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The Structure of Δ-8,14-Anhydrodigitoxigenin, $C_{23}H_{32}O_3$, by Direct Phase Determination

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Δ-8,14-Anhydrodigitoxigenin, a dehydration product of digitoxigenin, does not have any cardio-active properties. Two important properties of cardio-active aglycosides, namely a hydroxyl group on C(14) and the *cis C/D* ring junction, have been removed by the dehydration in the 8,14 positions. The double bond between the 8,14 positions has flattened the molecule in the vicinity of the *C* and *D* rings. In addition, although ring *D* assumes an envelope conformation, it is neither C(13) nor C(14), but C(17) which is out of the plane formed by the remaining four atoms. The packing of anhydrodigitoxigenin is quite different from that of digitoxigenin. In digitoxigenin there is head-to-tail hydrogen bonding between C=O and –OH groups, which links the molecules into infinite chains. Although the two ends of the anhydrodigitoxigenin molecule are quite similar to digitoxigenin, no advantage is taken of the C=O and –OH groups, and there is no hydrogen bonding. The material crystallizes in space group $P2_12_12_1$ with $a = 11{\cdot}199 \pm 0{\cdot}003$, $b = 23{\cdot}104 \pm 0{\cdot}005$, and $c = 7{\cdot}381 \pm 0{\cdot}002$ Å. Phases were determined directly from the structure factor magnitudes by the symbolic addition procedure for non-centrosymmetric crystals.

Introduction

Symptoms of heart failure are now commonly treated by rapid administration of a cardiotonic agent. Cardiotonic preparations, in proper dosage, increase the force of cardial contractions with no increase in oxygen consumption, causing the heart muscle to become a more efficient pump. These drugs generally contain a mixture of compounds called cardiac glycosides. The cardiac glycosides all contain a steroid residue linked to a sugar, and research has been concerned with the relationship of cardiac activity to molecular configuration and the effect of substituents.

Digitoxigenin is one of the active steroid residues contained in digitalis which is obtained from the purple foxglove, and its molecular and crystal structure was recently determined (Karle & Karle, 1969). Many variations of this steroid have been prepared and from their physiological action, several structural features appear to be simultaneously necessary. The hydroxyl at C(14), the unsaturated lactone ring at C(17), the *cis C/D* ring junction, and the presence of a hydroxyl or a sugar at C(3) are present in all known active cardiac agents.

A cardio-inactive dehydration product of digitoxigenin, Δ-8,14-anhydrodigitoxigenin (Fig. 1), was supplied to us by Dr U. Weiss of the National Institutes of Health. The total chemical change consisted of removal of the hydrogen and hydroxyl substituents at C(8) and C(14), respectively, but a major conformational change was suggested by a concurrent reversal in the direction of optical rotation (Burkhardt, Meier, Furst & Reichstein, 1967). A structure determination was undertaken to determine the changes which arise from the introduction of a double bond. The absence of a heavy atom in the crystal being investigated and the use of diffractometer intensity measurements afford the opportunity to obtain conformational parameters of high accuracy.

Experimental

The anhydrodigitoxigenin crystals were colorless orthorhombic prisms. A crystal was mounted along the longest axis of a prism, which was subsequently found to be the shortest unit-cell axis, *c*. Precession and Weissenberg photographs of this crystal exhibited axial extinctions only, indicating space group $P2_12_12_1$. The crystal was aligned on an automatic diffractometer, and reflections were measured manually along eleven independent axes of reciprocal space. Systematic errors due to alignment were minimized by measuring each reflection on the $+2\theta$ and on the -2θ side of the direct beam (Bond, 1960). The cell constants and other physical properties of the crystal are reported in Table 1.

Table 1. *Physical properties*

Molecular formula	$C_{23}H_{32}O_3$
Molecular weight	356·51
Crystal habit	Elongated prism
Crystal size	0·2 × 0·3 × 0·8 mm (**a**, **b**, **c** directions)
Space group	$P2_12_12_1$
a	11·199 ± 0·003 Å
b	23·104 ± 0·005
c	7·381 ± 0·002
V	1909·7 ± 1·4 Å^3
ϱ_{calc}	1·240 g.cm^{-3}
μ, linear absorption coefficient	6·4 cm^{-1}
$\mu r_{\max}$ ($r_{\max}$ = radius of sphere which circumscribes crystal)	0·25
No. independent reflections observed	1932

The standard deviations in the cell parameters indicated by the precision of the least-squares fit were all less than 0·001 Å. These estimates were arbitrarily increased fivefold to account for the possibility of small systematic errors in measurement. Errors in bond distance calculations attributable to cell constant errors are still negligible (± 0·0003 Å).

The X-ray intensity data were collected on a four-circle automatic diffractometer using the θ, 2θ (moving crystal, moving counter) technique. The intensities were corrected for Lorentz and polarization factors, approximately scaled to the proper absolute level and corrected for vibrational motion by means of a K curve, and normalized structure factor magnitudes ($|E|$ values) were derived.

Phase determination and refinement

The initial phases for a selected set of reflections with large $|E|$ values were determined by the symbolic addition procedure for noncentrosymmetric crystals (Karle & Karle, 1966). The details of the structure determination were essentially the same as those described in other papers using this method (Karle, Estlin & Karle, 1967; Karle & Karle, 1968). The first set of E maps generated for this structure revealed no recognizable portions of the asymmetric unit. Later examination revealed that for this case some of the first 25 phases determined were incorrect by more than one radian and the errors combined so that phases generated from them were incorrect by a value of π. When working with the strongest indications available in a data set,

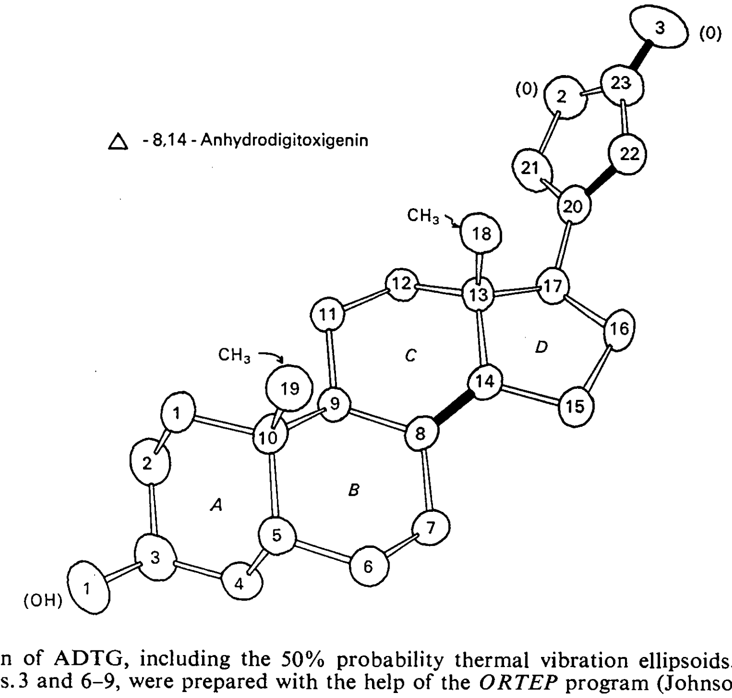


Fig. 1. The configuration of ADTG, including the 50% probability thermal vibration ellipsoids. This illustration, as well as Figs. 3 and 6–9, were prepared with the help of the *ORTEP* program (Johnson, 1965).

such accumulation of errors in the early stages of a phase determination can be expected to occur occasionally in noncentrosymmetric crystals. In such circumstances a new trial is made with a different set of reflections to initiate the phase determination. The assignments which were used in the second trial of this investigation are shown in Table 2. Using these assignments, 54 phases were determined with the relationship

$$\varphi_{\mathbf{h}} \simeq \langle \varphi_{\mathbf{k}} + \varphi_{\mathbf{h-k}} \rangle_{\mathbf{k}} \, . \qquad (1)$$

From multiple indications, it appeared that the symbol p had a value near $+\pi/2$. The tangent formula (Karle & Hauptman, 1956) was used to refine these phases and obtain phases for additional reflections with $|E| > 1{\cdot}35$.

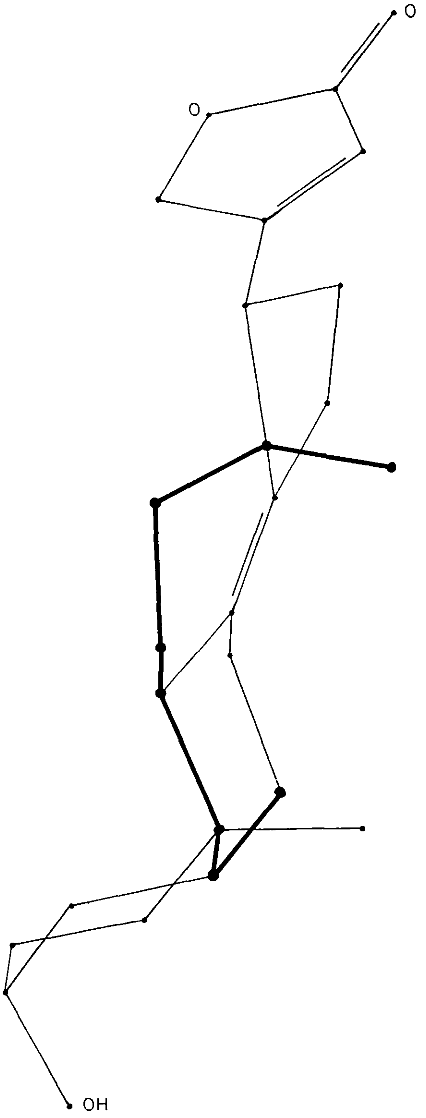


Fig.2. Outline of ADTG as it appears projected down the c axis. Atoms connected by heavily shaded lines constitute the initial portion of the structure found by the symbolic addition procedure (see text).

Table 2. *Phase assignments for implementing equation* (1)

$\|E\|$	$h\ k\ l$	φ*	
2·40	7 0 2	0	Origin assignment
2·11	2 5 0	0	
2·18	0 8 5	0	
2·10	1 4 0	$+\pi/2$	(enantiomorph assignment)
2·91	7 6 4	p	

* These values, except the first one, do not correspond to those listed in Table 5 since the origin was changed for convenience after the structure was known.

The E map based on phases obtained from the tangent formula revealed a group of peaks clustered in an area which was reasonable from packing considerations since this steroid was expected to be elongated and relatively planar. Eight peaks separated by chemically reasonable distances and angles were chosen as a trial partial structure. This part of the structure is emphasized by heavy lines in Fig.2. Phases based on this partial structure were used as input for a recycling procedure (Karle, 1968), employing the tangent formula, and the 26 carbon and oxygen atoms of the structure appeared in an E map at the end of only one cycle.

The initial R value, based on the coordinates of the atoms as obtained from this E map and an overall isotropic thermal factor of 3·5 Å^2, was 29·3%. Refinement proceeded to an R value of 13% with individual isotropic motion and 10% with one cycle of anisotropic refinement. At this stage, 28 hydrogen atoms were clearly visible in a difference map. The hydrogen atoms were given constant anisotropic thermal factors equal to those of the carbon atom to which they were attached, and no attempt was made to determine their individual motions. Their positions were refined, however, along with the positions and thermal factors of the heavier atoms, leading to an R value of 5·1%. Possible positions for the three methyl hydrogen atoms on C(19) and the hydroxyl hydrogen atom were indicated weakly in a subsequent difference map. Attempts to refine these positions by least-squares resulted in large oscillating shifts. Coordinates obtained from the difference map are reported for these four atoms along with least-squares results for all other atoms in Tables 3 and 4. The final R values computed with the reported parameters were 4·7% omitting unobserved reflections and 5·1% including unobserved reflections.

An empirical weighting scheme was used in which $w = 0{\cdot}25$ for $F_o = 0{\cdot}0$, $w = 1{\cdot}0$ for $|F_o| \leq 15{\cdot}0$, and $w = 15{\cdot}0/|F_o|$ for $|F_o| > 15{\cdot}0$. This empirical weighting scheme approximated closely a weighting curve based upon a statistical counting error, plus a random 1% error assumed for each intensity measurement. The least-squares refinement minimized the function $\Sigma w(|F_o| -$

Table 3. *Fractional atomic coordinates and thermal parameters for Δ-8,14-anhydrodigitoxigenin*

Thermal parameters are of the form $T=\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$. The β_{ij}'s are multiplied by 10^4.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B*
O(1)	−0·29197	0·70371	0·53117	55	26	277	7	−11	−10	4·0
O(2)	0·67382	0·63284	1·16522	83	28	202	1	−46	−22	4·3
O(3)	0·76745	0·54891	1·20805	113	32	300	0	100	16	5·4
C(1)	−0·10433	0·66484	0·79152	56	19	150	4	14	−6	3·1
C(2)	−0·12888	0·72682	0·72991	79	16	213	6	1	13	3·5
C(3)	−0·17290	0·72859	0·53378	71	15	233	6	−14	0	3·4
C(4)	−0·08792	0·69684	0·41199	65	17	160	5	−10	8	3·1
C(5)	−0·06192	0·63465	0·47214	51	14	140	0	−11	1	2·6
C(6)	0·02207	0·60410	0·34162	63	20	134	3	−8	−10	3·1
C(7)	0·15132	0·62665	0·35699	54	23	110	0	−2	−3	2·9
C(8)	0·19559	0·62631	0·55007	55	13	104	−3	10	−2	2·3
C(9)	0·11303	0·65678	0·68291	51	12	114	1	0	−1	2·3
C(10)	−0·01683	0·63128	0·67044	53	12	124	0	14	3	2·2
C(11)	0·16140	0·65873	0·87680	55	20	114	4	−4	−8	2·7
C(12)	0·29796	0·66094	0·88464	53	16	117	3	−10	−6	2·7
C(13)	0·35237	0·60915	0·78675	49	12	123	1	0	−2	2·3
C(14)	0·30183	0·60497	0·59674	55	14	116	−1	3	−5	2·4
C(15)	0·39630	0·58139	0·46752	59	24	153	6	−2	−14	3·5
C(16)	0·50944	0·57422	0·58555	58	23	161	6	8	−20	3·2
C(17)	0·48899	0·61650	0·74319	48	16	147	0	1	−2	2·7
C(18)	0·32977	0·55283	0·89095	65	16	169	0	0	9	3·0
C(19)	−0·01762	0·56754	0·73394	85	13	201	−3	9	17	3·2
C(20)	0·57121	0·60831	0·90077	45	17	156	−3	4	−8	3·0
C(21)	0·59262	0·65632	1·03343	74	23	249	8	−42	−18	4·2
C(22)	0·63686	0·56371	0·95017	64	18	188	−2	−8	−2	3·0
C(23)	0·70074	0·57736	1·11667	69	22	215	−4	−27	1	3·8
Standard deviations:										
O(1–2)	0·00025	0·00013	0·00043	2	1	7	1	4	2	0·15
O(3)	0·00030	0·00015	0·00048	3	1	8	1	5	2	0·20
C(1–23)	0·00033	0·00015	0·00055	3	1	8	1	4	2	0·20

* Thermal factor at the end of isotropic refinement.

Table 4. *Fractional atomic coordinates for the hydrogen atoms*

	x	y	z
H(1*a*)	−0·0756	0·6636	0·9245
H(1*b*)	−0·1852	0·6412	0·7909
H(2*a*)	−0·0537	0·7532	0·7467
H(2*b*)	−0·1925	0·7469	0·8151
H(3)	−0·1753	0·7727	0·4865
H(4*a*)	−0·0116	0·7194	0·4003
H(4*b*)	−0·1190	0·6951	0·2827
H(5)	−0·1412	0·6118	0·4707
H(6*a*)	−0·0099	0·6119	0·2144
H(6*b*)	0·0149	0·5621	0·3600
H(7*a*)	0·1585	0·6695	0·3066
H(7*b*)	0·2039	0·6028	0·2830
H(9)	0·1060	0·6996	0·6440
H(11*a*)	0·1314	0·6934	0·9435
H(11*b*)	0·1352	0·6242	0·9472
H(12*a*)	0·3278	0·6979	0·8296
H(12*b*)	0·3194	0·6611	1·0193
H(15*a*)	0·4095	0·6101	0·3629
H(15*b*)	0·3673	0·5429	0·4118
H(16*a*)	0·5856	0·5843	0·5169
H(16*b*)	0·5161	0·5293	0·6452
H(17)	0·5007	0·6583	0·6962
H(18*a*)	0·3720	0·5538	1·0110
H(18*b*)	0·3637	0·5195	0·8073
H(18*c*)	0·2404	0·5455	0·9044
H(19*a*)*	0·070	0·545	0·707
H(19*b*)*	−*·090	0·547	0·702
H(19*c*)*	−0·015	0·560	0·862
H(21*a*)	0·6270	0·6940	0·9635
H(21*b*)	0·5167	0·6659	1·0948
H(22)	0·6455	0·5248	0·8881
H(hydroxyl)*	−0·294	0·676	0·431
Standard deviations:	0·0035	0·0018	0·0058

* Indicated atoms were not refined by least-squares; their positions were estimated (±0·004) from a difference map.

$|F_c|)^2$. Observed and calculated structure factors for the weighted refinement are listed in Table 5.

Discussion

The conformations of Δ-8,14-anhydrodigitoxigenin (ADTG) and digitoxigenin (DTG) are compared in Fig. 3. The edge-on views of the steroid nuclei illustrate the normal *trans B/C* ring junction and *cis A/B* and *C/D* ring junctions in DTG in which the steroid nucleus is fully saturated and show the effect caused by the double bond at 8,14 in ADTG. Rings *A* and *B* (toward the left side of the illustration) are relatively undisturbed from their chair conformations in ADTG but major changes occur in rings *C* and *D* and the *C/D* ring junction.

Table 5. *Observed and calculated structure factors*

The columns represent the index l, $|F_o|$, $|F_c|$ and φ_{calc}(radians).

0 0 L			
2	3.8	6.7	0.00
4	8.6	7.4	-3.14
6	5.4	6.2	-3.14
8	2.7	1.4	0.00
0 1 L			
1	59.6	62.4	1.57
2	16.5	16.7	1.57
3	31.6	33.5	1.57
4	18.7	16.3	1.57
5	14.5	13.5	1.57
6	9.5	6.8	-1.57
7	1.7	0.9	-1.57
8	1.8	2.4	1.57
0 2 L			
2	23.3	20.6	-3.14
3	5.6	5.1	-0.00
4	15.6	15.1	-3.14
5	24.2	23.9	0.00
6	7.2	7.4	3.14
7	15.9	16.3	-3.14
8	0.0	0.7	0.00
0 3 L			
1	25.6	27.2	-1.57
2	19.2	16.2	-1.57
3	4.2	4.8	1.57
4	8.0	6.8	1.57
5	1.2	1.0	-1.57
6	14.6	15.1	1.57
7	7.3	7.3	1.57
8	10.7	10.6	1.57
0 4 L			
1	29.2	30.9	-3.14
2	17.3	17.8	0.00
3	24.6	25.8	0.00
4	25.2	27.1	0.00
5	14.6	14.3	0.00
6	6.9	7.3	-3.14
7	11.1	11.6	-3.14
8	4.8	1.1	-0.00
0 5 L			
1	10.5	6.9	1.57
2	13.0	12.8	1.57
3	9.9	9.9	1.57
4	1.7	1.0	1.57
5	3.2	4.3	-1.57
6	12.6	12.5	-1.57
7	0.0	1.1	-1.57
8	11.4	11.0	-1.57
0 6 L			
0	45.5	47.2	-3.14
1	4.2	6.8	-3.14
2	4.9	5.2	-3.14
3	19.7	19.2	0.00
4	14.3	13.8	-3.14
5	6.2	5.5	-3.14
6	16.8	17.2	0.00
7	11.6	10.7	0.00
8	2.3	1.4	-3.14
0 7 L			
1	68.7	70.9	-1.57
2	3.0	4.2	1.57
3	2.7	4.8	1.57
4	2.5	1.9	1.57
5	2.1	0.7	1.57
6	6.7	6.2	-1.57
7	6.1	5.8	-1.57
8	8.9	9.0	-1.57
0 8 L			
0	0.0	0.6	-3.14
1	8.1	5.4	0.00
2	28.4	29.0	-3.14
3	8.1	7.9	0.00
4	1.2	1.4	-3.14
5	31.2	30.9	-3.14
6	14.5	15.5	0.00
7	0.9	0.6	0.00
8	2.7	3.0	3.14
0 9 L			
1	22.9	23.3	-1.57
2	12.0	12.5	-1.57
3	1.1	1.1	1.57
4	23.9	23.8	-1.57
5	8.7	6.5	1.57
6	3.9	2.7	1.57
7	2.5	2.4	1.57
8	2.1	1.4	1.57
0 10 L			
0	35.7	35.0	-3.14
1	4.5	4.2	3.14
2	18.1	16.6	0.00
3	2.0	1.5	-3.14
4	1.6	2.2	0.00
5	17.3	16.1	0.00
6	9.3	10.8	-3.14
7	1.8	0.6	0.00
8	1.5	0.4	3.14
0 11 L			
1	58.3	60.2	1.57
2	23.1	21.6	1.57
3	3.4	2.9	1.57
4	22.1	21.4	-1.57
5	15.9	15.9	-1.57
6	17.0	17.2	1.57
7	6.4	6.6	1.57
8	3.0	2.9	1.57
0 12 L			
0	36.4	34.8	-3.14
1	15.4	15.4	-3.14
2	3.0	2.8	-0.00
3	1.7	1.1	-3.14
4	5.4	5.5	3.14
5	2.3	2.6	0.00
6	2.9	3.5	-3.14
7	1.6	2.2	-3.14
0 13 L			
1	18.5	17.7	-1.57
2	15.8	16.6	-1.57
3	7.0	7.4	-1.57
4	3.0	3.2	1.57
5	7.4	7.6	-1.57
6	[illegible]	0.2	1.57
7	1.0	0.7	1.57
0 14 L			
0	18.5	17.9	0.00
1	23.8	22.9	0.00
2	23.9	22.5	0.00
3	6.8	5.1	-3.14
4	8.0	8.5	0.00
5	13.3	12.9	-3.14
6	4.6	4.8	0.00
7	4.1	3.8	-3.14
0 15 L			
1	4.4	5.1	1.57
2	16.5	17.9	-1.57
3	4.3	4.2	1.57
4	16.1	16.2	1.57
5	12.3	11.5	1.57
6	3.0	3.9	1.57
7	5.4	5.4	-1.57
0 16 L			
0	8.9	9.4	0.00
1	21.8	21.7	-3.14
2	2.1	1.2	3.14
3	12.5	12.9	-3.14
4	4.6	4.2	0.00
5	5.3	5.2	-3.14
6	3.0	2.7	-3.14
7	7.7	7.7	0.00
0 17 L			
1	22.2	23.5	1.57
2	7.8	6.8	1.57
3	1.8	1.0	1.57
4	1.7	1.9	-1.57
5	2.2	1.2	-1.57
6	4.6	4.6	-1.57
0 18 L			
0	26.9	27.0	0.00
1	3.0	2.3	0.00
2	19.0	18.9	-3.14
3	6.1	7.0	-3.14
4	2.0	2.1	0.00
5	15.5	15.2	0.00
6	8.5	7.7	-3.14
0 19 L			
1	5.1	5.4	-1.57
2	21.0	21.0	1.57
3	1.7	1.9	-1.57
4	3.7	3.5	-1.57
5	2.8	2.5	1.57
6	5.2	5.3	-1.57
0 20 L			
0	3.7	2.9	-3.14
1	25.9	26.9	0.00
2	1.1	1.4	0.00
3	5.1	6.0	0.00
4	11.6	12.0	-3.14
5	5.7	4.9	0.00
0 21 L			
1	17.9	17.4	-1.57
2	1.3	0.6	1.57
3	8.1	7.7	-1.57
4	7.7	6.3	1.57
5	1.8	1.7	-1.57
0 22 L			
0	17.8	16.6	-3.14
1	2.0	1.1	0.00
2	4.9	4.9	0.00
3	4.9	5.3	0.00
4	2.6	2.1	0.00
5	1.4	2.2	-3.14
0 23 L			
1	1.9	1.6	1.57
2	7.1	7.3	-1.57
3	4.0	3.4	-1.57
4	2.3	1.4	1.57
0 24 L			
0	1.3	1.1	-3.14
1	11.2	11.2	-3.14
2	0.0	2.2	0.00
3	4.3	3.7	0.00
4	0.9	1.2	-3.14
0 25 L			
1	2.4	2.2	1.57
2	0.7	0.5	1.57
3	5.0	4.6	1.57
0 26 L			
0	8.7	8.0	0.00
1	2.7	2.5	-3.14
2	3.0	2.6	-3.14
0 27 L			
1	0.7	0.6	1.57
1 0 L			
1	1.6	2.9	1.57
2	78.5	79.1	0.00
3	44.1	45.4	1.57
4	25.9	25.0	-3.14
5	3.9	2.3	1.57
6	9.4	8.7	-3.14
7	15.4	15.5	-1.57
8	3.5	3.3	0.00
1 1 L			
0	1.3	1.7	-1.57
2	29.8	29.0	-2.73
3	39.9	39.1	-2.42
4	23.8	22.7	2.17
5	15.9	16.0	1.10
6	5.8	5.3	0.73
7	7.7	7.6	1.01
8	3.1	3.3	-1.76
1 2 L			
0	12.8	11.2	1.57
2	46.0	45.6	-1.36
3	39.4	39.1	3.01
4	21.9	21.0	-2.91
5	4.4	7.7	-0.25
6	27.4	26.6	1.65
7	2.4	2.5	2.61
8	6.3	6.3	-2.35
1 3 L			
0	9.4	7.8	1.57
2	27.1	27.7	-1.63
3	15.5	14.2	-0.31
4	22.8	22.4	-1.31
5	9.7	10.0	-2.16
6	8.8	8.3	-0.33
7	5.3	4.7	2.63
8	3.9	3.8	2.56
1 4 L			
0	89.8	90.4	-1.57
2	27.3	25.0	-2.10
3	14.0	13.1	0.71
4	27.0	27.1	0.44
5	14.1	14.4	-2.25
6	18.6	19.0	0.53
7	10.7	11.1	1.51
8	4.2	4.3	2.23
1 5 L			
0	68.1	69.3	1.57
1	20.1	20.1	2.00
2	30.5	30.4	0.80
3	37.9	39.8	0.85
4	22.3	22.1	1.26
5	14.5	14.5	2.24
6	12.6	12.5	-0.49
7	11.1	10.0	2.18
8	3.4	3.4	-0.80
1 6 L			
0	2.8	2.9	1.57
1	79.6	76.1	-2.65
2	38.4	35.9	-1.49
3	17.4	17.7	-1.49
4	19.0	19.1	0.74
5	11.9	12.4	0.78
6	25.7	25.9	-2.24
7	0.7	2.9	-2.39
8	3.8	3.9	1.41
1 7 L			
0	72.4	74.4	-1.57
1	40.4	41.5	-0.64
2	10.9	11.5	-2.01
3	8.4	7.7	-0.62
4	8.9	9.0	-3.07
5	16.0	15.9	0.95
6	9.4	9.8	2.34
7	7.9	7.8	0.67
8	6.6	5.7	-0.27
1 8 L			
0	25.2	25.4	1.57
1	14.9	12.1	1.67
2	10.8	10.2	-2.87
3	26.1	26.4	-1.40
4	19.3	21.3	3.08
5	33.0	34.2	0.18
6	0.9	1.3	-0.99
7	8.9	9.0	-2.60
8	4.0	4.2	-1.03
1 9 L			
0	0.0	0.9	-1.57
1	18.4	17.8	-0.68
2	23.6	21.8	0.87
3	22.6	22.2	-2.77
4	12.8	12.6	-1.78
5	9.2	9.7	-1.37
6	6.5	6.5	2.53
7	15.7	15.5	-1.54
8	8.2	7.8	2.22
1 10 L			
0	25.6	26.8	1.57
1	54.2	54.2	1.60
2	53.3	54.6	2.17
3	19.6	19.9	-2.98
4	6.6	6.9	-2.62
5	15.5	15.3	-3.09
6	20.2	20.2	0.42
7	4.7	4.8	0.05
8	7.7	7.3	-0.47
1 11 L			
0	26.5	26.2	-1.57
1	33.7	33.9	2.98
2	16.5	15.9	1.58
3	15.2	15.2	1.77
4	14.7	14.4	-1.38
5	19.0	18.9	-2.13
6	6.6	5.9	-2.04
7	6.2	6.3	-1.51
1 12 L			
0	26.4	25.0	-1.57
1	24.1	24.1	-1.45
2	24.8	23.3	1.71
3	3.0	3.6	0.22
4	27.8	28.3	-0.56
5	16.7	17.0	-2.57
6	6.8	6.4	2.61
7	2.4	2.6	0.77
1 13 L			
0	12.5	12.3	1.57
1	14.8	13.5	2.61
2	4.4	4.4	3.05
3	10.2	9.6	-0.51
4	10.7	11.3	0.59
5	7.5	8.4	0.24
6	4.7	4.6	-1.85
7	4.1	3.6	1.54
1 14 L			
0	5.0	3.7	-1.57
1	31.8	31.2	-1.67
2	24.5	24.6	-0.99
3	13.8	13.8	0.92
4	10.5	10.1	0.40
5	3.2	3.6	1.13
6	7.4	7.5	-2.87
7	3.7	3.5	2.42
1 15 L			
0	24.2	23.4	1.57
1	12.1	11.4	0.78
2	7.8	7.3	2.99
3	7.8	7.9	-2.20
4	12.2	12.9	-2.11
5	13.5	13.2	1.42
6	3.0	1.5	-0.39
7	2.8	2.0	1.95
1 16 L			
0	5.3	4.5	1.57
1	6.5	7.0	1.28
2	4.6	4.6	-2.11
3	8.5	8.8	2.27
4	17.1	16.9	3.10
5	7.3	6.8	1.59
6	7.7	7.2	-2.06
7	3.3	3.4	-0.16
1 17 L			
0	5.3	5.3	-1.57
1	12.1	12.4	0.72
2	9.0	9.1	-2.29
3	3.6	3.8	1.30
4	8.0	7.7	2.51
5	5.8	6.1	-1.37
6	3.0	2.2	0.62
1 18 L			
0	6.1	5.2	1.57
1	13.4	13.2	0.61
2	3.5	3.0	1.32
3	2.3	1.5	0.14
4	5.0	5.9	1.00
5	6.7	7.0	-2.41
6	0.0	0.3	-0.90
1 19 L			
0	16.6	16.6	-1.57
1	7.2	6.6	1.18
2	8.7	9.1	0.90
3	2.4	1.0	-0.63
4	15.0	14.6	1.20
5	2.7	2.7	3.04
6	3.4	3.2	0.54
1 20 L			
0	10.7	10.8	-1.57
1	9.8	10.6	1.62
2	8.5	8.4	-1.96
3	4.7	5.6	0.10
4	3.1	3.7	-0.38
5	2.1	2.6	0.38
1 21 L			
0	5.2	5.5	1.57
1	11.9	12.0	-1.16
2	2.1	0.5	-1.94
3	1.8	0.9	2.96
4	0.4	1.4	-3.01
5	0.7	1.3	2.12
1 22 L			
0	2.1	1.7	-1.57
1	8.3	8.1	-2.38
2	3.4	3.8	-0.02
3	2.7	2.7	-1.12
4	5.5	2.5	-3.10
5	2.7	2.2	-2.43
1 23 L			
0	3.6	3.0	1.57
1	3.1	3.7	2.43
2	11.0	10.9	-1.28
3	2.2	1.6	1.92
4	0.0	0.9	-1.00
1 24 L			
0	7.4	7.3	1.57
1	4.0	4.5	-1.67
2	6.6	6.4	0.54
3	5.2	5.7	-1.92
4	4.4	4.1	1.02
1 25 L			
0	4.8	4.5	-1.57
1	3.1	3.8	-3.10
2	0.0	1.3	-0.10
3	1.9	2.4	-1.73
1 26 L			
0	4.2	4.1	1.57
1	4.2	3.6	2.54
2	2.5	2.4	0.85
1 27 L			
0	1.6	1.5	1.57
1	4.8	4.8	-2.50
2 0 L			
0	12.8	12.7	-3.14
2	36.6	34.7	-3.14
3	46.1	45.6	1.57
4	14.7	14.6	0.00
5	15.9	16.1	-1.57
6	0.8	0.7	3.14
7	1.5	1.9	1.57
8	3.0	2.9	-3.14
2 1 L			
0	12.3	11.0	-3.14
1	40.8	41.9	0.23
2	26.9	26.4	0.50
3	60.1	60.2	-2.06
4	28.5	25.8	3.00
5	18.7	18.7	-3.11
6	14.3	14.6	0.27
7	9.8	10.0	2.75
8	4.2	4.9	1.91
2 2 L			
0	25.0	24.5	0.00
1	44.2	44.9	-0.13
2	37.5	38.6	-0.87
3	49.8	51.4	3.08
4	10.0	10.2	0.75
5	7.9	7.4	2.75
6	22.5	23.3	-1.50
7	4.9	5.1	3.12
8	2.9	2.4	-0.35
2 3 L			
0	41.5	43.0	0.00
1	65.0	70.7	1.99
2	6.2	5.4	-1.76
3	33.8	33.4	-0.69
4	29.0	28.2	-2.06
5	17.2	16.6	1.37
6	6.1	6.7	-1.46
7	2.2	2.5	2.40
8	1.1	2.2	-2.29
2 4 L			
0	48.2	47.0	-3.14
1	55.1	55.9	-0.37
2	25.0	24.1	1.18
3	10.1	10.6	-0.93
4	23.5	23.3	-3.08
5	20.4	20.7	0.71
6	11.6	11.6	2.17
7	9.7	10.1	-2.38
8	0.9	1.6	-0.75
2 5 L			
0	76.0	76.5	-3.14
1	31.3	32.9	2.69
2	27.2	26.9	-1.34
3	2.0	0.9	0.44
4	9.3	8.7	-0.15
5	18.7	19.2	-0.34
6	14.8	14.0	2.24
7	12.0	11.6	-1.10
8	3.0	2.7	-1.90
2 6 L			
0	21.9	19.1	-3.14
1	28.5	29.6	-1.64
2	15.8	13.8	-0.93
3	6.3	6.7	2.66
4	12.8	12.2	-1.03
5	9.8	10.1	-0.86
6	25.7	26.1	1.44
7	5.5	6.2	1.48
8	6.3	6.5	2.32
2 7 L			
0	9.1	8.6	0.00
1	21.8	20.0	1.13
2	23.6	21.9	-1.22
3	13.2	12.9	-0.35
4	25.4	24.6	0.26
5	17.1	17.5	-1.53
6	5.7	5.2	1.08
7	7.2	7.3	-0.59
8	1.4	1.9	-2.16
2 8 L			
0	17.8	17.5	0.00
1	14.7	13.9	0.22
2	23.4	22.1	-2.00
3	12.2	12.5	-2.48
4	5.7	5.9	1.00
5	3.5	4.2	2.47
6	9.7	8.3	-0.64
7	11.0	11.5	0.11
8	3.4	3.6	0.37
2 9 L			
0	15.9	16.4	0.00
1	27.1	27.3	0.15
2	41.6	41.8	1.76
3	18.5	18.5	-2.65
4	25.7	26.0	1.96
5	12.6	12.4	1.87
6	6.3	6.1	-1.35
7	6.7	6.8	0.70
8	2.1	1.9	-2.79
2 10 L			
0	16.2	15.3	0.00
1	4.4	3.7	1.42
2	22.2	22.9	2.37
3	18.5	18.1	-2.16
4	14.7	15.0	-3.02
5	21.1	22.1	-2.51
6	5.5	5.4	-2.05
7	4.8	4.8	-1.93
8	4.4	4.2	-0.55
2 11 L			
0	7.5	8.1	3.14
1	38.9	39.3	-2.01
2	9.6	8.9	1.20
3	6.5	6.0	-2.53
4	4.4	4.8	-1.29
5	14.7	15.7	1.38
6	19.6	19.8	-1.36
7	5.2	2.9	0.98
2 12 L			
0	16.3	16.0	0.00
1	25.2	25.0	2.67
2	11.9	11.1	0.27
3	13.5	13.6	1.11
4	11.5	11.3	0.09
5	8.9	9.1	-2.60
6	8.9	6.8	-1.42
7	6.1	5.7	1.66
2 13 L			
0	13.2	12.7	-3.14
1	7.6	7.6	-1.37
2	19.4	20.2	-1.48
3	16.1	15.8	1.00
4	7.9	6.2	-1.60
5	10.9	11.0	-0.11
6	0.0	1.2	2.70
7	6.4	5.5	2.30
2 14 L			
0	2.5	2.0	-0.00
1	22.4	22.6	2.64
2	3.8	3.1	2.96
3	11.9	12.6	-0.09
4	10.1	10.8	1.23
5	14.9	14.8	0.87
6	3.7	4.3	-2.62
7	3.1	3.1	-0.20
2 15 L			
0	8.5	6.4	0.00
1	10.0	9.6	2.43
2	8.6	8.3	-2.63
3	6.6	6.4	2.65
4	10.4	11.5	2.25
5	23.9	24.8	-2.63
6	2.5	1.8	1.76
7	3.7	2.8	3.07
2 16 L			
0	13.6	13.6	0.00
1	8.7	9.2	-0.34
2	17.2	16.1	-1.99
3	11.7	11.6	-0.47
4	12.5	12.2	-1.52
5	13.7	13.6	2.49
6	3.5	3.6	-2.89
2 17 L			
0	14.8	13.7	0.00
1	19.0	18.9	0.61
2	7.1	6.3	-2.69
3	4.2	4.2	2.41
4	0.0	1.7	2.01
5	2.3	1.7	-0.61
6	4.7	4.4	2.93
2 18 L			
0	8.4	7.4	-3.14
1	17.8	16.7	-0.28
2	10.7	9.8	2.55
3	10.0	10.6	1.32
4	3.7	4.2	-1.13
5	6.6	6.8	-2.33
6	5.5	5.1	1.22
2 19 L			
0	2.8	2.8	-3.14
1	5.1	4.7	-2.36
2	10.0	10.4	0.12
3	3.0	3.2	-0.69
4	9.7	9.3	-2.54
5	10.8	10.2	0.03
6	0.8	1.2	-1.51
2 20 L			
0	7.4	7.4	-3.14
1	4.1	3.1	-2.22
2	5.8	6.6	0.43
3	8.0	7.7	2.79
4	11.3	11.8	1.64
5	13.9	13.5	-0.83
2 21 L			
0	6.7	6.5	0.00
1	5.0	4.6	-2.30
2	9.4	9.7	0.66
3	5.9	5.7	-0.42
4	7.3	7.6	-0.13
5	1.1	1.3	2.86
2 22 L			
0	5.2	4.9	-3.14
1	9.3	9.4	3.01
2	6.9	6.4	0.23
3	5.9	5.7	-2.22
4	6.2	6.4	2.32
5	11.5	11.1	1.21
2 23 L			
0	11.9	11.8	-3.14
1	3.6	4.4	-0.14
2	3.8	3.8	-2.53
3	3.2	3.4	0.40
4	2.9	1.7	0.73
2 24 L			
0	4.1	4.1	-3.14
1	9.3	9.0	-1.70
2	2.4	2.2	1.23
3	1.3	1.3	-0.00
4	4.3	4.5	-1.08
2 25 L			
0	2.0	2.2	-1.00
1	5.6	5.3	2.58
2	4.7	4.1	-2.33
3	1.9	1.9	-2.42
2 26 L			
0	0.7	0.1	3.14
1	3.5	3.6	1.48
2	7.8	7.5	-1.75
2 27 L			
0	0.8	0.4	3.14
3 0 L			
1	18.8	19.8	1.57
2	37.5	37.5	-3.14
3	4.2	4.6	1.57
4	1.2	0.7	0.00
5	6.2	5.0	1.57
6	1.9	0.4	-3.14
7	4.6	5.8	1.57
8	6.3	6.5	0.00
3 1 L			
0	14.1	13.0	1.57
1	46.7	46.6	2.46
2	35.0	34.9	1.33
3	9.7	9.5	-0.59
4	14.1	13.9	-2.61
5	9.9	9.5	-0.78
6	16.5	17.0	-2.46
7	8.4	6.5	-1.10
8	1.5	1.6	-0.11
3 2 L			
0	55.4	56.0	1.57
1	39.6	39.2	-0.99
2	13.9	12.6	0.44
3	11.2	12.3	1.72
4	13.1	12.3	-0.84
5	6.7	7.3	-0.95
6	10.0	10.3	1.51
7	3.5	2.7	-0.13
8	1.7	1.4	-1.26
3 3 L			
0	59.2	58.9	-1.57
1	46.2	48.5	1.71
2	12.7	11.0	-1.80
3	45.0	45.1	1.90
4	16.1	16.4	-2.89
5	12.9	12.6	0.22
6	14.1	14.3	2.45
7	1.6	2.2	-2.61
8	1.8	1.0	-1.39
3 4 L			
0	64.2	64.0	1.57
1	21.1	21.5	-2.21
2	23.1	23.0	-1.75
3	18.4	17.8	-0.31
4	9.3	6.3	-2.66
5	14.0	14.3	-2.92
6	5.6	5.0	-2.26
7	4.7	5.5	-1.15
8	4.7	4.5	2.57
3 5 L			
0	2.1	2.0	1.57
1	33.9	32.9	1.09
2	57.4	58.2	-2.70
3	7.1	6.7	-0.96
4	2.8	3.7	-0.30
5	14.8	14.9	1.48
6	4.7	5.7	0.06
7	7.8	7.8	2.20
8	3.2	3.2	2.52
3 6 L			
0	9.7	6.7	1.57
1	14.9	14.1	0.47
2	34.6	33.9	2.18
3	35.5	34.4	-0.46
4	12.9	12.8	0.49
5	6.2	5.3	0.24
6	13.1	13.3	-2.06
7	4.1	3.7	0.08
8	6.4	6.4	1.30
3 7 L			
0	35.5	34.4	1.57
1	9.0	6.3	-0.48
2	38.7	38.5	2.16
3	32.4	31.6	-1.39
4	11.9	11.9	1.45
5	12.1	12.4	2.97
6	16.8	17.4	0.34
7	3.3	3.5	3.13
8	1.9	1.	1.74
3 8 L			
0	15.8	14.3	-1.57
1	25.2	25.2	1.39
2	30.5	30.0	0.39
3	16.0	15.1	-2.94
4	7.9	7.4	2.07
5	17.9	18.8	1.65
6	5.5	6.2	-0.97
7	7.6	7.2	2.56
8	2.9	3.5	2.71
3 9 L			
0	2.7	2.2	1.57
1	19.5	18.2	0.26
2	16.3	15.2	-0.58
3	5.0	5.2	-0.56
4	15.6	16.3	-2.82
5	20.1	20.3	-2.87
6	6.8	7.2	-2.52
7	6.7	6.9	-0.64
8	4.1	4.2	-0.38
3 10 L			
0	19.1	19.1	-1.57
1	22.4	21.7	-3.10
2	14.2	13.4	-1.07
3	6.2	6.2	-2.81
4	21.2	21.3	-2.44
5	14.8	14.5	-2.90
6	11.2	11.3	1.12
7	3.8	3.8	-0.67
3 11 L			
0	2.3	2.0	-1.57
1	24.9	25.1	-0.49
2	21.6	20.6	-0.83
3	3.8	3.7	1.88
4	18.1	17.7	-0.48
5	11.1	11.4	-1.89
6	4.9	5.2	-2.76
7	4.2	4.3	0.88
3 12 L			
0	6.9	6.7	1.57
1	12.1	12.3	1.83
2	3.1	2.6	-1.61
3	13.1	13.0	1.81
4	13.3	13.4	-0.10
5	12.6	12.3	-1.43
6	5.0	4.8	0.40
7	0.0	3.1	0.54
3 13 L			
0	4.9	4.2	1.57
1	17.5	17.4	-3.10
2	13.3	14.1	-1.97
3	13.8	13.5	1.83
4	24.9	26.0	0.53
5	6.1	5.9	0.59
6	1.6	1.9	0.98
7	4.5	1.3	-1.86
3 14 L			
0	24.1	23.7	-1.57
1	20.1	20.7	0.23
2	5.2	4.7	2.24
3	12.3	12.9	1.83
4	3.3	3.7	-2.08
5	6.9	6.8	-0.13
6	5.1	4.7	-1.71
7	5.1	4.5	-2.55
3 15 L			
0	2.9	2.7	-1.57
1	11.6	11.1	-2.42
2	3.3	3.5	0.53
3	9.3	9.5	-0.35
4	3.5	2.6	2.10
5	15.2	15.6	0.09
6	2.6	3.2	1.83
7	4.9	4.6	-2.09
3 16 L			
0	13.0	12.7	1.57
1	15.8	16.1	-2.02
2	3.7	3.1	-0.73
3	5.5	5.4	0.31
4	14.8	15.5	2.30
5	8.3	8.0	0.53
6	4.3	4.2	1.60
3 17 L			
0	9.6	9.3	1.57
1	15.9	16.0	-2.70
2	13.7	14.4	0.25
3	7.7	7.2	-2.62
4	20.1	20.6	3.12
5	2.1	1.7	-2.21
6	2.4	1.6	2.60

Table 5 (*cont.*)

	3	18	L
0	5,7	6,7	-1,57
1	11,8	11,5	-3,12
2	10,9	10,9	-1,72
3	11,1	11,4	-1,49
4	3,6	3,8	0,47
5	3,0	3,4	-2,92
6	5,0	4,5	1,80
	3	19	L
0	0,0	1,4	-1,57
1	13,3	13,8	0,79
2	9,1	9,1	2,18
3	7,0	5,9	1,88
4	10,9	10,3	-2,36
5	7,2	7,5	2,53
	3	20	L
0	3,6	4,3	1,57
1	15,3	15,2	-0,44
2	7,7	7,8	2,40
3	8,5	8,5	-1,91
4	2,9	3,3	1,67
5	12,0	11,6	-1,37
	3	21	L
0	1,5	1,7	-1,57
1	7,4	7,6	-0,76
2	6,6	6,9	2,54
3	3,5	3,0	2,08
4	14,6	14,6	-0,08
5	2,0	2,2	-2,34
	3	22	L
0	11,8	11,1	1,57
1	2,0	1,2	0,40
2	7,0	6,3	0,21
3	0,0	1,0	0,22
4	0,0	1,6	-2,42
	3	23	L
0	3,6	3,4	-1,57
1	1,7	2,1	2,52
2	6,2	5,6	-2,05
3	3,4	3,2	-1,43
4	4,7	4,4	1,47
	3	24	L
0	5,8	5,6	1,57
1	6,0	6,3	2,72
2	1,5	1,5	-2,54
3	1,3	0,6	1,80
	3	25	L
0	3,1	3,4	-1,57
1	3,8	3,6	2,53
2	3,0	3,0	0,00
	3	26	L
0	7,0	6,9	-1,57
1	7,1	7,0	1,60
	4	0	L
0	36,3	35,3	-3,14
1	46,4	47,0	1,57
2	24,3	23,9	-3,14
3	24,7	23,6	1,57
4	4,9	3,7	3,14
5	4,9	3,7	1,57
6	8,5	8,3	-3,14
7	4,5	4,4	-1,57
8	3,3	2,9	0,00
	4	1	L
0	32,8	32,2	-3,14
1	36,2	36,3	2,45
2	48,7	50,3	-1,69
3	28,6	28,2	-3,14
4	8,9	8,8	-2,18
5	10,0	9,9	0,47
6	11,5	10,6	-2,13
7	9,8	10,2	-0,26
8	6,2	6,3	1,42
	4	2	L
0	48,1	46,6	0,00
1	14,6	14,2	-1,91
3	17,0	17,0	-0,58
4	13,1	12,8	-1,23
5	10,0	10,6	0,78
6	9,0	7,5	-2,34
7	2,0	2,4	-2,89
8	1,5	1,1	-1,18
	4	3	L
0	5,3	6,3	3,14
1	33,8	33,9	0,85
2	6,9	5,4	2,04
3	18,2	18,4	-1,41
4	15,8	15,0	3,00
5	9,3	9,1	-3,01
6	10,6	10,7	-2,88
7	10,3	9,4	-1,88
8	2,3	2,0	-1,51
	4	4	L
0	3,5	3,3	0,00
1	25,9	25,3	-1,36
2	21,6	21,6	1,13
3	30,8	30,8	-1,94
4	2,1	1,1	-3,02
5	5,7	5,8	-0,94
6	10,7	9,0	-0,37
7	2,4	2,8	2,33
8	4,0	4,0	-2,05
	4	5	L
0	43,7	43,1	0,00
1	20,2	20,8	-0,22
2	16,0	16,0	1,57
3	17,6	17,1	0,27
4	6,0	6,3	2,50
5	16,6	16,6	-1,68
6	10,0	10,0	0,65
7	4,2	4,1	2,54
8	3,2	2,8	-2,01
	4	6	L
0	38,8	36,7	-3,14
1	39,4	40,2	2,38
2	29,5	29,2	-0,53
3	16,7	16,1	1,12
4	13,2	13,1	0,94
5	6,3	8,4	-1,72
6	5,2	6,1	-1,43
7	3,5	2,7	1,82
8	0,4	0,2	1,03
	4	7	L
0	6,6	6,5	-3,14
1	4,0	3,8	2,03
2	13,8	16,0	2,03
3	28,7	27,5	0,91
4	18,8	19,1	1,45
5	8,1	7,5	-0,37
6	11,9	12,0	0,79
7	6,3	6,4	2,28
8	2,1	1,6	-1,37
	4	8	L
0	2,8	3,3	-3,14
1	8,2	7,8	-2,93
2	15,0	15,4	-0,36
3	4,7	5,3	1,91
4	9,5	8,5	1,58
5	4,6	4,6	2,94
6	5,5	6,5	-1,19
7	0,0	0,2	-1,94
	4	9	L
0	0,0	0,2	3,14
1	19,6	19,1	-3,08
2	11,8	11,6	0,64
3	1,4	1,4	2,33
4	4,5	5,0	-0,26
5	4,9	5,2	3,08
6	6,3	6,6	2,91
7	0,0	1,4	1,60
	4	10	L
0	13,2	13,4	0,00
1	6,0	6,5	0,29
2	12,4	12,8	0,81
3	0,0	3,4	0,99
4	6,4	6,5	-1,99
5	11,2	11,6	2,92
6	9,9	10,2	0,84
7	5,8	4,9	-0,61
	4	11	L
0	6,8	6,4	-3,14
1	1,8	1,6	-0,75
2	17,2	16,4	2,96
3	9,5	8,7	-2,12
4	10,9	11,2	-2,12
5	10,6	11,2	2,00
6	6,9	7,0	-2,04
7	4,1	3,7	0,23
	4	12	L
0	18,0	17,9	-3,14
1	25,4	26,6	-1,48
2	5,1	4,9	-0,20
3	3,2	3,8	0,83
4	14,5	14,2	3,03
5	7,7	7,9	0,22
6	13,2	13,2	2,17
7	2,7	2,6	2,66
	4	13	L
0	35,4	36,6	0,00
1	9,2	9,1	-1,16
2	15,9	16,2	0,66
3	7,6	6,6	-1,72
4	7,7	8,2	-1,77
5	2,9	2,6	3,12
6	5,9	5,5	0,99
7	7,8	7,2	3,00
	4	14	L
0	0,0	1,6	3,14
1	23,3	24,5	3,01
2	11,8	11,9	-1,73
3	13,0	13,7	0,91
4	2,4	2,5	-1,90
5	7,8	7,5	0,60
6	10,4	9,9	-2,02
7	0,0	0,9	2,88
	4	15	L
0	7,6	7,1	3,14
1	2,9	3,3	-1,49
2	15,9	16,8	-1,48
3	4,4	4,6	0,74
4	9,1	8,8	-0,45
5	11,0	10,7	-0,53
6	4,2	2,5	-0,97
	4	16	L
0	15,0	16,4	-0,00
1	26,1	26,4	0,49
2	15,0	15,2	3,11
3	3,2	3,6	-2,00
4	9,9	10,0	-0,38
5	3,6	2,7	-0,01
6	2,1	1,2	2,22
	4	17	L
0	47,6	47,9	-3,14
1	0,0	2,0	-1,22
2	11,3	12,0	-2,61
3	4,6	4,5	-2,69
4	7,1	8,0	0,74
5	3,4	3,9	0,98
6	1,2	1,6	-1,41
	4	18	L
0	8,1	7,9	-3,14
1	19,9	19,6	-0,35
2	5,5	5,4	1,16
3	12,0	12,1	-2,18
4	2,9	2,5	-2,48
5	8,5	8,7	-2,48
6	3,0	2,4	1,98
	4	19	L
0	3,3	3,7	-0,00
1	4,6	5,5	1,76
2	10,2	9,7	0,60
3	2,2	2,7	-2,36
4	1,0	0,8	2,83
5	2,1	2,0	2,22
	4	20	L
0	3,8	3,9	3,14
1	9,2	9,1	2,55
2	1,3	1,8	1,50
3	3,0	2,7	-3,13
4	5,5	5,3	0,87
5	4,3	4,1	-0,34
	4	21	L
0	18,4	18,3	0,00
1	8,4	8,7	1,92
2	4,4	4,7	1,55
3	2,9	3,3	2,23
4	5,9	6,2	-3,11
	4	22	L
0	1,8	1,1	0,00
1	8,8	9,6	-2,92
2	2,5	3,0	-1,21
3	2,3	2,3	-2,23
4	4,9	4,9	-2,20
	4	23	L
0	12,9	11,3	0,00
1	1,7	2,2	0,00
2	2,4	2,4	-0,69
3	4,4	4,2	-0,73
	4	24	L
0	3,8	3,7	0,00
1	8,3	8,4	1,53
2	2,8	2,8	0,93
3	4,1	4,3	1,80
	4	25	L
0	12,7	12,5	-3,14
1	0,0	0,6	0,33
2	4,3	4,7	-2,91
	4	26	L
0	6,0	5,8	-3,14
	5	0	L
1	35,2	33,9	1,57
2	26,6	25,7	-3,14
3	7,1	5,9	-1,57
4	1,6	1,2	-3,14
5	5,1	5,2	1,57
6	8,0	8,2	0,00
7	2,5	2,3	-1,57
8	1,8	2,1	0,00
	5	1	L
0	52,2	53,0	1,57
1	13,5	14,1	1,56
2	13,5	12,9	-2,59
3	10,2	11,5	3,05
4	6,7	6,7	-0,59
5	14,8	15,4	-1,33
6	7,3	6,4	-0,63
7	6,7	6,8	-0,14
8	3,4	3,6	1,71
	5	2	L
0	30,1	29,0	-1,57
1	10,9	11,9	-2,71
2	19,0	18,9	0,82
3	14,9	15,4	1,93
4	14,9	14,4	1,53
5	7,1	6,2	-2,71
6	12,3	12,6	1,15
7	5,7	5,7	-3,09
8	4,6	5,1	-1,51
	5	3	L
0	27,3	24,6	-1,57
1	28,1	27,8	1,17
2	38,7	37,8	-2,50
3	20,0	20,3	0,05
4	16,2	16,0	2,53
5	5,9	5,8	-1,93
6	8,7	8,9	-0,34
7	4,0	4,0	-1,90
8	2,0	2,7	-0,30
	5	4	L
0	55,5	53,7	1,57
1	6,5	5,9	-1,30
2	20,2	20,2	-0,53
3	15,1	14,7	2,81
4	15,4	15,9	1,83
5	6,8	6,7	-0,90
6	7,0	6,1	1,97
7	4,7	5,0	1,76
8	3,5	3,4	-1,88
	5	5	L
0	16,3	15,6	-1,57
1	36,3	35,8	-2,43
2	12,9	11,6	2,88
3	3,6	4,6	1,65
4	20,1	20,7	-2,90
5	10,3	10,7	3,10
6	7,4	6,8	2,41
7	7,2	7,3	-2,48
	5	6	L
0	20,8	19,8	-1,57
1	10,4	10,4	0,82
2	21,4	22,8	-1,89
3	14,9	14,4	-2,51
4	7,1	5,2	1,93
5	8,1	8,3	-0,09
6	5,5	5,5	0,19
7	7,2	6,9	0,26
	5	7	L
0	16,8	16,7	1,57
1	21,0	19,6	-0,86
2	32,5	33,1	0,41
3	9,3	8,8	2,54
4	2,3	2,9	3,10
5	5,0	5,3	-2,47
6	8,4	8,1	2,28
7	5,3	5,5	-2,71
	5	8	L
0	4,9	4,1	-1,57
1	8,7	8,5	-2,26
2	20,8	20,7	2,56
3	17,1	17,6	-1,20
4	3,3	4,4	1,01
5	10,1	10,8	2,91
6	13,0	12,7	-2,47
7	13,1	12,7	-1,35
	5	9	L
0	16,8	16,5	-1,57
1	3,0	3,1	-1,22
2	23,8	24,2	0,63
3	1,4	3,0	0,41
4	18,7	18,0	-0,10
5	12,5	12,7	-0,53
6	5,9	6,0	0,01
7	4,6	4,4	0,04
	5	10	L
0	13,1	12,0	1,57
1	4,0	3,9	-2,34
2	5,2	5,1	1,54
3	5,9	5,7	-0,24
4	20,2	20,8	-1,38
5	5,0	5,2	0,94
6	8,9	9,5	-3,12
7	9,8	9,8	2,87
	5	11	L
0	4,6	5,0	-1,57
1	11,0	10,1	2,91
2	4,3	4,3	-2,60
3	0,8	1,9	-0,25
4	5,3	5,6	0,92
5	11,4	11,4	0,66
6	5,1	5,0	-1,34
7	6,6	6,4	1,30
	5	12	L
0	7,4	6,9	-1,57
1	13,1	13,8	0,91
2	13,9	13,3	-0,74
3	11,7	12,3	2,13
4	11,1	12,1	-1,48
5	6,7	7,4	0,18
6	4,7	5,1	1,44
7	10,7	9,7	1,71
	5	13	L
0	13,7	13,8	-1,57
1	14,6	14,3	0,61
2	12,0	12,9	3,13
3	3,0	4,0	0,94
4	3,2	3,5	-2,35
5	8,6	8,9	2,51
6	4,1	2,8	2,49
	5	14	L
0	2,0	3,3	-1,57
1	21,5	22,7	-0,79
2	17,4	16,2	1,42
3	5,1	5,0	1,43
4	5,1	5,0	1,24
5	3,2	3,6	1,06
6	3,5	3,1	-0,06
	5	15	L
0	9,1	9,1	1,57
1	1,4	1,8	-2,53
2	8,9	9,5	2,72
3	9,5	9,2	-3,00
4	3,9	4,5	1,58
5	3,1	3,4	-0,95
6	2,7	3,2	2,50
	5	16	L
0	4,4	3,8	-1,57
1	28,5	29,6	-2,39
2	12,0	12,7	-1,77
3	9,0	9,0	-0,61
4	7,3	7,8	1,15
5	4,6	4,3	-2,67
6	3,7	3,6	-1,17
	5	17	L
0	3,1	2,8	-1,57
1	8,0	8,1	-0,26
2	7,2	8,0	-1,29
3	11,3	11,7	-1,38
4	6,3	5,8	-2,00
5	4,8	4,6	0,92
6	0,0	0,8	-0,19
	5	18	L
0	10,5	10,8	1,57
1	21,1	21,5	2,00
2	4,4	4,8	2,36
3	6,4	6,5	-0,28
4	0,0	2,2	1,36
5	4,7	4,7	-1,46
	5	19	L
0	7,5	6,0	1,57
1	13,1	13,7	-3,12
2	5,2	4,8	-1,48
3	1,2	1,2	-2,55
4	2,1	1,9	-1,94
5	4,0	3,4	-2,83
	5	20	L
0	6,5	6,5	-1,57
1	11,1	10,7	0,98
2	2,9	3,1	1,55
3	8,6	8,8	2,25
4	4,2	3,7	3,01
	5	21	L
0	2,5	1,4	-1,57
1	10,2	9,8	1,88
2	5,1	5,1	2,88
3	0,5	1,2	0,30
4	2,1	2,2	1,16
	5	22	L
0	2,2	2,2	-1,57
1	8,5	9,2	-0,75
2	5,5	6,0	-1,79
3	5,3	5,3	-2,62
4	2,7	2,5	2,73
	5	23	L
0	0,0	0,4	-1,57
1	13,1	13,1	-0,15
2	6,0	5,8	1,42
3	2,4	2,7	2,56
	5	24	L
0	8,8	8,4	1,57
1	2,6	3,1	-3,09
2	2,5	2,6	-1,65
	5	25	L
0	4,1	3,8	1,57
1	2,4	2,3	-1,40
	6	0	L
0	60,8	58,6	0,00
1	23,7	23,5	-1,57
2	23,6	22,8	-3,14
3	26,7	27,0	-1,57
4	20,6	19,4	-3,14
5	0,0	0,4	1,57
6	3,4	1,5	-0,00
7	0,4	0,1	1,57
	6	1	L
0	5,5	4,9	0,00
1	15,3	15,1	0,25
2	5,6	5,8	-1,08
3	13,7	13,3	0,43
4	14,5	14,2	-0,68
5	5,7	6,8	2,45
6	6,4	6,5	-2,19
7	5,0	4,6	-2,56
	6	2	L
0	8,8	7,9	0,00
1	20,2	20,1	0,31
2	0,0	1,4	-2,69
3	9,4	9,3	0,59
4	27,4	27,5	-1,86
5	25,8	26,8	-0,15
6	10,3	9,3	2,26
7	3,6	3,9	3,08
	6	3	L
0	11,2	12,3	-3,14
1	10,6	9,3	-3,06
2	13,9	12,9	1,03
3	13,9	13,9	-1,66
4	10,5	10,5	2,97
5	19,6	20,4	-0,50
6	9,2	6,5	1,32
7	5,8	4,8	-0,66
	6	4	L
0	33,4	30,5	-3,14
1	22,7	22,7	-0,57
2	36,1	35,7	0,22
3	23,3	23,5	2,27
4	11,6	11,4	0,06
5	9,7	10,5	-0,69
6	2,4	2,3	2,90
7	2,1	1,7	1,76
	6	5	L
0	29,1	17,7	0,00
1	16,7	16,0	3,06
2	10,6	10,4	1,13
3	5,1	5,8	-1,53
4	8,8	6,9	2,59
5	3,3	2,9	2,31
6	4,6	4,0	-0,11
7	0,0	0,6	-0,68
	6	6	L
0	28,8	25,9	-3,14
1	19,4	20,0	-0,15
2	8,7	7,8	-1,37
3	13,9	13,4	-0,21
4	9,5	9,1	2,89
5	17,6	18,5	2,05
6	4,6	4,5	-0,20
7	5,7	3,9	-2,63
	6	7	L
0	16,9	16,6	-3,14
1	21,7	21,0	-1,37
2	6,2	8,0	0,73
3	12,8	11,9	2,58
4	12,8	13,0	1,29
5	21,3	22,0	2,06
6	4,3	5,1	-2,35
7	5,8	6,6	-2,09
	6	8	L
0	27,7	25,1	0,00
1	26,0	25,6	1,68
2	19,7	19,2	-2,84
3	9,3	9,4	0,15
4	11,0	11,5	-1,07
5	9,2	9,8	3,08
6	10,6	11,2	0,83
7	3,9	4,1	2,55
	6	9	L
0	30,4	28,9	-3,14
1	12,3	12,2	2,59
2	21,0	20,0	-1,94
3	8,2	8,5	2,53
4	11,0	12,7	-1,35
5	6,2	6,6	2,78
6	6,3	6,4	2,93
7	1,4	1,3	-1,25
	6	10	L
0	5,2	4,8	-3,14
1	2,0	2,4	-2,79
2	14,2	14,3	2,80
3	13,8	14,1	-2,81
4	19,6	19,0	0,07
5	13,1	13,1	-1,00
6	10,5	10,8	-1,15
7	6,0	5,7	-0,48
	6	11	L
0	24,9	23,7	0,00
1	13,0	11,7	0,70
2	5,0	4,7	-0,91
3	8,2	8,3	-0,94
4	9,7	9,4	-1,07
5	9,0	9,6	-1,07
6	5,7	6,2	1,12
	6	12	L
0	13,8	13,9	-3,14
1	6,8	6,8	-3,09
2	18,1	17,9	1,09
3	11,9	11,7	3,06
4	8,0	8,8	2,22
5	7,0	6,7	2,29
6	8,2	8,2	-2,70
	6	13	L
0	7,1	7,0	0,00
1	10,4	10,0	0,74
2	8,4	9,1	2,81
3	10,1	10,9	0,29
4	5,3	5,8	1,10
5	3,3	3,7	-1,65
6	6,2	6,2	-0,86
	6	14	L
0	6,6	6,2	0,00
1	10,6	11,3	-2,71
2	4,1	3,3	1,89
3	9,7	10,3	-0,86
4	11,0	10,3	2,32
5	5,3	5,6	2,67
6	9,2	9,0	1,92
	6	15	L
0	2,4	2,9	0,00
1	5,1	4,5	-0,54
2	10,2	11,3	-1,58
3	14,4	15,0	2,79
4	6,0	5,7	1,28
5	2,5	2,2	-0,39
6	2,3	2,3	-2,47
	6	16	L
0	14,9	15,4	0,00
1	2,6	2,7	-2,62
2	14,1	14,7	-1,99
3	9,1	9,0	-0,52
4	4,1	4,6	-0,66
5	4,7	3,3	-0,47
	6	17	L
0	3,1	3,4	0,00
1	7,7	8,1	-2,22
2	11,5	11,3	0,12
3	7,2	7,2	-1,26
4	9,2	9,3	2,93
5	3,8	3,7	-0,80
	6	18	L
0	10,6	10,5	0,00
1	2,6	3,0	0,05
2	10,4	10,6	-1,14
3	2,5	2,8	2,35
4	2,4	2,9	-0,10
5	7,4	5,4	0,21
	6	19	L
0	0,3	1,0	-3,14
1	8,4	8,4	1,27
2	14,9	14,8	1,91
3	6,8	6,7	-0,09
4	0,3	0,9	-1,07
	6	20	L
0	13,2	13,1	-3,14
1	4,5	4,7	-0,26
2	3,9	3,7	1,49
3	5,0	4,8	2,54
4	5,6	5,8	-1,91
	6	21	L
0	6,8	6,9	-3,14
1	3,3	3,5	-2,07
2	0,0	0,7	2,68
3	4,4	4,0	1,27
4	2,5	2,4	-0,95
	6	22	L
0	0,1	0,4	-3,14
1	5,7	5,8	1,13
2	8,7	8,9	1,06
3	7,8	6,9	1,45
	6	23	L
0	2,3	1,9	-3,14
1	5,1	4,9	3,07
2	8,2	7,7	-2,88
	6	24	L
0	3,4	3,1	-3,14
1	4,5	4,6	-2,14
	7	0	L
1	3,5	3,2	-1,57
2	39,8	41,7	0,00
3	4,4	3,6	-1,57
4	19,5	21,0	-3,14
5	3,9	3,1	1,57
6	9,9	10,2	-3,14
7	2,6	2,4	1,57
	7	1	L
0	10,7	9,7	-1,57
1	6,5	6,6	-1,66
2	4,3	3,7	1,89
3	13,2	13,9	-3,12
4	4,3	4,0	0,63
5	15,4	16,2	-0,08
6	14,1	15,0	0,55
7	6,4	6,1	1,61
	7	2	L
0	16,6	15,4	1,57
1	17,5	17,9	2,36
2	8,9	7,2	2,60
3	16,3	16,4	1,84
4	25,3	25,7	-1,58
5	10,8	10,9	2,70
6	6,6	6,8	2,40
7	3,6	3,2	-0,60
	7	3	L
0	7,6	7,3	1,57
1	9,8	9,7	-0,15
2	10,8	10,3	2,72
3	24,3	24,1	-1,28
4	0,0	2,0	2,85
5	13,7	13,3	-2,49
6	8,5	8,5	-1,33
7	1,4	1,8	-2,39
	7	4	L
0	28,2	27,2	-1,57
1	11,5	11,7	-1,12
2	17,5	16,9	-2,78
3	10,1	13,8	2,08
4	29,4	29,8	-0,15
5	9,6	9,5	-1,14
6	5,5	6,4	-0,14
7	5,1	5,3	-0,49
	7	5	L
0	7,0	6,8	-1,57
1	13,7	13,7	0,94
2	12,4	12,9	0,31
3	14,5	17,3	-0,28
4	5,2	5,6	0,01
5	5,2	6,0	1,64
6	7,8	8,1	-3,12
7	5,0	4,2	-1,95
	7	6	L
0	7,2	7,1	-1,57
1	18,8	18,8	-2,49
2	11,5	10,7	-0,29
3	14,3	14,5	-1,26
4	33,6	33,6	1,83
5	2,4	3,6	1,51
6	2,1	1,6	-1,05
7	0,4	0,9	2,10
	7	7	L
0	5,4	6,1	-1,57
1	18,8	19,1	2,89
2	16,8	17,1	-1,35
3	18,2	17,9	-2,96
4	12,9	12,7	-0,58
5	12,9	12,9	2,03
6	4,5	4,1	1,61
7	1,7	1,8	1,09
	7	8	L
0	13,1	12,1	-1,57
1	13,5	13,8	2,54
2	10,0	10,0	-2,32
3	23,2	24,5	-0,63
4	13,5	13,9	-2,93
5	2,6	1,5	1,92
6	2,7	2,1	-1,83
	7	9	L
0	7,8	7,4	1,57
1	8,4	8,4	-0,46
2	12,2	12,1	2,42
3	9,1	9,1	-2,82
4	1,5	2,9	-2,67
5	3,0	2,8	-2,25
6	3,6	4,0	0,24
	7	10	L
0	0,0	0,5	-1,57
1	16,3	16,8	0,66
2	11,1	12,0	2,77
3	19,4	19,8	-1,91
4	10,1	9,2	-1,12
5	7,3	6,9	-1,85
6	4,9	5,1	0,38
	7	11	L
0	4,4	4,1	-1,57
1	2,2	2,6	2,93
2	3,5	3,2	0,63
3	17,0	17,0	0,67
4	4,6	4,6	1,56
5	7,4	7,4	-1,51
6	7,3	7,5	-1,90
	7	12	L
0	0,0	1,0	-1,57
1	18,1	17,9	-0,85
2	18,9	18,7	1,46
3	6,5	6,8	1,98
4	7,1	7,1	-1,80
5	3,2	3,6	1,83
6	0,0	2,0	0,47
	7	13	L
0	16,9	17,2	1,57
1	10,2	10,1	-2,67
2	4,9	5,9	3,07
3	8,6	9,3	0,50
4	6,0	6,6	3,07
5	2,8	3,2	-0,24
6	0,0	1,7	-2,83
	7	14	L
0	20,7	21,6	1,57
1	15,3	15,7	-2,65
2	6,8	7,0	0,48
3	18,6	18,7	1,60
4	2,2	1,5	2,05
5	5,9	4,1	-2,44
	7	15	L
0	17,6	18,3	1,57
1	1,2	1,4	2,49
2	10,2	10,3	-1,47
3	2,0	2,5	2,95
4	2,8	2,3	-1,87
5	3,1	3,3	1,74
	7	16	L
0	1,7	0,9	-1,57
1	6,8	6,9	1,44
2	10,6	10,2	-1,60
3	7,6	7,9	2,12
4	7,7	7,6	1,38
5	1,9	1,4	2,59
	7	17	L
0	11,7	11,0	-1,57
1	7,3	7,1	0,80
2	6,8	6,7	0,46
3	4,2	4,2	-3,07
4	1,9	1,7	-0,35
5	0,0	2,1	-1,71
	7	18	L
0	9,0	9,5	-1,57
1	3,3	3,3	0,30
2	12,1	11,6	-1,32
3	6,6	6,9	-2,29
4	1,2	0,9	-2,75
	7	19	L
0	21,0	19,7	-1,57
1	7,4	6,7	-0,80
2	4,5	4,3	-2,75
3	4,7	4,3	0,25
4	6,2	6,2	2,47
	7	20	L
0	4,0	3,8	1,57
1	3,9	4,5	-2,38

Table 5 (*cont.*)

2	6.3	6.4	1.31
3	13.0	13.0	-1.06
7 21 L			
0	0.0	0.0	1.57
1	4.2	3.9	0.65
2	1.5	1.7	1.13
3	3.9	3.7	-2.48
7 22 L			
0	0.0	1.1	1.57
1	3.3	3.2	-1.30
2	5.1	5.0	2.24
7 23 L			
0	5.2	4.6	1.57
1	0.6	1.0	2.38
8 0 L			
0	1.7	1.4	-3.14
1	0.0	0.7	-1.57
2	36.2	37.2	-3.14
3	3.9	3.3	-1.57
4	20.5	21.1	0.00
5	14.2	14.6	1.57
6	2.1	0.8	-0.00
8 1 L			
0	0.2	0.6	-3.14
1	23.5	23.3	-0.13
2	6.6	6.7	3.09
3	27.5	28.0	-1.91
4	20.1	19.1	2.91
5	4.8	5.1	-2.17
6	2.7	2.2	1.90
8 2 L			
0	15.0	14.1	0.00
1	21.5	20.9	-0.85
2	24.9	25.5	1.10
3	17.9	18.0	3.12
4	6.0	5.8	0.41
5	4.4	2.3	0.49
6	0.8	1.0	-2.95
8 3 L			
0	11.0	10.1	0.00
1	14.7	14.6	2.08
2	13.2	13.3	0.18
3	9.8	9.6	-1.49
4	4.1	3.7	-1.99
5	7.5	6.9	-1.42
6	9.4	9.6	-0.31
8 4 L			
0	9.3	8.8	0.00
1	10.7	11.0	1.97
2	24.4	24.8	-1.00
3	10.8	10.9	0.74
4	7.2	7.8	-3.08
5	1.8	2.6	0.44
6	5.3	5.0	3.11
8 5 L			
0	8.3	8.5	-3.14
1	16.5	16.6	3.13
2	9.0	9.6	-0.98
3	16.8	16.7	0.77
4	12.9	12.4	0.31
5	5.1	5.7	-0.35
6	4.3	3.7	0.78
8 6 L			
0	9.7	9.4	-3.14
1	15.5	15.4	2.00
2	6.2	6.6	-2.02
3	20.8	21.2	-0.96
4	11.3	11.2	2.11
5	4.4	4.5	-1.54
6	12.1	7.6	1.12
8 7 L			
0	11.3	9.5	0.00
1	3.1	3.0	2.53
2	10.7	10.4	-2.70
3	6.1	6.5	2.58
4	5.0	4.5	-0.60
5	13.0	10.3	-2.80
6	7.0	6.7	-2.85
8 8 L			
0	15.8	14.2	-3.14
1	1.6	2.3	1.67
2	14.9	16.0	2.79
3	9.3	8.6	0.49
4	6.4	6.4	-2.49
5	4.7	5.5	-1.82
6	2.9	3.3	-0.58
8 9 L			
0	1.6	1.8	-3.14
1	18.3	18.5	-0.17
2	14.2	14.7	2.14
3	12.7	12.9	-1.07
4	2.1	2.1	3.08
5	2.0	1.8	0.40
6	2.8	2.8	-0.84
8 10 L			
0	6.5	6.9	-3.14
1	10.4	11.4	-1.39
2	5.3	4.7	-1.36
3	22.4	22.7	2.13
4	0.0	1.0	2.06
5	3.8	3.7	-3.03
6	4.7	3.8	-0.88
8 11 L			
0	8.6	8.7	-3.14
1	16.6	17.8	-2.30
2	2.4	2.6	1.45
3	3.0	1.6	1.33
4	8.0	8.0	-2.26
5	6.6	6.6	0.63
6	3.5	3.1	0.62
8 12 L			
0	9.1	9.4	0.00
1	12.3	12.7	-2.74
2	13.4	14.4	-0.41
3	13.2	13.3	-2.13
4	3.6	3.7	-0.23
5	6.4	6.4	-1.53
8 13 L			
0	9.5	9.4	0.00
1	18.4	19.2	2.69
2	3.8	3.9	-1.21
3	15.2	15.2	2.21
4	3.0	2.9	2.10
5	1.5	2.3	0.31
8 14 L			
0	3.0	2.8	0.00
1	5.9	6.2	1.36
2	5.7	5.5	1.34
3	7.6	7.3	-2.06
4	6.6	6.4	-2.53
5	3.2	3.3	0.84
8 15 L			
0	0.0	1.0	0.00
1	10.3	10.4	0.47
2	2.2	2.4	1.75
3	3.3	3.5	-0.10
4	4.6	1.1	2.63
5	0.8	1.3	2.74
8 16 L			
0	1.3	0.8	0.00
1	7.4	7.2	-0.13
2	6.9	6.4	1.51
3	16.6	16.7	0.36
4	4.7	4.6	2.06
8 17 L			
0	0.0	0.4	0.00
1	7.6	7.4	-0.51
2	5.0	5.1	-0.15
3	4.4	4.1	-1.91
4	5.2	5.0	0.42
8 18 L			
0	5.3	5.6	0.00
1	8.6	8.8	0.34
2	7.4	7.4	3.04
3	0.0	2.5	1.14
8 19 L			
0	4.7	4.6	-3.14
1	0.6	0.5	3.02
2	4.3	4.6	-1.28
3	5.6	5.5	-2.48
8 20 L			
0	4.5	4.6	-3.14
1	3.0	3.4	-1.30
2	3.0	2.7	0.91
8 21 L			
0	0.0	0.9	-3.14
1	2.2	2.9	0.86
9 0 L			
1	4.9	4.8	-1.57
2	14.9	15.3	0.00
3	3.5	4.0	1.57
4	9.6	9.6	-3.14
5	5.5	0.9	-1.57
6	0.0	2.2	0.00
9 1 L			
0	2.2	2.1	-1.57
1	19.6	19.3	2.48
2	7.0	6.9	0.68
3	13.1	13.9	1.55
4	11.0	10.6	2.69
5	7.8	5.0	-1.95
6	6.5	6.1	-2.02
9 2 L			
0	1.9	1.3	-1.57
1	9.5	8.8	2.92
2	24.3	25.2	-1.56
3	11.6	11.8	-1.25
4	4.7	4.3	-1.66
5	2.2	2.4	-1.23
6	4.6	4.2	1.48
9 3 L			
0	18.2	18.7	1.57
1	7.5	7.2	1.44
2	1.9	1.7	1.08
3	21.0	21.1	1.16
4	4.9	4.9	2.15
5	7.2	8.1	-0.72
6	7.9	7.6	0.01
9 4 L			
0	5.4	5.2	1.57
1	11.6	11.9	2.94
2	15.6	15.5	2.86
3	4.8	4.9	1.38
4	1.5	2.4	-1.69
5	8.5	8.4	0.37
6	2.5	2.0	2.84
9 5 L			
0	3.7	3.2	-1.57
1	7.4	7.8	0.09
2	25.5	26.7	-2.38
3	8.5	8.5	-2.10
4	4.6	4.7	-2.38
5	4.6	4.4	2.35
6	8.7	8.1	0.50
9 6 L			
0	0.0	0.5	1.57
1	20.4	20.4	-0.08
2	6.6	7.1	-2.54
3	7.8	8.2	0.95
4	1.3	1.8	0.60
5	3.3	3.8	-2.69
6	5.5	5.5	-1.22
9 7 L			
0	6.4	6.4	-1.57
1	12.0	12.2	-0.18
2	8.1	8.0	1.21
3	2.3	2.8	-0.31
4	8.1	7.9	-1.77
5	6.0	5.6	1.96
6	3.1	2.5	2.33
9 8 L			
0	9.1	9.5	1.57
1	3.1	2.5	0.48
2	15.0	15.4	-0.03
3	7.9	7.8	-2.21
4	9.1	5.8	1.02
5	9.9	5.6	2.88
9 9 L			
0	11.7	13.3	-1.57
1	10.2	10.7	-3.08
2	16.0	16.3	0.31
3	2.0	2.7	2.44
4	3.4	3.1	-3.11
5	1.4	0.3	-2.61
9 10 L			
0	1.4	2.3	1.57
1	5.4	5.2	2.31
2	13.2	12.8	0.14
3	2.4	2.9	-1.12
4	10.1	9.7	-1.00
5	3.3	3.3	1.20
9 11 L			
0	8.3	8.0	-1.57
1	9.4	9.7	-0.64
2	7.8	8.3	2.29
3	0.0	1.2	2.07
4	1.8	2.1	-1.08
5	7.4	7.0	-1.64
9 12 L			
0	3.1	2.7	1.57
1	4.2	3.8	-2.02
2	16.8	17.2	2.27
3	11.1	11.3	1.92
4	3.9	2.9	-2.55
5	6.3	5.7	-1.09
9 13 L			
0	11.7	11.3	1.57
1	8.9	8.6	-1.11
2	7.2	7.2	-2.14
3	10.3	10.5	-3.04
4	7.1	7.2	0.24
9 14 L			
0	6.2	5.8	-1.57
1	5.7	6.0	-2.88
2	12.0	12.1	-2.53
3	5.0	5.3	2.24
4	7.8	7.2	1.95
9 15 L			
0	3.2	3.2	1.57
1	8.1	8.6	2.49
2	7.1	6.9	-0.60
3	6.4	6.0	-1.56
4	5.7	5.0	1.45
9 16 L			
0	10.5	10.5	-1.57
1	2.4	2.6	0.43
2	5.7	5.9	-0.69
3	8.1	8.0	-1.16
9 17 L			
0	5.6	5.4	1.57
1	8.4	8.0	1.89
2	6.9	7.1	1.19
3	5.1	5.7	0.23
9 18 L			
0	4.4	4.5	-1.57
1	2.9	3.3	-2.13
2	1.3	1.7	-0.19
9 19 L			
0	6.2	6.1	-1.57
1	5.0	4.9	0.28
2	2.7	2.6	2.53
9 20 L			
0	2.0	2.3	1.57
10 0 L			
0	27.1	27.6	0.00
1	15.5	16.6	-1.57
2	8.7	9.1	0.00
3	6.2	5.9	1.57
4	1.0	1.0	3.14
5	0.6	0.2	1.57
10 1 L			
0	2.3	1.8	-3.14
1	10.0	10.0	1.31
2	23.8	23.9	-0.88
3	5.1	5.0	2.85
4	4.5	4.7	-1.38
5	0.0	0.8	-0.62
10 2 L			
0	6.6	6.7	-3.14
1	15.7	16.5	0.70
2	6.0	6.1	1.72
3	6.7	6.2	1.80
4	6.4	6.1	-2.03
5	1.9	2.7	-0.71
10 3 L			
0	9.9	9.6	-3.14
1	10.8	10.7	2.36
2	6.9	7.0	1.29
3	3.3	3.9	-2.94
4	6.8	4.2	2.78
5	2.3	2.5	1.94
10 4 L			
0	12.2	11.7	-3.14
1	8.3	8.6	2.31
2	5.5	5.3	1.54
3	9.0	9.0	-1.79
4	5.7	5.7	-1.83
5	2.4	2.9	-0.95
10 5 L			
0	11.5	11.8	0.00
1	9.8	10.1	2.20
2	17.4	17.0	1.11
3	6.0	5.5	1.48
4	8.9	9.1	3.05
5	0.0	0.5	-2.30
10 6 L			
0	2.3	2.3	0.00
1	7.9	8.1	-2.83
2	5.6	5.7	2.94
3	7.6	7.9	2.98
4	5.4	5.0	0.45
5	1.8	2.0	-1.67
10 7 L			
0	8.2	7.9	0.00
1	3.0	3.3	-1.42
2	2.0	2.7	-2.47
3	10.4	9.6	0.20
4	2.6	2.0	2.36
5	3.9	3.8	-0.57
10 8 L			
0	12.0	11.5	-3.14
1	11.6	11.8	-0.60
2	4.1	3.7	2.51
3	6.4	6.2	-2.75
4	9.2	8.7	1.35
5	2.5	1.5	2.43
10 9 L			
0	11.7	11.7	-3.14
1	17.6	17.3	-0.80
2	5.2	5.4	-1.36
3	7.5	7.9	-1.38
4	6.6	6.4	0.29
10 10 L			
0	6.1	5.8	0.00
1	6.2	6.1	-1.10
2	11.2	11.5	0.52
3	9.0	9.0	0.04
4	6.8	6.6	-1.74
10 11 L			
0	2.9	1.6	3.14
1	9.1	9.1	1.23
2	6.3	6.5	1.38
3	4.9	5.1	-0.14
4	1.8	2.6	1.07
10 12 L			
0	11.2	11.2	0.00
1	4.1	4.5	3.06
2	4.0	4.2	-2.31
3	6.6	7.5	0.84
4	4.1	2.3	-2.50
10 13 L			
0	1.5	0.2	0.00
1	3.9	4.0	-2.39
2	11.2	11.2	2.93
3	6.6	6.6	-2.84
10 14 L			
0	4.3	4.1	0.00
1	1.7	2.4	2.92
2	12.5	12.5	-1.60
3	5.0	4.8	-1.93
10 15 L			
0	3.0	3.1	0.00
1	3.9	3.7	-2.21
2	6.0	6.2	-1.75
3	0.0	1.8	2.47
10 16 L			
0	4.2	4.5	-3.14
1	8.3	8.3	1.69
2	3.4	3.1	2.26
10 17 L			
0	1.0	1.3	-3.14
1	4.9	4.3	0.44
10 18 L			
0	2.4	2.2	-3.14
11 0 L			
1	5.5	6.4	-1.57
2	1.3	2.2	0.00
3	0.7	0.1	1.57
4	8.2	8.0	0.00
11 1 L			
0	2.5	2.7	-1.57
1	4.0	3.9	1.89
2	7.1	7.3	-2.28
3	6.7	6.4	-2.12
4	4.7	4.5	-0.85
11 2 L			
0	8.5	8.3	-1.57
1	8.7	7.7	-0.35
2	2.9	3.1	-0.52
3	3.8	4.1	1.18
4	0.0	4.3	2.21
11 3 L			
0	5.6	5.0	1.57
1	7.4	6.9	2.87
2	1.3	4.1	2.28
3	8.5	8.6	-2.27
4	2.7	3.3	-1.22
11 4 L			
0	8.2	8.1	-1.57
1	9.5	9.7	0.88
2	1.6	2.0	-0.99
3	1.8	2.2	0.59
4	6.6	6.2	2.33
11 5 L			
0	11.2	11.5	1.57
1	10.7	10.4	0.50
2	8.0	7.7	1.70
3	3.9	4.4	0.35
4	3.7	3.9	1.70
11 6 L			
0	7.0	6.9	1.57
1	4.9	5.3	-2.49
2	11.2	10.8	2.43
3	7.6	7.8	-3.10
4	4.7	4.5	-0.73
11 7 L			
0	11.6	10.7	-1.57
1	4.4	4.0	0.76
2	4.1	4.2	-2.46
3	7.4	7.6	1.20
4	4.6	4.6	-2.61
11 8 L			
0	1.9	1.5	-1.57
1	3.2	2.8	-1.28
2	6.6	6.5	-2.36
3	8.3	8.3	-1.36
4	3.8	3.7	-3.10
11 9 L			
0	10.9	11.0	-1.57
1	2.4	2.3	-0.44
2	6.4	6.1	-0.60
3	5.4	5.2	-0.79
11 10 L			
0	0.0	1.0	-1.57
1	5.5	5.2	1.78
2	10.6	10.7	0.84
3	9.5	9.1	0.38
11 11 L			
0	1.2	0.3	-1.57
1	6.1	6.1	-2.71
2	4.4	4.3	1.00
3	2.1	2.2	-1.22
11 12 L			
0	3.2	2.9	1.57
1	4.2	3.8	3.07
2	3.2	3.4	-0.97
3	6.7	6.3	2.94
11 13 L			
0	4.9	5.0	1.57
1	4.4	4.4	-2.21
2	3.4	3.5	-2.19
11 14 L			
0	1.4	2.2	-1.57
1	3.5	4.0	-0.35
2	5.2	5.6	-1.14
11 15 L			
0	8.3	8.0	1.57
1	0.7	0.8	2.84
12 0 L			
0	5.3	5.4	0.00
1	3.1	3.3	-1.57
2	3.6	3.3	3.14
3	3.0	2.7	-1.57
12 1 L			
0	3.7	4.0	-3.14
1	9.9	9.4	-0.37
2	6.3	6.2	1.23
3	1.5	1.6	0.84
12 2 L			
0	2.4	3.0	0.00
1	0.4	1.3	-2.19
2	9.7	10.0	-1.94
3	4.8	5.0	-2.20
12 3 L			
0	0.0	2.0	-3.14
1	2.9	3.4	-2.62
2	3.9	3.3	-1.48
3	2.1	2.1	2.67
12 4 L			
0	4.8	4.7	-3.14
1	9.6	9.3	0.43
2	5.9	5.7	0.19
3	8.1	8.1	0.67
12 5 L			
0	1.8	1.7	-3.14
1	8.5	8.5	2.13
2	9.8	10.2	-3.08
3	1.5	2.0	2.54
12 6 L			
0	1.9	0.4	-3.14
1	3.7	2.9	-1.71
2	1.4	2.0	-1.50
3	5.9	5.6	0.56
12 7 L			
0	2.1	0.5	3.14
1	1.1	0.6	0.74
2	4.0	3.9	-1.22
3	2.1	2.1	-0.64
12 8 L			
0	3.6	3.1	0.00
1	1.2	2.0	-2.71
2	5.9	5.7	-1.68
12 9 L			
0	3.3	3.1	0.00
1	4.2	4.3	-2.19
2	7.2	7.5	0.32
12 10 L			
0	2.6	2.9	-3.14
1	4.5	4.6	2.13
12 11 L			
0	1.4	1.5	0.00
1	5.5	5.3	-1.81
13 0 L			
1	12.6	12.2	1.57
13 1 L			
0	2.2	2.1	-1.57
1	2.0	1.5	0.31
13 2 L			
0	2.4	1.8	-1.57
1	1.5	1.3	1.07
13 3 L			
0	4.7	4.4	-1.57
1	5.5	4.6	1.69
13 4 L			
0	1.6	1.6	-1.57
1	9.5	9.4	-2.49
13 5 L			
0	1.6	2.2	1.57

Table 6. *Bond lengths and angles in ADTG*

Bond	Distance	Angle	θ
O(2)—C(21)	1·438 Å	C(21)O(2)C(23)	108·4°
O(2)—C(23)	1·365		
C(1)—C(2)	1·527	C(2)C(1)C(10)	114·5
C(1)—C(10)	1·536		
C(2)—C(3)	1·530	C(1)C(2)C(3)	111·4
O(1)—C(3)	1·453	O(1)C(3)C(2)	107·3
C(3)—C(4)	1·501	O(1)C(3)C(4)	112·4
		C(2)C(3)C(4)	110·5
C(4)—C(5)	1·532	C(3)C(4)C(5)	113·9
C(5)—C(6)	1·520	C(4)C(5)C(6)	111·7
C(5)—C(10)	1·550	C(4)C(5)C(10)	112·5
		C(6)C(5)C(10)	111·9
C(6)—C(7)	1·543	C(5)C(6)C(7)	112·2
C(7)—C(8)	1·509	C(6)C(7)C(8)	112·1
C(8)—C(9)	1·521	C(7)C(8)C(9)	114·0
C(8)—C(14)	1·333	C(7)C(8)C(14)	122·6
		C(9)C(8)C(14)	123·2

Table 6 (*cont.*)

Bond	Distance	Angle	θ
C(9)—C(10)	1·572	C(8)C(9)C(10)	110·6
C(9)—C(11)	1·531	C(8)C(9)C(11)	113·7
		C(10)C(9)C(11)	113·2
		C(1)C(10)C(5)	108·4
		C(1)C(10)C(9)	111·5
C(10)-C(19)	1·546	C(1)C(10)C(19)	107·5
		C(5)C(10)C(9)	109·8
		C(5)C(10)C(19)	109·4
		C(9)C(10)C(19)	110·2
C(11)-C(12)	1·531	C(9)C(11)C(12)	112·9
C(12)-C(13)	1·525	C(11)C(12)C(13)	110·8
C(13)-C(14)	1·515	C(12)C(13)C(14)	109·8
C(13)-C(17)	1·573	C(12)C(13)C(17)	113·6
C(13)-C(18)	1·533	C(12)C(13)C(18)	111·3
		C(14)C(13)C(17)	100·4
		C(14)C(13)C(18)	110·4
		C(17)C(13)C(18)	110·8
		C(8)C(14)C(13)	123·3
C(14)-C(15)	1·525	C(8)C(14)C(15)	126·1
		C(13)C(14)C(15)	110·0
C(15)-C(16)	1·547	C(14)C(15)C(16)	104·7
C(16)-C(17)	1·536	C(15)C(16)C(17)	103·7
		C(13)C(17)C(16)	103·4
C(17)-C(20)	1·495	C(13)C(17)C(20)	115·2
		C(16)C(17)C(20)	114·6
C(20)-C(21)	1·499	C(17)C(20)C(21)	120·9
C(20)-C(22)	1·317	C(17)C(20)C(22)	131·1
		C(21)C(20)C(22)	108·0
		O(2)C(21)C(20)	105·3
C(22)-C(23)	1·457	C(20)C(22)C(23)	109·8
O(3)—C(23)	1·202	O(2)C(23)O(3)	120·2
		O(2)C(23)C(22)	108·5
		O(3)C(23)C(22)	131·3

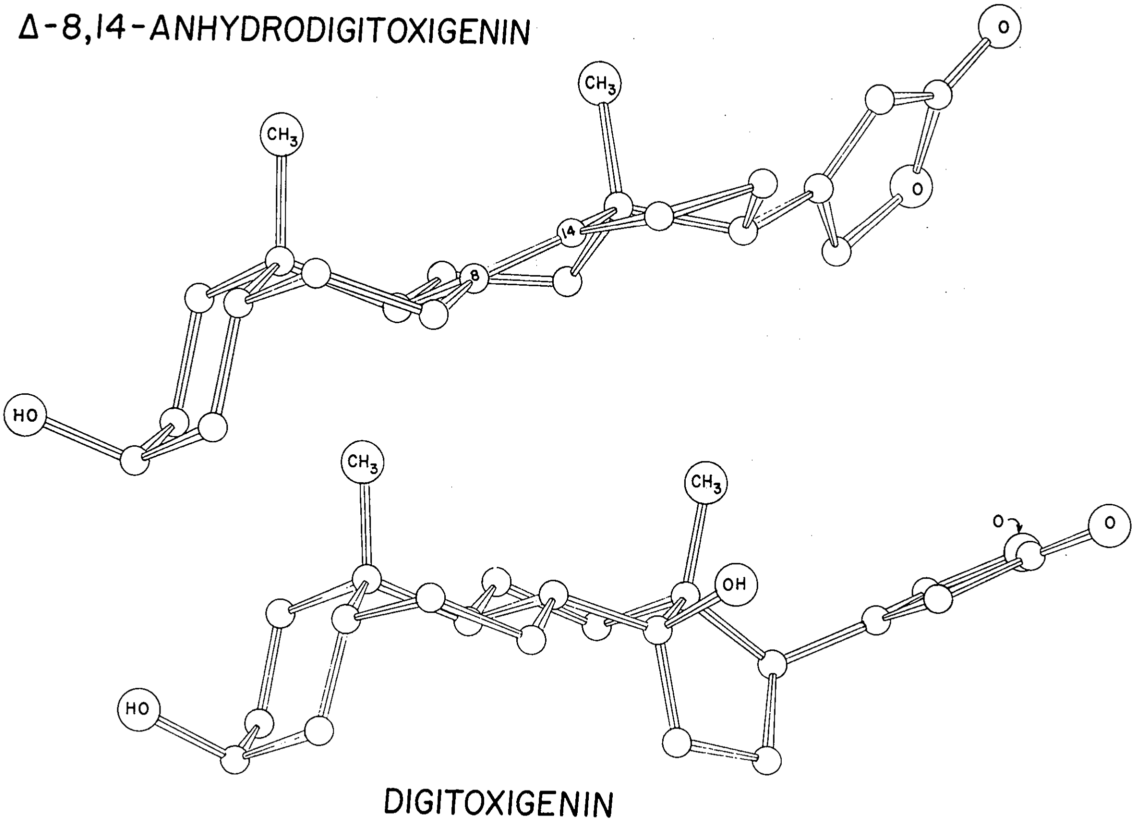


Fig. 3. A comparison of the conformations of ADTG and DTG.

The overall lengths of the two steroids are almost equal despite local differences. The calculated distances between the hydroxyl oxygen atom on ring *A* and the carbonyl oxygen atom of the lactone ring are 13·21 Å for DTG and 13·36 Å for ADTG. One measure of the length of the steroid nucleus is the C(3)···C(16) distance. The folded nucleus of DTG is significantly shorter, 7·25 Å, than that of ADTG, 8·44 Å. A detailed discussion of the conformations of six steroids has been published (Norton, 1965) in which the steroid nuclei contained only *trans* ring junctions and therefore were relatively planar. Their C(3)···C(16) distances, 9·1 ± 0·2 Å, were necessarily longer than those reported here.

Fractional coordinates and thermal parameters are listed in Table 3. Values for bond lengths are presented in Fig. 4 and bond angles are shown in Fig. 5. The bond lengths and angles are also tabulated in Table 6. The standard deviations indicated by the least-squares refinement alone are 0·005 Å for the bonds and 0·4° for the angles except in the lactone ring where the indicated standard deviations are slightly larger, 0·006 Å for bonds and 0·7° for angles.

There seem to be significant deviations in the single bond lengths from the average value of 1·533 Å for this molecule. They range from a minimum value of 1·501 Å for C(3)–C(4) to a maximum of 1·573 Å for C(13)–C(17). There are at least three reasonable explanations for bond lengthening in steroids:

(*a*) *Gauche* interactions between nonbonded neighboring substituents. For example, there are such interactions between the methyl group C(18) and atoms C(20) and C(16) which could be used to explain the length (1·573 Å) of the C(13)–C(17) bond.

(*b*) Intramolecular van der Waals interactions. A possible effect between rings *A* and *C* may occur through hydrogen–hydrogen repulsions. The van der

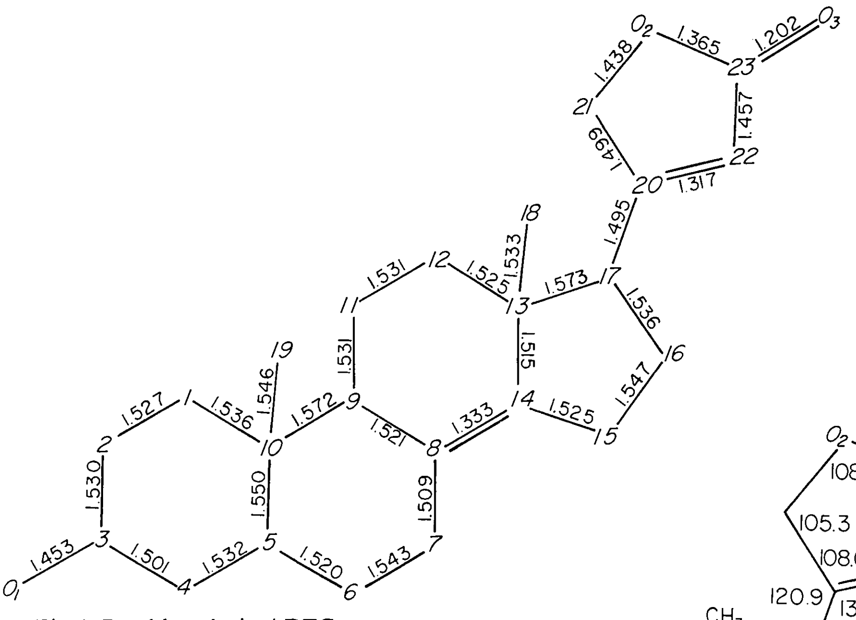


Fig. 4. Bond lengths in ADTG.

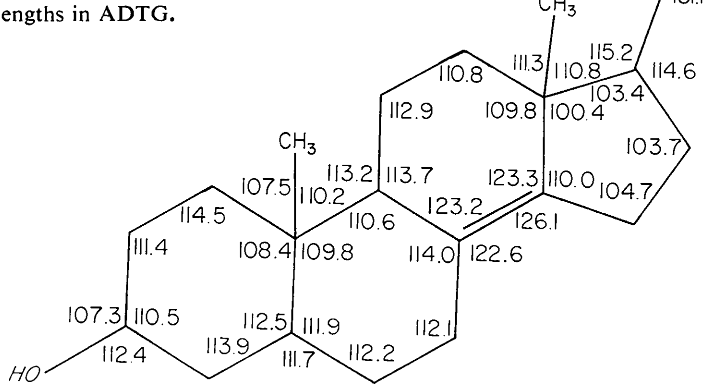


Fig. 5. Bond angles in ADTG. Four angles not shown in the Figure are: C(1)C(10)C(9), 111·5°; C(5)C(10)C(19), 109·4°; C(12)C(13)C(17), 113·6°; and C(14)C(13)C(18), 110·4°.

Table 7. *Torsion angles about ring bonds in ADTG*

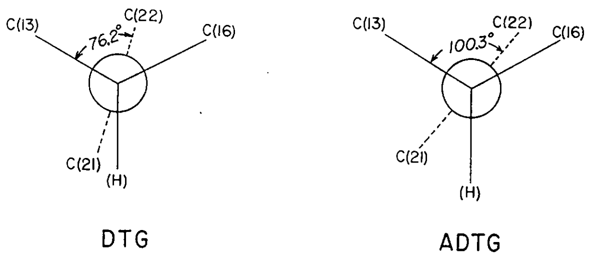
Bonded atoms	θ	
1, 2	−55·3°	Ring *A*
2, 3	53·3	
3, 4	−54·1	
4, 5	54·5	
5, 10 (*A*)*	−51·4	
1, 10	53·1	
5, 6	54·5	Ring *B*
6, 7	−51·5	
7, 8	52·1	
8, 9 (*B*)	−54·2	
9, 10	54·9	
5, 10 (*B*)	−56·1	
8, 9 (*C*)	2·1	Ring *C*
9, 11	−30·9	
11, 12	57·5	
12, 13	−52·9	
13, 14 (*C*)	25·4	
8, 14	0·5	
13, 14 (*D*)	−26·6	Ring *D*
14, 15	2·8	
15, 16	23·1	
16, 17	−39·9	
13, 17	40·5	

* Where a bond is common to two rings, the notation 5,10(*A*) indicates that the adjacent atoms of ring *A* were used in computing this particular torsion angle. Thus, torsion angle 5,10(*A*) involves the torsion of bonds (4,5) and (1,10) about bond (5,10).

Waals H···H contact has been reported as 2·34 A (Kitaigorodskii, 1961). In order for the separations between H(9) and H(2*B*) and between H(9) and H(4*A*) to be as large as 2·30 and 2·28 Å, respectively, the C(9)–C(10) bond which is 1·572 Å may have been lengthened.

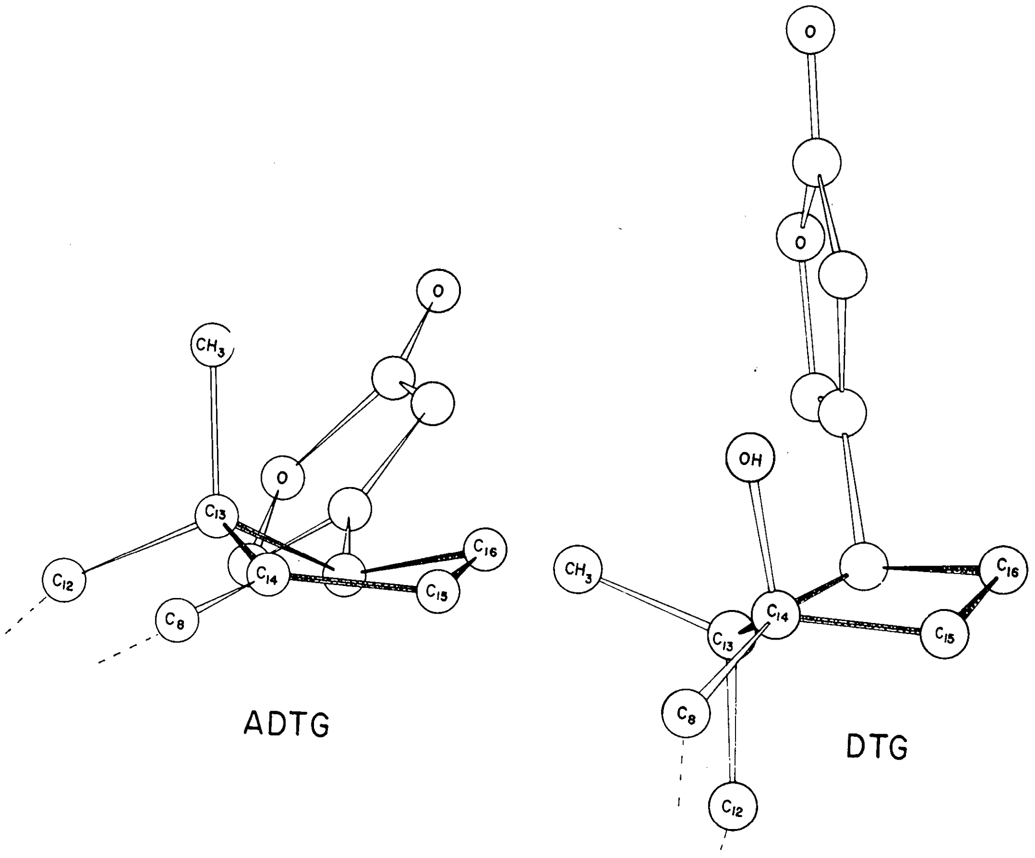
(*c*) Effect of ring closure. Closure of rings containing five atoms or less generally leads to smaller-than-normal bond angles within the ring, and this circumstance may lead to bond lengthening (Dewar, 1962).

Comparisons of the conformations of steroids are facilitated by the computation of torsion angles about ring bonds (Brutcher & Leopold, 1966). The torsion angles for ADTG are presented in Table 7, using the



DTG ADTG

Fig.6. Newman projections down the C(17)–C(20) bond in ADTG and DTG.



ADTG DTG

Fig.7. Comparison of the conformations of rings *D* and the neighboring lactone chromophores in DTG and ADTG.

sign convention of Brutcher & Leopold. The ideal chair form of cyclohexane has torsion angles of 60° which alternate in sign. Rings *A* and *B* are readily seen to be in a slightly flattened chair form.

Ring *C* of the steroid presents an unusual conformation. Atoms C(8), C(9), C(11), C(13) and C(14) are almost planar; this is reflected by the negligible torsion about bonds C(8)–C(14) and C(8)–C(9). The cyclohexene ring generally exhibits a half-chair conformation, which consists of four atoms in a plane with the remaining two atoms puckered above and below the plane. Ring *C* has four atoms fitting a plane to within ±0·002 Å, with atom C(11) located only 0·06 Å above this plane, and C(12) 0·62 Å below this plane.

Ring *D* is present in the envelope configuration; *i. e.* four atoms in a plane and the fifth one more than 0·5 Å out of the plane. Torsion angles have been calculated for several steroidal ring *D* envelopes (Brutcher & Leopold, 1966) from X-ray data. In all examples previously reported, atom C(13) or C(14) (as in DTG with a *cis* *C*/*D* ring junction) is out of the plane of the other four. In ADTG, atoms C(13) to (16) fit a plane to within ±0·015 Å, and it is C(17) which is displaced 0·637 Å below this plane. The torsion angles computed are

Table 8. *Least-squares planes.*

Atoms	Plane	Maximum deviation
8, 9, 13, 14	$4{\cdot}7680x+20{\cdot}219y-1{\cdot}6971z=$ 12·660	±0·002 Å
8, 9, 11, 13, 14	$4{\cdot}7158x+20{\cdot}376y-1{\cdot}5638z=$ 12·829	±0·020
13, 14, 15, 16	$3{\cdot}1097x+21{\cdot}730y-1{\cdot}4441z=$ 13·207	±0·016
17, 20, 21, 22, 23, O_2, O_3	$-8{\cdot}6064x-7{\cdot}6310y+4{\cdot}0449z=-5{\cdot}9189$	±0·02
7, 8, 9, 13, 14, 15	$4{\cdot}5540x+20{\cdot}723y-1{\cdot}2816z=$ 13·209	+0·04 (9, 15) +0·01 (7, 13) −0·04 (8) −0·06 (14)

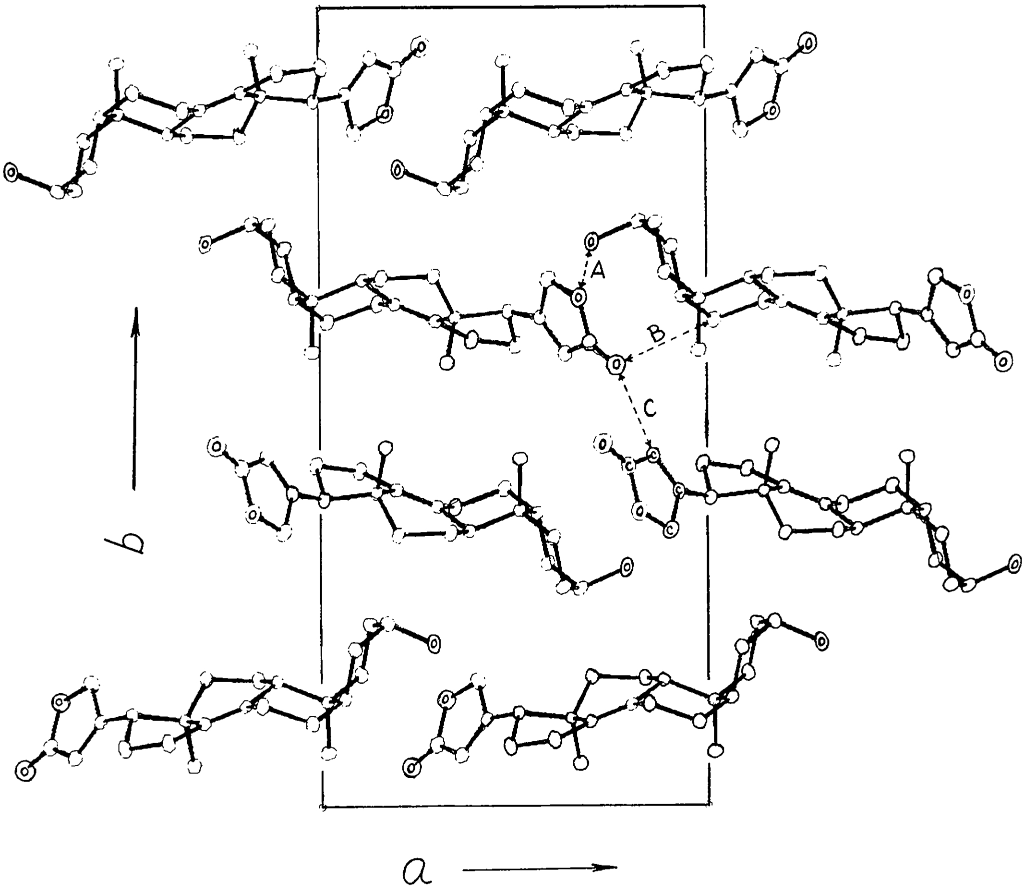


Fig. 8. Contents of the unit cell viewed down the *c* axis. Closest approaches are (*A*) O(1′)· · ·O(2), 3·182 Å; (*B*) O(3)· · ·C(6′), 3·276 Å; and (*C*) O(3)· · ·C(22″), 3·334 Å.

similar to those found by Brutcher & Leopold for steroidal envelopes, when suitably permuted to account for a different out-of-plane atom.

Equations for the least-squares planes passing through the *C* and *D* rings are presented in Table 8. The lactone ring together with C(17) forms a seven-atom planar grouping with 0·02 Å maximum deviation. The atoms adjacent to the double bond C(8)–C(14) deviate slightly from planarity, forming a shallow boat with carbon atoms 7, 9, 13 and 15 all lying slightly above and the double bond below the least-squares plane for these six atoms.

A comparison of the conformation about the C(17)–C(20) bond for DTG and ADTG is shown in Fig. 6. Atom C(17) is of interest because it is the asymmetric carbon closest to the optically absorbing lactone moiety which is referred to as a chromophore. ADTG dissolved in dioxane exhibits a weak negative Cotton effect in its optical rotatory dispersion spectrum, whereas a strong positive Cotton effect is observed for DTG in dioxane; both substances absorb only in the ultraviolet region, and the Cotton effect is accordingly in the ultraviolet at 250 to 300 nm (Burkhardt, Meier, Furst & Reichstein, 1967).

Changes in the optical rotatory dispersion are often explicable in terms of conformational changes in groups close to a chromophore in the molecule. However, Fig. 6 illustrates that the orientation of the lactone group with respect to atoms C(13), C(17) and C(16) is similar in DTG and ADTG in the crystalline state. Fig. 7 illustrates the *D* rings plus the lactone groups of the two molecules and reveals that a considerable difference does occur in the orientation of next-nearest neighbors with respect to the lactone group.

The packing of the ADTG molecule is illustrated in Figs. 8 and 9. The most surprising feature is the lack of a strong hydrogen bond despite the presence of a hydroxyl group and a carbonyl group at opposite ends of the molecule. In the DTG crystal, molecules were linked by head-to-tail hydrogen bonds (OH···O at 2·94 Å) in endless chains along the axis of intermediate length, *b*. Fig. 8 illustrates the similar alignment of ADTG along the intermediate axis (*a*), but in this case, the heads and tails are not in position to form a hydrogen bond.

The nearest intermolecular contact (labelled *A* in Figs. 8 and 9), is 3·18 Å between the hydroxyl oxygen atom and the oxygen atom in the lactone ring. The next nearest intermolecular approaches are O(3)···C(6′) at 3·28 Å and O(3)···C(22″) at 3·33 Å, labelled *B* and *C* in Fig. 8. All other C···O distances are greater than 3·4 Å and all C···C distances are greater than 3·6 Å.

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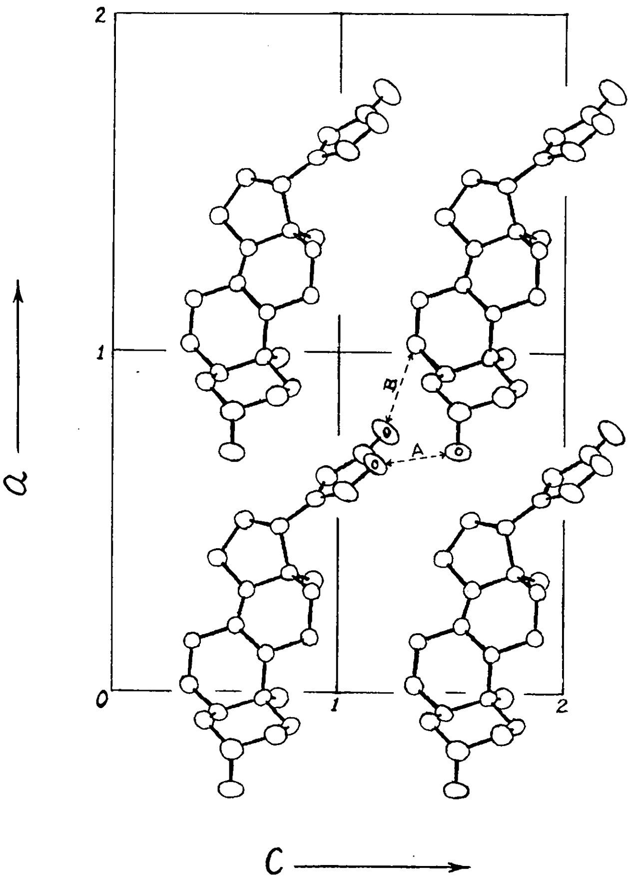

Fig. 9. Partial contents of four unit cells viewed down the *b* axis. The only molecules shown are those occurring in the region $0{\cdot}5 \le y \le 0{\cdot}75$.

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