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The Crystal and Molecular Structure of Dibromoeriostoic Acid

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Eriostoic acid is a plant product with the constitution 5-methoxy-2,2,8,8-tetramethyl-2*H*,8*H*[1,2*b*,5,4-*b*′]-dipryram-10-2-propionic acid. The crystal structure of its 3,7-dibromo derivative, $C_{20}H_{22}O_5Br_2$, has been determined by a three-dimensional X-ray analysis. The nucleus of the molecule consists of two chemically equivalent units which are independent of each other in the crystal structure. A comparison of the geometries of the two units has provided an internal check on the accuracy of the structure determination. Small differences which exist are consistent with a distortion of the molecule by packing forces.

Introduction

Eriostoic acid is one of a group of plant products which has been studied by Dr P. R. Jefferies and his coworkers at the Department of Chemistry, University of Western Australia. The compounds are extracted by distillation from the roots of plants of the family *Rutaceæ*, which are found in the desert areas of Western Australia. Eriostoic acid has been isolated from *Eriostemon difformis*, *Eriostemon coccineus* and *Eriostemon deserti.* It exists in 'ordinary', 'hydrogenated ordinary', 'isometric' and 'hydrogenated isometric' forms. Initially only the empirical formulae of these compounds were known from chemical evidence, and an investigation by X-ray diffraction methods was undertaken to determine their structural formulae, as well as their molecular geometries. Bromo derivatives of all four were prepared and crystallized. The dibromide of the ordinary form gave the best crystals, and was selected for a first analysis. In the course of this investigation its formula was determined by chemical methods to be 3,7-dibromo-5-methoxy-2,2,8,8-tetramethyl-2*H*, 8*H* [1,2*b*,5,4-*b*′]-dipryram-10-2-propionic acid, and its relation to the other forms was established (Duffield, Jefferies & Lucich, 1962).

The structure of this form, shown diagrammatically in Fig. 1, is of particular interest in that, neglecting side chains, it may be regarded as consisting of two chemically equivalent units. Because of the freedom of rotation around the single bonds in the side chains it is unlikely that the two units would be crystallographically equivalent. However, apart from any distortions due to packing the bond lengths and interbond angles in the two equivalent units are expected to be identical. This provides a means for assessing the validity of the method used for calculating the standard deviations on the parameters obtained from the refinement. In view of bond length anomalies reported recently for similar compounds (*e.g.* Hall & Maslen, 1965, Oh & Maslen, 1965) this verification of accuracy estimates is of considerable importance.

Experimental

The crystals of the dibromide of eriostoic acid, which were kindly prepared by Mr A. M. Duffield of the Department of Chemistry, University of Western Australia, were colourless, thick plates of irregular shape, of approximately 0·1 mm² in area and between 0·1 and 0·2 mm thick. The axis perpendicular to the plate was later assigned to be c^*.

The crystal data are given in Table 1. The cell dimensions were determined by the θ method of Weisz, Cochran & Cole (1948). The cell constants listed first are those of the Delaunay cell (Balashov & Ursell, 1957), taking $a<b<c$, which was taken as standard for this

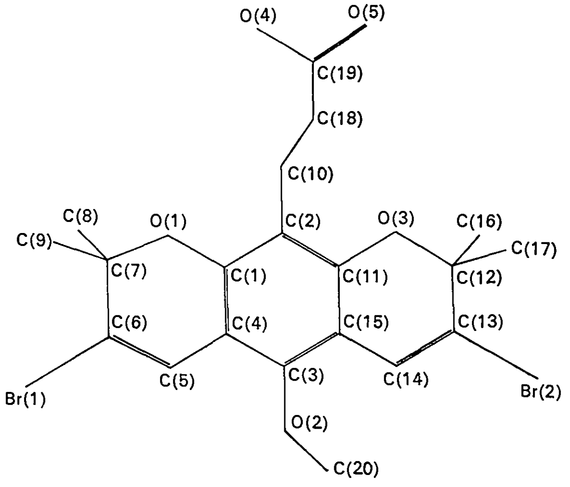

Fig. 1. Molecular formula of dibromoeriostoic acid.

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analysis. The dimensions of the Dirichlet cell, which is defined by an alternative convention, are also included. The crystal density was measured by flotation in a solution of potassium mercuri-iodide in water.

The intensity data were recorded by taking multiple film and multiple exposure Weissenberg photographs of the layers perpendicular to **a** with h from 0 to 7, and those perpendicular to **b** with k from 0 to 4. They were estimated visually. Film factors were determined from a comparison of the relative intensities of common reflections on neighbouring films. Out of approximately 4850 independent reflexions within the Cu $K\alpha$ sphere 4160 were recorded, but 1273 of these were too weak to be measured. 2561 observed reflexions were estimated from the a-axis photographs and 1642 from the b-axis data, of which 1316 were common to both sets. The crystal used for the a-axis data collection was roughly a rectangular parallelepiped, with dimensions approximately $0{\cdot}35 \times 0{\cdot}25 \times 0{\cdot}15$ mm^3. The variations in the cross sections are not extreme, so there are no sudden changes in the absorption factor. Absorption corrections accurate to approximately five per cent, which were satisfactory for this analysis, were obtained as follows. The absorption factors for 285 reflexions chosen at appropriate intervals through reciprocal space were evaluated by the method of Busing & Levy (1957) with the extension by Wells (1960) to compute the direction cosines of the incident and diffracted rays for the three-dimensional data. Corrections for the remaining reflexions could be calculated by interpolation from a three-dimensional plot of the absorption factor. After these had been applied the data were reduced to a common scale by evaluating the average of the reciprocal point-to-point ratio between the reflexions common to each pair of intersecting layers. The resulting matrix was then reduced by row and column multiplication by scale factors until all elements lay as close as possible to unity. The final set of intensity data was obtained by applying these scale factors and averaging the results. The R index on the common reflexions, defined as $R=2\Sigma||F_a|-|F_b||/\Sigma|F_a|+|F_b|$, where $|F_a|$ and $|F_b|$ are the structure factor amplitudes for reflexions with the same indices recorded on Weissenberg photographs taken about the a and b axes respectively, was 0·12.

Structure analysis

The positions of the bromine atoms were determined from Patterson syntheses, sharpened to point atoms at rest, for the [100] and [010] projections. These could be arranged as two centrosymmetrically related pairs, suggesting that the structure as a whole was centrosymmetric, and conformed to space group $P\bar{1}$. An attempt at solving the structure from bromine-phased electron density projections down [100] and [010] was unsuccessful, so a three-dimensional electron density map was evaluated, using the observed magnitudes and the phases of the bromine contributions to the structure factors. The peaks were well resolved, and every non-hydrogen atom was placed from this synthesis. The oxygen atoms were readily distinguished by their peak heights, which had a mean value of 7·8 e.Å^{-3} compared with an average of 5·4 e.Å^{-3} for the carbon atoms. There were few spurious peaks.

Structure factors for the observed reflexions were evaluated by means of the atomic scattering factor curves of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for carbon and oxygen and of Thomas & Umeda (1957) for bromine, the latter being modified by the real part of the dispersion correction by Dauben & Templeton (1955). A mean isotropic temperature factor coefficient, obtained from a Wilson plot, was applied.

The R index* of 0·44 was rather high, but there was close agreement for the inner terms, indicating a basically correct structure. Approximate corrections for the positional parameters were evaluated from two projection difference syntheses. Three-dimensional difference syntheses were then used to refine positional and isotropic thermal parameters. After three cycles R had fallen to 0·25, at which stage the predominant features in the difference maps could be interpreted in terms of anisotropic thermal motions of the bromine and other atoms. It was therefore decided to introduce anisotropic thermal parameters, and to continue refinement by the method of least-squares.

The structure-factor least-squares program, which minimizes $\Sigma w(|F_o|-|F_c|)^2$, uses the block diagonal approximation to the full matrix, and consists of a 3×3 and 6×6 matrix for each atom's positional and thermal parameters respectively, and a 2×2 matrix for refinement of the scale, allowing for an interaction with the mean temperature factor coefficient. For the first six rounds a weighting scheme was chosen where $w=1$ for $|F_o|<F^*$ and $w=(F^*/|F_o|)^2$ for $|F_o|<F^*$ for the observed reflexions.

The unobserved reflexions were given zero weight. F^* was set equal to 2·3 electrons. This scheme, suggested by Abrahams (1955) assumes that the standard deviation in F_o is proportional to $|F_o|$ for all observations greater than F^*, while those which are less are all equally reliable. Abrahams based his assumption on careful observations on a set of visually measured intensity data, and his conclusions were largely confirmed by the work of Donohue & Marsh (1962).

After three cycles of least-squares refinement R had fallen to 0·154, but there were still some significant discrepancies in the structure factors of low order reflexions which could not be accounted for solely in terms of experimental factors, such as extinction. As the twenty-two hydrogen atoms in the molecule account for almost nine per cent of the electrons in the structure it seemed possible that their scattering was responsible for these discrepancies. The standard devia-

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* All R indices calculated during the refinement were of the form $\Sigma\ ||F_o|-|F_c||/\Sigma\ |F_o|$ for the observed reflexions only.

tion in the electron density at this stage of the refinement was 0·3 e.Å^{-3}. Since hydrogen atoms give rise to peaks of the order of 0·5 e.Å^{-3} they may easily be confused with features arising from shifts in other parameters, or from errors in the data. However, if normal molecular geometries are assumed, the positions of the two hydrogen atoms attached to C(5) and C(14) and the four attached to C(10) and C(18) may be determined uniquely from the positions of the carbon atoms. The fifteen hydrogen atoms in the five methyl groups at C(8), C(9), C(16), C(17) and C(20) are restricted to positions on circles traced out by the ends of a rotating C–H bond, shown in Fig. 2(*a*). A difference synthesis was evaluated, and the difference electron density on the restricting circles was plotted as a function of angle for the five methyl groups. Around C(8), C(17) and C(20) there were three maxima at intervals of 120°, and around C(9) and C(16) there were two peaks 120° apart. In both the last two cases the difference synthesis near the expected third position was obviously affected by slightly incorrect coordinates assigned to C(9) and C(16). Confidence in these positions was strengthened when it was found that the hydrogen atoms in the *gem* dimethyl groups at C(8), C(9), C(16) and C(17) have the staggered configuration shown in Fig. 2(*b*). This arrangement is favoured energetically unless an interaction with another neighbouring group perturbs the system.

This accounted for twenty-one of the twenty-two hydrogen atoms in the molecule. These were included in the structure factor calculation but not the refinement in the subsequent least-squares rounds, giving them, for lack of better values, the anisotropic temperature factor coefficients of the carbon atoms to which they were attached. The scattering factor used was that by McWeeny (1951). On the fourth cycle there was an immediate drop of the R value to 0·133, and there were noticeable increases in the shifts of several atoms.

The remaining hydrogen atom, which was that attached to the carboxyl group, could not be located from the early difference maps, and was omitted from the structure factor calculations until the tenth cycle of refinement, when it was identified. It lay on a rather elongated peak, 0·6 e.Å^{-3} in height, half way between the atoms O(4) and O(5) in neighbouring molecules. It was symmetrical about the point half way along the contact, and the hydrogen atom was placed in this position for the purpose of structure factor calculations.

After six cycles of least-squares refinement R had fallen to 0·123. During these computations considerable difficulty was encountered in refining the scale factor. The changes indicated for this parameter were often in the opposite sense to that indicated by the ratio $\Sigma|F_c|/\Sigma|F_o|$, and were also unreasonably large. An examination of the structure factor agreement for ranges of $|F_o|$ indicated that a revision of the weighting scheme was necessary. Hodgson & Rollett (1963) have drawn attention to the considerable changes in parameters which may result from the use of different weighting schemes, and the need to choose the one best suited to the experimental data. Assessments of the reliability of the $|F_o|$ values were made in two different ways. The first was obtained by considering the reflexions which had been measured independently in the two sets of data. The reciprocal of the mean value of $||F_{oa}|-|F_{ob}||^2$ where a and b denote the rotation axis, was plotted as a function of $|F_o|$ for ranges of $|F_o|$. As $\sigma|F_o|$ is proportional to $\{\overline{||F_{oa}|-|F_{ob}||}\}^{1/2}$ this graph gives the square root of the required weighting function. The second assessment was made by comparing the observed and calculated structure factors in the same manner. The results obtained by the two methods were remarkably similar. The original weighting scheme gave too much weight to the weak terms and not enough to the intermediate terms, but it was not possible to obtain a better approximation to the correct weighting merely by altering F^*. However, close correspondence was given by a function of the form

$$w=\frac{1}{1+\left\{\dfrac{|F_o|-g}{f}\right\}^2}$$

where f and g were 4·56 electrons and −4·00 electrons respectively. The change in the weighting scheme gave a rapid improvement in the refinement, and consequently in the standard deviations on the parameters.

This type of variation of standard deviation with intensity, although different from those reported by

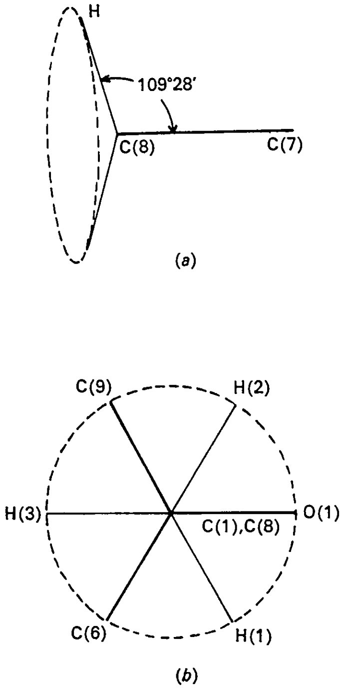

Fig. 2. Arrangement of hydrogen atoms in a *gem* dimethyl group. (*a*) The atoms are restricted to the circle shown by the dashed line. (*b*) The atoms tend to adopt the staggered configuration shown.

Table 1. *Crystal data*

Reciprocal cell	Real cell (Delaunay)	Real cell (Dirichlet)
$a^*=0{\cdot}1243\pm0{\cdot}0003$ Å^{-1}	$a=9{\cdot}68\pm0{\cdot}06$ Å	9·68 Å
$b^*=0{\cdot}1049\pm0{\cdot}0002$	$b=11{\cdot}33\pm0{\cdot}07$	10·35
$c^*=0{\cdot}0881\pm0{\cdot}0001$	$c=11{\cdot}66\pm0{\cdot}02$	11·66
$\alpha^*=80°59'\pm13'$	$\alpha=93°48'\pm30'$	76°36′
$\beta^*=77\ \ 16\ \pm4$	$\beta=99\ \ 48\ \pm28$	80 12
$\gamma^*=57\ \ 27\ \pm20$	$\gamma=121\ \ 36\ \pm36$	68 54
	$U=1060\pm10$ Å^3	

Empirical formula $C_{20}H_{22}O_5Br_2$

F.W. 502·3
D_x $=1{\cdot}57\pm0{\cdot}02$ g.cm^{-3}
D_m $=1{\cdot}58\pm0{\cdot}01$ g.cm^{-3}
μ $=53{\cdot}65$ cm^{-1} for Cu $K\alpha$ radiation

Triclinic
Space group $P1$ or $P\bar{1}$ (The analysis indicates $P\bar{1}$)
$Z=2$

Table 2. *Atomic coordinates of non-hydrogen atoms*

	x/a	y/b	z/c
Br(1)	0·33822	−0·06128	1·33048
Br(2)	0·86943	0·58460	0·69853
O(1)	0·5369	0·3585	1·3022
O(2)	0·5275	0·1477	0·9328
O(3)	0·7634	0·6432	1·0170
O(4)	1·0155	0·8491	1·5089
O(5)	0·8897	0·9096	1·3689
C(1)	0·5773	0·3704	1·1946
C(2)	0·6552	0·5026	1·1624
C(3)	0·5664	0·2638	1·0070
C(4)	0·5292	0·2485	1·1176
C(5)	0·4453	0·1130	1·1606
C(6)	0·4391	0·1117	1·2729
C(7)	0·5295	0·2448	1·3616
C(8)	0·4345	0·2377	1·4559
C(9)	0·7041	0·2817	1·4122
C(10)	0·7019	0·6303	1·2457
C(11)	0·6913	0·5127	1·0511
C(12)	0·8744	0·6744	0·9369
C(13)	0·7975	0·5494	0·8413
C(14)	0·6950	0·4189	0·8579
C(15)	0·6490	0·3957	0·9722
C(16)	0·8888	0·8032	0·8911
C(17)	1·0405	0·7056	1·0040
C(18)	0·8661	0·6871	1·3312
C(19)	0·9225	0·8227	1·4053
C(20)	0·3626	0·0740	0·8595

Table 3. *Atomic coordinates of hydrogen atoms*

	Bonded to	x/a	y/b	z/c
H(1)	C(5)	0·401	0·020	1·101
H(2)	C(14)	0·650	0·335	0·788
H(3)	C(10)	0·710	0·708	1·199
H(4)	C(10)	0·611	0·604	1·293
H(5)	C(18)	0·857	0·613	1·386
H(6)	C(18)	0·958	0·701	1·283
H(7)	C(8)	0·410	0·147	1·498
H(8)	C(8)	0·310	0·209	1·410
H(9)	C(8)	0·491	0·325	1·515
H(10)	C(9)	0·767	0·377	1·475
H(11)	C(9)	0·765	0·296	1·344
H(12)	C(9)	0·700	0·202	1·455
H(13)	C(16)	0·936	0·887	0·960
H(14)	C(16)	0·765	0·776	0·846
H(15)	C(16)	0·962	0·832	0·830
H(16)	C(17)	1·118	0·733	0·942
H(17)	C(17)	1·026	0·621	0·036
H(18)	C(17)	1·095	0·795	0·071
H(19)	C(20)	0·311	−0·024	0·812
H(20)	C(20)	0·354	0·137	0·799
H(21)	C(20)	0·275	0·060	0·910
H(22)	O(4) or O(5)	0·953	0·880	0·439

Abrahams and Donohue & Marsh, is similar to that found by some other investigators. It is clear that the reliability of visually estimated data does not always depend on the intensity in the same manner, but varies with different investigators and different compounds. If the best parameters are to be obtained it appears necessary to make an independent assessment of the best weighting scheme for every analysis. Refinement continued for eight further cycles of structure-factor and least-squares computations, at which stage R was 0·095. There were no significant changes in the atomic positions or in the temperature factor coefficients indicated, so the refinement was terminated. The final parameters are listed in Tables 2, 3 and 4, and the structure factors in Table 5. In the final data there is a tendency for $|F_o|$ to exceed $|F_c|$ for large values of $|F|$, and conversely for small values. This is consistent with a slight underestimation of the weaker reflexions in the intensity measurements. The effect is presumably small compared with random error for a single observation, but the cumulative effect of the resulting film factor errors would give rise to significant errors in the extreme values. This also explains the shape of the weighting function which was found to be the optimum for this analysis.

Accuracy of the analysis

The standard deviations of the structural parameters and the corresponding values for the bond lengths and angles were evaluated from the least-squares matrix variances and covariances by the formulae of Ahmed & Cruickshank (1953) and Darlow (1960). The latter are included in Tables 6 and 7. The errors in the coordinates resulting from thermal librations were calculated, but were found to be very much less than the respective standard deviations and therefore no corrections were applied.

The estimate of accuracy provided by the standard deviations from the least-squares was checked by an analysis of the molecular symmetry. The quantity

$$t=\frac{|l-l'|}{|(\sigma_l^2+\sigma_l^2)^{\frac{1}{2}}},$$

where l and l' denote the lengths of chemically equivalent but crystallographically distinct bonds, was evaluated for each pair of bonds. For values of t less than 1·96 there is more than ninety-five per cent probability that the differences result from pure chance, and have no physical significance. In no case did t exceed 1·5, indicating that the bonds on either side were almost certainly equivalent. The r.m.s. deviation between the equivalent bonds is 0·010 Å, which is slightly less than the average standard deviation from the least-squares of 0·012 Å, suggesting that, if anything, the accuracy of the structure determination has been underestimated. Similar results are obtained from an analysis of the bond angles.

The atomic coordinates themselves may be compared by transforming to an orthogonal molecular axis system, X, Y, Z. The origin was chosen at the centre of mass of the benzene ring, with X along the length of the ring system and Z perpendicular to the plane of the central ring. The atomic coordinates in this system are listed in Table 8. For an exactly symmetrical molecule the magnitudes of X, Y and Z for each pair of atoms would be equal, the X coordinates having opposite signs. The coordinates of the related pairs in this molecule do not match exactly in this way, but the differences show a regular pattern. The atoms on the same side of Br(2) have, in general, larger Z coordinates than their symmetric opposites, and there is also a tendency in the XY plane for these atoms to be bent away from the methoxyl group. These regular variations are consistent with a very slight bending of the molecule due to packing, but they may also be explained partly in terms of errors in the measurement of the cell angles. Kitajgorodskij (1965) has recently shown that the effects of intermolecular interaction on molecular shape are in general small, but that the packing can influence the molecular geometry in some cases. In view of the close correspondence between equivalent bond lengths and angles it seems probable that the deviations in this structure result from molecular distortion rather than errors in the analysis.

A further guide to the accuracy of the structure determination may be obtained by considering the geometry of the part of the molecule which is expected to be planar. This is the central benzene ring plus the atoms bonded to it directly. Least-squares planes were calculated for the whole system, and for the benzene ring alone, by the method of Schomaker, Waser, Marsh & Bergman (1959). As all the atoms have comparable standard deviations their coordinates were given equal weights in the calculations, the results of which are included in Table 10. None of the atoms in

Table 4. *Thermal parameters of non-hydrogen atoms*

The B_{ij} are defined as coefficients of the expression:

Temperature factor $= 2^{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{23}kl+B_{31}hl+B_{12}hk)}$

	B_{11}	B_{22}	B_{33}	B_{23}	B_{31}	B_{12}
Br(1)	0·04739	0·02233	0·01788	0·01681	0·01677	0·02431
Br(2)	0·05939	0·02959	0·01858	0·01115	0·03339	0·02266
O(1)	0·03481	0·02049	0·01216	0·00388	0·01341	0·02998
O(2)	0·02543	0·01507	0·01392	−0·00161	0·00370	0·02217
O(3)	0·03072	0·01380	0·01608	0·00635	0·01068	0·02247
O(4)	0·04230	0·02082	0·01532	−0·00050	−0·00334	0·03652
O(5)	0·05410	0·02643	0·02079	−0·01564	−0·02333	0·05922
C(1)	0·02573	0·01774	0·01233	0·00116	0·00507	0·02519
C(2)	0·02829	0·01719	0·01344	0·00164	0·00688	0·02703
C(3)	0·02483	0·01295	0·01184	0·00091	0·00436	0·02049
C(4)	0·02722	0·01584	0·01305	0·00666	0·01197	0·02460
C(5)	0·02666	0·01770	0·01430	0·00574	0·00767	0·02581
C(6)	0·03088	0·02005	0·01489	0·01479	0·01234	0·02494
C(7)	0·03234	0·02063	0·01336	0·00749	0·01110	0·02785
C(8)	0·04872	0·03084	0·01593	0·01253	0·02589	0·03755
C(9)	0·03493	0·02736	0·01714	0·00800	0·00220	0·03101
C(10)	0·02821	0·01705	0·01434	−0·00445	0·00169	0·02463
C(11)	0·02579	0·01271	0·01443	0·00612	0·00630	0·02170
C(12)	0·02505	0·01568	0·01649	0·00563	0·00686	0·01838
C(13)	0·02891	0·02382	0·01393	0·01121	0·01271	0·02976
C(14)	0·02535	0·01744	0·01252	0·00296	0·00670	0·02124
C(15)	0·02422	0·01737	0·01169	0·00498	0·00584	0·02370
C(16)	0·03445	0·01807	0·02296	0·01137	0·01708	0·02661
C(17)	0·02952	0·02591	0·02214	0·00681	0·00151	0·03040
C(18)	0·03772	0·01868	0·02082	−0·01077	−0·00804	0·03148
C(19)	0·03431	0·01783	0·01383	−0·00757	0·00229	0·02455
C(20)	0·03068	0·02075	0·01939	−0·01188	−0·00602	0·02563

Table 5. *Observed and calculated structure factors*

l	Fo	Fc
0	0	
2	-20.09	-19.22
3	47.18	52.42
4	-7.47	-6.73
5	-28.14	-26.31
6	34.23	31.27
7	9.24	9.32
8	-10.33	-10.80
9	1.86	1.48
10	3.00	2.58
11	-5.00	-4.42
12	1.43	1.49
13	1.71	1.65
0	1	
-13	-4.38	-4.42
-12	4.52	4.82
-11	4.05	4.31
-10	-10.09	-9.19
-9	3.43	3.21
-8	9.14	7.62
-7	-19.76	-17.44
-6	-16.19	-13.77
-5	1.86	1.38
-4	-32.52	-27.66
-3	-3.14	-3.69
-2	10.43	11.09
-1	-13.38	-12.58
0	-14.43	-12.99
1	-47.09	-44.30
2	6.38	5.15
3	1.19	1.08
4	-21.09	-18.67
5	-3.67	-3.04
6	21.23	17.75
7	-19.33	-16.89
9	11.09	10.21
11	-3.90	-3.77
12	3.29	3.23
14	-1.14	-1.07
0	2	
-14	-1.14	-.34
-13	1.29	1.39
-12	5.43	5.24
-11	-5.00	-4.52
-10	-4.67	-5.04
-9	15.00	14.63
-8	-7.71	-7.66
-7	-12.95	-12.85
-6	29.37	26.93
-5	-.86	-.88
-4	-43.99	-42.24
-3	18.90	17.57
-2	-2.81	-2.35
-1	-42.23	-47.13
0	7.81	7.25
1	40.04	36.18
2	-70.46	-70.21
3	10.05	9.43
4	21.00	19.54
5	-28.66	-25.80
6	5.71	5.92
7	11.38	11.05
8	-10.28	-9.42
9	-12.76	-12.69
10	-2.09	-1.98
11	- .09	-2.04
12	-2.71	-2.30
0	3	
-14	1.76	1.59
-13	-2.67	-2.87
-11	5.43	4.90
-10	-6.38	-6.17
-9	-2.29	-1.83
-8	11.43	10.59
-7	.81	.79
-6	-5.71	-5.16
-5	13.85	13.32
-4	4.57	5.16
-3	-2.86	-2.98
-2	-6.47	-8.02
-1	-6.90	-7.46
0	10.95	9.55
1	6.28	7.68
2	-17.04	-15.02
3	64.51	54.10
4	7.67	7.01
5	-6.57	-6.97
6	21.52	17.59
8	-9.09	-8.91
9	17.38	14.96
10	5.57	5.33
11	-2.95	-2.73
0	4	
-13	-3.33	-3.07
-12	2.05	2.12
-11	1.81	1.97
-10	-10.43	-10.45
-9	8.24	8.47
-8	12.09	12.37
-7	-20.95	-20.45
-6	10.71	10.55
-5	34.56	31.73
-4	-40.42	-39.73
-3	2.95	2.42
-2	41.13	41.52
-1	-32.80	-33.27
0	-24.42	-24.64
1	36.14	34.75
2	-13.54	-12.54
3	-19.61	-17.41
4	7.19	8.66
5	-8.43	-7.78
6	-10.05	-10.36
7	8.66	8.33
8	-2.62	-2.17
9	2.43	2.63
11	1.52	1.51
12	1.57	.35
0	5	
-14	3.14	2.44
-12	-3.33	-2.76
-11	3.90	3.55
-10	2.95	2.11
-8	7.00	6.32
-7	-2.14	-2.05
-6	-3.00	-2.53
-5	4.57	4.97
-3	4.57	5.27
-2	2.05	1.85
-1	-8.95	-8.98
0	1.29	.05
1	2.14	2.47
2	-13.00	-12.02
3	-4.00	-3.61
4	9.47	9.03
5	-15.90	-14.16
6	-4.81	-4.22
7	8.43	8.40
8	-5.05	-4.28
10	3.81	3.55
11	-1.90	-1.48
12	-1.86	-1.33
0	6	
-14	1.29	1.19
-13	-5.19	-3.62
-11	6.00	4.80
-10	-6.28	-5.26
-9	-10.76	-8.78
-8	4.90	3.94
-7	-13.24	-12.69
-6	-12.09	-12.39
-5	16.71	17.05
-4	1.24	1.03
-3	-14.76	-14.28
-2	23.33	24.76
0	-15.57	-16.69
1	14.57	14.38
2	7.52	8.03
3	-12.19	-11.46
4	7.28	6.34
5	3.62	3.38
6	-6.76	-6.28
7	-3.95	-3.65
10	2.19	1.43
11	-1.43	-1.28
0	7	
-13	2.09	1.34
-12	-3.14	-1.50
-10	2.57	2.40
-9	-4.71	-4.31
-8	3.86	3.1
-6	-2.52	-2.19
-5	3.61	3.28
-3	-3.00	-3.71
-2	12.33	12.39
-1	-8.24	-10.40
0	-4.95	-5.31
1	9.09	9.45
2	-3.76	-3.35
3	-5.05	-4.36
4	8.47	7.35
5	-5.33	-4.17
6	-4.61	-4.12
7	4.24	3.60
9	-4.24	-3.25
10	2.90	2.14
0	8	
-12	-4.90	-3.28
-11	7.52	5.60
-10	2.05	1.22
-9	-7.71	-6.92
-8	7.09	6.24
-7	3.57	3.20
-6	-9.43	-8.35
-5	8.57	8.30
-4	9.52	9.41
-3	-12.33	-11.93
-2	2.19	1.28
-1	8.57	8.20
0	-4.19	-3.56
1	4.67	4.66
2	8.90	8.46
3	-4.24	-2.96
4	3.76	3.62
5	5.52	4.03
6	-2.05	-1.02
8	1.95	1.28
9	-1.38	-1.42
0	9	
-11	2.14	1.66
-9	-2.81	-2.19
-7	2.24	2.60
-6	-4.52	-4.97
-5	-2.62	-3.58
-4	-2.24	-2.47
-3	-4.86	-5.13
-1	2.90	2.43
0	-6.52	-6.73
3	-4.99	-4.41
4	2.71	2.26
5	4.24	3.71
6	-1.33	-1.07
0	10	
-10	2.90	1.85
-9	-6.09	-3.99
-7	6.33	5.86
-6	-5.14	-4.55
-4	5.71	6.18
-3	-3.24	-2.77
-2	-3.90	-3.50
-1	5.48	5.80
0	-3.05	-2.27
1	-3.62	-3.30
4	-3.38	-2.54
0	11	
-7	2.71	2.64
-6	-2.90	-1.95
0	12	
-5	-4.09	-2.70
-4	2.71	2.11
0	2.62	1.51
1	-2.43	-1.78
1	0	
-14	1.05	.96
-13	1.29	1.18
-12	-4.52	-3.99
-11	-1.71	-1.91
-10	10.85	10.52
-9	-11.52	-11.37
-8	-2.05	-2.04
-7	20.85	20.09
-6	-27.04	-24.74
-5	-21.85	-20.68
-4	44.85	44.50
-3	-4.52	-5.38
-2	-6.95	-6.50
-1	11.38	13.00
0	-23.90	-24.82
1	-44.42	-43.70
2	22.80	22.28
3	18.85	16.31
4	-23.28	-20.88
5	9.19	9.11
6	11.38	11.05
7	-12.52	-11.38
8	5.00	4.92
10	2.05	1.96
12	2.05	1.96
1	1	
-14	-2.24	-2.27
-11	-6.00	-5.78
-10	2.38	2.40
-9	1.19	.58
-8	-2.86	-2.34
-7	.86	.73
-6	4.28	3.35
-5	28.14	27.96
-4	22.33	21.36
-3	-26.76	-26.54
-2	32.61	30.87
-1	-2.24	-2.13
0	-44.13	-37.74
1	-4.52	-4.09
2	28.14	22.34
3	-20.55	-18.60
4	-25.23	-19.85
5	17.42	15.72
6	-6.86	-6.96
7	-14.95	-13.90
8	14.52	13.85
10	-2.00	-2.02
11	5.09	4.74
13	-3.62	-3.11
1	2	
-14	-1.57	-1.53
-13	5.81	5.64
-12	-2.48	-2.29
-11	-3.52	-3.09
-10	12.52	12.37
-9	.90	.26
-8	-23.76	-20.86
-7	21.28	18.32
-6	5.33	7.38
-5	-38.47	-36.71
-4	30.18	28.59
-3	30.33	32.55
-2	-40.18	-40.32
-1	3.33	3.83
0	23.19	22.56
1	-34.99	-29.56
2	2.43	1.66
3	32.47	27.29
4	-3.38	-3.67
5	-2.38	-2.67
6	5.62	5.80
7	-6.28	-6.62
8	2.62	2.41
9	5.67	5.34
10	-2.19	-2.41
11	1.29	1.37
1	3	
-14	-.81	-1.04
-13	-.71	-1.10
-12	.71	.20
-10	-3.24	-3.18
-9	2.43	2.25
-8	-6.24	-6.62
-7	3.14	3.96
-6	-5.28	-5.56
-5	-4.67	-6.13
-4	15.62	18.49
-3	6.14	7.86
-2	-8.58	-10.92
-1	31.18	34.10
0	-12.57	-13.26
1	-8.71	-8.80
2	22.71	21.39
3	-2.62	-2.00
4	-28.09	-23.27
5	5.86	5.44
6	6.62	6.18
7	-15.00	-13.89
8	-2.43	-3.33
9	2.30	3.20
10	-7.33	-7.17
12	1.86	2.01
1	4	
-14	-3.33	-3.50
-13	2.38	2.77
-12	4.28	4.84
-11	-8.57	-8.54
-10	4.46	4.58
-9	8.24	8.67
-8	-26.42	-24.01
-7	-1.19	-1.49
-6	18.71	19.62
-5	-17.04	-16.24
-4	-12.24	-14.41
-3	19.04	20.99
-2	-30.14	-28.02
-1	-15.38	-17.26
0	14.09	14.29
1	5.52	6.71
2	-14.19	-14.93
3	8.62	8.64
4	8.57	8.14
5	-3.29	-3.69
6	-2.81	-2.69
7	5.00	4.70
8	-2.90	-2.86
1		5
-12	1.62	1.67
-10	3.09	2.89
-8	3.19	3.65
-7	10.95	10.99
-5	-17.14	-17.50
-4	6.67	7.51
-3	7.14	8.75
-2	-17.14	-16.59
-1	15.71	14.32
0	22.85	19.68
1	-23.80	-20.15
3	15.71	15.32
4	-8.57	-7.67
5	2.51	3.68
6	8.76	8.15
7	-2.38	-2.26
8	-4.67	-4.35
9	3.67	3.32
11	-1.81	-1.84
1	6	
-13	-2.43	-1.89
-12	6.05	5.99
-11	-3.05	-2.80
-10	-7.33	-6.62
-9	11.43	9.87
-8	-2.90	-2.28
-7	-18.09	-15.89
-6	16.19	15.11
-4	-17.14	-16.21
-3	5.24	6.11
-2	4.52	4.63
-1	-13.22	-14.19
0	9.52	9.36
1	4.81	5.40
6	4.43	4.30
7	2.62	2.62
1	7	
-9	6.19	6.08
-8	-2.05	-2.03
-6	10.09	9.49
-5	-7.33	-7.99
-3	12.38	12.07
-2	-4.24	-3.88
-1	-5.48	-6.56
0	10.43	10.56
1	-15.47	-14.01
2	-19.04	-17.30
3	3.95	3.34
5	-5.62	-5.30
6	4.00	3.80
8	-2.33	-2.26
9	-1.19	-1.34
1	8	
-12	3.29	3.41
-11	1.90	1.27
-10	-7.62	-7.24
-9	2.86	2.46
-8	5.48	4.64
-7	-7.24	-6.89
-5	7.09	7.72
-4	-5.33	-4.89
-2	4.09	4.57
-1	-2.71	-2.85
0	-3.05	-3.04
1	3.09	3,13
2	3.14	3.53
1	9	
-11	-1.95	-1.57
-10	-2.76	-2.72
-9	3.05	2.52
-7.	-6.52	-5.80
-6	5.57	4.66
-4	-9.57	-8.88
-3	5.76	5.49
-2	2.33	3.47
-1	-5.43	-5.09
0	3.29	2.84
1	4.19	3.93
2	-5.28	-4.58
5	-3.00	-3.24
1	10	
-8	4.48	4.60
-7	-2.62	-2.42
-6	-1.62	-1.78
-5	4.33	3.88
-2	2.76	2.60
1	2.57	2.18
5	-1.24	-1.43
1	11	
-6	-3.67	-.69
-5	3.09	2.69
-4	-3.52	-2.97
-2	4.05	3.78
-1	-2.62	-2.42
0	-1.95	-1.61
1	3.29	2.87
1	-1	
-14	-1.52	-1.70
-13	2.05	2.44
-12	1.10	1.78
-11	-1.29	-1.76
-10	3.14	3.70
-7	.71	.37
-6	3.29	2.27
-5	4.71	5.99
-4	-1.33	-2.19
-3	-17.42	-16.85
-2	-10.76	-10.78
-1	18.00	16.15
1	-6.67	-6.56
2	43.75	38.21
3	-28.99	-27.35
4	15.66	14.30
5	22.85	19.59
6	-23.14	-19.74
8	15.76	14.37
9	-8.66	-8.25
10	-1.19	-1.86
11	4.76	4.37
12	-5.09	-4.81
13	-1.52	-1.87
14	1.14	1.26
1	-2	
-14	2.14	2.20
-12	-4.48	-4.39
-11	5.62	5.59
-10	3.71	3.76
-9	-6.71	-6.26
-8	18.04	16.14
-7	6.19	6.79
-6	-27.04	-24.05
-5	8.00	8.32
-4	7.38	6.86
-3	-57.61	-45.91
-2	-24.28	-18.72
-1	34.66	33.85
0	-37.61	-29.25
1	-39.99	-32.88
2	56.18	55,98
3	-18.04	-19.65
4	-19.04	-17.75
5	28.90	25.42
6	-5.76	-5.37
8	2.57	2.28
9	-2.71	-2.76
10	-1.33	-1.48
11	3.19	3.41
12	-3.52	-2.61
1	-3	
-13	1.57	1.81
-12	-1.10	-1.18
-10	-4.00	-3.93
-9	-6.05	-6.63
-8	-.71	-.79
-7	3.19	3.13
-5	2.76	3.09
-4	-6.09	-6.04
-3	5.62	5.49
-2	10.57	10.37
-1	-5.43	-4.52
0	2.19	2.60
1	67.13	52.81
2	-7.19	-6.42
3	1.10	1.59
4	23.33	22.24
5	4.38	3.13
6	-28.71	-25.00
7	15.95	16.08
8	1.43	1.46
9	-10.90	-10.44
10	5.09	4.91
11	5.14	5.84
12	-2.57	-2.78
13	2.71	2.89
14	4.38	2.59
1	-4	
-11	3.67	3.29
-10	-5.05	-5.12
-9	-2.71	-3.18
-8	3.86	3.62
-7	-4.28	-4.21
-6	-12.57	-12.07
-5	16.28	15.61
-4	6.19	4.85
-3	-29.66	-27.87
-2	7.43	9.37
-1	39.28	33.88
0	-33.52	-34.20
1	27.38	28.35
2	8.19	7.59
3	-18.38	-18.44
4	8.61	11.21
5	10.47	11.46
6	-13.04	-12.88
7	2.38	2.48
8	4.05	4.66
9	-6.81	-7.77
12	- .24	-2.52
1	-5	
-8	-3.09	-2.72
-7	3.95	4.71
-5	-3.09	-3.08
-3	2.62	2.53
-2	1.38	1.75
-1	-1.81	-2.41
0	-2.14	-1.99
1	1.09	3.54
2	-26.66	-25.40
3	-33.33	-31.59
4	4.43	5.80
5	-20.00	-19.86
6	-6.00	-6.70
7	17.62	15.52
8	-7.14	-7.70
9	-14.28	-12.42
10	7.62	6.97
11	-2.57	-2.30
12	-2.81	-3.17
13	3.90	3.73
1	-6	
-10	-3.05	-2.98
-8	5.62	5.59
-7	-5.24	-4.82
-5	12.38	12.41
-4	-9.28	-9.74
-3	-2.38	-2.05
-2	30.47	26.75
-1	-17.62	-17.17
0	-2.48	-1.61
1	31.42	27.30
2	2.48	2.34
3	-19.52	-18.05
4	20.00	19.41
5	-1.67	-2.48
6	-14.28	-13.09
7	13.81	13.96
8	10.47	11.18
10	9.52	6.32
1	-7	
-11	-1.29	-.58
-10	1.29	1.31
-8	2.81	3.76
-6	2.00	2.53
-3	-4.57	-4.69
-2	3.29	3.55
0	10.47	10.53
1	1.95	1.82
2	-6.90	-7.60
3	5.48	7.16
4	3.62	3.82
5	-9.38	-10.89
6	8.28	7.95
7	3.09	3.21
8	-12.38	-12.69
10	3.29	3.43
11	-6.86	-5.64
12	2.48	.91
1	-8	
-9	1.95	1.15
-7	-5.38	-4.81
-5	-2.00	-2.65
-4	-8.00	-7.52
-3	1.95	2.50
-1	-29.33	-24.45
0	-12.35	-13.30
1	6.81	7.17
2	-12.85	-13.45
4	14.38	12.99
5	-10.00	-11.15
7	7.47	6.84
8	-5.48	-5.03
10	3.95	3.43
11	-2.86	-3.01
1	-9	
-2	6.95	7.01
-1	7.62	7.73
0	2.33	2.85

Table 5 (*cont.*)

ℓ	F_o	F_c
2	-2.71	-3.24
3	3.86	4.70
6	7.43	7.78
8	-6.14	-5.60
9	4.05	4.18
11	-3.90	-3.99
1	-10	
-3	5.05	5.88
-1	-3.57	-3.52
0	7.14	7.59
2	-6.19	-6.28
3	9.00	10.00
5	-7.14	-7.18
6	6.19	5.04
8	-6.33	-5.10
9	3.09	2.72
10	2.19	1.62
11	-2.81	-2.19
1	-11	
-4	-3.33	-2.80
4	-3.05	-2.95
7	-3.43	-2.86
10	-1.62	-1.00
1	-12	
0	2.19	2.09
1	-3.67	-4.11
3	3.62	3.28
4	-2.48	-2.04
5	-1.90	-1.75
6	2.67	2.60
7	-2.76	-2.09
2	0	
-14	3.67	3.83
-13	-3.14	-3.53
-12	-4.19	-4.45
-11	10.52	10.63
-10	-1.19	-.65
-9	-13.09	-13.42
-8	16.28	15.67
-7	-3.29	-3.51
-6	-22.52	-20.78
-5	4.71	4.66
-4	9.47	9.94
-3	-23.66	-23.18
-2	38.13	41.44
-1	7.24	7.88
0	6.14	6.43
1	-12.90	-12.01
2	-17.14	-15.19
3	3.76	4.00
4	6.52	6.14
5	-14.66	-13.35
6	5.76	5.66
8	-5.05	-5.27
9	1.95	1.89
10	5.48	5.82
11	-.67	-.51
13	1.43	1.60
2	1	
-12	4.38	4.92
-11	4.33	5.33
-10	-6.86	-7.14
-9	5.67	5.49
-8	8.52	9.80
-7	-12.00	-13.14
-6	-4.52	-4.71
-5	22.23	21.79
-4	-11.57	-13.43
-3	-32.85	-34.04
-2	58.42	53.61
-1	-21.66	-18.83
0	-28.95	-25.28
1	51.66	42.35
2	-9.47	-9.25
3	-40.09	-32.26
4	33.95	27.74
5	3.19	3.49
6	-8.00	-8.43
7	8.00	7.04
8	6.24	6.69
9	-12.95	-12.51
10	-4.71	-4.79
11	-.95	-1.28
12	-1.48	-1.67
2	2	
-14	2.90	2.88
-12	-7.05	-7.26
-11	2.24	1.80
-10	3.71	3.67
-9	-12.38	-13.79
-7	19.61	18.90
-6	-21.09	-19.51
-5	-4.52	-4.86
-4	7.95	8.66
-3	-18.14	-17.14
-2	-12.47	-14.68
-1	2.38	2.74
0	-9.33	-9.25
1	3.62	4.53
2	-9.57	-8.86
4	19.76	17.05
6	4.00	4.30
7	5.67	5.48
8	-6.00	-5.51
9	-2.29	-2.84
10	4.24	4.13
2	3	
-13	-1.14	-1.22
-12	-1.81	-2.04
-11	5.00	5.10
-10	-3.62	-3.49
-9	-7.38	-8.31
-8	16.81	17.61
-7	-1.67	-1.32
-6	-15.71	-17.29
-5	26.04	26.73
-4	-2.90	-2.62
-3	-36.42	-36.67
-2	7.43	9.44
-1	22.57	22.72
0	-40.71	-39.03
1	9.66	9.92
2	10.05	10.71
3	-18.19	-17.30
4	2.05	1.84
5	4.43	4.43
6	-7.09	-7.06
7	3.67	3.55
8	1.00	1.02
9	.71	.58
10	-.52	-.42
11	1.00	1.10
2	4	
-13	4.19	4.83
-12	-4.86	-4.66
-11	-1.67	-1.60
-10	7.57	7.76
-8	5.52	7.02
-7	16.09	17.56
-6	1.05	.94
-5	-4.24	-4.70
-4	8.24	9.47
-3	2.95	3.26
-2	2.76	3.43
-1	14.04	15.55
0	-2.86	-3.19
1	3.90	5.05
2	-.86	-.73
3	-9.86	-10.13
4	2.14	1.51
5	4.05	4.49
6	-6.38	-6.34
7	6.28	6.66
8	3.00	3.30
2	5	
-12	-4.14	-3.65
-11	1.90	2.11
-10	2.05	2.51
-9	-9.76	-9.99
-8	-4.95	-5.96
-6	-20.19	-21.26
-4	15.52	17.79
-3	-15.04	-16.35
-2	-2.09	-3.67
-1	17.19	18.86
0	-9.76	-11.07
1	-9.28	-9.62
2	20.47	17.03
3	-5.81	-5.34
4	-11.24	-11.21
5	7.09	7.45
6	-2.09	-2.38
7	-2.76	-2.60
2	6	
-13	4.28	4.24
-11	-5.81	-6.34
-10	4.62	4.36
-8	-6.81	-6.66
-7	5.14	5.35
-5	-5.05	-4.54
-4	2.71	2.70
0	-4.57	-5.04
1	-4.76	-5.99
3	-6.05	-5.73
6	-4.95	-5.01
7	-1.19	-1.92
9	-1.05	-1.71
2	7	
-12	-2.52	-2.27
-10	5.62	6.49
-9	-4.86	-4.35
-8	-3.29	-3.48
-7	7.95	8.69
-5	-4.38	-4.33
-4	15.23	16.00
-2	-8.86	-9.12
-1	6.71	6.79
0	3.81	3.98
2	12.43	12.43
3	6.00	5.46
7	-1.67	-1.77
8	2.24	2.44
2	8	
-11	-2.43	-2.18
-9	2.95	3.05
-8	-3.52	-3.58
-6	2.81	3.07
-5	-6.19	-6.68
-4	-2.86	-3.43
-3	-2.48	-2.70
-2	-4.52	-4.23
5	1.81	1.83
7	-1.57	-1.98
2	9	
-10	2.71	2.26
-8	-5.33	-5.66
-7	3.57	3.24
-6	2.52	2.66
-5	-5.81	-6.41
-3	5.19	5.14
-2	-6.76	-6.97
0	4.95	4.65
1	-3.48	-3.69
3	2.09	1.80
4	-2.33	-2.28
5	-1.76	-2.04
2	-1	
-11	-3.52	-4.06
-8	-1.81	-1.76
-7	-16.28	-16.91
-6	19.81	19.60
-5	11.00	11.04
-4	-46.09	-42.50
-3	36.80	36.35
-2	37.71	35.47
-1	-80.55	-65.28
0	81.17	68.39
1	91.22	83.53
2	-29.57	-25.93
3	-2.62	-2.01
4	24.04	23.18
5	-16.33	-16.35
6	-5.81	-6.47
7	19.52	17.66
8	-3.29	-3.91
9	-4.81	-5.24
10	2.48	2.36
13	1.76	1.34
2	-2	
-13	-3.81	-4.05
-12	1.81	1.71
-11	4.00	4.10
-10	-7.52	-7.38
-9	.90	.67
-8	16.33	17.17
-7	-14.76	-14.74
-6	-16.14	-14.47
-5	11.04	14.53
-4	-13.81	-14.04
-3	-9.14	-7.45
-2	26.76	23.70
-1	-22.23	-21.28
1	-18.71	-18.43
2	-8.76	-9.04
3	4.09	3.52
4	-3.81	-3.79
5	-3.24	-3.40
6	-10.90	-11.25
7	-9.33	-8.86
8	-5.43	-5.51
9	5.62	5.90
11	-2.00	-2.11
12	3.33	3.24
14	-1.95	-2.12
2	-3	
-14	-.33	-.31
-12	-2.71	-2.89
-9	.90	.56
-8	-12.52	-13.69
-7	-2.29	-2.38
-6	20.57	18.66
-5	-4.09	-4.34
-4	-15.33	-14.24
-3	46.28	40.52
-2	-28.76	-26.28
-1	-40.85	-31.44
0	28.33	24.22
1	5.67	5.16
2	-40.13	-36.37
3	32.99	27.81
4	8.09	7.62
5	-27.42	-24.81
6	14.52	15.08
7	15.04	13.79
8	-14.52	-13.90
9	4.28	4.43
10	6.71	6.48
11	-5.00	-4.27
12	-1.57	-2.10
13	2.62	3.23
14	-1.29	-1.26
2	-4	
-13	-1.24	-1.31
-12	3.09	3.39
-10	-6.86	-6.11
-9	18.00	17.99
-8	8.09	8.06
-7	-17.76	-16.47
-6	16.14	15.14
-5	10.66	10.59
-4	-21.23	-18.80
-3	38.52	37.30
-2	30.28	21.50
-1	-24.99	-23.65
0	-4.86	-4.87
1	6.67	8.29
2	-6.86	-6.85
3	6.81	7.81
4	8.52	9.99
5	4.95	4.86
6	1.76	2.08
7	-1.57	-2.37
8	-.95	-.89
9	5.00	5.90
10	-1.76	-2.06
12	1.19	1.34
14	-1.05	-1.01
2	-5	
-7	2.52	2.73
-5	-11.95	-11.36
-3	-8.86	-8.11
-2	-38.52	-31.29
0	17.28	16.53
1	-42.09	-38.36
3	44.70	41.73
4	-14.19	-17.53
5	-7.28	-8.20
6	21.04	21.72
7	-5.86	-6.05
8	-7.57	-7.79
9	11.09	10.22
11	-6.05	-5.99
12	2.67	2.68
2	-6	
-11	-3.67	-4.26
-9	3.95	3.66
-8	-6.52	-6.85
-6	11.62	11.38
-5	-9.76	-10.15
-4	-8.43	-9.21
-3	10.19	10.83
-1	-17.28	-16.58
0	17.76	17.14
2	-15.04	-14.99
3	2.90	3.52
4	2.43	2.71
5	-9.28	-9.05
6	5.38	5.77
7	-3.48	-3.69
8	-4.52	-4.01
12	1.95	1.89
2	-7	
-5	-4.67	-4.68
-4	7.90	7.68
-2	-7.24	-8.30
-1	12.30	14.14
0	10.19	11.56
1	-8.86	-11.01
2	18.62	20.15
3	6.67	7.95
4	-6.19	-7.72
5	2.67	2.82
6	6.67	8.65
7	-10.62	-10.65
9	3.86	3.74
10	-7.09	-6.00
12	4.24	3.69
13	-1.76	-1.59
2	8	
-11	-.71	-1.52
-8	-3.43	-3.26
-7	5.52	5.35
-6	6.00	6.90
-5	-7.24	-7.50
-4	2.57	2.73
-3	4.09	3.96
-2	-12.38	-12.92
-1	5.95	7.50
0	15.04	14.91
1	-11.09	-12.72
3	5.14	5.23
4	-9.76	-10.23
5	-3.00	-3.12
6	3.29	3.81
9	3.29	2.64
10	-3.14	-3.44
2	-9	
-4	3.43	3.46
-2	-2.95	-2.29
0	-4.71	-4.94
2	3.14	3.75
3	-3.00	-3.46
4	-6.67	-7.61
5	7.24	8.29
7	-4.76	-4.69
8	5.76	5.09
9	1.95	2.02
10	-4.71	-4.24
11	3.67	3.80
12	1.62	1.67
2	-10	
-7	3.14	3.22
-4	5.14	4.58
-2	-3.57	-3.34
-1	5.33	5.40
4	-5.62	-5.47
7	-3.62	-3.19
8	3.90	3.52
10	-3.24	-3.12
2	-11	
2	2.43	2.67
3	-3.09	-3.67
5	4.86	5.30
8	4.00	3.99
9	-2.90	-1.69
2	-12	
2	3.62	4.00
3	-2.76	-2.74
4	-1.71	-1.61
5	4.00	3.18
6	-2.24	-1.80
7	-3.95	-1.07
2	-13	
2	2.76	2.70
4	1.71	1.96
3	0	
-14	-.76	-.47
-13	-4.00	-3.72
-12	5.19	4.99
-11	-2.29	-2.12
-10	-7.14	-7.74
-9	4.14	3.98
-8	7.33	7.62
-7	-2.38	-2.77
-6	1.95	2.81
-5	26.04	26.47
-4	15.04	16.45
-3	-5.43	-7.07
-2	7.00	8.37
-1	3.62	3.71
0	3.52	3.89
1	-11.62	-11.37
2	3.71	3.63
3	-1.48	-1.37
4	-12.95	-11.40
5	-6.14	-6.07
6	10.95	10.97
7	-5.62	-5.17
8	.95	.42
9	3.71	3.78
10	-2.48	-2.46
11	-1.81	-1.98
12	2.29	2.30
13	-.81	-1.15
3	1	
-14	-2.24	-2.45
-13	1.38	1.44
-12	4.14	4.09
-11	-8.66	-7.98
-9	13.38	13.59
-8	-10.43	-10.57
-7	-8.57	-9.74
-6	36.52	34.07
-5	-10.00	-10.65
-4	-18.57	-19.04
-3	32.61	34.17
-2	1.19	1.34
-1	-30.18	-29.96
0	18.76	18.59
1	16.95	15.59
2	-19.04	-18.65
3	16.57	14.07
4	19.90	17.46
5	-9.28	-9.05
6	9.81	9.63
7	.90	.87
9	6.19	6.13
10	4.81	4.65
11	.62	.96
3	2	
-14	2.33	2.43
-13	-3.71	-3.28
-12	-1.81	-2.05
-11	4.28	3.90
-10	-6.81	-5.99
-9	-1.57	-1.52
-8	3.38	3.35
-7	-5.09	-5.23
-6	.81	.26
-5	-6.76	-7.59
-4	1.24	1.78
-3	3.57	4.61
-2	-4.19	-4.39
-1	5.67	6.71
0	9.43	9.36
1	-10.05	-9.29
2	-3.09	-3.24
3	13.71	12.48
4	-17.38	-14.83
5	-21.66	-17.97
6	4.57	4.34
7	-4.28	-4.24
8	-6.00	-6.39
9	2.86	2.72
10	-.76	-1.19
11	-2.95	-3.23
3	3	
-14	-2.24	-2.24
-13	-2.38	-2.52
-12	6.57	6.63
-10	-10.14	-9.67
-9	14.57	13.80
-8	-.81	-.52
-7	-20.71	-23.51
-6	10.52	10.50
-5	16.38	17.71
-4	-23.09	-24.90
-3	8.38	9.52
-2	13.14	14.88
-1	-24.52	-24.08
0	-4.24	-4.65
1	22.80	21.98
2	-4.76	-4.97
3	-7.95	-7.83
4	9.33	8.80
5	-2.43	-2.73
6	-8.86	-8.98
7	4.62	3.93
8	-1.14	-1.03
10	.67	.75
11	-.48	-.88
3	4	
-14	2.05	2.00
-12	-1.95	-2.33
-11	3.43	3.03
-10	2.43	2.80
-9	-3.38	-3.47
-8	-2.43	-3.27
-7	2.48	2.83
-5	-3.00	-3.48
-4	-6.19	-7.81
-2	11.71	12.34
-2	-3.76	-4.29
-1	-5.86	-6.52
0	10.24	9.95
1	4.52	4.97
2	-4.95	-5.40
3	6.05	6.90
4	6.95	7.35
5	-2.19	-1.96
7	4.28	4.21
8	-4.48	-4.29
10	1.62	1.89
3	5	
-13	-3.67	-3.55
-12	2.67	2.35
-11	7.09	6.29
-10	-8.66	-7.57
-9	-2.09	-2.23
-8	11.28	11.96
-7	-11.09	-10.58
-6	-4.62	-5.73
-5	17.04	16.54
-4	17.76	-8.31
-3	-10.71	-11.70
-2	8.81	9.35
-1	-5.05	-5.17
0	-8.38	-9.02
1	8.66	9.01
2	2.86	2.94
8	1.43	1.46
3	6	
-12	-1.67	-1.43
-8	2.29	2.40
-7	-1.90	-1.80
-6	3.86	4.35
-5	2.90	3.05
-4	-3.29	-3.53
-3	2.71	2.85
-2	6.19	6.96
-1	-9.81	-9.44
0	2.24	2.05
1	4.71	5.10
2	-9.90	-10.27
3	-4.09	-3.46
4	5.00	4.89
7	1.67	1.28
3	7	
-11	6.43	5.46
-10	-1.43	-1.30
-9	-6.71	-6.06
-8	7.86	6.84
-7	1.81	2.17
-6	-8.33	-7.58
-5	4.48	3.61
-4	3.29	3.40
-3	-8.57	-9.26
-2	2.24	1.73
-1	2.57	2.53
0	-5.71	-5.92
1	-2.86	-3.25
2	2.29	2.09
3	-1.86	-1.96
3	8	
-10	-2.29	-1.82
-9	-1.81	-1.48
-8	2.09	2.11
-7	-1.76	-1.71
-6	-2.48	-2.40
-5	4.48	4.38
-3	-2.57	-2.41
-2	5.33	4.86
0	-3.09	-2.95
1	2.52	2.38
3	-2.86	-2.83
4	2.00	2.02
3	9	
-8	2.24	1.82
-7	3.67	3.41
-6	-4.43	-3.89
-4	3.24	2.87
-1	2.86	2.85
3	10	
-5	1.57	1.18
-3	-2.67	-2.24
-2	2.09	1.63
-1	2.48	2.23
3	-1	
-14	-.52	-.67
-13	1.90	2.01
-11	-6.47	-6.62
-10	6.33	6.64
-9	4.28	4.34
-8	-16.43	-17.14
-7	9.81	11.33
-6	4.33	5.21
-5	-52.08	-47.09
-4	-7.33	-8.53

Table 5 (*cont.*)

ℓ	F_o	F_c
-3	13.90	14.67
-2	-18.19	-19.90
-1	-21.42	-20.18
0	34.23	30.26
1	-75.51	-65.64
2	-47.94	-37.22
3	23.19	21.70
4	-18.23	-15.63
5	-11.85	-11.67
6	16.04	14.21
7	-2.38	-2.39
8	-6.57	-7.10
9	2.29	2.21
11	-1.43	-1.85
12	.62	.34
3 -2		
-14	-3.00	-3.17
-12	4.67	4.90
-11	-1.48	-1.16
-10	-2.09	-2.15
-9	6.43	6.97
-8	-1.00	-.87
-7	-5.28	-5.65
-6	13.00	12.86
-5	-3.38	-3.51
-4	-9.14	-9.86
-3	-2.33	-1.49
-2	-14.47	-14.62
-1	14.90	15.46
0	33.04	39.91
1	21.38	19.82
2	16.19	16.29
3	10.71	10.14
4	-15.76	-13.92
5	22.14	19.72
6	7.86	8.34
7	-4.00	-3.82
8	7.09	6.60
9	3.48	4.15
10	-6.81	-6.74
11	2.14	1.77
12	-.71	-.54
13	-1.90	-1.98
3 -3		
-14	1.81	1.67
-13	3.09	3.03
-12	-3.67	-3.42
-10	7.62	7.19
-9	-2.05	-1.57
-8	6.28	7.06
-7	19.23	19.12
-6	-6.86	-6.08
-5	-15.33	-14.61
-4	9.05	9.06
-3	9.86	9.07
-2	-44.04	-39.94
-1	43.09	40.15
0	18.09	17.04
1	-24.85	-27.00
2	3.86	4.71
3	23.71	22.67
4	-23.23	-21.30
5	5.52	5.92
6	7.52	8.13
7	-6.19	-6.34
9	3.52	3.19
10	-5.67	-5.86
11	2.86	3.04
12	1.86	2.18
13	-1.48	-1.58
3 -4		
-14	-1.81	-1.79
-13	1.48	1.31
-11	2.90	-3.10
-10	-1.52	-1.71
-9	-5.43	-5.61
-8	-16.00	-18.04
-7	-1.86	-1.60
-6	3.14	3.88
-5	-4.95	-5.71
-4	-11.66	-10.60
-3	9.38	9.67
-2	-14.47	-15.40
-1	1.05	-.95
0	1.10	1.64
1	3.05	3.86
2	8.28	8.56
3	-1.00	-1.12
4	-6.71	-7.62
5	6.05	7.62
6	-6.43	-6.18
7	-6.81	-7.99
8	3.90	4.62
9	-3.05	-3.06
10	-3.67	-4.40
11	2.38	2.57
3 -5		
-12	-1.62	-1.44
-11	1.14	1.35
-10	1.24	1.10
-9	-2.52	-.04
-7	6.05	6.54
-6	-12.81	-11.72
-5	-7.90	-6.79
-4	34.95	28.34
-3	-3.38	-1.55
-2	-6.24	-6.89
-1	26.80	26.16
0	-4.67	-6.47
1	-23.90	-23.05
2	15.52	18.32
3	-10.62	-11.59
4	-12.38	-13.66
5	17.28	18.18
7	-12.38	-11.72
8	10.14	9.46
9	-2.81	-2.93
10	-4.76	-4.27
3 -6		
-9	4.24	1.03
-7	2.67	2.20
-6	1.81	3.63
-5	-4.05	-5.52
-4	11.14	11.50
-2	3.95	4.71
-1	5.00	5.61
0	-4.81	-5.52
1	-10.19	-11.16
2	7.52	8.64
3	-19.47	-21.03
4	-7.52	-7.91
5	3.81	4.13
6	-7.76	-8.74
8	11.09	10.26
9	-5.90	-5.97
11	2.67	3.10
12	-2.05	-1.71
3 -7		
-9	-2.71	-2.61
-8	5.67	5.36
-6	-3.86	-3.50
-5	5.24	4.91
-4	3.86	4.16
-3	-9.95	-10.01
-2	8.90	8.73
-1	5.24	6.27
0	-14.52	-15.19
2	20.38	21.57
3	-8.62	-10.68
4	1.57	1.58
5	14.62	14.36
6	-9.28	-8.71
8	9.28	9.22
9	2.86	3.78
10	4.43	4.27
11	3.76	3.12
3 -8		
-9	-2.19	-.55
-7	2.67	2.37
-6	-2.76	-2.88
-4	4.86	5.42
-3	-4.48	-4.72
-2	-5.43	-6.28
-1	2.14	1.93
0	-4.71	-5.62
1	2.05	2.54
2	2.95	3.87
3	-2.86	-3.58
4	5.09	6.31
5	2.19	2.76
6	-4.52	-5.64
7	2.52	2.84
8	-3.19	-3.36
9	-7.24	-7.57
12	-1.95	-2.13
3 -9		
-7	-2.71	-2.23
-6	-3.67	-3.53
-5	2.71	2.23
-4	-2.71	-2.00
-3	-6.71	-7.44
-2	3.62	3.56
-1	-1.76	-2.22
0	-23.47	-25.58
1	1.71	1.13
3	-8.00	-9.25
4	8.33	8.09
6	-9.28	-9.53
7	3.14	2.86
9	-3.67	-2.60
10	2.95	2.50
11	1.67	1.49
12	-2.95	-2.70
3 -10		
-9	-1.10	-1.20
-7	1.43	1.22
-6	-1.62	-1.90
-5	1.76	1.49
-2	4.19	4.50
-1	8.86	9.12
0	3.90	4.36
1	8.66	9.46
4	5.57	6.07
5	2.67	2.11
7	5.00	5.68
8	-2.43	-2.77
9	-1.90	-2.03
10	1.62	1.98
3 -11		
-2	2.86	3.61
-1	-5.14	-4.68
1	5.33	5.50
2	-5.19	-5.12
4	3.62	3.88
5	-5.52	-5.41
6	-3.81	-4.28
7	3.81	3.40
8	-1.67	-1.25
9	-2.24	-2.18
10	2.71	2.43
3 -12		
-5	1.05	1.23
-4	-2.24	-2.02
-3	-3.86	-4.45
1	2.09	2.00
2	-2.38	-2.11
3	-1.67	-1.75
5	-2.48	-2.78
3 -13		
-3	2.29	2.27
-1	-2.29	-2.50
0	2.81	2.38
2	-2.71	-2.98
4	2.05	2.34
5	-3.00	-3.00
4 0		
-14	-.62	-.14
-13	-.71	-.68
-12	2.95	2.82
-11	4.28	4.79
-10	2.14	2.70
-9	-1.76	-1.89
-8	4.95	4.86
-7	1.43	1.25
-6	-7.28	-7.96
-5	1.62	2.03
-4	18.38	20.94
-3	-20.52	-22.51
-2	10.28	12.02
-1	10.24	11.01
0	-18.52	-18.29
1	2.48	3.65
2	25.95	23.92
3	-9.43	-9.52
4	-2.52	-2.29
5	14.90	12.81
6	-4.14	-3.97
7	-4.67	-4.73
8	8.66	7.31
9	-1.29	-1.06
10	-2.71	-2.70
11	-.71	-.86
12	-.95	-.83
4 1		
-14	-1.10	-1.25
-13	5.19	5.24
-12	-3.09	-2.81
-11	-6.47	-6.16
-10	9.24	8.04
-9	-2.19	-2.38
-8	-17.14	-15.89
-7	13.19	12.86
-6	4.90	5.19
-5	-26.90	-24.58
-4	10.14	11.66
-3	1.52	1.58
-2	-18.71	-17.24
-1	2.29	2.71
0	3.24	3.48
1	-8.33	-8.65
2	13.66	12.43
3	-1.14	-1.33
4	3.71	3.37
5	4.00	3.79
6	1.10	1.46
9	-2.71	-2.99
10	-1.10	-1.51
4 2		
-14	-.90	-.64
-12	-.81	-1.03
-11	2.38	2.26
-10	1.62	1.98
-9	-4.90	-5.06
-8	-1.76	-2.04
-7	5.38	5.68
-6	-9.62	-11.07
-5	-3.62	-3.93
-4	14.62	15.07
-3	-10.95	-11.47
-2	-23.09	-22.97
-1	12.38	12.11
0	-7.52	-8.37
1	-15.71	-14.24
2	10.05	9.08
5	2.33	2.01
6	1.14	1.00
7	-3.29	-3.42
4 3		
-14	-2.67	-2.54
-13	3.57	3.30
-12	2.62	2.62
-11	-6.90	-6.84
-10	3.19	2.71
-9	8.00	7.92
-8	-3.09	-2.10
-7	11.38	12.02
-6	17.42	15.83
-5	-7.05	-6.92
-4	-3.43	-3.72
-3	12.28	12.86
-2	-3.52	-4.26
-1	5.67	5.83
0	6.71	6.83
1	-3.09	-2.73
2	-3.43	-3.63
3	-.90	-.89
4	-2.90	-2.72
5	3.48	3.57
4 4		
-13	-1.10	-.90
-12	-.76	-1.01
-11	-.71	-1.19
-10	3.38	3.44
-8	-5.86	-6.13
-7	1.38	1.10
-6	-4.95	-5.43
-5	-9.71	-11.04
-4	6.76	7.95
-3	5.57	6.18
-2	-14.04	-13.32
-1	5.48	6.55
0	6.43	6.59
1	-13.47	-13.02
2	3.14	2.67
3	8.86	8.53
4	-7.67	-7.95
5	3.19	3.27
6	2.57	2.41
4 5		
-12	5.33	5.18
-11	-4.52	-4.21
-10	-5.09	-4.78
-9	7.67	6.91
-8	-2.86	-2.73
-7	-5.43	-4.98
-6	7.90	7.76
-4	-5.24	-5.31
-3	5.09	5.50
-2	2.48	2.52
0	.43	3.42
1	-5.81	-5.73
2	-7.62	-7.41
3	-2.81	-3.05
4	-3.38	-3.17
7	-2.81	-1.96
8	-2.67	-1.58
4 6		
-11	-2.81	-2.55
-9	2.19	2.37
-8	-5.38	-5.45
-6	4.95	5.35
-5	-5.19	-5.22
-3	9.09	8.45
-2	-2.52	-2.66
-1	-3.62	-3.21
0	4.76	4.30
3	7.43	6.31
5	-2.05	-1.97
6	1.90	2.14
4 7		
-10	-3.43	-3.22
-9	3.81	3.45
-8	2.81	2.58
-7	-5.00	-4.68
-6	1.48	1.57
-5	1.52	1.61
-4	-5.14	-5.19
-3	-2.29	-2.36
4 8		
-9	3.90	3.21
-8	-1.00	-1.00
-7	-3.19	-3.05
-6	4.38	4.28
-4	-4.33	-4.66
-3	4.52	4.55
-1	-3.09	-3.61
0	3.57	3.68
1	2.19	1.89
2	-1.52	-1.32
4 9		
-5	1.57	1.33
-1	-1.38	-1.37
4 -1		
-14	2.19	2.01
-13	2.05	2.21
-12	-6.24	-6.32
-10	10.09	9.57
-9	-13.04	-12.28
-8	-5.19	-5.76
-7	11.09	10.92
-6	-11.38	-11.79
-5	-3.57	-3.68
-4	23.19	24.45
-3	-4.19	-5.73
-2	-5.33	-5.66
-1	10.19	10.83
0	-1.43	-1.41
1	3.24	3.70
2	-3.62	-3.55
3	.95	.23
4	-4.00	-4.28
5	-4.48	-5.36
6	-5.90	-6.18
7	-4.19	-3.94
10	1.33	1.71
11	2.05	2.60
4 -2		
-14	-.90	-.93
-13	1.24	1.19
-11	-2.95	-3.05
-8	-1.05	-.97
-7	-5.86	-6.03
-6	-9.62	-10.05
-5	21.19	19.89
-4	-12.62	-12.60
-3	-8.19	-8.20
-2	20.23	22.52
-1	-1.71	-1.41
0	-29.52	-28.75
1	32.37	31.91
2	29.04	23.96
3	-12.28	-14.02
4	2.57	2.59
5	5.09	5.09
6	-13.04	-10.45
7	3.00	2.89
8	4.38	4.28
11	1.05	1.11
12	-1.00	-.66
4 -3		
-13	-.86	-.99
-12	-4.09	-4.27
-11	6.14	6.22
-9	-9.71	-9.44
-8	9.81	9.46
-7	12.95	13.03
-6	-23.80	-21.51
-5	16.28	16.37
-4	26.18	21.83
-3	-14.81	-14.32
-2	4.00	5.37
-1	18.95	19.49
0	-24.99	-23.98
1	-17.66	-15.16
2	5.86	6.45
3	-6.57	-7.12
4	-.71	-.22
5	8.24	7.44
6	-8.57	-8.66
8	-.95	-1.46
10	3.24	3.10
12	-.62	-1.08
4 -4		
-13	1.29	1.72
-12	-2.05	-2.08
-11	-1.29	-1.34
-9	4.52	4.41
-8	.81	.91
-7	-6.14	-6.20
-6	7.90	8.38
-5	8.47	9.05
-4	-15.53	-15.69
-3	-3.52	-3.85
-2	6.67	6.47
-1	-24.52	-21.93
0	-8.14	-7.45
1	21.61	21.96
2	-18.76	-18.96
3	-9.66	-9.68
4	7.67	7.77
5	-5.71	-6.73
6	-6.52	-7.35
7	11.05	11.23
8	1.57	2.00
9	-5.28	-5.90
10	3.14	2.91
12	-4.57	-3.80
4 -5		
-13	-2.24	-2.16
-11	4.62	4.88
-10	-5.57	-6.26
-9	-2.05	-2.00
-8	17.95	16.73
-7	-4.48	-4.25
-6	-5.52	-5.59
-5	14.76	13.03
-4	-8.43	-8.94
-3	-15.71	-14.90
-2	22.28	19.60
-1	5.00	5.32
0	-17.42	-17.53
1	7.24	7.42
2	3.71	4.91
3	-3.05	-2.76
4	6.57	6.95
5	3.05	2.60
6	1.86	2.85
9	-1.62	-1.28
4 -6		
-10	1.52	1.83
-9	-2.57	-3.38
-7	2.67	3.02
-5	-3.14	-2.72
-4	-2.86	-3.17
-3	-2.90	-2.61
-2	-6.19	-7.09
-1	-13.00	-13.67
0	18.23	18.52
1	1.62	2.21
2	-10.38	-11.08
3	6.47	7.57
4	15.90	18.85
5	-6.86	-6.97
6	4.48	4.81
7	9.43	9.93
8	-2.62	-2.18
9	-2.00	-2.49
10	5.48	5.58
11	-2.57	-2.00
4 -7		
-12	1.71	1.81
-10	-4.24	-3.95
-9	2.95	2.80
-7	-9.81	-9.26
-6	2.09	1.88
-5	5.28	5.37
-4	-14.47	-13.88
-3	-2.19	-2.24
-2	20.95	19.14
-1	-11.66	-11.27
0	2.81	3.39
1	10.71	10.67
2	-10.05	-9.32
3	-16.00	-15.92
4	2.43	2.19
5	-6.47	-6.80
6	-5.48	-5.85
7	5.33	5.01
8	-4.05	-4.06
9	-7.71	-7.54
11	-2.24	-1.98
4 -8		
-11	2.14	2.25
-5	-5.90	-6.47
-3	5.05	5.50
-2	-2.29	-2.97
0	8.05	11.11
3	7.14	6.32
5	-4.19	-4.69
6	3.14	2.91
7	2.43	2.57
8	-3.76	-3.61
9	4.67	4.05
11	-2.90	-2.38
12	1.14	.72
4 -9		
-9	2.14	2.27
-6	10.28	9.12
-4	-3.48	-3.46
-3	9.76	9.42
-2	-2.76	-2.87
-1	-1.71	-1.61
0	9.66	10.47
1	7.05	8.65
2	-7.95	-8.18
3	2.33	2.22
4	1.76	1.69
5	-6.57	-5.94
7	4.71	4.21
8	-3.67	-3.06
9	2.62	2.27
11	-1.14	-.95
4 -10		
-9	.81	1.11
-3	2.67	2.48
-1	-4.19	-4.65
0	-9.52	-10.52
1	-3.33	-3.63
2	-2.29	-2.70
4	-1.86	-2.15
5	-2.00	-2.31
6	2.38	2.43
7	-2.48	-1.87
8	-2.29	-2.68
9	4.00	3.87
4 -11		
-8	-2.48	-2.58
-7	1.10	1.35
-5	-2.86	-2.54
-4	1.71	1.68
-3	3.24	3.09
-2	-1.62	-1.36
0	4.05	3.57
1	-2.33	-1.80
2	-4.09	-4.05
3	5.05	4.32
5	-2.00	-1.76
6	5.38	4.66
7	-1.67	-1.43
8	-1.90	-1.59
9	2.81	2.31
10	-1.14	-.90
4 -12		
1	-3.86	-3.90
3	1.86	1.97
5	1.48	.86
6	2.76	3.23
7	-1.71	-1.79
9	1.33	1.56
4 -13		
0	1.43	1.83
1	-1.62	-1.30
2	2.71	2.56
3	2.14	1.99
4	-2.95	-2.53
6	1.81	1.43
7	-2.52	-2.25
4 -14		
0	1.38	1.35
1	-.71	-.63
2	1.10	.95
3	2.43	2.10
5 0		
-14	-1.19	-.85
-13	-1.81	-1.71
-12	2.57	2.63
-11	-1.14	-1.04
-10	-9.38	-8.42

Table 5 (*cont.*)

ℓ	F_o	F_c
-9	6.52	5.73
-8	6.67	6.76
-7	-11.24	-10.82
-6	6.71	7.33
-5	16.81	15.89
-4	-12.71	-12.69
-3	-10.19	-9.08
-2	24.85	22.90
-1	-12.85	-12.33
0	-18.85	-15.82
1	15.62	13.36
2	-7.05	-6.56
3	-11.38	-10.28
4	18.57	15.21
5	2.05	2.01
6	2.43	2.58
7	4.14	4.08
9	-1.14	-.87
10	3.09	3.31
11	2.24	2.50
5	1	
-14	4.00	3.40
-12	-5.52	-5.10
-11	2.24	1.81
-10	2.38	2.86
-9	-5.48	-5.42
-8	3.09	4.15
-7	5.14	5.72
-6	-3.52	-4.23
-5	-2.38	-2.32
-4	1.71	2.18
-3	-1.52	-1.46
-2	2.52	3.21
-1	4.43	4.98
0	6.43	7.00
1	.90	.45
2	-5.19	-5.13
3	1.38	1.82
4	3.81	3.91
5	-8.43	-7.43
6	-1.05	-1.22
8	-.95	-1.33
9	-.76	-1.22
10	1.00	1.23
5	2	
-13	-3.33	-3.07
-11	5.24	4.66
-10	-6.24	-5.60
-9	-2.76	-2.64
-8	16.19	14.25
-7	-6.62	-6.60
-6	-9.66	-9.61
-5	15.62	14.88
-4	-.71	-1.03
-3	-10.33	-10.15
-2	14.66	14.28
-1	8.14	7.32
0	-12.71	-10.82
1	5.28	5.97
2	6.19	7.68
3	-12.43	-11.02
4	-1.86	-1.66
5	1.86	1.68
6	-4.67	-4.56
5	3	
-13	2.52	2.67
-12	-3.61	-3.58
-11	-1.62	-1.89
-10	5.52	4.87
-9	-1.67	-1.17
-8	-6.62	-6.53
-7	-2.05	-2.69
-6	-3.67	-4.02
-5	-3.67	-4.35
-4	-3.29	-3.85
-3	-.62	-.96
-2	1.00	1.51
-1	-1.14	-.65
0	-4.38	-4.32
1	2.86	3.01
2	.62	.63
3	-4.90	-4.81
4	2.81	2.36
5	2.14	1.96
6	-2.95	-2.93
7	2.00	2.24
9	-1.14	-2.03
5	4	
-12	-1.67	-1.84
-11	4.90	5.02
-10	1.43	1.58
-9	-7.62	-6.73
-8	3.48	3.44
-7	7.19	7.41
-6	-9.24	-9.25
-5	3.90	4.51
-4	8.33	8.01
-3	-9.09	-9.53
-2	-1.43	-1.63
-1	6.19	6.36
0	-4.00	-4.27
2	5.57	5.39
3	1.57	1.52
4	-1.24	-1.50
5	2.00	1.91
6	-1.14	-1.12
7	-.86	-.44
8	1.57	1.54
5	5	
-11	-2.38	-2.18
-10	2.24	1.88
-8	-1.57	-1.31
-7	1.62	1.63
-5	2.62	2.96
-2	2.62	2.88
0	-2.33	-2.06
1	5.24	5.09
2	2.95	2.99
5	2.14	2.10
5	6	
-10	4.86	4.39
-9	-4.28	-3.55
-8	-1.43	-1.29
-7	5.95	5.69
-6	-1.52	-1.50
-5	-4.71	-4.66
-4	3.67	3.24
-3	-4.24	-4.11
-2	-7.28	-7.05
-1	1.57	1.46
1	-4.33	-4.09
3	-1.48	-1.40
4	-1.95	-1.77
5	7	
-4	2.90	3.14
-1	2.67	2.43
2	1.90	1.98
5	8	
-5	-2.48	-2.31
-4	2.09	2.09
-3	2.76	1.94
-2	-.86	-.84
5	-1	
-14	2.48	2.36
-13	-3.43	-3.22
-12	-.90	-1.15
-11	6.86	6.75
-10	-4.00	-4.02
-9	-7.62	-7.26
-8	10.90	10.54
-7	3.05	2.76
-6	-9.71	-10.10
-5	6.67	7.61
-4	14.14	13.29
-3	-5.48	-6.63
-2	3.43	4.82
-1	-1.24	-1.06
0	-5.09	-5.33
1	-3.19	-3.74
2	-8.33	-7.82
3	-3.24	-3.78
4	1.90	2.13
5	-5.90	-6.03
6	.67	.57
7	3.86	4.29
8	-3.52	-3.95
11	-2.33	-2.98
5	-2	
-14	-1.29	-1.08
-12	3.52	2.80
-11	-3.67	-2.93
-9	8.71	8.09
-8	-5.28	-4.85
-7	-8.28	-8.47
-6	9.14	9.36
-5	-10.28	-10.07
-4	-33.52	-31.78
-3	8.33	10.13
-2	5.86	6.32
-1	-21.09	-20.67
0	15.33	14.03
1	-.61	-.17
2	-37.85	-34.31
3	3.48	3.28
4	8.90	8.24
5	-4.57	-4.23
6	-1.29	-.80
7	6.95	6.81
8	-6.14	-5.96
9	-1.71	-1.78
10	1.71	1.47
5	-3	
-13	-3.14	-3.54
-12	2.71	2.54
-11	5.05	5.20
-10	-4.14	-4.01
-9	2.14	1.88
-8	6.43	6.78
-7	-7.95	-6.43
-6	-2.09	-2.39
-5	18.04	15.95
-4	-8.47	-9.96
-3	2.33	2.81
-2	3.19	3.81
-1	-3.57	-4.56
0	8.52	8.35
1	33.42	32.42
2	12.57	11.95
3	17.81	17.00
5	1.62	1.58
6	6.62	7.14
7	2.57	2.82
9	3.67	4.11
10	-.57	-1.11
5	-4	
-13	2.90	2.54
-11	-1.19	-.85
-10	2.00	1.42
-9	1.86	1.57
-8	-2.24	-1.29
-7	6.52	7.14
-6	5.81	5.60
-5	-7.43	-7.53
-4	-6.43	-6.73
-3	19.38	19.81
-2	-7.81	-8.61
-1	-9.52	-10.16
0	10.28	11.16
1	-4.00	-4.22
2	-23.42	-21.23
3	10.14	9.98
4	3.48	4.42
5	-15.66	-14.73
6	2.76	2.75
7	-4.24	-4.24
8	-7.33	-7.11
9	2.71	2.41
11	-.86	-.92
12	1.71	2.13
5	-5	
-12	2.05	2.00
-11	-1.05	-1.45
-10	-4.38	-4.37
-8	-13.38	-13.48
-7	-20.09	-19.48
-6	5.71	5.86
-5	2.81	2.68
-4	-9.76	-8.99
-3	5.57	5.61
-2	-2.62	-1.70
-1	-22.38	-20.98
0	5.00	4.48
2	1.05	1.63
3	6.47	5.91
4	-1.76	-.79
5	-7.43	-8.11
6	1.95	1.75
7	-4.76	-4.85
8	-2.33	-2.36
5	-6	
-10	1.57	1.34
-9	2.43	2.74
-8	1.71	2.07
-7	5.48	4.78
-6	6.14	5.39
-5	-9.90	-8.41
-4	14.47	12.45
-3	16.33	14.82
-2	2.29	2.33
-1	3.29	3.04
0	15.33	14.22
1	-17.81	-15.51
2	2.86	2.78
3	11.19	11.06
4	-13.38	-11.70
5	4.09	3.52
6	11.00	10.42
7	-7.14	-6.58
8	2.43	2.11
9	3.71	3.39
5	-7	
-12	1.52	1.65
-11	-1.24	-1.27
-10	1.52	1.69
-9	2.38	2.56
-8	-2.14	-1.35
-7	-1.76	-1.64
-6	7.00	7.47
-3	5.28	5.76
-2	-5.19	-4.58
-1	-4.33	-4.96
0	5.52	6.27
1	-11.09	-10.54
2	-1.62	-1.28
3	6.95	6.58
4	-7.95	-8.29
5	-2.33	-2.29
6	1.67	1.74
7	-4.62	-5.03
8	4.24	4.49
9	3.00	3.28
5	-8	
-12	-1.05	-1.03
-11	-1.86	-2.04
-7	1.95	1.37
-4	-1.57	-2.03
-3	-2.09	-1.75
-2	-9.38	-9.03
-1	4.24	3.99
1	-11.66	-12.15
2	5.81	5.85
3	2.14	3.20
4	-6.90	-7.71
5	4.19	2.96
7	-5.00	-4.38
9	3.19	3.02
11	2.09	1.89
5	-9	
-8	-1.57	-1.40
-7	3.81	3.15
-5	-5.19	-5.63
-3	1.43	2.35
-2	-12.09	-10.53
-1	4.43	4.08
0	1.52	1.41
1	-4.62	-4.25
2	7.47	7.73
3	2.81	2.74
4	-3.09	-2.66
5	6.86	7.48
10	-3.05	-3.33
5	-10	
-4	1.71	2.31
-3	-4.86	-4.26
-2	-3.81	-4.65
-1	10.28	9.81
0	-4.52	-4.36
1	-4.52	-5.39
2	2.62	2.77
3	-2.38	-2.15
4	-3.09	-3.06
5	4.57	4.53
6	-3.52	-3.09
8	2.52	2.20
5	-11	
-5	-2.24	-2.28
-4	1.67	1.17
-1	5.62	5.31
0	2.38	2.70
1	5.28	5.61
2	3.86	3.77
3	-2.09	-2.02
8	2.19	1.78
9	-1.90	-2.23
5	-12	
-4	1.76	2.19
-3	-1.52	-1.53
-2	1.90	1.64
0	-2.29	-2.35
3	-3.00	-3.58
6	-2.71	-3.08
5	-13	
-3	-3.29	-3.59
3	-3.52	-3.39
7	1.10	.96
5	-14	
0	-1.71	-1.12
3	-2.29	-2.33
6	0	
-13	1.90	1.56
-12	3.67	3.46
-11	-5.47	-5.57
-9	5.76	6.02
-8	-7.38	-7.12
-7	-5.81	-5.34
-6	13.57	13.62
-5	-8.47	-9.81
-4	-9.81	-8.59
-3	7.76	7.09
-2	-6.05	-7.59
-1	-4.28	-4.81
0	8.05	7.47
1	-1.14	-1.19
3	2.95	2.85
4	-2.05	-1.82
5	-3.81	-3.68
7	-1.05	-.87
9	-.76	-.44
10	-1.62	-2.05
6	1	
-13	-1.14	-1.32
-11	2.29	2.54
-10	1.14	1.22
-8	-1.52	-1.88
-7	-2.38	-2.84
-6	.57	.86
-5	-5.67	-6.54
-4	4.19	5.10
-3	4.67	4.69
-2	-8.62	-8.69
-1	-5.76	-5.38
0	3.67	3.71
1	-2.00	-1.30
2	1.29	2.08
3	4.24	3.87
4	1.33	1.80
5	-.86	-1.05
6	2.76	2.56
9	1.33	1.34
6	2	
-13	-.81	-.78
-12	3.95	3.72
-11	-.76	-.95
-10	-5.38	-4.80
-9	5.62	5.11
-8	.81	.57
-7	-3.81	-2.39
-6	10.71	11.10
-5	6.67	6.46
-4	-9.86	-9.46
-3	1.33	1.98
-2	4.38	3.90
-1	-5.95	-6.40
0	4.00	3.70
1	3.62	3.39
2	-3.19	-2.98
5	-1.38	-1.36
6	.95	.57
7	1.33	1.59
6	3	
-12	-.90	-.94
-10	.90	1.02
-5	-1.90	-2.09
-4	-3.09	-2.92
-3	5.52	5.89
-2	-3.33	-4.22
-1	-6.81	-6.27
0	3.52	3.44
1	-2.00	-2.59
2	-3.00	-2.72
3	4.67	4.50
5	-1.48	-1.39
6	4	
-11	2.43	2.47
-10	-5.14	-5.41
-8	4.95	4.84
-7	-4.43	-4.57
-5	6.24	6.04
-4	-2.86	-3.02
-2	4.28	4.29
1	2.05	1.95
2	-3.62	-3.75
3	-2.52	-2.42
4	-1.43	-1.54
6	5	
-10	-.95	-1.06
-7	-2.19	-2.13
-6	1.86	2.12
-4	-1.71	-1.64
-3	1.81	2.07
-2	3.86	3.32
-1	-2.38	-2.43
0	-1.14	-1.18
1	1.33	1.17
2	-2.24	-2.29
3	2.09	1.96
4	2.29	2.32
6	6	
-8	4.00	3.47
-6	-3.48	-3.75
-5	2.00	2.13
-3	-3.19	-3.39
0	-1.14	-.96
6	7	
-5	1.6[illegible]	1.65
-4	-2.24	-2.50
-2	2.38	2.63
6	-1	
-14	.67	.77
-13	-1.62	-2.17
-12	1.10	1.24
-11	.95	1.05
-5	-1.38	-1.64
-4	1.10	1.16
-2	-3.14	-3.57
-1	2.43	2.88
0	.71	.59
1	-5.38	-5.26
2	3.19	3.61
3	3.57	3.79
4	-5.86	-5.54
5	1.48	1.72
6	1.52	1.96
7	-2.09	-2.31
9	1.95	2.09
6	-2	
-14	-.90	-.89
-13	3.00	2.84
-12	-.76	-.66
-11	-6.47	-5.68
-10	2.14	1.73
-9	2.29	1.85
-8	-9.05	-10.14
-7	5.00	5.50
-6	4.38	4.07
-5	-4.33	-4.47
-4	9.19	10.50
-3	17.00	13.82
-2	-1.90	-1.59
-1	4.09	4.41
0	12.52	11.44
1	2.81	2.99
3	7.28	6.37
4	-5.24	-4.21
5	-1.71	-1.44
6	1.14	.71
7	-2.24	-1.93
8	-1.05	-1.17
9	1.81	1.66
6	-3	
-14	-1.10	-1.40
-12	1.24	1.45
-11	-1.62	-1.99
-10	-1.38	-1.59
-9	1.43	1.74
-6	-3.24	-3.18
-5	-3.19	-3.52
-3	-5.24	-6.11
-2	-2.62	-3.07
-1	12.76	14.82
0	-8.71	-8.85
1	-13.04	-13.61
2	2.33	2.19
3	-1.57	-1.59
4	-7.38	-6.97
5	2.48	2.49
9	1.00	1.94
10	-1.24	-1.85
6	-4	
-12	-3.24	-3.29
-10	6.28	5.49
-9	-4.05	-3.54
-8	-2.33	-2.24
-7	10.14	9.83
-6	-2.33	-2.39
-5	-8.28	-8.44
-4	10.28	9.69
-3	2.90	3.45
-2	-11.81	-11.61
-1	10.24	11.55
0	1.14	1.13
1	-12.52	-12.64
3	-3.48	-3.66
4	-5.67	-5.28
5	4.76	4.49
6	1.38	1.36
7	-1.52	-1.04
8	-1.29	-.17
9	1.33	.32
10	1.19	.35
6	-5	
-13	.95	1.25
-12	1.05	1.10
-9	3.14	3.64
-8	7.05	6.61
-7	3.29	3.71
-5	2.52	2.34
-4	-1.52	-1.76
-3	-6.67	-7.17
-1	2.24	1.84
0	-1.24	-1.75
1	1.76	1.94
2	1.52	1.85
3	-4.09	-4.29
5	1.76	2.44
8	4.76	4.99
9	-1.43	-1.89
6	-6	
-12	-1.62	-1.79
-11	2.76	2.75
-10	1.29	1.85
-9	-5.38	-5.82
-7	5.09	5.08
-6	-7.09	-6.22
-5	-3.48	-3.40
-4	8.28	7.42
-3	-16.23	-12.85
-2	-2.29	-2.71
-1	6.24	7.57
0	-2.43	-1.97
1	-4.43	-5.72
2	7.52	7.09
3	2.76	4.17
4	2.76	3.78
5	4.09	3.76
6	3.86	5.17
7	-3.09	-3.58
8	2.38	1.72
9	-1.57	-1.66
11	1.57	1.47
6	-7	
-10	2.00	2.28
-8	-2.57	-3.21
-5	-2.38	-2.53
-4	2.57	2.64
-3	-1.52	-1.72
-2	1.95	2.15
-1	-4.86	-5.66
0	-1.48	-1.26
1	3.38	4.22
2	1.62	1.26
3	-7.90	-8.20
4	4.90	5.34
5	6.81	6.76
6	-2.52	-2.51
7	2.14	2.05
8	2.24	2.95
9	-2.67	-2.94
11	1.05	1.44
6	-8	
-11	1.29	1.41
-9	-1.90	-1.73
-8	2.86	2.69
-7	-4.67	-4.45
-6	-6.81	-7.35
-5	4.43	4.71
-3	-3.90	-3.74
-2	9.38	7.38
-1	4.19	5.16
0	-4.24	-4.22
1	1.86	1.09
2	2.29	3.04
3	-9.52	-8.29
4	-5.76	-7.75
6	-10.66	-9.59
9	-4.57	-4.14
10	-2.09	-2.38
6	-9	
-10	1.10	1.99
-4	-3.09	-2.83
-3	3.86	4.33
1	2.86	3.43
3	3.00	3.52
4	2.33	2.21
5	1.86	2.42
6	-2.05	-2.38
7	2.09	1.99
9	1.43	1.55

Table 5 (*cont.*)

5

l	F_o	F_c
10	3.48	3.70
6 -10		
-10	-1.90	-1.63
-6	2.14	2.24
-5	7.86	7.39
-3	2.86	2.40
-2	2.09	1.67
-1	-1.57	-.84
0	-3.05	-4.08
1	9.71	8.88
2	3.05	3.68
3	-3.86	-4.04
4	4.28	3.37
6	-3.19	-3.34
7	2.57	1.95
6 -11		
-6	-1.90	-2.12
-3	-2.14	-2.04
-1	-2.48	-2.37
0	-11.05	-10.50
1	-6.67	-7.55
2	-3.24	-3.91
3	-2.29	-2.77
4	2.67	2.54
5	-2.81	-2.87
6	-2.38	-2.49
8	-2.48	-2.94
6 -12		
-5	-2.95	-.91
0	3.09	3.09
1	3.24	3.04
4	2.81	3.25
6	2.86	2.25
7	3.33	2.86
6 -14		
-3	-1.86	-2.21
0	1.48	1.46
3	1.43	1.05
7 0		
-13	4.38	2.98
-12	-2.05	-1.88
-11	-2.71	-2.45
-10	4.38	3.91
-8	-3.62	-3.05
-7	5.57	5.15
-5	-5.57	-4.96
-4	3.09	3.47
-2	-3.00	-2.47
0	1.76	1.78
1	-1.76	-1.65
3	-1.52	-1.18
4	2.14	2.12
5	1.10	1.12
6	-1.81	-1.61
7	-1.52	-1.27
7 1		
-12	-1.24	-1.26
-11	2.05	1.97
-9	-5.05	-4.37
-8	4.05	3.93
-7	8.38	6.72
-6	-1.90	-1.84
-5	1.29	1.92
-4	8.09	6.77
-1	12.95	9.97
0	2.62	2.48
1	-3.19	-3.10
2	6.38	5.39
4	-2.52	-2.18
7 2		
-12	.52	.51
-11	-4.67	-4.02
-10	.71	.88
-9	4.14	3.09
-8	-4.00	-3.05
-7	-5.09	-4.48
-6	-2.62	-2.96
-5	-6.24	-5.81
-4	-1.67	-1.78
-1	1.57	2.04
0	-1.90	-2.12
1	-4.76	-4.05
5	1.57	1.66
7 3		
-10	3.19	2.90
-9	-1.29	-1.34
-8	-3.57	-3.32
-7	4.48	3.93
-5	-4.00	-3.79
-4	3.76	3.66
-3	.62	.35
-2	-4.00	-3.78
-1	1.52	1.88
0	1.86	1.66
1	-3.33	-2.83
3	1.86	1.09
4	-1.90	-1.72
5	.81	1.07
7 4		
-10	-1.19	-.89
-9	2.48	2.25
-8	-.95	-1.07
-7	-.95	-.75
-6	1.00	.98
-3	2.24	1.98
-2	1.81	1.85
2	2.33	2.35
3	2.95	3.14
7 5		
-8	-1.86	-1.61
-7	1.05	1.23
-6	2.95	2.54
-5	-2.09	-2.09
-4	-1.33	-1.18
-2	-3.52	-3.70
-1	-1.86	-1.68
0	.86	.70
1	-2.05	-.78
7 -1		
-13	-1.43	-1.25
-11	1.24	1.13
-10	-3.76	-3.57
-9	-3.86	-3.82
-8	3.24	2.61
-6	-4.19	-3.98
-5	4.62	5.14
-4	7.67	7.15
-3	-16.81	-13.35
-1	2.62	2.36
0	-13.61	-13.10
1	-1.71	-1.74
2	3.09	2.74
3	-5.09	-4.72
5	4.52	3.98
8	1.52	1.58
9	-1.29	-1.18
7 -2		
-13	.67	.69
-12	-2.95	-2.68
-11	2.57	2.53
-10	5.95	5.61
-9	-5.62	-4.95
-8	-1.14	-1.09
-7	8.66	7.62
-6	-2.48	-2.61
-5	-3.19	-2.81
-4	7.90	7.64
-3	2.33	2.43
-2	-2.43	-2.72
-1	4.24	3.76
0	-4.19	-4.16
1	1.86	2.06
2	1.00	.75
4	1.38	1.22
5	1.14	.81
6	-2.52	-2.60
7	1.95	2.12
8	.71	.51
7 -3		
-14	-.95	-.64
-12	2.19	2.05
-10	-.86	-.66
-9	3.09	2.68
-8	1.90	1.41
-7	-4.33	-4.17
-6	-2.09	-2.27
-5	9.81	8.24
-4	-11.14	-10.54
-3	-4.09	-4.52
-2	3.38	3.29
-1	-3.29	-2.98
0	-2.57	-2.25
1	12.05	9.81
2	-1.48	-1.43
3	-8.57	-7.35
4	2.33	2.54
5	2.19	2.80
6	-4.48	-3.79
7	1.33	1.74
9	-1.14	-1.16
7 -4		
-12	-2.43	-2.57
-11	2.86	3.79
-9	-4.57	-4.70
-8	2.29	2.48
-7	1.05	.84
-6	-11.05	-10.03
-5	5.57	6.27
-4	3.14	3.60
-3	-8.62	-9.10
-2	1.24	1.47
-1	-1.10	-1.41
0	-7.38	-6.69
1	8.33	8.36
2	16.28	12.52
3	3.57	4.14
4	2.48	2.25
5	-1.67	-2.36
6	-1.81	-1.59
7	1.57	1.84
8	1.43	1.36
9	.95	1.32
7 -5		
-13	1.14	1.44
-6	7.95	5.80
-4	-3.09	-3.16
-3	1.90	1.46
-2	13.62	10.37
-1	-3.29	-3.63
0	-1.05	-.96
1	7.09	7.45
2	-9.43	-7.89
3	-8.00	-6.96
4	7.81	6.74
5	-5.62	-5.32
6	-2.57	-2.26
8	-4.14	-3.27
10	1.67	1.21
7 -6		
-13	-1.38	-2.05
-10	-3.43	-3.37
-8	2.38	2.31
-7	-16.43	-11.78
-6	-3.90	-3.68
-5	7.33	5.76
-3	-4.09	-3.72
-2	6.43	5.40
-1	-7.05	-5.65
0	-5.90	-4.47
1	5.57	4.94
4	4.24	3.27
5	-4.81	-4.47
7 -7		
-11	-1.00	-.87
-8	3.76	3.96
-7	7.38	5.77
-6	5.09	4.30
-4	-3.00	-2.73
-3	3.38	3.10
-2	7.90	6.69
-1	-1.33	-.48
0	6.52	5.67
1	-3.29	-3.26
2	-8.66	-7.63
3	3.29	2.76
4	-3.19	-2.44
5	-3.62	-3.02
6	5.14	4.07
7	1.33	.70
8	-1.19	-1.14
10	.86	.93
7 -8		
-10	-1.10	-.96
-9	1.95	1.64
-7	-2.24	-1.43
-5	4.76	4.69
-4	-4.71	-4.23
-3	1.19	.75
-2	1.95	2.35
-1	-9.86	-8.54
0	2.71	1.79
1	2.43	1.98
2	-10.47	-8.32
3	3.19	3.07
4	2.48	1.91
5	-2.43	-1.02
6	1.71	1.47
7	1.86	1.02
9	1.19	1.53
10	1.81	1.52
7 -9		
-11	-.81	-.87
-10	-1.71	-1.64
-4	-4.71	-4.51
-2	-2.81	-2.78
0	4.48	4.32
1	-1.71	-1.50
2	-3.43	-4.17
3	2.29	2.72
4	-2.38	-1.70
6	2.57	1.97
8	-3.09	-2.85
10	-1.38	-1.00
7 -10		
-10	1.14	1.23
-9	1.24	1.23
-6	1.33	1.07
-5	-6.28	-4.73
-4	-4.81	-5.13
-3	4.76	3.90
-2	-6.14	-4.63
0	4.33	3.11
1	-3.95	-2.82
3	3.81	3.36
6	1.90	1.75
7 -11		
-6	1.71	2.07
-3	1.90	2.03
-2	-2.52	-2.59
-1	2.33	1.62
0	5.10	5.13
4	-1.90	-1.43
7	-2.19	-1.71
7 -12		
-7	-1.24	-1.52
-5	-2.09	-1.78
2	2.38	1.98
3	1.81	1.34
6	2.19	1.56
7	-1.57	-.97
7 -13		
-4	2.86	2.69
1	-1.52	-2.24
7 -14		
0	-1.10	-.89
1	-2.00	-1.50
3	-1.57	-1.35
4	-1.71	-1.31
8 0		
-12	-2.00	-1.44
-11	1.29	1.12
-10	1.95	1.66
-9	-.62	-.16
-8	.95	.46
-7	-2.09	-1.94
-6	-2.00	-2.13
-5	-3.14	-3.37
-4	-1.71	-1.25
-3	1.81	1.70
-2	1.57	1.08
-1	-1.95	-1.56
0	-1.71	-1.24
1	1.05	.87
4	1.00	.71
5	-.67	-.48
6	.71	.71
8 1		
-11	1.48	1.38
-10	-1.52	-1.79
-9	-1.05	-.73
-8	3.76	2.92
-7	-2.29	-2.83
-6	-.81	-.60
-5	6.43	5.42
-3	-4.67	-4.29
-2	3.43	3.37
0	-.76	-1.25
1	2.29	2.27
3	-1.95	-2.53
8 2		
-10	2.29	1.89
-7	1.29	1.53
-1	-3.00	-3.11
3	-1.90	-.16
8 3		
-9	-3.24	-2.85
-8	1.14	1.44
-7	1.10	1.09
-6	-2.81	-2.56
-5	1.29	1.74
-4	1.48	1.18
-3	-1.67	-1.95
-1	.95	1.04
1	.67	1.16
2	.57	.53
8 4		
-3	-1.24	-1.04
8 -1		
-12	2.09	1.83
-10	-4.28	-3.30
-9	2.95	2.93
-8	2.67	2.16
-7	-5.24	-4.50
-6	1.24	1.90
-5	2.05	1.62
-4	-8.24	-7.56
-3	-1.05	-1.04
-2	1.48	1.61
-1	-1.33	-1.48
1	2.67	2.60
2	-1.57	-1.54
5	-1.48	1.62
6	-1.00	-1.46
8 -2		
-12	-1.38	-1.22
-11	1.43	1.11
-10	-1.29	-1.36
-8	2.43	2.34
-6	-2.14	-1.78
-5	4.48	3.88
-2	3.95	3.98
2	-2.19	-1.90
3	2.14	1.76
4	1.33	1.14
6	1.29	1.08
7	1.52	1.54
8	-.81	-1.06
8 -3		
-12	1.62	1.45
-11	-2.29	-1.99
-10	-2.29	-1.97
-9	1.95	1.16
-8	-2.57	-2.54
-7	-.95	-1.31
-6	3.86	2.82
-3	9.81	8.44
-2	6.52	6.49
-1	-1.00	-1.13
0	3.90	3.31
1	1.24	2.13
2	-2.81	-2.72
3	3.57	3.61
8	-1.57	-1.92
8 -4		
-12	1.62	1.50
-8	1.05	1.18
-7	-1.62	-1.80
-5	-3.24	-3.22
-4	-4.62	-4.82
-3	-1.24	-1.81
-2	-5.38	-5.81
1	-7.05	-7.88
2	-8.76	-9.51
3	-2.95	-3.83
4	-1.71	-1.77
5	-1.14	-1.73
8	-1.10	-1.16
9 0		
-10	.48	.24
-9	-2.00	-1.59
-8	-1.62	-1.01
-7	2.29	1.97
-6	4.81	3.95
-5	.95	1.17
-4	1.71	1.70
-3	2.09	1.48
-2	-1.57	-1.34
-1	.81	.99
0	4.67	3.76
1	.90	.55
4	-1.00	-.86
9 1		
-9	1.67	1.54
-8	.76	.89
-7	-1.62	-1.67
-5	-1.24	-1.90
-4	-1.62	-1.75
-3	.67	1.14
1	-.71	-1.38
2	-.48	-.87
9 2		
-8	-1.62	-1.35
-6	1.14	1.02
-3	1.24	1.04
-2	-.71	-.64
-1	-.62	-.75
0	1.29	1.45
9 -1		
-11	-2.29	-1.77
-9	2.09	1.95
-8	-1.00	-1.20
-6	1.86	1.97
-5	-2.48	-2.52
-4	-1.00	-1.05
-3	1.19	1.17
-2	-1.90	-2.23
-1	-1.62	-2.04
5	.62	1.19
9 -2		
-9	-1.90	-1.43
-8	-2.19	-1.66
-7	2.33	-1.98
-4	4.33	3.54
-2	-5.90	-4.81
1	-1.86	-1.42
3	.71	.74
4	-2.67	-2.11
5	.76	.68
9 -3		
-11	-1.00	-1.02
-10	2.62	2.61
-9	2.90	2.60
-8	-3.00	-2.67
-7	1.48	1.48
-6	1.90	2.11
-5	-2.24	-2.41
-3	.95	1.60
9 -4		
-6	-2.67	-2.80
-3	-2.09	-1.82
-1	1.29	1.24
2	4.33	4.66
3	-1.24	-1.02
4	-1.29	-1.39
5	1.10	1.50
10 0		
-6	-4.43	-3.03
-5	-1.19	-.82
-4	1.05	.38
-3	-1.52	-1.39
-2	-1.29	-.73
-1	1.14	.72
0	-.90	-.99
1	-1.57	-1.24
10 1		
-6	.62	1.20
10 -1		
-5	-.95	-1.60
10 -2		
-10	-1.05	-.96
-8	3.52	2.18
-7	.71	.63
-5	1.95	1.53
-3	-2.57	-2.01
-2	.95	.69
-1	1.33	1.22
1	1.95	1.86
2	.67	.61
4	.48	.48
10 -3		
-9	-2.14	-2.17
-6	-1.57	-1.67
-5	1.52	1.45
-4	2.86	2.60
0	-1.48	-1.36
10 -4		
-5	.95	1.13
-4	-.81	-.81
-3	1.10	1.36
-2	2.57	2.49
3	-.95	-.12
11 -2		
-5	-1.00	-.73
-4	-1.81	-1.39
0	-.57	-.93
11 -3		
-1	-1.24	-1.45
11 -4		
-4	-1.24	-1.32
-3	-.81	-.59

the benzene ring deviate by more than one and a half times the standard deviation, so that it may be regarded as planar, within the limits of error. For the benzene ring and its substituents there are small but significant deviations from the mean plane, the largest being that of O(3), which is 0·05 Å. However the atoms which are displaced from the mean plane are the substituent atoms only, and this appears to result from the molecular distortion, described above, which has been attributed to packing forces.

Discussion

The bond lengths and angles calculated from the final model are listed in Tables 6 and 7. The mean values for symmetric pairs are included in the Tables. These have appropriately reduced standard deviations.

In general the 3σ significance level of differences in bond length is approximately 0·04 Å, which corresponds to a difference in bond order of 0·3, and it is not possible to regard differences as unequivocally real below this limit.

Table 6. *Bond lengths*

		σ	Weighted mean length	σ
C(1)—C(2)	1·393 Å	0·015 Å	1·396 Å	0·008 Å
C(2)—C(11)	1·397	0·010		
C(1)—C(4)	1·396	0·012	1·389	0·009
C(11)-C(15)	1·383	0·012		
C(3)—C(4)	1·395	0·008	1·398	0·007
C(3)—C(15)	1·406	0·012		
C(4)—C(5)	1·483	0·013	1·476	0·008
C(14)-C(15)	1·473	0·008		
C(5)—C(6)	1·322	0·010	1·325	0·009
C(13)-C(14)	1·332	0·016		
C(6)—C(7)	1·487	0·016	1·486	0·011
C(12)-C(13)	1·485	0·015		
Br(1)-C(6)	1·907	0·010	1·902	0·006
Br(2)-C(13)	1·899	0·007		
C(8)—C(7)	1·529	0·012	1·531	0·009
C(16)-C(12)	1·533	0·013		
C(9)—C(7)	1·505	0·016	1·505	0·011
C(17)-C(12)	1·504	0·015		
O(1)—C(7)	1·477	0·010	1·469	0·007
O(3)—C(12)	1·462	0·009		
O(1)—C(1)	1·371	0·008	1·377	0·007
O(3)—C(11)	1·386	0·011		
O(2)—C(3)	1·356	0·010		
O(2)—C(20)	1·421	0·015		
O(4)—C(19)	1·288	0·012		
O(5)—C(19)	1·259	0·010		
C(2)—C(10)	1·490	0·013		
C(10)-C(18)	1·497	0·016		
C(18)-C(19)	1·479	0·016		

Table 7. *Bond angles*

		σ	Weighted mean value	σ
C(2)—C(1)—O(1)	118·8°	0·8°	118·7°	0·5°
C(2)—C(11)-O(3)	118·5	0·7		
C(2)—C(1)—C(4)	122·1	0·6	122·0	0·5
C(2)—C(11)-C(15)	122·0	0·8		
O(1)—C(1)—C(4)	119·0	0·8	119·2	0·5
O(3)—C(11)-C(15)	119·4	0·6		
C(1)—C(2)—C(10)	120·7	0·6	120·8	0·5
C(11)-C(2)—C(10)	121·0	0·8		
C(4)—C(3)—O(2)	118·5	0·7	119·0	0·5
C(15)-C(3)—O(2)	119·1	0·5		
C(3)—C(4)—C(5)	125·0	0·8	124·9	0·5
C(3)—C(15)-C(14)	124·9	0·8		
C(3)—C(4)—C(1)	117·5	0·8	117·7	0·5
C(3)—C(15)-C(11)	117·8	0·6		
C(5)—C(4)—C(1)	117·5	0·6	117·5	0·5
C(14)-C(15)-C(11)	117·4	0·8		
C(1)—O(1)—C(7)	118·8	0·5	118·7	0·4
C(11)-O(3)—C(12)	118·5	0·5		
Br(1)-C(6)—C(7)	117·4	0·5	117·0	0·5
Br(2)-C(13)-C(12)	116·0	0·8		
Br(1)-C(6)—C(5)	120·8	0·9	121·3	0·6
Br(2)-C(13)-C(14)	121·7	0·7		
C(5)—C(6)—C(7)	121·2	1·0	121·8	0·6
C(14)-C(13)-C(12)	122·1	0·7		
O(1)—C(7)—C(6)	108·9	0·6	108·9	0·5
O(3)—C(12)-C(13)	108·8	0·9		
O(1)—C(7)—C(8)	103·5	0·6	103·8	0·4
O(3)—C(12)-C(16)	103·9	0·5		
O(1)—C(7)—C(9)	109·6	1·0	109·7	0·6
O(3)—C(12)-C(17)	109·7	0·7		
C(6)—C(7)—C(8)	112·4	1·1	112·8	0·7
C(13)-C(12)-C(16)	112·9	0·7		
C(6)—C(7)—C(9)	108·7	0·7	109·0	0·5
C(13)-C(12)-C(17)	109·2	0·7		
C(8)—C(7)—C(9)	113·5	0·8	113·0	0·7
C(16)-C(12)-C(17)	112·1	1·0		
C(4)—C(5)—C(6)	120·4	0·9	120·2	0·6
C(15)-C(14)-C(13)	120·0	0·8		
C(3)—O(2)—C(20)	113·3	0·6		
C(2)—C(10)-C(18)	110·6	0·6		
C(10)-C(18)-C(19)	110·9	0·7		
O(4)—C(19)-O(5)	122·0	1·0		
O(4)—C(19)-C(18)	114·8	0·7		
O(5)—C(19)-C(18)	123·2	0·9		
C(1)—C(2)—C(11)	118·3	0·8		
C(4)—C(3)—C(15)	122·3	0·7		

Table 8. *Atomic coordinates referred to molecular axes*

	X	Y	Z
C(1)	−1·197 Å	−0·683 Å	−0·015 Å
C(11)	1·199	−0·452	−0·001
C(4)	−1·227	0·708	0·004
C(15)	1·228	0·695	−0·008
C(5)	−2·556	1·366	−0·007
C(14)	2·551	1·345	−0·036
O(1)	−2·382	−1·378	0·038
O(3)	2·391	−1·394	0·071
C(7)	−3·581	−0·782	−0·589
C(12)	3·575	−0·832	−0·580
Br(1)	−5·363	1·501	−0·299
Br(2)	5·361	1·422	−0·413
C(6)	−3·653	0·658	−0·222
C(13)	3·643	0·621	−0·278
C(10)	−0·005	−2·894	0·021
C(2)	−0·001	−1·404	0·011
C(3)	−0·002	1·377	0·006
O(2)	−0·005	2·733	−0·038

Aromatic ring

The mean length of the bonds in the benzene ring is $1{\cdot}394 \pm 0{\cdot}005$ Å, which agrees with the mean value of 1·397 Å given by Pauling (1960). The standard deviations are too large for the differences between the individual bond lengths of the benzene ring to be regarded as having any definite significance. Nevertheless it is interesting to note that the pairs related by the approximate molecular symmetry are in very close agreement.

The bond angles in the aromatic ring differ significantly from the 120° required for perfect sixfold symmetry, but are symmetric, within the limits of error, about the line joining C(2) and C(3). The differences may be accounted for in terms of the difference between the C–C and C–O bonds. Since oxygen is more electronegative than carbon the C–O bond has considerable ionic character, and the bonding electrons are expected to be attracted towards the oxygen atom, distorting the orbitals slightly from a trigonal configuration and reducing the C–C–O angle.

The six C–C–O angles from the aromatic ring agree well within the limits of error, and have a mean value of 118·9°. The three C–C–C angles associated with the C–C–O angles are also in good agreement, with a mean value of 122·1°. The angles centred at C(2) are nearly trigonally symmetric, but those centred at C(4) and C(15) are not. This difference may be caused by steric hindrance between hydrogen atoms attached to the C(5) and C(14) carbons and O(2).

Methoxyl group

The bond lengths C(3)–O(2) and O(2)–C(20) agree with the values expected for sp^2 and sp^3 carbon–oxygen bonds, and the angle C(3)–O(2)–C(20) is similar to the C–O–C value obtained from an electron diffraction investigation of $(CH_2)_2O$ (Sutton, 1958).

Aliphatic chain and carboxyl group

The lengths of the C(2)–C(10) and C(10)–C(18) are somewhat shorter than those normally associated with sp^2–sp^3 and sp^3–sp^3 bonds, though the discrepancies do not exceed 3σ. The bond C(18)–C(19), on the other hand, is only $1{\cdot}48 \pm 0{\cdot}01_6$ Å and is significantly shorter than the lengths of most C–C bonds attached to carboxyl groups. Brown (1959) holds that the carbon in a carboxyl group is sp^3 hybridized and supports this with evidence from acetic and oxalic acids, where the C–C bonds have the characteristic single-bond length of 1·54 Å. The shortening in this case may be due to an unusually large amount of resonance, for this group shows a number of other unusual features. The O–H···O distance is 2·59 Å, and is equal, within the limits of error, to the usual hydrogen bond length in carboxylic acids, but the O(5)–C(19) bond is not significantly shorter than the O(4)–C(19) bond and the hydrogen is symmetrically placed between the two oxygen atoms, suggesting that the two bonds may be equivalent. On the other hand the O(4)–C(19)–C(18) angle is smaller than the angle O(5)–C(19)–C(18), which is consistent with the C(19)–O(5) bond having more double bond character. However the distance between O(5) and the C(20) atom of a neighbouring molecule is unusually small, and it seems possible that the bond angles are altered by the packing, so the evidence of the bond lengths is to be preferred. It was noted that the hydrogen peak in the difference map was extended along the bond, which would be consistent with its occupying alternative sites on either side of the centre at random. However this would also require that the oxygen peaks should be extended along the O–H···O bond, and as there was no evidence for this in the electron density maps a random distribution seems unlikely.

It is interesting to compare the carboxyl group in eriostoic acid with those of other carboxylic acids, for which bond lengths and angles have been tabulated by Vaughan & Donohue (1952) and Nardelli, Fava & Giraldi (1962). These reviews show that, in general, the two carbon–oxygen bonds are different, and there is a similar lack of equivalence in the C–C–O bond angles, and the O–H···O linkage. When two carboxyl groups are linked together, so that the molecules become dimers, the two bonds become more alike (Karle & Brockway, 1944), but none of the compounds shows equivalence to the degree exhibited by eriostoic acid. Acetylenecarboxylic acid dihydrate (Dunitz & Robertson, 1947) has bond lengths of 1·26 and 1·27 Å, but its hydrogen bonding system involves the water molecules, and is very different from that in the present compound. Equivalent bonds are reported for allokainic acid (Cruickshank, 1959) but these should be regarded as belonging to a carbonyl, rather than a carboxyl group.

It is also of interest to note that the hydrogen bonded carboxyl groups are coplanar, within the limits of experimental error (Table 10), since Jeffrey & Sax (1963) have recently shown that this is the exception, rather than the rule, in such systems.

The heterocyclic rings and their substituents

The bond pairs C(4)–C(5):C(14)–C(15), C(5)–C(6):C(13)–C(14) and C(6)–C(7):C(12)–C(13) have mean lengths in agreement with the values generally accepted for sp^2–sp^2, $sp^2{=}sp^2$ and sp^2–sp^3 hybridization. The means of the pairs O(1)–C(1):O(3)–C(11) and O(1)–C(7):O(3)–C(12) are longer than the standard values for these bonds of 1·43 and 1·36 Å respectively (*International Tables for X-ray Crystallography*, 1962). The angles C(1)–O(1)–C(7) and C(11)–O(3)–C(12) are larger than that observed in the methoxyl group, and the angles C(6)=C(5)–C(4) and C(13)=C(14)–C(15) are considerably less than the 125° usual for single bond–double bond angles (Pauling, 1960).

The C–Br bond lengths agree closely with other values reported for this bond in olefinic compounds (Sutton, 1958). The single bond–double bond angles

C(5)=C(6)–C(7) and C(14)=C(13)–C(12) are 121, 122°, which are also smaller than normal value, but are larger than the single bond–single bond angle of 117°.

In the *gem* dimethyl groups the bonds C(7)–C(8) and C(12)–C(16), which are approximately in the benzene ring plane, are equal to the usual value of an sp^3–sp^3 bond, but C(7)–C(9) and C(12)–C(17), which are almost perpendicular to the plane, are 0·02 Å shorter. This difference is only just within the limits of error, and may be a real effect resulting from the packing.

The ionic character of the carbon–oxygen bonds is expected to influence the bond angles in the heterocyclic rings in a manner similar to that observed for the aromatic ring. The angles O(1)–C(7)–C(8) and O(3)–C(12)–C(16) are indeed smaller than the tetrahedral angle, but none of O(1)–C(7)–C(9), O(1)–C(7)–C(6), O(3)–C(12)–C(17) and O(3)–C(12)–C(13) appears to have been affected. It is possible that these angles are prevented from decreasing by steric forces on C(8), C(9), C(16) and C(17).

Packing

The three rings in the molecule form an approximately planar system, with the side chains rising and descending step-like on either side, and a methyl group protruding perpendicularly at each end. The structure consists of molecules stacked together in layers roughly perpendicular to the *a* axis (Fig. 3) with the centrosymmetrically related molecules partly overlapping. Neighbouring molecules are hydrogen bonded through the carboxyl groups. The lines joining the centres of benzene rings in adjacent molecules are in the [110] and [1$\bar{1}$0] directions, which correspond to the preferred directions of growth in the crystal. The long axis of the molecule lies in the [001] direction which, as expected, is the direction of slow growth that gives rise to the plate-like character of the crystals.

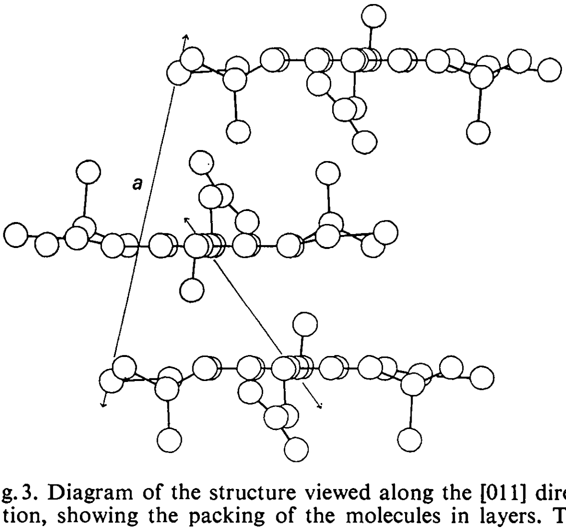

Fig. 3. Diagram of the structure viewed along the [011] direction, showing the packing of the molecules in layers. The line joining the centres of two benzene rings which corresponds to one of the principal growth directions is shown.

The intermolecular distances between non-hydrogen atoms of less than 3·8 Å are given in Table 9. The side of the molecule containing Br(2) is packed tightly

Table 9. *Intermolecular contacts less than* 3·8 Å

Br(1)–O(2′)	3·79 Å
Br(1)–O(4)	3·78
Br(2)–O(5)	3·66
O(1)—C(16′)	3·71
O(2)—O(2′)	3·61
O(2)—C(5′)	3·24
O(2)—C(17′)	3·51
O(3)—C(1′)	3·69
O(3)—C(2′)	3·63
O(3)—C(4′)	3·79
O(3)—C(11′)	3·69
O(4)—O(4′)	3·60
O(4)—O(5′)	2·60*
O(4)—C(9′)	3·74
O(4)—C(19′)	3·49
O(5)—O(5′)	3·23
O(5)—C(8′)	3·74
O(5)—C(19′)	3·31
O(5)—C(20′)	3·38
C(1)—C(16′)	3·76
C(2)—C(11′)	3·74
C(3)—C(17′)	3·66
C(4)—C(16′)	3·75
C(5)—C(16′)	3·79
C(5)—C(20′)	3·50
C(10)–C(14′)	3·55
C(10)–C(15′)	3·74
C(11)–C(11′)	3·54
C(14)–C(17′)	3·72
C(15)–C(17′)	3·72

* Hydrogen bond.

Atoms at the equivalent position $\bar{x},\bar{y},\bar{z}$ are shown dashed.

Table 10. *Mean plane parameters and deviations of atoms from the plane*

(i) Benzene ring and adjacent atoms

$$0·9181x+0·0720y+0·3897z-6·241=0$$

	Deviation		Deviation
C(1)	0·025 Å	O(1)	0·017 Å
C(2)	0·010	O(2)	0·007
C(3)	−0·020	O(3)	−0·049
C(4)	−0·010	C(5)	−0·007
C(11)	0·013	C(10)	0·020
C(15)	0·003	C(14)	0·024

(ii) Benzene ring

$$0·9221x+0·0629y+0·3818z-6·141=0$$

	Deviation
C(1)	0·013 Å
C(2)	−0·011
C(3)	−0·006
C(4)	−0·004
C(11)	0·001
C(15)	0·008

(iii) Carboxyl groups

$$0·7804x+0·5153y-0·3542z+2·074=0$$

	Deviation		Deviation
O(4)	0·007 Å	O(4′)	−0·007 Å
O(5)	0·007	O(5′)	−0·007
C(18)	0·004	C(18′)	−0·004
C(19)	−0·016	C(19′)	0·016

Atoms at the equivalent position $\bar{x},\bar{y},\bar{z}$ are shown dashed.

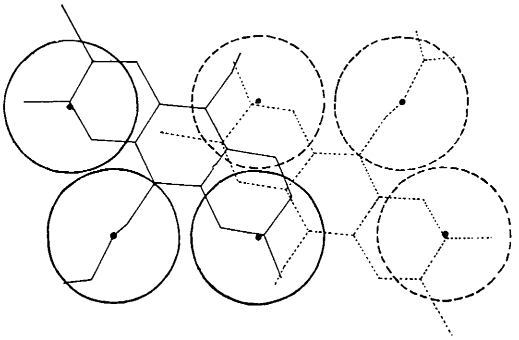

Fig. 4. Diagram of the structure viewed along the *a* axis showing the close packing in the plane midway between the overlapping molecules. The circles round each of the methyl groups are 3·5 Å in diameter.

against its nearest neighbour. This appears to give rise to a bending of the molecule away from the neighbour, resulting in the molecular distortion mentioned earlier. The side of the molecule containing Br(1) is not as close to another molecule in the stack, and consequently is more nearly in the plane of the benzene ring. The Br(1) atoms itself interacts slightly with the C(9) atom in another stack, and is bent slightly towards the methoxyl group.

The projecting methyl groups of C(17) and C(19) and the 'elbow' of the aliphatic chain at C(10) interlock with their symmetric equivalents. These six atoms are not quite coplanar, but are closely packed, as is shown in Fig. 4. Since the spacing between the planar sections of the molecules of 3·5 Å is close to the nonbonded separation of aromatic rings (Pauling, 1960), the structure as a whole is closely packed, which accounts for the comparatively high density of 1·58 of the crystal.

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References

ABRAHAMS, S. C. (1955). *Acta Cryst.* **8**, 661.
AHMED, F. R. & CRUICKSHANK, D. W. J. (1953). *Acta Cryst.* **6**, 385.
BALASHOV, V. & URSELL, H. D. (1957). *Acta Cryst.* **10**, 582.
BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.
BUERGER, M. J. (1942). *X-ray Crystallography.* New York: John Wiley.
BROWN, M. G. (1959). *Trans. Faraday Soc.* **55**, 694.
BUSING, W. R. & LEVY, H. A. (1957). *Acta Cryst.* **10**, 180.
CRUICKSHANK, D. W. J. (1959). *Acta Cryst.* **12**, 1052.
DARLOW, S. F. (1960). *Acta Cryst.* **13**, 683.
DAUBEN, C. H. & TEMPLETON, D. H. (1955). *Acta Cryst.* **8**, 841.
DONOHUE, J. & MARSH, R. E. (1962). *Acta Cryst.* **15**, 941.
DUFFIELD, A. M., JEFFERIES, P. R. & LUCICH, P. H. (1962). *Aust. J. Chem.* **15**, 812.
DUNITZ, J. D. & ROBERTSON, J. M. (1947). *J. Chem. Soc.* p. 148.
HALL, S. R. & MASLEN, E. N. (1965). *Acta Cryst.* **18**, 265.
HODGSON, L. I. & ROLLETT, J. S. (1963). *Acta Cryst.* **16**, 329.
International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.
JEFFERY, G. A. & SAX, M. (1963). *Acta Cryst.* **16**, 430.
KARLE, J. & BROCKWAY, L. O. (1944). *J. Amer. Chem. Soc.* **46**, 574.
KITAJGORODSKIJ, A. I. (1965). *Acta Cryst.* **18**, 585.
MCWEENY, R. (1951). *Acta Cryst.* **4**, 513.
NARDELLI, M., FAVA, G. & GIRALDI, G. (1962). *Acta Cryst.* **15**, 737.
OH, Y. L. & MASLEN, E. N. (1965). *Acta Cryst.* **20**, 852.
PAULING, L. (1960). *The Nature of the Chemical Bond.* Ithaca: Cornell Univ. Press.
SCHOMAKER, V., WASER, J., MARSH, R. E. & BERGMAN, G. (1959). *Acta Cryst.* **12**, 600.
SUTTON, L. E. (1958). *Tables of Interatomic Distances and Configurations in Molecules and Ions.* Special Publication No. 11. London: The Chemical Society.
THOMAS, L. H. & UMEDA, K. (1957). *J. Chem. Phys.* **26**, 293.
VAUGHAN, P. & DONOHUE, J. (1952). *Acta Cryst.* **5**, 530.
WEISZ, O., COCHRAN, W. & COLE, W. F. (1948). *Acta Cryst.* **1**, 83.
WELLS, M. (1960). *Acta Cryst.* **13**, 722.