered heterocycle the C—C bonds are longer and the C—O bonds shorter in the hexafluoro derivative.

Introduction. Perfluoroalkylpolyketones, unlike simple monoketones, react in the presence of electron-donor molecules such as water, ethanol, tetrahydrofuran and pyridine to form heterocyclic compounds containing a fluorinated 6,8-dioxabicyclo[3.2.1]octane framework. The stability of the heterocycle is dependent on the

length of the perfluoroalkylether group (Chen & Tamborski, 1984). For example, bicyclic structures originating from the hydration of the ketone were not observed when a longer chain $-(O)C(CF_2)_4C(O)-$ or $-(CF_2)_4-$ group replaced the $-(CF_2)_3-$ group.

The structure of the 6,8-dioxabicyclo[3.2.1]octane framework was first reported by Mundy, Dirks, Larsen & Caughlan (1978) in their paper on the X-ray analysis of the *exo* isomer of 5,7-dimethyl-7-phenyl-6,8-dioxabicyclo[3.2.1]octane. Prior to this, spectrometric and stereospecific synthetic methods had been used to make the stereochemical assignments of the possible isomeric structures. The assignments were then verified by lanthanide-induced shift experiments (Gore & Armitage, 1976).

The framework has been shown to be a structural component of sex pheromones and marine toxins. In particular, this skeletal system is found in two oxidation products obtained from N-(p-bromobenzyl)palytoxin (Uemura, Ueda, Hirata, Katayama & Tanaka, 1980). The parent compound, palytoxin, a powerful toxin, is derived from marine animal and plant sources. Unfortunately, Uemura *et al.* did not report crystallographic results or compare their framework structure with the earlier structure published by Mundy *et al.* (1978).

Chen, Fratini & Tamborski (1986) have shown that a 6,8-dioxabicyclo[3.2.1]octane is produced when a tetraketone, $C_6H_5C(O)C(O)(CF_2)_3C(O)C(O)C_6H_5$, cyclizes in water. A bis hydroxy[3.2.1]octane in which the methylene $-CH_2-$ groups are replaced by $-CF_2-$ groups (I) has been crystallized and subjected to an X-ray analysis which is reported here.
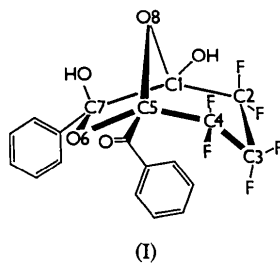
(I)

Experimental. For the X-ray studies, a nicely shaped hexagonal prism, elongated along **a**, was chosen from a batch recrystallized from a diethyl ether/petroleum ether (1:1 volume) solution at 303–333 K. The space group was initially determined by *Crystalytics** and confirmed by structure analysis to be $P2_1/n$. The data

crystal, $0.2 \times 0.2 \times 0.6$ mm, mosaic spread $0.03°$ (FWHM), was mounted with the long dimension parallel to the φ axis of the four-circle diffractometer. Reported cell constants are from least-squares fit of $2\theta,\omega,\chi$ values for 15 reflections ($45 < 2\theta < 48°$) measured at $\pm 2\theta$ with Mo $K\alpha_1$ radiation.

Intensity data, 14 724 reflections, were measured to a limit of $(\sin\theta)/\lambda = 0.7035$ Å^{-1} with Mo $K\alpha$ radiation from a graphite monochromator ($\pm$ hkl and h$\bar{k}$l with $40 < 2\theta < 60°$ and $\pm h \pm k \pm l$ with $2\theta < 40°$). Picker FACS-I software (Lenhert, 1975) measured 2θ step scans of $1.05°$ (plus a dispersion term) with $0.02°$ steps, 1 s each, 20 s backgrounds at scan ends and applied a coincidence correction. Four reflection standards ($\bar{1}03$, 180, 122, 202), measured at intervals, declined 10% in intensity after 596 h of X-ray exposure. The decline was corrected by scaling each interval group. Lorentz–polarization and absorption corrections, made with *ORABS* (Wehe, Busing & Levy, 1962), used an $8 \times 8 \times 8$ Gaussian grid. Maximum, minimum and average transmission factors were 0.97, 0.96 and 0.97. Symmetry-related reflections were averaged ($R_{int} = 0.050$) to give 5325 F_o (including 518 with zero intensity).

The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1971). After preliminary refinement of the heavier atoms, H-atom positions were calculated, then confirmed with a difference synthesis. Refinement was by full-matrix least squares with anisotropic thermal motion for heavy atoms, isotropic for H atoms. The quantity minimized was $\sum w(|F_o| - |F_c|)^2$ where $w = 1/\sigma^2(F_o)$ and the variance, σ^2, was based on counting statistics and included the usual instability term (4%). Atomic scattering factors were from Cromer & Mann (1968) except for Stewart's H values (Stewart, Davidson & Simpson, 1965). Anomalous-dispersion factors (all atoms except H) were those of Cromer & Liberman (1970). The final R factor (all reflections) was 0.074, $wR = 0.050$. If $I < 3\sigma(I)$ data are omitted, the values are 0.040 and 0.039, respectively, for 3302 reflections. The maximum shift-to-e.s.d. ratio for the final refinement cycle was 0.19. Maximum and minimum $\Delta\rho$ values were 0.26 and -0.28 e Å^{-3}. The standard error of an observation of unit weight was 2.06.

The atomic parameters in Table 1 were used to calculate the bond distances and angles given in Table 2.* Fig. 1 is a stereographic drawing (Johnson, 1976) of the molecule showing the atom-numbering scheme.

Table 1. Fractional atomic coordinates and B or B equivalent thermal parameters ($\mathring{A}^2$)

$B_{eq} = \frac{8}{3}\pi^2(U_{11}^2 + U_{22}^2 + U_{33}^2)$ where the U_{ii} are the r.m.s. principal axis deviations.

	x	y	z	B or B_{eq}
F(1)	0·16916 (14)	0·05495 (4)	0·07346 (7)	5·57
F(2)	−0·10421 (12)	0·07840 (4)	0·13695 (8)	5·81
F(3)	0·21380 (14)	0·16146 (4)	0·10214 (8)	6·33
F(4)	0·05188 (13)	0·16451 (3)	0·24980 (8)	5·42
F(5)	0·52943 (12)	0·12470 (4)	0·22084 (8)	5·46
F(6)	0·41548 (13)	0·18188 (3)	0·34187 (8)	5·34
O(2)	0·58992 (13)	0·07971 (4)	0·43229 (10)	4·16
O(3)	0·29819 (14)	0·03234 (4)	0·53120 (9)	3·62
O(6)	0·06963 (11)	0·05724 (3)	0·36802 (7)	3·23
O(8)	0·35565 (11)	0·03238 (3)	0·30080 (7)	3·27
O(9)	−0·09805 (15)	−0·03704 (4)	0·27381 (9)	5·20
C(1)	0·39964 (17)	0·08134 (5)	0·37485 (12)	3·25
C(2)	0·38344 (20)	0·13143 (5)	0·28685 (13)	4·02
C(3)	0·18391 (23)	0·13366 (6)	0·20116 (13)	4·42
C(4)	0·09444 (21)	0·07437 (6)	0·16868 (13)	4·15
C(5)	0·14710 (18)	0·03292 (5)	0·27160 (11)	3·18
C(7)	0·23377 (17)	0·07631 (6)	0·45246 (11)	2·98
C(9)	−0·06359 (20)	−0·02763 (5)	0·24531 (11)	3·62
C(10)	0·17411 (22)	−0·07123 (6)	0·18880 (12)	3·96
C(11)	0·08964 (31)	−0·12500 (7)	0·17752 (15)	5·57
C(12)	0·18462 (44)	−0·16812 (8)	0·12533 (20)	7·33
C(13)	0·35943 (41)	−0·15788 (10)	0·08484 (18)	7·32
C(14)	0·44293 (34)	−0·10560 (9)	0·09529 (16)	6·31
C(15)	0·35226 (26)	−0·06198 (7)	0·14678 (14)	4·93
C(16)	0·18259 (19)	0·12924 (5)	0·51550 (11)	3·32
C(17)	0·33094 (25)	0·15428 (6)	0·59529 (14)	4·54
C(18)	0·29284 (32)	0·20374 (7)	0·65253 (16)	5·65
C(19)	0·10609 (33)	0·22728 (7)	0·63222 (16)	5·82
C(20)	−0·04263 (30)	0·20194 (6)	0·55595 (17)	5·35
C(21)	−0·00559 (23)	0·15296 (6)	0·49646 (14)	4·11
H(2)	0·6054 (25)	0·0497 (8)	0·4646 (17)	7·0 (5)
H(3)	0·2358 (22)	0·0328 (7)	0·5831 (14)	5·1 (4)
H(11)	−0·0309 (21)	−0·1309 (6)	0·2041 (13)	4·4 (4)
H(12)	0·1184 (27)	−0·2002 (9)	0·1187 (17)	7·7 (5)
H(13)	0·4274 (29)	−0·1885 (9)	0·0466 (19)	9·1 (5)
H(14)	0·5581 (29)	−0·0997 (8)	0·0650 (18)	8·0 (6)
H(15)	0·4078 (21)	−0·0251 (7)	0·1512 (14)	5·6 (4)
H(17)	0·4604 (22)	0·1379 (6)	0·6105 (13)	5·1 (3)
H(18)	0·3919 (24)	0·2206 (7)	0·7039 (15)	6·1 (4)
H(19)	0·0867 (23)	0·2600 (8)	0·6740 (15)	6·8 (4)
H(20)	−0·1674 (26)	0·2171 (7)	0·5443 (15)	6·5 (4)
H(21)	−0·1037 (20)	0·1377 (6)	0·4413 (12)	4·5 (3)

Table 2. Bond distances ($\mathring{A}$) and angles (°)

C(4)—F(1)	1·355 (2)	C(3)—F(4)	1·342 (2)
C(4)—F(2)	1·344 (2)	C(2)—F(5)	1·348 (2)
C(3)—F(3)	1·355 (2)	C(2)—F(6)	1·347 (1)
C(1)—O(2)	1·356 (1)	C(1)—C(2)	1·546 (2)
C(1)—O(8)	1·436 (1)	C(1)—C(7)	1·547 (2)
C(5)—O(8)	1·403 (1)	C(2)—C(3)	1·545 (2)
C(5)—O(6)	1·419 (2)	C(3)—C(4)	1·545 (2)
C(7)—O(6)	1·430 (1)	C(4)—C(5)	1·532 (2)
C(7)—O(3)	1·399 (2)	C(5)—C(9)	1·547 (2)
C(9)—O(9)	1·214 (2)	C(7)—C(16)	1·509 (2)
		C(9)—C(10)	1·480 (2)

C(2)—C(1)—C(7)	116·85 (10)	C(4)—C(5)—C(9)	113·77 (10)
O(2)—C(1)—C(2)	107·72 (10)	O(6)—C(5)—C(4)	105·95 (10)
O(8)—C(1)—C(2)	103·81 (10)	O(8)—C(5)—C(4)	107·15 (10)
O(2)—C(1)—C(7)	116·21 (11)	O(6)—C(5)—C(9)	110·80 (10)
O(8)—C(1)—C(7)	100·21 (9)	O(8)—C(5)—C(9)	111·32 (10)
O(2)—C(1)—O(8)	111·05 (10)	O(6)—C(5)—O(8)	107·50 (9)
C(1)—C(2)—C(3)	114·06 (11)	C(5)—O(6)—C(7)	108·14 (9)
F(5)—C(2)—C(1)	107·14 (10)	O(3)—C(7)—C(1)	104·32 (9)
F(6)—C(2)—C(1)	112·12 (11)	O(6)—C(7)—C(1)	101·16 (9)
F(5)—C(2)—C(3)	107·10 (12)	C(1)—C(7)—C(16)	117·16 (10)
F(6)—C(2)—C(3)	109·25 (10)	O(3)—C(7)—O(6)	109·71 (9)
F(5)—C(2)—F(6)	106·77 (11)	O(3)—C(7)—C(16)	111·93 (10)
C(2)—C(3)—C(4)	113·28 (11)	O(6)—C(7)—C(16)	111·79 (9)
F(3)—C(3)—C(2)	108·62 (12)	C(1)—O(8)—C(5)	104·04 (8)
F(4)—C(3)—C(2)	109·22 (11)	O(9)—C(9)—C(5)	115·78 (11)
F(3)—C(3)—C(4)	109·82 (12)	C(5)—C(9)—C(10)	121·98 (12)
F(4)—C(3)—C(4)	109·09 (12)	O(9)—C(9)—C(10)	122·24 (12)
F(3)—C(3)—F(4)	106·60 (11)	F(1)—C(4)—C(5)	109·64 (11)
C(3)—C(4)—C(5)	110·76 (11)	F(2)—C(4)—C(5)	110·92 (12)
F(1)—C(4)—C(3)	108·49 (12)	F(1)—C(4)—F(2)	106·96 (11)
F(2)—C(4)—C(3)	109·96 (12)		

Least-squares refinement, structure factors, electron density, least-squares planes, bond distances and angles were calculated with the XRAY67 programs (Stewart, 1967) as implemented and updated on the Vanderbilt DEC-1099 computer.

Discussion. The molecular parameters of the fluorinated bicyclic system are generally in agreement with the corresponding values reported by Mundy et al. (1978) for the protonated structure. The five-membered ring of the bicyclic system displays the typical bent configuration with C(1) deviating 0·634 Å from the best plane of the other four atoms, which are planar to better than 0·02 Å. The six-membered ring of the bicyclic system assumes an approximate half-chair conformation with C(3) 0·421 and O(8) −0·835 Å out of the best plane of the other four ring atoms. This distortion from an ideal half-chair is to be expected in order to preclude a perfectly eclipsed arrangement of C—F bonds in the —(CF$_2$)$_3$— group. In the protonated structure of Mundy et al. (1978), one finds all best-plane deviations within 0·05 Å of those mentioned above.

The C(sp^3)—C(sp^3) bond lengths in the six-membered ring are longer [1·532 (2)–1·546 (2) Å] than the corresponding bonds in the protonated structure [1·507 (6)–1·528 (7) Å]. The expected paraffinic value is 1·537 (5) Å (Sutton, 1965). The C(5)—O(8) and C(5)—O(6) bridgehead distances of 1·403 (1) and 1·419 (2) Å, however, are shorter than the protonated values of 1·432 (4) and 1·456 (5) Å. This apparent bond shortening is in part ascribed to the effect of the different substituent attached to C(5). The expected C(sp^3)—O bond length is 1·426 (5) Å (Sutton, 1965). The average C—F bond distance we report is 1·349 Å, close to the expected value of 1·345 (5) Å (Sutton, 1965). Bond distances in the phenyl groups* range from 1·353 to 1·388 Å and average 1·377 Å.
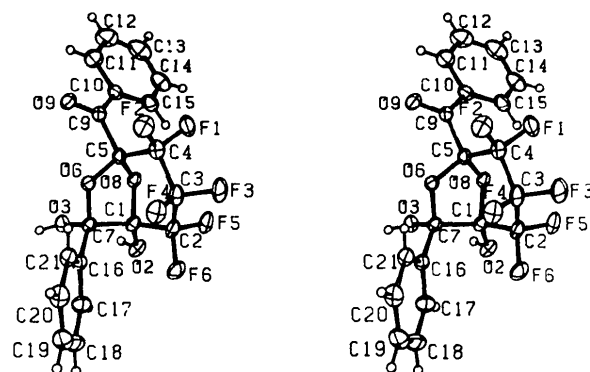
* See deposition footnote.

Fig. 1. Stereoview of the molecule showing atom numbering. Thermal ellipsoids at 25% probability.

$C_{19}H_{12}F_6O_5$

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Presence of Conformational Rotamers in the Structures of Two Diaxially Substituted Dimeric Methylcyclohexanols

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Abstract. The structures of (1*S*,3*R*)-1-[(1*S*)-1-hydroxy-3-methylcyclohexyl]-3-methyl-1-cyclohexanol (referred to as 3-*M* hereinafter) and *trans*-1-(*trans*-1-hydroxy-4-methylcyclohexyl)-4-methyl-1-cyclohexanol (referred to as 4-*M* hereinafter) have been determined so as to provide unequivocal support for results of an ongoing study of metal-catalyzed pinacol coupling reactions. Both compounds have the chemical formula $C_{14}H_{26}O_2$. Compound 3-*M*: $M_r = 226.358$, space group P1, $a = 10.453$ (3), $b = 10.616$ (3), $c = 11.057$ (3) Å, $\alpha = 97.47$ (3), $\beta = 104.23$ (3), $\gamma = 118.72$ (3)°, $V = 997.6$ (10) Å^3, $Z = 3$, $D_m = 1.14$ (2), $D_x = 1.131$ g cm^{-3}, $\lambda = 0.71069$ Å (graphite-monochromatized Mo $K\alpha$ radiation), $\mu = 0.068$ mm^{-1}, $F(000) = 378$, $T = \sim297$ K, $R = 0.064$ for 2579 observed data $(F > 2.5\sigma_F)$ of 3508 unique reflections. Compound 4-*M*: $M_r = 226.358$, space group $P2_1/n$, $a = 10.349$ (2), $b = 18.992$ (6), $c = 11.143$ (3) Å, $\beta = 108.86$ (2)°, $V = 2067.9$ (8) Å^3, $Z = 6$, $D_m = 1.11$ (2), $D_x = 1.089$ g cm^{-3}, $\lambda = 0.71069$ Å (graphite-monochromatized Mo $K\alpha$ radiation), $\mu = 0.066$ mm^{-1}, $F(000) = 756$, $T = \sim297$ K, $R = 0.064$ for 1457 observed data $(F > 4.0\sigma_F)$ of 3643 unique reflections. The structural results reported here verify the NMR-derived conclusions as to the stereochemistry of pinacol coupling products. The pinacol coupling reactions were carried out in the presence of Al–Hg amalgam; the products are all axial although this is the less energetically favored configuration compared to the equatorial product. The lower-yield product (4-*M*) (produced in 64.6% yield of the diol as compared to the 75.8% yield of the 3-*M* diol) appears to be the energetically more favored molecule as there are fewer possible diaxial interactions. This evidence strongly suggests that the steric interactions in the intermediates formed from the Al–Hg methylcyclohexanone reaction are the determining factors with respect to product formation.

Introduction. The structural work on these two compounds was undertaken to verify the three-dimensional structures of two molecules produced in an ongoing study of pinacol coupling reactions (Mundy, Srinivasa, Kim, Dolph & Warnet, 1982; Mundy, Bruss, Kim, Larsen & Warnet, 1985). Nuclear magnetic resonance studies on these two compounds (3-*M*: Mundy *et al.,*

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