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The Structure of Davallol Iodoacetate

By Yow-Lam Oh and E. N. Maslen

Department of Physics, The University of Western Australia, Nedlands, Western Australia

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The structure and the absolute configuration of davallol iodoacetate, $C_{32}H_{51}O_2I$, which crystallizes in colourless prismatic needles belonging to the space group $P2_12_12_1$ (D_2^4) with cell axes $a=7{\cdot}171$, $b=13{\cdot}222$, $c=31{\cdot}205$ Å, were determined by the direct method of anomalous dispersion phasing and refined by the block-diagonal least-squares method to a final R value of 0·101 for all observed reflexions. Anomalous long bonds to fully substituted carbon atoms have been observed and hydrogen atoms were located approximately in a three-dimensional difference synthesis.

1. Introduction

Davallic acid (Nakanishi, Lin, Hsu & Hsiu, 1963) is a triterpene with a novel rearranged hopane skeleton. The acid is isolated from the rhizome of the Chinese fern *Davallia divaricata* which is used widely as a tonic and diuretic in Taiwan. It is of chemical interest to elucidate the stereochemistry and to establish the absolute configuration of its structure. Nakanishi and his co-workers propose on spectrochemical grounds that davallic acid is stereochemically as shown in Fig. 1.

The present work also forms a part of a programme currently undertaken at this laboratory to investigate the carbon–carbon bonding and molecular packing in strained structures. It has been observed that in various terpenoid structures the fully substituted carbon atoms tend to form long carbon–carbon bonds (Hall & Maslen, 1965; O'Connell, 1965).

2. Experimental and crystal data

Davallol iodoacetate crystallizes in colourless prismatic needles, elongated along the shortest crystallographic axis. The crystal data are as follows:

Chemical formula $C_{32}H_{51}O_2I$
Molecular weight 594·67
$a = 7{\cdot}171 \pm 0{\cdot}007$ Å
$b = 13{\cdot}222 \pm 0{\cdot}010$
$c = 31{\cdot}205 \pm 0{\cdot}030$
$U = 2959$ Å^3
$D_x = 1{\cdot}334$ g.cm^{-3}
$D_m = 1{\cdot}32 \pm 0{\cdot}01$ g.cm^{-3}
$\mu = 85{\cdot}16$ cm^{-1} for Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å)
Space group $P2_12_12_1$ (D_2^4)
$Z = 4$

The cell parameters were measured from precession photographs which were corrected for film shrinkage. The density was determined by flotation in an aqueous solution of potassium mercuric iodide. Weissenberg photographs showed spectral absences of $h00$, $0k0$ and $00l$ with h, k and l odd. This uniquely determined the space group as $P2_12_12_1$ (D_2^4).

The intensity data were recorded by multiple-film equi-inclination Weissenberg technique with Cu $K\alpha$ radiation. Layers 0–6 were collected along the a axis, 0–2 along the b axis and the zero layer only on c axis rotation. The intensities were estimated by visual comparison with a calibrated standard strip.

Iodine has an absorption edge near the Cu $K\alpha$ wavelength and anomalous dispersion effects lead to non-equivalence of the hkl and $\bar{h}\bar{k}\bar{l}$ reflexions in non-equatorial zones. The non-equivalent intensities $I(hkl)$ and $I(\bar{h}\bar{k}\bar{l})$ were severally indexed according to the method of Peerdeman & Bijvoet (1956).

For the purpose of refinement, $I(hkl)$ and $I(\bar{h}\bar{k}\bar{l})$ were averaged. There were then 2008 reflexions, representing 62% of the data in the full copper sphere. The complete data could not be collected in view of the high temperature-factor coefficient of 4·0 Å^2. Of the recorded 2008 reflexions 380 were too weak to be measured and they were assigned the minimum observable values.

The b-axis correlation data were collected some time after the a-axis data and in the preliminary analysis it was necessary to apply Wilson scaling to the a axis layer by layer. However, the final data were correlated by calculating the interlayer scale factors after the application of Lorentz-polarization and absorption corrections. Absorption corrections were calculated following a procedure similar to that described by Busing & Levy (1957)*.

The value of κ, the correlation disagreement index defined as

$$\kappa = 100 \times \frac{|F_1 - F_2|}{\frac{1}{2}|F_1 + F_2|} \quad \%$$

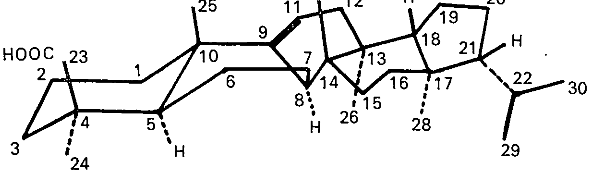

Fig. 1. Dreiding model of davallic acid.

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* A general absorption program for an IBM 1620 computer written in SPS II using exponential-table-look-up, capable of a speed of 4½ seconds per crystal face per reflexion, is available on request.

where F_1 and F_2 are two independently measured values of a single structure factor for the present set of data is 10·9% for the observed reflexions only. The averaged standard deviation $\sigma(F_o)$ is therefore approximately 9·7% (Ibers, 1956).

During the refinement, it was noticed that the values of large F_o were consistently lower than the values of the corresponding F_c, which was considered to be due to secondary extinction. An empirical plot of $\ln(F_o^2/F_c^2)$ *versus* F_c^2 was made and a good straight line was obtained. Corrections ($\varepsilon = 1{\cdot}5 \times 10^{-6}$) for secondary extinction were applied by a procedure described by Hamilton (1957) for $F_o^2/F_c^2 > 0{\cdot}7$.

The complete expression by Zachariasen (1963) was not necessary since all terms affected were of low θ values.

3. Structure analysis

Patterson projections

The coordinates of the iodine atom were determined from sharpened Patterson projections on (100) and (001). The coordinates were

$$\frac{x}{a} = 0{\cdot}0912\,, \quad \frac{y}{b} = 0{\cdot}1101\,, \quad \frac{z}{c} = 0{\cdot}0652\,.$$

Compared with the final values (Table 1) there are errors in the coordinates of 0·10, 0·02 and 0·02 Å in x, y and z respectively. The relatively large error in the x direction was due to overlap in the (001) projection.

Solution of the structure

Structure factors were calculated from the iodine coordinates and the residual index R was 0·36. The phases were calculated directly by the method of anomalous dispersion as described by Hall & Maslen (1965).

Following the notation of Hall & Maslen,

$$\alpha = \alpha' + \pi/2 \pm \theta$$

the ambiguity in α arises from the correction term θ which is evaluated from

$$\cos\theta = \frac{\Delta F_o^2}{4|F'||F_A''|}\,.$$

To resolve this ambiguity α was always chosen so that it was nearest to α'. This is reasonable since the iodine atom provides 82% of the total scattering power of the structure and therefore α is more likely to lie closer to α' than $\alpha' + \pi$*.

From equation (2) it is clear that the data have to be scaled absolutely. This was accomplished by Wilson

Table 1. *Coordinates of atoms*

Atom	x/a	y/b	z/c	$\sigma(x/a)$	$\sigma(y/b)$	$\sigma(z/c)$
C(1)	0·85633	0·64856	0·04476	0·00271	0·00168	0·00060
C(2)	0·95796	0·54942	0·03186	0·00357	0·00194	0·00081
C(3)	0·97771	0·48498	0·06825	0·00289	0·00194	0·00085
C(4)	0·80963	0·45175	0·09465	0·00298	0·00160	0·00063
C(5)	0·71394	0·55221	0·10740	0·00279	0·00158	0·00059
C(6)	0·52656	0·53607	0·13356	0·00338	0·00162	0·00070
C(7)	0·41659	0·62653	0·14057	0·00319	0·00147	0·00067
C(8)	0·52663	0·72161	0·13712	0·00253	0·00144	0·00063
C(9)	0·61943	0·73158	0·09220	0·00281	0·00173	0·00060
C(10)	0·67359	0·62824	0·07146	0·00261	0·00171	0·00056
C(11)	0·64177	0·81889	0·07232	0·00477	0·00167	0·00069
C(12)	0·58722	0·92098	0·09019	0·00368	0·00151	0·00063
C(13)	0·55447	0·91631	0·13867	0·00289	0·00152	0·00060
C(14)	0·41398	0·82581	0·14707	0·00253	0·00157	0·00054
C(15)	0·35502	0·82316	0·19433	0·00273	0·00153	0·00062
C(16)	0·26026	0·92349	0·20777	0·00267	0·00167	0·00073
C(17)	0·37836	0·01799	0·20062	0·00248	0·00141	0·00054
C(18)	0·44664	0·01289	0·15375	0·00299	0·00155	0·00062
C(19)	0·53293	0·11736	0·14557	0·00373	0·00160	0·00071
C(20)	0·40464	0·18642	0·17052	0·00402	0·00185	0·00076
C(21)	0·27768	0·12085	0·19779	0·00285	0·00174	0·00057
C(22)	0·20201	0·17077	0·23916	0·00318	0·00193	0·00075
C(23)	0·68863	0·37768	0·06980	0·00270	0·00164	0·00071
C(24)	0·87634	0·40186	0·13697	0·00454	0·00212	0·00082
C(25)	0·51784	0·60219	0·03804	0·00348	0·00186	0·00067
C(26)	0·74225	0·90217	0·16089	0·00300	0·00176	0·00086
C(27)	0·24065	0·82419	0·11905	0·00351	0·00188	0·00077
C(28)	0·53296	0·02544	0·23643	0·00355	0·00202	0·00072
C(29)	0·06736	0·10396	0·26650	0·00354	0·00234	0·00083
C(30)	0·10420	0·27258	0·22755	0·00337	0·00204	0·00089
C(31)	0·71235	0·21619	0·04123	0·00293	0·00160	0·00056
C(32)	0·83926	0·13565	0·02499	0·00377	0·00151	0·00063
I	0·07734	0·11189	0·06448	0·00024	0·00014	0·00006
O(1)	0·80044	0·29182	0·05828	0·00172	0·00115	0·00049
O(2)	0·54828	0·21245	0·03760	0·00218	0·00133	0·00057

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* A note on weighting the structure factors using both α_1 and α_2 came to our notice only after the structure was solved (Sim, 1964).

Table 2. Anisotropic temperature factor coefficients*†

Atom	B_{11}	B_{22}	B_{33}	B_{23}	B_{13}	B_{12}
C(1)	0·01502	0·00760	0·00098	−0·00078	0·00292	−0·00147
*	0·00405	0·00161	0·00020	0·00093	0·00140	0·00385
C(2)	0·02729	0·00759	0·00169	−0·00172	0·00425	0·00879
*	0·00570	0·00170	0·00032	0·00124	0·00233	0·00524
C(3)	0·01171	0·00991	0·00227	−0·00450	0·00262	0·00090
*	0·00411	0·00184	0·00035	0·00148	0·00205	0·00416
C(4)	0·02010	0·00495	0·00119	−0·00080	−0·00135	−0·00183
*	0·00465	0·00136	0·00024	0·00089	0·00179	0·00407
C(5)	0·01905	0·00612	0·00082	−0·00018	−0·00030	0·00111
*	0·00436	0·00140	0·00020	0·00089	0·00157	0·00401
C(6)	0·02507	0·00543	0·00143	0·00076	0·00164	−0·00238
*	0·00505	0·00142	0·00028	0·00104	0·00203	0·00438
C(7)	0·02749	0·00440	0·00142	0·00101	0·00460	−0·00177
*	0·00530	0·00130	0·00026	0·00096	0·00212	0·00462
C(8)	0·01031	0·00459	0·00137	0·00110	0·00075	0·00382
*	0·00365	0·00121	0·00025	0·00090	0·00149	0·00335
C(9)	0·01659	0·00755	0·00091	0·00059	0·00159	−0·00161
*	0·00413	0·00151	0·00022	0·00090	0·00155	0·00403
C(10)	0·01466	0·00943	0·00075	0·00054	0·00160	−0·00590
*	0·00375	0·00175	0·00020	0·00094	0·00136	0·00405
C(11)	0·05872	0·00455	0·00098	0·00042	0·00433	−0·00021
*	0·00910	0·00141	0·00026	0·00098	0·00265	0·00600
C(12)	0·03525	0·00483	0·00092	0·00037	0·00315	0·00733
*	0·00628	0·00137	0·00022	0·00083	0·00226	0·00488
C(13)	0·01892	0·00634	0·00095	0·00040	0·00056	0·00167
*	0·00448	0·00137	0·00022	0·00084	0·00168	0·00417
C(14)	0·01151	0·00758	0·00088	−0·00168	−0·00051	0·00605
*	0·00353	0·00140	0·00019	0·00086	0·00146	0·00384
C(15)	0·01788	0·00501	0·00105	0·00046	0·00233	0·00417
*	0·00424	0·00130	0·00022	0·00088	0·00154	0·00366
C(16)	0·01130	0·00761	0·00167	−0·00141	0·00114	0·00094
*	0·00409	0·00169	0·00030	0·00109	0·00178	0·00412
C(17)	0·01345	0·00488	0·00080	−0·00128	−0·00145	0·00616
*	0·00373	0·00119	0·00019	0·00077	0·00133	0·00323
C(18)	0·01934	0·00548	0·00121	−0·00025	0·00263	0·00153
*	0·00463	0·00133	0·00023	0·00089	0·00179	0·00408
C(19)	0·03515	0·00467	0·00144	0·00033	0·00449	0·00624
*	0·00630	0·00140	0·00027	0·00108	0·00223	0·00538
C(20)	0·03630	0·00840	0·00147	0·00278	0·00793	0·00369
*	0·00693	0·00183	0·00030	0·00124	0·00272	0·00623
C(21)	0·01935	0·00801	0·00082	−0·00102	0·00030	0·00527
*	0·00449	0·00157	0·00020	0·00099	0·00155	0·00469
C(22)	0·02304	0·00700	0·00142	−0·00021	−0·00028	0·00793
*	0·00535	0·00164	0·00028	0·00111	0·00209	0·00498
C(23)	0·01414	0·00724	0·00162	−0·00181	−0·00115	0·00600
*	0·00419	0·00160	0·00029	0·00121	0·00184	0·00408
C(24)	0·04941	0·00871	0·00150	0·00055	−0·00185	0·02328
*	0·00882	0·00202	0·00032	0·00132	0·00277	0·00764
C(25)	0·02663	0·00735	0·00107	−0·00074	−0·00302	0·00077
*	0·00544	0·00158	0·00025	0·00105	0·00188	0·00517
C(26)	0·01539	0·00680	0·00231	−0·00158	0·00234	0·00483
*	0·00456	0·00168	0·00038	0·00133	0·00208	0·00468

Table 2 (*cont.*)

C(27)	0·02543	0·00763	0·00152	−0·00149	−0·00279	0·00798
*	0·00545	0·00176	0·00031	0·00121	0·00212	0·00534
C(28)	0·02760	0·00894	0·00136	−0·00104	−0·00331	−0·00016
*	0·00581	0·00198	0·00028	0·00119	0·00214	0·00556
C(29)	0·02740	0·01210	0·00164	0·00041	0·00049	−0·00190
*	0·00618	0·00240	0·00033	0·00148	0·00244	0·00763
C(30)	0·02206	0·00851	0·00217	−0·00327	−0·00143	0·01215
*	0·00532	0·00191	0·00039	0·00148	0·00250	0·00565
C(31)	0·02112	0·00584	0·00067	0·00014	0·00002	−0·00395
*	0·00463	0·00139	0·00019	0·00083	0·00152	0·00401
C(32)	0·03886	0·00433	0·00084	−0·00048	0·00306	0·00048
*	0·00648	0·00132	0·00019	0·00084	0·00202	0·00484
I	0·03122	0·01035	0·00181	−0·00216	−0·00407	0·01508
*	0·00042	0·00012	0·00002	0·00010	0·00018	0·00040
O(1)	0·00947	0·00929	0·00147	−0·00199	−0·00032	−0·00077
*	0·00256	0·00111	0·00019	0·00080	0·00122	0·00261
O(2)	0·01670	0·00915	0·00222	−0·00150	0·00000	−0·00300
*	0·00357	0·00131	0·00026	0·00091	0·00160	0·00352

* The second line of each entry is the estimated standard deviation.

† $T=\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\}$.

scaling of each layer of the *a*-axis data after the application of Lorentz-polarization corrections but not the absorption correction (see §2), which could not be made at the time because the general absorption program was still being developed.

A three-dimensional Fourier synthesis was calculated with sections along the *c* axis using the set of directly phased structure factors. There were 35 peaks with electron densities greater than 3·5 e.Å^{-3}, other than that due to the iodine atom and some obvious diffraction ripple. A search was made for bond lengths less than 1·7 Å, treating all the 35 peaks as possible atomic sites. Pairs of 'atoms' with an interatomic separation between 1·15 and 1·70 Å were mapped, making appropriate transformation of coordinates according to the space-group symmetry. 30 out of the 35 peaks appeared to form a molecule. Using Nakanishi's proposed structure (Fig. 1) as a working model a search was made for C(11), C(19), C(25) and C(30), the crucial ones being C(11) and C(19) since these were required to complete the ring system.

On re-examination of the Fourier sections, peaks corresponding to C(11), C(19) and C(25) were identifiable with peak heights of 3·3, 3·4 and 3·1 Å respectively. At this point it appeared very probable that Nakanishi's model was correct if an atom could be found to bond to C(22). There were two peaks each of height of about 2·6 e.Å^{-3} that were tetrahedrally directed to C(22). One of these was arbitrarily assumed to be C(30).

One round of structure factors was calculated with the use of all the 35 non-hydrogen atoms, each being given an isotropic temperature factor coefficient of 3·85 Å^2 except for the iodine atom, which was assigned a value of 4·0 Å^2. The *R* index decreased by 0·08 to 0·28. A difference synthesis using $|F_o-F_c|$ as coefficients was evaluated. The chosen site for C(30) appeared as a hollow and a sharp peak appeared at the alternative position.

The correct site for C(30) was selected and minor positional shifts were applied to the other 34 atoms. Thermal anisotropy was evident for most atoms in the difference synthesis. However, since the final set of data was not yet available, only isotropic temperature factor coefficients were used in the calculation of the structure factors at this stage. *R* fell to 0·26, indicating that the trial structure was approximately correct.

While the *b*-axis correlation data were being collected two rounds of block-diagonal least-squares calculation were performed to refine the anisotropic thermal and positional parameters of the iodine atom alone. *R* was lowered to 0·20.

Refinement

The structure was refined principally through the use of a block-diagonal least-squares (BDLS) program for the IBM 1620 computer written by Dr G.A. Mair of the Royal Institution, London. The analytical *f* curves used in the structure factor calculation were taken from *International Tables for X-ray-Crystallography* (1962) and were adjusted for the real component of the anomalous scattering factor $\Delta f'$ but not for the imaginary part $\Delta f''$. (Dauben & Templeton, 1955). Refinement procedures involving $\Delta f''$ (Patterson, 1963; Ibers & Hamilton, 1964) were not followed since the extra labour involved in computation is not justified in the present analysis where $(f^\circ+\Delta f')$ is much larger than $\Delta f''$ and where the accuracy of the data is not sufficiently high.

During the refinement, each reflexion was weighted according to a scheme suggested by Mills & Rollett (1961);

$$\omega^{\frac{1}{2}} = [1 + (F_o - b)^2/a^2]^{-\frac{1}{2}}$$

where a and b are constants to be derived from a plot of $[F_o - F_c - 1]^{\frac{1}{2}}$ *versus* F_o. However, during the initial stages of refinement, it was found satisfactory to put $a = 8\,|F_{\min}|$ and $b = 5|F_{\min}|$. In this instance $5|F_{\min}|$ corresponded to the most reliable value in visual estimation of intensities.

Unobserved reflexions were included in the evaluation of all structure factors but only reflexions with $F_o < F_c$ were included in the least-squares calculations.

After nine rounds of block-diagonal least-squares (BDLS) calculations, the R index for all the observed reflexions fell to 0·126. An analysis of the structure factors showed that the F_o values were consistently less than the corresponding F_c values for large F_o, indicating secondary extinction. Correction factors were evaluated and applied.

Location of hydrogen atoms

BDLS calculations were continued for two more rounds after the application of secondary extinction corrections. A three-dimensional difference synthesis was computed to locate the hydrogen atoms where possible. There are 51 hydrogen atoms in the asymmetric unit. Out of these 30 could be fixed approximately from the basic skeleton. Their positions were determined by assuming a C–H bond of approximately 1·09 Å in an ideal tetrahedral configuration. All atomic sites except that of H(072) were located in positive areas with heights ranging from 0·1 to 0·6 e.Å^{-3}. The site of H(072) was in a shallow of about −0·15 e.Å^{-3}.

The remaining 21 hydrogen atoms belong to seven methyl groups. Six of these groups are in close contact (within the sum of the van der Waals radii) either with one another or with hydrogen-bearing carbon atoms in the basic molecular skeleton, some of the contacts being intramolecular and others intermolecular. It would be expected that such close contacts would hinder free rotation of these methyl groups and that the hydrogen atoms belonging to them would occupy fixed sites in the cell. These groups were those with carbon atoms C(25), C(26), C(27), C(28), C(29) and C(30). The seventh methyl group with carbon C(24) has no contact closer than 4·0 Å and free rotation about the C(4)–C(24) bond seems possible.

The hydrogen atoms for each methyl group are restricted to the circumference of a circle of radius of 1·03 Å in the plane having the C–C bond as its normal. Sections for each methyl plane were taken from the difference synthesis, and for each of the six hindered methyl groups three positive peaks or areas at approximately 120° apart were present, indicating clearly the positions of the three hydrogen atoms. However, this evidence was absent for the C(24) methyl group where free rotation was possible.

Structure factors were evaluated on all 86 atoms giving each hydrogen atom an isotropic temperature factor coefficient approximately 1·5 times that of its bonding carbon atom. The R index was lowered by 0·009 to 0·109. This was particularly encouraging in view of the low contribution of the hydrogen atoms to the structure factors and one could infer with some confidence that most of the hydrogen atoms were correctly located. A list of the coordinates of all the hydrogen atoms is given in Table 3*.

Table 3. *Coordinates of hydrogen atoms**

Atom	x/a	y/b	z/c	B
H(11)	0·8249	0·6907	0·0162	6·0
H(12)	0·9520	0·6959	0·0629	6·0
H(21)	0·8820	0·5071	0·0077	8·3
H(22)	0·0957	0·5622	0·0189	8·3
H(31)	0·0557	0·4185	0·0613	7·8
H(32)	0·0713	0·5222	0·0915	7·8
H(51)	0·8065	0·5989	0·1259	5·1
H(61)	0·4433	0·4785	0·1165	7·2
H(62)	0·5575	0·5018	0·1634	7·2
H(71)	0·3017	0·6272	0·1157	5·9
H(72)	0·3425	0·6201	0·1699	5·9
H(81)	0·6362	0·7152	0·1606	4·9
H(111)	0·7250	0·8250	0·0417	8·5
H(121)	0·6854	0·9776	0·0819	7·2
H(122)	0·4554	0·9457	0·0746	7·2
H(151)	0·2690	0·7584	0·2002	5·7
H(152)	0·4804	0·8121	0·2138	5·7
H(161)	0·1283	0·9299	0·1892	6·2
H(162)	0·2138	0·9181	0·2405	6·2
H(181)	0·3104	0·0120	0·1384	5·7
H(191)	0·5453	0·1373	0·1125	7·8
H(192)	0·6773	0·1216	0·1594	7·8
H(201)	0·3143	0·2325	0·1494	8·5
H(202)	0·4701	0·2399	0·1920	8·5
H(211)	0·1510	0·1049	0·1786	5·7
H(221)	0·3250	0·1900	0·2600	8·0
H(231)	0·6307	0·4147	0·0419	7·3
H(232)	0·5715	0·3568	0·0898	7·3
H(241)	0·7592	0·3661	0·1528	10·0
H(242)	0·9800	0·3438	0·1275	10·0
H(243)	0·9366	0·4564	0·1580	10·0
H(251)	0·4505	0·6711	0·0286	7·8
H(252)	0·4126	0·5484	0·0506	7·8
H(253)	0·5769	0·5672	0·0091	7·8
H(261)	0·7267	0·8625	0·1875	7·4
H(262)	0·8373	0·9571	0·1489	7·4
H(263)	0·7800	0·8375	0·1433	7·4
H(271)	0·1500	0·7650	0·1290	7·8
H(272)	0·2750	0·8075	0·0858	7·8
H(273)	0·1666	0·8950	0·1225	7·8
H(281)	0·4700	0·0560	0·2646	7·7
H(282)	0·6200	0·0950	0·2317	7·7
H(283)	0·5836	0·9477	0·2441	7·7
H(291)	0·0733	0·1450	0·2958	7·8
H(292)	0·1080	0·0225	0·2660	7·8
H(293)	0·9280	0·1126	0·2558	7·8
H(301)	0·0437	0·3125	0·2541	7·8
H(302)	0·1834	0·3238	0·2108	7·8
H(303)	0·9961	0·2300	0·2192	7·8
H(321)	0·7589	0·0638	0·0226	8·0
H(322)	0·8789	0·1507	0·9925	8·0

* The first two digits identify the carbon atom to which the hydrogen atom is bonded.

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* No adjustment was made to the hydrogen positional coordinates for the shifts in the coordinates of their associated carbon atoms in the subsequent rounds of BDLS refinement, in view of the approximate nature of the hydrogen coordinates.

Table 4. *Observed and calculated structure factors*

H	K	L	FO	FC	AO	BO
0	0	2	164.6	143.1	164.6	0.0
		4	96.2	97.5	-96.2	0.0
		6	171.5	178.2	-171.5	0.0
		8	177.6	180.7	-177.6	0.0
		10	203.5	213.5	-203.5	0.0
		12	34.1	30.6	-34.1	0.0
		14	129.4	123.9	129.4	0.0
		16	65.7	71.4	65.7	0.0
		18	22.4	18.4	-22.4	0.0
		20	8.9U	8.2	8.9	0.0
		22	44.8	42.0	-44.8	0.0
		24	56.9	54.0	-56.9	0.0
		26	10.5U	5.2	-10.5	0.0
		28	10.8U	14.9	10.8	0.0
		30	55.4	43.9	55.4	0.0
		32	10.2U	4.0	10.2	0.0
	1	1	82.7	76.8	0.0	82.7
		2	106.0	108.5	0.0	106.0
		3	126.6	128.4	0.0	126.6
		4	58.5	45.4	0.0	-58.5
		5	40.1	33.7	0.0	40.1
		6	101.6	108.5	0.0	101.6
		7	135.2	140.5	0.0	-135.2
		8	16.1	13.1	0.0	-16.1
		9	120.1	125.1	0.0	-120.1
		10	96.3	103.6	0.0	-96.3
		11	46.7	44.2	0.0	-46.7
		12	56.8	85.9	0.0	-86.8
		13	30.0	25.0	0.0	30.0
		14	32.5	30.2	0.0	-32.5
		15	35.6	36.1	0.0	35.6
		16	44.9	45.3	0.0	44.9
		17	80.3	75.0	0.0	80.3
		18	28.4	31.8	0.0	28.4
		19	19.0	16.4	0.0	19.0
		20	50.1	49.8	0.0	50.1
		21	28.9	29.2	0.0	-28.9
		22	39.4	33.9	0.0	39.4
		23	40.5	36.5	0.0	-40.5
		24	32.2	30.0	0.0	-32.2
		25	23.5	21.4	0.0	-23.5
		26	13.3	8.2	0.0	-13.3
		27	10.9U	10.6	0.0	-10.9
		28	17.8	19.4	0.0	-17.8
		29	11.7U	10.1	0.0	11.7
		30	14.0	12.5	0.0	-14.0
		31	13.8	14.4	0.0	13.8
		32	11.1U	5.2	0.0	-11.1
	2	0	53.7	44.1	53.7	0.0
		1	103.5	94.7	-103.5	0.0
		2	23.6	17.5	-23.6	0.0
		3	150.5	138.1	-150.5	0.0
		4	44.2	40.9	-44.2	0.0
		5	246.0	235.1	-246.0	0.0
		6	21.5	24.2	-21.5	0.0
		7	110.8	110.2	-110.8	0.0
		8	20.1	18.4	20.1	0.0
		9	37.5	31.1	-37.5	0.0
		10	28.7	26.1	28.7	0.0
		11	95.9	93.9	95.9	0.0
		12	29.8	27.6	29.8	0.0
		13	61.9	63.1	61.9	0.0
		14	34.9	34.1	34.9	0.0
		15	56.0	46.2	56.0	0.0
		16	7.2U	3.9	7.2	0.0
		17	32.7	31.5	-32.7	0.0
		18	12.4U	9.3	-12.4	0.0
		19	63.7	55.3	-63.7	0.0
		20	9.2U	1.2	9.2	0.0
		21	39.1	33.6	-39.1	0.0
		22	27.4	23.4	-27.4	0.0
		23	10.0U	1.7	10.0	0.0
		24	12.3U	9.3	-12.3	0.0
		25	39.6	35.8	39.6	0.0
		26	10.6U	2.6	-10.6	0.0
		27	30.5	28.1	30.5	0.0
		28	10.9U	2.6	10.9	0.0
		29	25.0	17.7	25.0	0.0
		30	13.8	11.1	13.8	0.0
		31	13.8	12.4	-13.8	0.0
		32	10.9U	.4	-10.9	0.0
	3	1	80.3	67.2	0.0	80.3
		2	126.3	117.9	0.0	-126.3
		3	23.6	21.0	0.0	23.6
		4	88.3	82.8	0.0	-88.3
		5	112.6	103.2	0.0	-112.6
		6	43.6	42.0	0.0	-43.6
		7	92.5	96.0	0.0	-92.5
		8	25.5	26.4	0.0	-25.5
		9	84.0	86.3	0.0	-84.0
		10	36.7	36.9	0.0	36.7
		11	39.3	36.6	0.0	39.3
		12	9.1	7.9	0.0	9.1
		13	70.4	76.0	0.0	70.4
		14	31.9	30.8	0.0	31.9
		15	112.3	116.2	0.0	112.3
		16	7.5U	5.0	0.0	7.5
		17	41.8	39.1	0.0	41.8
		18	31.9	30.9	0.0	-31.9
		19	9.2U	.6	0.0	-9.2
		20	27.2	28.0	0.0	-27.2
		21	31.2	31.7	0.0	-31.2
		22	10.0U	12.2	0.0	-10.0
		23	57.9	54.9	0.0	-57.9
		24	12.4	12.9	0.0	12.4
		25	32.2	28.8	0.0	-32.2
		26	21.4	20.8	0.0	21.4
		27	10.9U	8.2	0.0	-10.9
		28	17.5	14.4	0.0	17.5
		29	10.9U	6.1	0.0	10.9
		30	11.3	7.7	0.0	11.3
		31	23.3	19.7	0.0	23.3
	4	0	185.2	192.8	-185.2	0.0
		1	32.7	26.7	-32.7	0.0
		2	126.7	100.0	-126.7	0.0
		3	33.3	27.5	-33.3	0.0
		4	32.7	22.3	32.7	0.0
		5	48.4	44.4	-48.4	0.0
		6	75.6	65.6	75.6	0.0
		7	6.1U	4.8	6.1	0.0
		8	123.0	116.7	123.0	0.0
		9	24.4	25.4	24.4	0.0
		10	92.8	88.8	92.8	0.0
		11	20.3	20.3	20.3	0.0
		12	6.8	6.6	-6.8	0.0
		13	59.7	52.4	59.7	0.0
		14	86.5	84.9	-86.5	0.0
		15	12.4	9.8	12.4	0.0
		16	87.2	81.4	-87.2	0.0
		17	38.9	36.3	-38.9	0.0
		18	22.4	18.0	-22.4	0.0
		19	45.9	44.0	-45.9	0.0
		20	18.9	19.4	18.9	0.0
		21	31.3	29.2	-31.3	0.0
		22	51.2	44.5	51.2	0.0
		23	10.3U	8.5	10.3	0.0
		24	45.6	40.7	45.6	0.0
		25	46.5	41.2	46.5	0.0
		26	10.9U	10.6	10.9	0.0
		27	10.9U	3.5	10.9	0.0
	5	1	53.3	48.4	0.0	-53.3
		2	81.8	70.7	0.0	-81.8
		3	15.8	11.3	0.0	-15.8
		4	118.0	111.7	0.0	-118.0
		5	30.0	20.7	0.0	30.0
		6	41.0	40.9	0.0	-41.0
		7	6.9U	4.3	0.0	6.9
		8	49.9	40.4	0.0	49.9
		9	11.3	10.5	0.0	11.3
		10	100.9	92.9	0.0	100.9
		11	7.8U	1.8	0.0	7.8
		12	78.6	70.6	0.0	78.6
		13	7.5U	2.7	0.0	-7.5
		14	41.7	37.2	0.0	41.7
		15	17.5	17.7	0.0	-17.5
		16	43.7	36.7	0.0	-43.7
		17	14.0	11.7	0.0	-14.0
		18	46.8	44.2	0.0	-46.8
		19	9.7U	8.0	0.0	-9.7
		20	65.3	58.5	0.0	-65.3
		21	10.3U	7.4	0.0	10.3
		22	22.7	21.4	0.0	-22.7
		23	10.6U	11.5	0.0	10.6
		24	15.2	14.2	0.0	-15.2
		25	29.5	25.3	0.0	29.5
		26	27.8	25.1	0.0	27.8
		27	22.0	20.1	0.0	22.0
		28	32.2	28.0	0.0	32.2
		29	11.4U	4.8	0.0	-11.4
		30	21.7	19.7	0.0	21.7
	6	0	64.5	53.4	-64.5	0.0
		1	64.1	49.4	64.1	0.0
		2	51.0	40.5	-51.0	0.0
		3	107.4	90.0	107.4	0.0
		4	22.0	19.4	22.0	0.0
		5	120.3	101.2	120.3	0.0
		6	61.6	49.0	61.6	0.0
		7	32.7	26.9	32.7	0.0
		8	32.5	27.5	32.5	0.0
		9	78.6	65.3	-78.6	0.0
		10	8.1U	4.8	8.1	0.0
		11	87.7	82.5	-87.7	0.0
		12	8.6U	7.8	-8.6	0.0
		13	88.2	75.4	-88.2	0.0
		14	40.3	32.8	-40.3	0.0
		15	9.2U	3.2	-9.2	0.0
		16	9.5U	1.9	-9.5	0.0
		17	47.6	36.5	47.6	0.0
		18	10.0U	2.4	10.0	0.0
		19	53.4	44.9	53.4	0.0
		20	12.7	13.7	12.7	0.0
		21	53.1	43.6	53.1	0.0
		22	10.6U	3.8	-10.6	0.0
		23	13.5	13.0	13.5	0.0
		24	13.5	10.4	13.5	0.0
		25	23.6	21.6	-23.6	0.0
		26	20.9	13.3	20.9	0.0
		27	20.6	18.6	-20.6	0.0
		28	13.0	12.0	-13.0	0.0
		29	17.2	15.9	-17.2	0.0

H	K	L	FO	FC	AO	BO
0	7	1	111.0	94.3	0.0	-111.0
		2	19.5	12.7	0.0	19.5
		3	39.2	31.6	0.0	-39.2
		4	8.6U	2.4	0.0	-8.6
		5	52.1	43.9	0.0	52.1
		6	8.6U	3.0	0.0	8.6
		7	73.8	60.6	0.0	73.8
		8	8.9U	1.3	0.0	-8.9
		9	71.7	62.9	0.0	71.7
		10	12.7	12.9	0.0	12.7
		11	25.3	24.1	0.0	25.3
		12	9.1	8.7	0.0	-9.1
		13	22.3	13.4	0.0	-22.3
		14	9.5U	6.3	0.0	-9.5
		15	85.3	84.2	0.0	-85.3
		16	9.9	7.8	0.0	-9.9
		17	31.3	32.9	0.0	-31.3
		18	10.3U	5.0	0.0	10.3
		19	10.6U	.5	0.0	10.6
		20	10.6U	16.7	0.0	10.6
		21	33.9	31.1	0.0	33.9
		22	33.3	30.4	0.0	33.3
		23	43.4	39.7	0.0	43.4
		24	11.7U	2.1	0.0	11.7
		25	21.1	19.9	0.0	21.1
		26	11.4U	3.1	0.0	-11.4
		27	11.1U	14.4	0.0	-11.1
		28	10.9U	14.6	0.0	-10.9
		29	10.6U	9.6	0.0	-10.6
		30	19.5	17.5	0.0	-19.5
	8	0	76.0	56.4	76.0	0.0
		1	9.2U	3.9	-9.2	0.0
		2	45.7	38.2	45.7	0.0
		3	68.7	59.5	68.7	0.0
		4	8.6U	2.2	8.6	0.0
		5	45.4	40.3	45.4	0.0
		6	42.0	26.9	-42.0	0.0
		7	8.9U	10.6	8.9	0.0
		8	61.1	53.9	-61.1	0.0
		9	40.1	34.3	-40.1	0.0
		10	60.1	49.3	-60.1	0.0
		11	31.6	28.2	-31.6	0.0
		12	10.3U	.4	10.3	0.0
		13	16.7	13.4	-16.7	0.0
		14	54.8	47.2	54.8	0.0
		15	10.9U	.6	-10.9	0.0
		16	39.9	34.6	39.9	0.0
		17	24.4	19.6	24.4	0.0
		18	17.5	12.1	17.5	0.0
		19	13.8	13.7	13.8	0.0
		20	11.4U	1.1	-11.4	0.0
		21	11.7U	.8	-11.7	0.0
		22	25.5	21.2	-25.5	0.0
		23	11.4U	8.8	-11.4	0.0
		24	24.1	23.7	-24.1	0.0
		25	22.4	14.8	-22.4	0.0
		26	16.1	8.1	-16.1	0.0
		27	15.5	8.4	-15.5	0.0
		28	11.1U	.5	-11.1	0.0
	9	1	9.5U	14.9	0.0	9.5
		2	40.3	30.9	0.0	40.3
		3	15.5	15.0	0.0	-15.5
		4	61.3	57.0	0.0	61.3
		5	9.5U	14.9	0.0	9.5
		6	45.4	38.8	0.0	45.4
		7	9.6	10.9	0.0	-9.6
		8	15.5	13.3	0.0	15.5
		9	15.8	7.7	0.0	15.8
		10	32.2	31.1	0.0	-32.2
		11	10.0U	2.4	0.0	10.0
		12	18.1	14.7	0.0	-18.1
		13	11.1U	4.8	0.0	11.1
		14	23.0	19.1	0.0	-23.0
		15	11.4U	3.5	0.0	11.4
		16	11.4U	1.9	0.0	-11.4
		17	11.4U	8.1	0.0	-11.4
		18	11.7U	0.0	11.7	0.0
		19	11.7U	2.8	0.0	11.7
		20	27.6	26.7	0.0	27.8
	10	0	61.0	52.3	61.0	0.0
		1	61.0	56.5	-61.0	0.0
		2	10.0U	14.8	10.0	0.0
		3	56.9	51.5	-56.9	0.0
		4	10.0U	6.2	-10.0	0.0
		5	10.3U	9.3	-10.3	0.0
		6	16.4	14.7	-16.4	0.0
		7	23.3	23.7	-23.3	0.0
		8	49.8	43.0	-49.8	0.0
		9	10.6U	5.7	-10.6	0.0
		10	38.9	34.2	-38.9	0.0
		11	10.6U	8.3	10.6	0.0
		12	10.6U	5.2	10.6	0.0
		13	41.4	39.4	41.4	0.0
		14	41.7	35.5	41.7	0.0
		15	10.9U	2.6	-10.9	0.0
		16	27.2	25.5	27.2	0.0
	11	1	53.2	55.5	0.0	53.2
		2	52.6	47.0	0.0	52.6
		3	10.6U	5.8	0.0	10.6
		4	10.6U	1.4	0.0	-10.6
		5	10.6U	9.2	0.0	-10.6
		6	16.7	17.1	0.0	-16.7
		7	46.2	43.3	0.0	-46.2
		8	21.4	19.2	0.0	-21.4
		9	35.8	33.8	0.0	-35.8
		10	15.2	14.8	0.0	-15.2
		11	10.9U	9.1	0.0	-10.9
		12	20.6	13.8	0.0	-20.6
		13	10.9U	7.1	0.0	10.9
		14	10.9U	10.7	0.0	10.9
		15	28.6	27.9	0.0	28.6
		16	18.6	18.5	0.0	18.6
	12	0	25.5	25.8	-25.5	0.0
		1	10.9U	11.6	-10.9	0.0
		2	30.6	26.4	-30.6	0.0
		3	10.9U	.7	-10.9	0.0
		4	10.9U	.5	-10.9	0.0
		5	10.9U	16.6	-10.9	0.0
		6	10.9U	8.0	10.9	0.0
		7	10.9U	1.4	10.9	0.0
		8	13.0	14.8	13.0	0.0
		9	14.7	15.4	14.7	0.0
		10	15.2	17.1	15.2	0.0
		11	16.7	18.6	16.7	0.0
		12	15.0	12.1	15.0	0.0
1	0	1	67.4	80.3	0.0	-67.4
		2	38.4	39.6	38.4	0.0
		3	54.3	60.9	0.0	54.3
		4	123.8	153.0	123.8	0.0
		5	244.2	260.0	0.0	244.2
		6	33.4	39.9	-33.4	0.0
		7	11.8	16.2	0.0	11.8
		8	52.4	55.3	52.4	0.0
		9	78.1	95.8	0.0	-78.1
		10	16.4	17.1	16.4	0.0
		11	80.8	97.0	0.0	-80.8
		12	24.9	28.3	24.9	0.0
		13	56.1	62.4	0.0	-56.1
		14	69.6	71.8	69.6	0.0
		15	47.1	48.4	0.0	-47.1
		16	19.2	20.9	-19.2	0.0
		17	30.4	33.6	0.0	30.4
		18	32.0	33.5	-32.0	0.0
		19	97.6	112.7	0.0	97.6
		20	32.6	36.6	-32.6	0.0
		21	37.9	45.6	0.0	37.9
		22	23.6	25.3	-23.6	0.0
		23	6.7U	.5	0.0	-6.7
		24	6.9U	15.1	6.9	0.0
		25	19.9	22.4	0.0	-19.9
		26	7.8U	3.0	-7.8	0.0
		27	24.0	25.9	0.0	-24.0
		28	12.4	10.7	12.4	0.0
		29	24.0	21.0	0.0	-24.0
		30	9.9	9.9	9.9	0.0
	1	0	201.3	200.2	0.0	201.3
		1	63.0	60.6	43.8	-45.2
		2	139.4	152.8	-138.6	14.2
		3	83.7	101.7	83.6	4.4
		4	88.6	102.7	-87.4	-14.5
		5	87.9	94.3	-70.6	-52.3
		6	77.1	87.0	-13.3	-75.9
		7	75.3	73.9	-73.0	18.5
		8	76.3	87.6	33.7	-68.4
		9	82.7	91.8	-71.2	42.1
		10	47.4	56.9	47.3	2.8
		11	66.9	71.8	-1.6	66.9
		12	96.2	102.7	93.6	-22.1
		13	14.1	9.5	13.2	-4.9
		14	45.6	47.4	32.1	32.3
		15	64.3	73.0	64.2	-3.8
		16	66.8	73.4	-47.5	47.0
		17	60.1	62.4	59.4	-9.0
		18	43.4	45.1	-40.7	14.9
		19	25.9	25.5	4.2	-25.5
		20	29.1	27.6	-24.4	15.9
		21	43.4	47.6	-42.0	-10.8
		22	36.3	36.1	-24.6	-26.7
		23	20.1	21.6	-20.0	-1.5
		24	19.8	17.4	-.5	-19.8
		25	25.2	24.5	-24.9	3.9
		26	25.4	26.6	25.2	-3.1
		27	8.6U	7.8	5.7	6.5
		28	23.2	21.5	23.0	3.1
		29	19.1	17.1	16.0	10.4
		30	13.3	16.3	6.3	11.7
	2	0	111.0	124.8	0.0	111.0
		1	60.7	70.4	-60.1	-8.6
		2	98.2	113.6	11.7	97.5
		3	96.8	98.2	19.6	94.8
		4	71.1	75.0	-56.0	43.7
		5	68.6	69.0	57.5	37.4
		6	153.1	160.6	-67.5	-137.4
		7	78.3	83.1	63.1	46.4
		8	138.0	142.8	-25.8	-135.5
		9	108.0	108.4	103.8	-29.8
		10	47.1	49.8	25.9	-39.3
		11	16.4	15.7	-1.4	-18.4
		12	42.4	40.6	19.4	37.7
		13	57.3	62.3	-57.2	4.0

H	K	L	FO	FC	AO	BO
1	2	14	79.3	78.1	34.2	71.5
		15	57.9	60.0	-57.7	4.9
		16	65.2	76.1	-12.9	63.9
		17	42.5	40.2	-40.4	13.2
		18	33.2	31.4	10.2	31.6
		19	14.6	9.9	-11.2	9.4
		20	17.4	18.9	-6.6	-16.1
		21	10.9U	7.9	2.8	-10.5
		22	46.2	46.0	6.2	-45.8
		23	26.3	21.6	24.9	-8.3
		24	38.3	39.5	1.4	-38.3
		25	22.1	20.6	20.1	-9.2
		26	13.8	11.4	-4.1	-13.2
		27	26.3	22.0	21.3	-15.5
	3	0	91.0	83.5	0.0	-91.0
		1	82.6	75.8	-76.6	-31.0
		2	120.4	119.3	-120.2	-6.8
		3	91.4	95.1	-47.5	-78.1
		4	153.1	163.1	-153.1	3.1
		5	70.3	71.3	36.4	-60.1
		6	79.0	74.9	-51.7	59.7
		7	84.0	88.1	67.0	-50.7
		8	65.8	58.0	-26.7	60.1
		9	39.8	42.6	33.0	22.2
		10	91.3	91.5	80.7	42.7
		11	41.2	43.3	4.1	41.0
		12	58.9	66.5	58.8	-3.3
		13	57.9	59.6	-40.1	41.8
		14	58.7	57.0	54.3	-22.2
		15	48.3	49.0	-31.2	36.9
		16	64.5	63.4	-28.2	-58.0
		17	25.4	22.8	-23.9	-8.5
		18	45.6	45.9	-41.3	-19.4
		19	23.5	19.5	.8	-23.5
		20	34.3	32.3	-34.1	-3.5
		21	31.8	30.8	16.1	-27.4
		22	10.9U	7.3	3.0	10.4
		23	30.2	30.1	30.1	1.8
		24	14.3	12.3	3.8	13.8
		25	16.3	18.3	9.4	13.3
		26	26.0	27.0	25.9	2.3
		27	8.8	9.4	8.7	.9
		28	21.3	21.3	20.0	7.4
		29	9.1	9.0	-8.1	4.1
		30	8.9U	3.8	-6.1	-6.4
	4	0	45.7	50.3	0.0	45.7
		1	76.9	77.0	-44.3	-62.8
		2	62.0	61.9	35.7	50.7
		3	75.5	77.7	17.5	-73.4
		4	56.6	60.3	56.4	4.7
		5	94.3	101.1	13.2	-93.4
		6	48.6	50.5	34.5	-34.2
		7	34.9	30.7	-17.5	-30.2
		8	37.5	42.5	-20.4	-31.5
		9	21.6	25.0	7.8	20.1
		10	34.6	34.2	-28.9	-19.0
		11	62.6	64.0	-3.7	62.5
		12	23.8	26.9	-21.5	10.2
		13	53.5	51.2	9.0	52.7
		14	47.3	43.4	-46.7	7.5
		15	33.2	28.2	-6.7	32.5
		16	13.5	13.5	-11.7	6.7
		17	36.9	36.0	26.1	-26.0
		18	14.3	14.0	12.4	7.1
		19	41.0	42.8	4.9	-40.7
		20	31.2	29.4	19.6	-24.3
		21	36.9	33.7	-12.1	-34.9
		22	26.3	23.2	25.7	-5.5
		23	8.8	7.6	-8.1	-3.4
		24	12.5U	6.2	12.4	-2.1
		25	9.9	9.8	-2.9	9.4
		26	13.0	10.1	-5.5	-11.8
		27	16.0	15.2	-2.7	15.8
		28	16.6	13.0	-14.8	7.6
		29	24.0	22.2	7.0	23.0
		30	11.6	9.9	-8.1	8.3
	5	0	25.4	24.5	0.0	-25.4
		1	129.6	138.3	-129.5	2.9
		2	49.9	48.8	0.0	-49.9
		3	65.5	66.5	-65.1	7.3
		4	48.0	41.0	29.4	-37.9
		5	82.6	75.6	4.7	82.5
		6	91.9	91.7	63.8	66.2
		7	132.5	136.3	128.8	30.9
		8	63.4	66.5	29.4	56.2
		9	114.5	119.6	111.9	-24.4
		10	17.4	16.3	-4.8	16.7
		11	43.6	41.8	17.8	-39.8
		12	25.4	19.5	-19.4	16.3
		13	40.0	38.9	-29.5	-27.0
		14	37.1	37.6	-19.7	-31.4
		15	52.9	53.0	-49.7	-18.0
		16	33.5	28.7	-4.3	-33.2
		17	44.3	48.1	-44.3	-1.4
		18	16.6	16.3	12.1	-11.3
		19	20.2	16.0	-16.3	11.9
		20	26.6	23.8	20.8	16.9
		21	38.8	39.5	38.1	7.4
		22	18.5	19.1	13.1	13.0
		23	44.9	43.5	44.9	0.0
		24	21.1	20.8	-19.0	9.1
		25	12.2	8.4	6.4	10.4
		26	11.0	11.7	-10.4	-3.8
		27	13.0	13.3	-13.0	.4
	6	0	118.1	131.8	0.0	-118.1
		1	62.2	64.3	46.3	-41.8
		2	58.4	56.8	-31.0	-49.5
		3	22.4	15.2	-18.7	-12.3
		4	35.2	36.9	34.0	-9.3
		5	17.4	20.2	-6.3	-16.2
		6	80.6	81.5	40.7	73.5
		7	28.3	27.3	-26.1	-10.9
		8	67.0	69.1	-7.5	67.4
		9	30.5	35.2	-16.4	25.7
		10	45.8	49.5	-16.2	42.8
		11	46.1	50.5	-20.2	41.4
		12	18.2	14.6	-17.9	-3.4
		13	24.6	23.9	-3.7	24.3
		14	33.5	32.5	-9.8	-32.0
		15	30.5	27.2	29.4	-8.2
		16	45.0	46.7	8.3	-44.2
		17	30.2	31.9	16.8	-25.3
		18	33.8	32.0	15.0	-30.3
		19	37.1	32.5	9.0	-36.0
		20	19.4	16.4	16.1	10.8
		21	20.8	20.1	0.0	-20.8
		22	19.6	18.2	-11.8	15.7
		23	15.4	15.7	-10.5	11.2
		24	21.1	19.5	-2.1	21.0
		25	28.8	23.8	-4.9	28.4
		26	16.6	16.8	-7.5	14.8
	7	0	22.6	21.4	0.0	22.6
		1	39.7	34.7	33.5	21.2
		2	53.6	61.1	52.8	9.2
		3	45.6	44.8	27.3	36.5
		4	69.0	77.3	68.2	10.7
		5	23.2	23.3	1.3	23.1
		6	55.8	56.6	54.8	-10.4
		7	18.0	19.2	-14.0	11.3
		8	32.1	28.7	6.7	-31.4
		9	36.0	33.1	-13.2	-33.5
		10	47.1	46.6	-39.9	-25.0
		11	26.8	24.7	-14.8	-22.4
		12	42.7	46.7	-42.2	-6.6
		13	20.8	21.1	-6.2	-19.8
		14	23.2	21.1	-22.0	7.4
		15	9.9	9.0	-5.3	-8.3
		16	12.7	10.1	1.1	12.6
		17	7.8U	10.3	5.6	5.4
		18	28.5	25.9	28.2	4.4
		19	10.3U	10.8	-2.2	10.1
		20	24.6	23.2	24.0	5.5
		21	12.2	13.1	-1.4	12.1
		22	10.8	4.2	9.1	5.8
		23	10.2	7.8	2.2	10.0
		24	10.8	7.7	-8.3	7.0
		25	13.0	14.0	-12.5	-3.6
		26	17.4	16.4	-13.5	11.0
		27	6.9U	4.2	-6.9	.9
		28	16.0	17.5	-16.0	-.9
		29	14.6	10.7	0.0	-14.6
	8	0	25.2	26.5	0.0	-25.2
		1	26.6	27.3	21.1	16.2
		2	22.9	22.4	-22.6	-3.9
		3	39.2	39.0	1.3	39.2
		4	39.9	40.6	-36.1	16.9
		5	51.2	56.2	-12.7	49.6
		6	41.9	44.1	-13.1	39.8
		7	16.8	17.3	2.1	16.7
		8	28.8	30.7	7.3	27.8
		9	35.2	32.9	-22.3	-27.2
		10	19.1	17.9	19.0	1.7
		11	36.0	34.5	-1.6	-36.0
		12	34.9	36.0	16.5	-30.7
		13	29.4	28.3	3.7	-29.2
		14	42.9	42.1	18.8	-38.6
		15	48.9	27.3	34.9	-34.2
		16	32.6	29.7	2.4	-32.5
		17	19.4	16.6	14.4	13.0
		18	9.7U	7.7	1.2	-9.7
		19	29.7	31.1	0.0	29.7
		20	21.6	16.5	-14.8	15.7
		21	17.1	17.9	-10.5	13.5
		22	30.2	28.0	-16.6	25.2
		23	14.3	13.8	-11.8	8.0
		24	13.3	12.7	-5.4	12.2
		25	8.8	9.9	-7.8	-4.1
	9	0	13.0	12.8	0.0	13.0
		1	53.7	55.7	53.0	-8.3
		2	23.8	27.2	10.3	21.5
		3	19.1	20.2	18.9	-2.7
		4	6.9U	3.6	-6.7	-1.9
		5	35.7	33.4	-32.7	-14.3
		6	24.3	24.9	.0	-24.3
		7	41.8	44.5	-39.8	-12.7
		8	38.5	41.2	-8.5	-37.5
		9	38.8	42.0	-38.5	4.6
		10	14.3	14.2	-6.6	-12.7
		11	10.2	6.9	0.0	-10.2
		12	9.9	10.7	-5.0	6.5

Table 4 (*cont.*)

H	K	L	FO	FC	AC	BO
1	9	13	30.5	27.7	16.1	25.9
		14	36.9	37.2	3.4	36.7
		15	36.9	37.6	32.1	18.2
		16	29.7	29.7	12.8	26.8
		17	15.7	14.0	15.0	4.6
		18	8.5U	5.8	-6.8	4.8
		19	8.9U	5.2	-4.0	8.0
		20	11.9	9.5	-7.4	-9.3
		21	19.9	16.6	-15.1	-12.9
		22	11.9	13.3	.7	-11.9
		23	10.2	13.0	-9.7	-3.1
		24	13.5	13.8	-9.4	-9.7
		25	10.8	12.5	-10.6	-1.8
		26	6.7U	8.4	1.4	-6.5
		27	9.6	5.3	1.5	-9.5
	10	0	27.1	26.0	0.0	-27.1
		1	12.4	14.1	-11.2	5.4
		2	24.9	27.7	-10.4	22.6
		3	27.1	24.4	10.9	24.8
		4	22.9	22.5	-11.2	20.0
		5	19.9	19.8	-.9	19.9
		6	16.0	15.9	-2.8	-15.8
		7	22.2	21.1	18.5	-12.2
		8	31.1	31.8	13.6	-28.0
		9	28.5	28.1	11.8	-25.9
		10	11.0	7.2	7.8	-7.7
		11	27.7	28.9	1.3	-27.7
		12	9.5U	8.5	-9.3	1.7
		13	24.0	23.3	7.8	-22.7
		14	9.9	8.8	-2.6	-9.6
		15	72.4	31.3	-72.4	0.0
		16	18.2	19.1	-4.8	17.5
		17	23.2	23.0	-9.7	21.1
		18	28.5	31.2	0.0	28.5
		19	27.4	27.4	-11.8	24.7
		20	8.9U	8.2	-6.6	-6.0
		21	11.9	11.8	2.4	11.7
		22	12.7	13.2	0.0	-12.7
		23	11.6	13.2	11.4	1.9
	11	0	7.8U	1.6	0.0	-7.8
		1	12.7	13.0	-8.7	-9.2
		2	19.6	19.7	-13.6	-14.1
		3	23.2	22.3	23.2	-.9
		4	35.5	40.5	-33.7	11.0
		5	8.5	5.6	6.6	-5.4
		6	21.6	22.7	-15.6	14.9
		7	18.5	19.4	-16.7	-7.9
		8	7.8U	11.9	-1.3	7.7
		9	14.3	17.5	.4	14.3
		10	21.6	18.9	21.2	-4.3
		11	7.2U	6.3	6.2	3.7
		12	21.1	24.0	19.1	-9.0
		13	9.4	12.0	-3.5	8.7
		14	16.3	19.9	16.2	-1.9
		15	9.9	9.8	-9.9	-.9
		16	7.8U	3.2	-6.7	-3.9
		17	10.0U	11.0	5.7	-8.2
		18	17.7	19.9	-17.1	-4.7
		19	8.9U	8.8	-.9	-8.8
		20	15.7	18.4	-15.3	-3.3
		21	10.8	13.9	-6.5	-8.6
	12	0	11.3	14.4	0.0	11.3
		1	15.2	19.3	-15.2	-1.1
		2	11.3	12.1	-3.5	10.7
		3	8.3U	10.0	-1.2	-8.2
		4	7.2U	4.5	2.6	-6.7
		5	13.8	14.3	0.0	-13.8
		6	18.0	22.3	-.7	-18.0
		7	11.0	13.6	8.9	-6.4
2	0	0	85.0	110.2	85.0	0.0
		1	105.4	117.7	0.0	105.4
		2	44.8	58.6	44.8	0.0
		3	76.2	89.5	0.0	76.2
		4	16.2	17.8	-16.2	0.0
		5	107.2	133.0	0.0	-107.2
		6	20.6	24.3	-20.6	0.0
		7	131.9	159.8	0.0	-131.9
		8	12.1	13.8	-12.1	0.0
		9	59.8	68.1	0.0	-59.8
		10	85.5	115.6	-85.5	0.0
		11	12.6	16.5	0.0	-12.6
		12	11.0	13.6	11.0	0.0
		13	60.4	75.8	0.0	60.4
		14	62.8	69.4	62.8	0.0
		15	40.3	49.1	0.0	40.3
		16	21.0	25.0	21.0	0.0
		17	53.8	68.6	0.0	53.8
		18	20.1	19.7	-20.1	0.0
		19	7.3U	3.6	0.0	-7.3
		20	23.6	25.0	-23.6	0.0
		21	25.5	31.1	0.0	-25.5
		22	8.2U	4.6	8.2	0.0
		23	25.4	23.4	0.0	-25.4
		24	23.8	24.7	-23.8	0.0
		25	20.4	23.8	0.0	-20.4
		26	9.4U	5.7	-9.4	0.0
		27	9.6U	5.5	0.0	9.6
		28	16.9	17.1	16.9	0.0
		29	15.2	17.0	0.0	15.2
		30	11.9	13.2	11.9	0.0
		31	13.3	16.3	0.0	13.3
	1	0	71.7	88.8	-71.7	0.0
		1	45.7	58.3	-40.5	21.2
		2	38.1	45.4	-16.8	34.2
		3	104.7	113.7	-104.6	-4.0
		4	93.7	105.3	-50.7	78.8
		5	92.6	107.4	-89.8	-22.6
		6	46.4	45.7	43.6	-16.0
		7	34.5	41.5	6.0	-34.0
		8	63.5	68.8	56.0	-30.0
		9	22.2	20.3	0.0	-22.2
		10	92.6	105.5	64.7	-66.2
		11	75.0	89.3	70.9	24.3
		12	54.3	64.7	26.1	-47.6
		13	49.2	53.1	48.5	8.3
		14	30.8	28.3	-30.7	1.8
		15	21.5	27.6	15.9	14.5
		16	32.4	38.8	-31.8	6.0
		17	30.9	31.5	-16.5	26.1
		18	34.0	37.2	-24.5	23.6
		19	34.0	33.0	-33.2	7.4
		20	24.1	28.3	-8.0	22.7
		21	31.2	35.8	-6.8	-30.5
		22	23.1	23.7	11.5	20.0
		23	26.8	27.2	-22.6	-14.4
		24	24.2	23.5	23.9	-3.8
		25	9.4U	2.0	7.2	-5.9
		26	24.8	23.9	-7.9	-23.5
		27	17.9	20.1	16.0	8.1
		28	10.7	7.2	-6.0	-8.9
		29	13.8	10.7	13.1	4.3
	2	0	86.9	77.6	86.9	0.0
		1	82.5	80.9	-81.8	-10.5
		2	83.0	85.7	31.9	-76.6
		3	91.9	99.4	-91.9	1.8
		4	93.2	105.8	10.3	-92.6
		5	63.1	64.9	-62.7	-6.6
		6	67.7	64.2	-40.2	-54.4
		7	41.5	42.1	-40.7	8.3
		8	23.2	23.6	-20.8	10.2
		9	35.4	30.1	12.5	-33.1
		10	87.4	93.7	-51.8	70.4
		11	61.1	68.9	60.4	8.9
		12	82.5	90.4	7.3	82.2
		13	48.6	55.9	48.5	2.2
		14	53.7	58.2	16.7	51.0
		15	19.2	17.8	2.4	19.0
		16	26.8	28.0	25.7	-7.7
		17	27.3	27.6	-15.2	22.7
		18	33.5	39.0	0.0	-33.5
		19	34.1	36.2	-34.0	2.5
		20	46.0	47.7	-9.2	-45.1
		21	14.0U	15.3	-12.6	-6.0
		22	36.2	35.1	-7.1	-35.5
		23	9.1U	8.8	4.9	-7.7
		24	10.5U	7.4	-2.2	10.3
		25	14.2U	17.8	11.9	-7.8
		26	22.0	26.3	7.2	20.8
		27	15.4	17.4	15.2	2.4
		28	19.2	16.6	-2.1	19.1
	3	0	82.4	72.0	-82.4	0.0
		1	75.6	58.4	30.7	69.1
		2	74.9	66.0	-70.9	-24.1
		3	80.2	75.8	79.5	-10.5
		4	71.6	67.5	5.7	-71.4
		5	76.8	79.1	58.3	-49.9
		6	77.2	79.6	68.6	-34.9
		7	59.7	66.3	24.8	-54.3
		8	88.2	96.9	86.3	-17.9
		9	54.7	60.2	6.9	-54.3
		10	74.7	77.8	60.3	44.0
		11	46.8	45.9	-46.3	-7.0
		12	48.7	49.2	-20.5	44.2
		13	78.6	85.0	-63.6	46.2
		14	54.3	59.4	-47.5	26.2
		15	56.5	61.1	-28.6	48.7
		16	59.0	63.4	-56.1	-18.2
		17	36.5	39.6	4.2	36.3
		18	41.5	43.6	-38.7	-14.9
		19	27.4	27.4	17.7	20.9
		20	23.4	23.6	10.9	-20.7
		21	38.4	38.5	26.1	-28.2
		22	28.5	27.1	26.1	4.6
		23	28.3	29.2	7.4	-27.3
		24	25.9	25.7	24.5	-8.4
		25	10.5U	9.5	1.3	-10.4
		26	21.2	21.6	13.2	16.5
		27	10.8U	9.5	-7.4	7.8
		28	9.4U	8.5	-3.3	8.8
		29	12.7	10.9	-3.0	12.3
	4	0	13.0	6.8	-13.0	0.0
		1	87.4	89.7	-30.7	-81.8
		2	65.7	60.1	-65.3	-8.5
		3	43.6	43.2	18.8	-39.3
		4	29.7	29.8	10.4	-27.8
		5	71.9	69.2	-47.8	53.6
		6	45.7	47.5	45.5	3.7
		7	96.9	108.2	-10.2	96.3
		8	39.7	41.3	37.3	13.5
		9	93.4	99.4	-4.6	93.2

H	K	L	FO	FC	AC	BO
2	4	10	32.2	35.7	25.1	20.2
		11	32.2	29.9	32.0	-3.1
		12	14.9	16.9	-3.7	14.4
		13	38.8	44.8	2.8	-38.7
		14	23.1	27.6	-22.7	-4.0
		15	66.9	80.3	-14.5	-65.3
		16	20.3	22.1	-20.3	1.1
		17	43.9	50.0	-2.9	-43.8
		18	28.3	30.0	-14.5	-24.3
		19	24.2	22.5	1.7	-24.1
		20	22.8	25.1	-.5	-22.8
		21	32.5	33.5	-3.4	32.3
		22	17.2	14.9	2.4	17.0
		23	37.6	41.9	7.4	36.9
		24	16.3	16.5	16.2	2.1
		25	16.6	18.2	7.5	14.8
		26	14.6	14.1	7.8	12.3
	5	0	95.7	89.9	95.7	0.0
		1	95.0	89.8	91.1	-26.9
		2	56.0	59.1	18.4	-52.9
		3	49.7	51.1	47.5	-14.6
		4	109.2	97.7	-53.2	-95.3
		5	44.1	35.0	-11.1	42.7
		6	40.8	35.7	-36.2	18.8
		7	14.9	15.0	6.2	-13.5
		8	38.0	40.8	-29.5	23.9
		9	29.7	33.3	-24.0	17.4
		10	42.7	49.4	-16.9	39.2
		11	51.4	56.4	-50.7	8.6
		12	49.6	52.9	-2.5	49.5
		13	45.9	48.5	-45.5	6.2
		14	32.7	36.6	21.0	25.0
		15	16.0	15.3	10.8	-11.8
		16	31.9	37.6	18.8	-25.8
		17	20.6	23.4	20.3	-3.4
		18	44.4	45.4	5.1	-44.1
		19	16.0	14.9	15.8	2.8
		20	30.6	35.5	27.9	-12.6
		21	22.8	23.4	22.8	0.0
		22	9.4U	7.6	9.3	.6
		23	24.8	23.4	18.9	-16.1
		24	13.0	15.1	-12.7	2.4
		25	9.1U	9.8	-5.5	7.2
		26	22.3	23.5	-12.8	18.2
		27	16.9	13.6	-16.7	2.8
		28	9.4U	8.8	-4.9	8.0
		29	13.3	13.6	-13.3	0.0
	6	0	38.5	41.8	-38.5	0.0
		1	60.5	61.5	0.0	-60.5
		2	48.2	45.7	-38.7	28.7
		3	33.6	29.4	31.1	12.6
		4	43.6	44.4	-2.3	43.5
		5	24.5	23.1	24.5	-.6
		6	57.6	55.5	38.9	42.4
		7	18.9	21.0	-1.8	18.8
		8	13.8	13.2	11.6	-7.5
		9	32.5	30.8	-15.6	28.5
		10	53.0	56.5	17.1	-50.2
		11	41.1	43.4	-41.0	-1.9
		12	49.9	55.5	0.0	-49.9
		13	16.6	17.4	-15.7	-5.4
		14	27.7	32.8	-12.0	-25.0
		15	13.8	13.3	.6	-13.8
		16	24.8	23.3	-23.4	8.3
		17	11.6U	11.0	-.9	11.6
		18	29.1	37.6	8.5	27.8
		19	18.6	22.9	17.7	-5.6
		20	40.4	43.9	16.3	36.9
		21	15.4	15.5	15.1	-3.2
		22	10.2U	9.1	-.6	10.2
		23	12.2	10.2	-.7	12.2
		24	11.3U	9.1	7.4	-8.5
		25	13.8	13.8	-13.5	3.0
		26	14.0	15.3	-2.2	-13.8
	7	0	64.8	65.4	64.8	0.0
		1	31.3	34.0	-1.2	-31.3
		2	38.5	40.5	38.4	-2.9
		3	17.5	14.5	1.0	-17.5
		4	22.8	24.8	-9.5	-20.7
		5	21.2	21.4	-10.1	18.6
		6	52.1	51.7	-52.1	-1.3
		7	32.2	31.1	2.4	32.1
		8	53.3	62.0	-51.9	12.1
		9	35.4	36.3	-2.6	35.3
		10	32.7	32.8	-30.3	12.3
		11	18.6	20.7	16.4	8.7
		12	18.6	18.4	15.1	-10.8
		13	31.9	33.6	14.3	-28.5
		14	32.2	37.6	32.2	.8
		15	27.4	31.7	15.9	-22.3
		16	37.9	39.9	37.9	.9
		17	14.6	17.1	9.2	-11.4
		18	29.1	31.8	27.8	-8.5
		19	13.5	14.3	-13.1	-3.1
		20	12.2	12.7	-11.5	-4.2
		21	12.2	13.8	-5.8	10.7
		22	22.3	24.8	-21.9	-4.3
		23	19.7	17.8	-15.8	11.8
		24	15.4	15.7	-15.4	0.0
		25	14.3	14.8	-5.3	13.3
	8	0	39.0	37.8	39.0	0.0
		1	42.5	45.8	18.4	38.3
		2	25.1	26.2	4.8	24.6
		3	40.4	37.6	36.9	16.5
		4	40.0	42.0	-7.3	39.3
		5	43.2	41.0	38.5	-19.6
		6	40.7	37.4	-26.1	31.2
		7	47.1	48.5	17.1	-43.9
		8	18.1	18.2	-6.0	17.1
		9	47.3	48.9	-12.9	-45.5
		10	22.1	29.2	-13.6	-17.4
		11	35.4	32.4	-35.2	-3.6
		12	15.4	12.7	-1.0	-15.4
		13	26.3	27.3	-19.1	18.1
		14	17.5	18.4	8.7	-15.2
		15	22.3	23.1	1.8	22.2
		16	14.3	15.0	10.4	9.6
		17	28.0	32.0	11.5	25.5
		18	15.7	15.7	15.3	3.3
		19	15.4U	22.2	13.3	7.7
		20	11.2	14.4	6.9	8.8
		21	11.0U	13.9	9.5	-5.6
		22	7.9U	7.7	-8.5	-5.0
		23	11.6U	16.2	-2.9	-11.2
		24	9.9U	13.5	-7.5	-6.5
		25	15.4	18.3	-10.5	-11.3
	9	0	13.5	13.8	-13.5	0.0
		1	16.9	17.8	-14.9	-8.0
		2	22.6	22.0	-12.1	19.3
		3	31.6	37.9	-31.3	4.6
		4	32.5	33.9	7.0	31.7
		5	19.5	19.5	-19.5	0.0
		6	21.5	22.1	9.8	19.1
		7	19.5	20.9	-19.3	2.3
		8	8.2U	4.5	8.2	-.5
		9	8.5U	4.7	8.0	3.1
		10	29.1	32.5	22.3	-18.7
		11	26.8	32.8	26.0	-6.7
		12	27.4	29.4	1.4	-27.4
		13	29.1	34.4	29.0	1.6
		14	8.8U	11.5	-3.1	-8.2
		15	11.0U	17.8	8.4	-7.2
		16	14.6	13.7	-10.1	10.5
		17	12.8U	14.6	-12.4	3.3
		18	26.8	27.6	-12.9	23.5
		19	17.2	19.9	-16.8	3.8
		20	15.2	16.2	-1.9	15.1
		21	16.0	20.4	-13.6	8.5
	10	0	28.0	30.6	28.0	0.0
		1	23.4	29.4	-12.2	20.0
		2	26.8	30.2	17.5	-20.3
		3	22.1	24.4	-13.4	17.6
		4	43.9	50.1	-6.7	-43.4
		5	12.8U	10.9	3.5	-12.3
		6	22.1	25.1	-20.3	-8.7
		7	18.6	18.9	5.1	-17.9
		8	14.3	15.0	-14.2	1.2
		9	22.8	26.5	-17.0	-15.3
		10	25.1	27.2	-5.6	24.4
		11	18.9	22.1	18.6	-2.0
		12	21.2	25.2	6.3	20.2
		13	10.2U	13.2	9.5	3.8
		14	11.5	12.1	8.7	7.5
	11	0	20.0	23.1	-20.0	0.0
		1	10.9	12.3	-.4	10.9
		2	21.2	25.3	-20.3	6.1
		3	8.8U	6.3	-6.9	5.5
		4	8.8U	6.3	6.4	6.0
		5	8.8U	8.7	-4.8	-7.4
		6	19.5	24.2	19.5	0.0
		7	18.1	19.9	16.3	-7.9
		8	17.2	20.7	15.0	8.3
		9	16.3	17.1	4.5	-15.7
		10	12.8U	13.8	12.4	-3.1
		11	8.8U	1.7	8.3	3.0
		12	8.8U	13.4	-5.1	-7.2
		13	19.2	19.6	-5.2	18.5
		14	10.4	13.7	-10.3	-1.4
		15	10.4	11.0	-9.4	4.5
		16	13.8	16.7	-8.0	11.2
	12	0	8.8U	.5	-8.8	0.0
		1	17.2	18.0	-12.5	-11.8
		2	8.8U	9.7	6.5	-5.9
		3	16.6	17.2	-16.5	-1.8
		4	11.5	13.6	-1.7	-11.4
		5	10.9	11.5	-10.9	0.0
		6	10.9	11.8	-6.0	-9.1
		7	13.0	13.2	-6.1	11.5
		8	9.4U	8.0	-8.6	-3.6
		9	11.9	16.5	1.1	11.8
		10	10.4	7.2	9.2	4.0
		11	13.5	16.8	10.8	8.0
		12	13.0	14.1	6.9	11.0
3	0	1	10.8	10.2	0.0	-10.8
		2	57.2	83.3	-57.2	0.0
		3	9.9	9.9	0.0	9.9
		4	68.0	94.6	-68.0	0.0
		5	22.8	22.1	0.0	22.8
		6	53.5	63.6	-53.5	0.0
		7	6.6U	3.6	0.0	-6.6

H	K	L	FO	FC	AO	BO
3	0	8	21.6	20.3	-21.6	0.0
		9	95.2	115.4	0.0	-95.2
		10	97.4	121.2	97.4	0.0
		11	19.2	14.9	0.0	-19.2
		12	79.9	93.3	79.9	0.0
		13	9.4U	6.5	0.0	9.4
		14	38.4	42.5	38.4	0.0
		15	9.9U	16.2	0.0	9.9
		16	6.8U	3.8	-6.8	0.0
		17	23.1	26.1	0.0	23.1
		18	33.9	39.7	-33.9	0.0
		19	19.9	22.8	0.0	19.9
		20	61.6	74.6	-61.6	0.0
		21	11.5U	14.0	0.0	11.5
		22	27.8	30.6	-27.8	0.0
		23	29.0	31.1	0.0	-29.0
		24	8.9U	11.0	8.9	0.0
		25	20.8	22.4	0.0	-20.8
		26	28.3	32.1	28.3	0.0
	1	0	71.6	87.2	0.0	71.6
		1	39.0	48.3	1.1	-39.0
		2	55.9	65.0	14.0	54.1
		3	81.6	94.5	-10.2	-80.9
		4	14.8	11.9	12.9	7.3
		5	90.9	103.3	3.2	-90.8
		6	25.4	31.9	20.4	-15.2
		7	17.4	14.9	-15.3	-8.4
		8	84.6	93.8	-15.7	-83.1
		9	46.4	49.9	1.9	46.3
		10	64.1	71.9	-4.0	-64.0
		11	55.0U	59.0	9.3	54.2
		12	15.2	15.5	3.5	14.8
		13	45.2	49.7	-13.8	43.0
		14	45.0	48.5	9.1	44.1
		15	26.7	28.1	17.8	19.9
		16	42.3	45.0	-7.7	41.6
		17	22.9	19.6	-16.8	-15.5
		18	20.9	24.2	4.2	20.5
		19	38.4	49.7	2.9	-38.3
		20	15.9	12.4	3.8	-15.4
		21	16.7	14.2	4.8	-16.0
		22	29.0	34.3	14.0	-25.4
		23	11.3U	14.0	9.8	-5.7
		24	21.6	20.9	0.0	-21.6
	2	0	15.5	11.8	0.0	-15.5
		1	95.9	98.4	-95.9	2.0
		2	25.6	20.5	-23.0	-11.2
		3	37.0	36.3	-29.7	22.1
		4	47.5	42.8	-33.1	-34.1
		5	86.8	91.4	77.6	38.9
		6	27.0	29.7	15.0	-22.5
		7	76.0	85.8	73.8	18.1
		8	16.1	15.1	13.6	-8.7
		9	66.4	64.9	66.3	-3.5
		10	31.9	30.8	22.4	22.7
		11	10.8U	9.2	10.7	-.9
		12	24.0	25.1	-13.9	19.5
		13	40.0	41.1	-30.8	-25.4
		14	23.6	21.8	6.0	23.1
		15	75.6	79.5	-75.1	-8.3
		16	13.8U	9.6	-9.2	10.3
		17	47.1	48.7	-46.8	5.6
		18	11.4U	5.7	3.6	10.8
		19	14.8U	17.7	-7.2	12.9
		20	22.9	15.8	-18.1	-14.0
		21	33.9	35.5	32.9	8.0
		22	12.1U	9.9	-3.8	-11.5
		23	20.2	21.1	19.9	-3.4
		24	11.4U	10.5	11.3	-1.7
		25	31.2	29.9	30.6	-6.0
		26	14.2U	1.9	13.8	-3.4
		27	14.2U	8.9	5.6	-13.1
	3	0	38.0	32.0	0.0	-38.0
		1	26.5	23.4	-6.4	-25.7
		2	40.4	35.0	-17.4	-36.5
		3	74.9	75.1	2.0	-74.9
		4	34.5	33.5	-33.6	7.8
		5	102.1	103.5	-10.7	-101.5
		6	53.3	50.4	-37.7	37.7
		7	32.5	27.4	6.8	-31.8
		8	51.3	52.0	10.4	48.2
		9	42.0	40.7	21.7	36.0
		10	42.3	37.9	33.8	25.5
		11	50.7	53.7	6.2	50.3
		12	29.9	23.7	22.4	-19.8
		13	53.5	49.7	6.6	53.1
		14	23.3	20.8	16.7	-16.2
		15	7.7U	3.6	4.7	6.0
		16	23.6	22.1	-11.0	-20.9
		17	34.8	30.7	-3.1	-34.7
		18	32.5	28.5	-18.0	-28.8
		19	38.0	34.4	-8.2	-37.1
		20	8.6U	4.3	-8.5	-1.2
		21	22.7	23.7	-4.9	-22.2
		22	8.9U	5.8	8.0	3.9
		23	9.2U	2.7	2.8	8.8
		24	14.1	15.9	6.7	12.4
		25	16.5	16.1	-9.3	13.6
		26	14.1	12.2	.9	14.1
		27	21.7	22.6	-9.4	19.6
		28	8.9U	2.9	-5.4	-7.1
		29	8.6U	12.0	1.1	8.5
	4	0	45.6	39.1	0.0	45.6
		1	54.8	51.9	-53.4	-12.2
		2	67.5	64.1	65.9	14.8
		3	6.3U	4.6	6.2	.6
		4	107.3	105.2	107.3	-2.6
		5	20.5	19.4	20.5	0.0
		6	41.7	40.8	39.6	-12.9
		7	43.8	41.6	39.6	18.8
		8	19.1	17.2	14.7	-12.2
		9	31.3	29.2	16.7	26.5
		10	68.9	70.5	-68.3	8.8
		11	33.6	31.2	15.5	29.8
		12	64.9	71.3	-64.8	2.3
		13	21.7	20.1	-20.9	5.7
		14	25.4	28.2	-25.4	0.0
		15	40.5	35.4	-39.0	-10.9
		16	20.5	15.1	17.6	10.4
		17	24.1	23.8	8.3	-22.6
		18	48.4	46.9	45.9	-15.4
		19	22.7	21.5	-4.5	-22.2
		20	35.6	37.6	35.5	-1.8
		21	8.9U	6.3	-8.5	-2.5
		22	14.1	13.4	12.3	-6.8
		23	17.0	16.8	14.7	8.5
		24	9.2U	8.0	1.5	-9.0
		25	14.1	14.4	9.4	10.5
		26	20.5	24.1	-20.2	3.2
	5	0	60.1	58.9	0.0	-60.1
		1	31.9	23.9	6.6	-31.2
		2	73.7	67.6	-12.8	-72.6
		3	37.7	37.2	-12.6	35.5
		4	34.2	27.3	6.8	-33.5
		5	41.2	39.2	7.7	40.5
		6	76.7	79.6	-2.0	76.7
		7	12.8	13.8	7.8	10.1
		8	59.6	59.7	-10.0	58.7
		9	17.3	13.8	2.7	-17.1
		10	52.7	49.7	3.3	52.6
		11	26.6	27.0	-6.2	-27.3
		12	31.9	26.3	28.6	-14.1
		13	19.1	17.4	-8.6	-17.0
		14	30.2	26.4	16.5	-25.3
		15	37.0	34.3	14.1	-34.2
		16	57.8	56.7	-21.4	-53.7
		17	9.5U	4.8	-3.6	-8.8
		18	44.8U	45.8	-21.7	-39.2
		19	39.3U	41.5	0.0	39.3
		20	31.6U	26.4	-1.2	31.6
		21	14.6U	16.6	4.5	13.9
		22	24.3U	27.1	0.0	24.3
		23	16.1U	2.3	10.5	-12.2
		24	24.3U	24.3	2.4	24.2
	6	0	21.2U	16.4	0.0	21.2
		1	72.1U	66.3	72.0	-3.0
		2	28.5U	27.8	3.5	28.2
		3	42.8U	38.8	41.1	-12.0
		4	62.6U	54.7	61.6	11.2
		5	58.0U	48.5	-46.2	-35.1
		6	22.4U	22.9	21.6	-5.7
		7	52.5U	51.6	-52.3	4.2
		8	22.7U	18.4	-15.4	-16.6
		9	49.1U	47.4	-49.0	-3.0
		10	28.5U	26.7	-28.0	-5.0
		11	39.3U	36.3	-35.9	16.0
		12	28.7U	26.5	-26.7	-10.7
		13	31.6U	32.7	31.3	-4.8
		14	25.6U	23.1	-13.9	-21.4
		15	42.8U	40.1	42.6	4.1
		16	22.4	22.9	-16.1	-15.5
		17	26.5	30.1	25.8	5.9
		18	42.7	40.4	39.5	16.1
		19	13.8U	11.7	-1.1	-13.7
		20	28.0	27.7	24.5	13.5
		21	12.6U	9.6	-11.4	-5.4
		22	10.3U	3.1	-6.6	7.9
		23	13.1	16.3	-13.0	1.4
		24	11.4U	13.5	-11.3	-1.4
		25	21.4	26.1	-21.4	0.0
	7	0	36.8	31.2	0.0	36.8
		1	41.7	39.9	-33.9	24.2
		2	24.1	18.8	16.9	17.2
		3	50.6	49.7	-7.6	50.0
		4	27.0	20.9	25.2	9.8
		5	75.6	78.4	15.8	73.9
		6	33.9	30.5	25.1	-22.8
		7	23.6	21.0	23.5	-1.8
		8	30.5	27.3	-14.3	-26.9
		9	39.9	33.9	24.0	-31.9
		10	15.6	14.6	-14.0	-6.9
		11	49.9	53.5	10.7	-48.7
		12	11.8U	11.6	-2.1	-11.6
		13	40.1	41.7	-24.5	-31.7
		14	8.6U	8.9	0.0	8.6
		15	14.3U	15.9	-14.0	-3.1
		16	10.0U	8.4	-4.8	8.6
		18	15.9	17.2	3.2	15.6
		19	26.8	28.4	4.5	26.4
		20	10.6U	11.2	-1.3	10.5

Table 4 (*cont.*)

H	K	L	FO	FC	AO	BO
3	7	21	15.6	18.9	6.7	14.1
	8	0	38.5	34.7	0.0	-38.5
		1	25.4	29.5	25.4	-.5
		2	37.7	34.8	-36.1	-10.8
		3	9.8U	12.6	9.3	-1.8
		4	44.3	43.8	-44.0	-4.9
		5	17.9	19.2	-17.5	3.7
		6	37.7	35.9	-27.8	25.4
		7	25.4	26.5	-22.4	-11.9
		8	17.9	15.5	2.5	17.7
		9	24.8	22.9	-18.5	-16.5
		10	26.2	25.1	19.7	17.2
		11	9.7U	7.6	-8.3	-5.1
		12	43.0	43.2	42.0	-9.2
		13	12.9U	13.4	12.4	-3.5
		14	23.9	24.0	19.6	-13.6
		15	24.8	23.7	24.8	0.0
		16	22.0	18.0	-11.6	-18.7
		17	10.3U	7.7	8.2	6.2
		18	23.0	22.6	-22.8	-2.8
		19	9.2U	10.5	-8.5	3.5
		20	15.6	19.9	-14.4	5.9
	9	0	45.7	48.9	0.0	45.7
		1	10.0U	2.2	2.1	9.8
		2	23.6	31.1	6.8	22.6
		3	8.6U	1.8	8.0	3.2
		4	22.0	20.0	19.6	-10.0
		5	8.6U	4.7	7.7	-3.9
		6	41.9	40.5	0.0	-41.9
		7	10.3U	9.1	1.8	-10.1
		8	26.2	32.7	1.8	-26.1
		9	8.9U	7.4	2.2	-8.6
		10	15.9	15.9	-3.1	-15.6
		11	8.9U	12.6	-8.8	1.1
		12	12.1U	11.7	-8.0	9.1
		13	8.6U	4.7	-6.7	5.4
		14	16.1U	17.1	7.3	14.4
		15	8.6U	6.7	2.1	8.4
		16	21.7	24.0	-1.5	21.6
		17	8.6U	7.8	4.6	7.3
		18	17.9	19.6	6.3	16.7
	10	0	8.9U	9.6	0.0	-8.9
		1	11.7	12.9	-11.0	4.0
		2	21.1	22.8	-18.1	-10.9
		3	17.9	18.3	-16.7	8.5
		4	23.3	24.0	-21.8	8.3
		5	14.1	15.7	2.2	13.9
		6	17.0	19.9	-16.7	-3.4
		7	15.1	15.2	14.8	2.7
		8	8.6U	8.2	-4.8	-7.2
		9	26.5	30.8	24.4	-10.2
		10	26.2	31.1	21.8	14.6
		11	11.8U	14.0	7.4	-9.2
		12	16.5	19.5	16.5	0.0
	11	0	9.2U	8.3	0.0	9.2
		1	16.5	19.3	14.4	-8.0
		2	9.2U	7.7	-2.7	-8.8
		3	19.9	26.4	7.6	-18.4
		4	8.6U	6.1	-3.2	-8.0
		5	22.4	25.6	-.6	-22.4
		6	8.6U	7.0	-3.7	7.8
		7	20.8	21.4	-17.2	-11.1
		8	8.6U	8.9	8.3	-2.3
		9	15.3	14.9	-10.6	11.0
		10	10.0U	1.9	6.1	-8.0
		11	19.4	22.8	4.4	18.9
		12	8.2U	11.6	-5.5	6.1
		13	17.6	20.0	1.7	17.5
4	0	0	10.5	9.6	-10.5	0.0
		1	71.3	90.9	0.0	71.3
		2	18.9	20.8	-18.9	0.0
		3	30.8	37.2	0.0	30.8
		4	8.2U	10.2	-8.2	0.0
		5	28.3	30.8	0.0	-28.3
		6	18.3	19.8	18.3	0.0
		7	60.7	73.2	0.0	-60.7
		8	35.5	42.0	35.5	0.0
		9	39.5	50.9	0.0	-39.5
		10	8.0U	6.1	8.0	0.0
		11	9.1U	18.9	0.0	-9.1
		12	10.5U	12.5	-10.5	0.0
		13	10.5U	11.6	0.0	10.5
		14	10.8U	17.4	-10.8	0.0
		15	34.4U	54.2	0.0	34.4
		16	15.3	14.7	-15.3	0.0
		17	15.6	20.1	0.0	15.6
		18	10.8	12.7	-10.8	0.0
		19	5.4U	1.0	0.0	5.4
		20	5.4U	8.9	-5.4	0.0
		21	5.7U	7.6	0.0	-5.7
		22	5.7U	1.0	-5.7	0.0
		23	14.5	14.5	0.0	-14.5
		24	16.7	16.8	16.7	0.0
		25	13.4	22.8	0.0	-13.4
		26	13.6	14.7	13.6	0.0
		27	12.8	13.3	0.0	-12.8
		28	13.1	12.1	13.1	0.0
	1	0	69.2	78.0	-69.2	0.0
		1	38.7	41.4	-37.6	-9.2
		2	47.1	54.3	-44.7	-14.7
		3	65.0	65.7	-64.9	3.2
		4	39.2	40.2	0.0	-39.2
		5	69.1	73.8	-69.1	1.5
		6	47.1	49.8	42.9	-19.3
		7	8.1U	12.5	-7.7	-2.4
		8	47.8	49.9	47.8	0.0
		9	31.1	32.6	30.7	4.7
		10	37.0	39.8	33.7	15.3
		11	41.9	48.5	38.1	17.3
		12	8.3U	5.3	-5.9	5.9
		13	40.1	43.1	40.0	-3.2
		14	40.6	44.1	-35.6	19.4
		15	10.8	7.3	0.0	-10.8
		16	22.3	24.8	-22.2	2.5
		17	38.2	42.4	-32.5	-20.1
		18	11.0U	17.0	-10.8	-2.3
		19	32.6	36.6	-31.9	-6.8
		20	13.1	11.6	5.2	-12.0
		21	22.2	24.4	-15.6	15.8
		22	26.4	28.9	25.0	-9.5
		23	6.8U	3.5	4.5	5.1
		24	20.1	27.1	20.1	-.9
		25	22.2	25.4	20.2	9.3
		26	6.0U	7.7	2.9	7.4
		27	18.1	20.3	17.2	5.5
		28	9.5U	8.9	-3.2	8.9
	2	0	34.2	28.3	34.2	0.0
		1	11.0U	11.1	9.6	-5.1
		2	57.0	49.1	-3.2	-56.9
		3	40.2	31.8	38.4	-11.8
		4	79.3	77.9	-6.9	-78.7
		5	34.5	33.6	31.9	-13.3
		6	56.7	49.3	-15.2	-54.6
		7	27.4	23.1	25.2	-10.6
		8	11.5U	12.2	-5.8	-9.9
4	2	9	10.3U	12.3	-9.2	4.6
		10	43.9	46.4	-2.6	43.8
		11	28.0	29.9	-26.6	8.6
		12	52.9	54.0	17.8	49.8
		13	30.5	27.8	-25.0	17.4
		14	31.0	32.3	4.6	30.6
		15	14.8U	17.0	-13.7	5.6
		16	23.6	23.2	-7.3	-22.4
		17	10.3U	8.4	-10.0	2.5
		18	30.6	29.9	3.6	-30.4
		19	30.5	31.0	27.2	-8.8
		20	32.5	35.4	-3.2	-32.3
		21	18.2	19.7	18.2	0.0
		22	8.6U	5.7	-3.5	-7.9
		23	9.5U	6.4	4.7	8.2
		24	15.6	17.1	-2.9	15.3
		25	8.6U	8.4	8.6	.3
		26	15.3	18.8	1.3	15.2
		27	9.1	7.8	-8.8	-2.1
	3	0	94.7	68.3	-94.7	0.0
		1	51.5	40.1	13.7	-49.6
		2	45.2	34.2	-45.2	-1.6
		3	42.9	37.3	41.0	-12.5
		4	23.3	15.8	10.4	20.8
		5	22.7	15.8	22.7	-1.4
		6	51.5	49.7	48.8	16.4
		7	23.6	21.4	15.9	17.4
		8	48.7	50.4	46.8	13.3
		9	39.5	38.9	-30.3	25.3
		10	33.0	29.1	19.4	-26.7
		11	24.5	24.5	-20.6	13.2
		12	28.8	27.3	-18.2	-22.3
		13	25.4	23.4	-20.5	15.0
		14	29.4	29.4	-29.4	-1.6
		15	13.4	11.7	13.3	-1.9
		16	29.4	31.0	-29.4	0.0
		17	19.1	20.0	19.0	-2.2
		18	16.7	15.4	-11.5	12.1
		19	21.7	19.8	12.6	-17.7
		20	16.2	16.5	8.4	13.9
		21	11.4	14.1	11.4	.5
		22	25.6	26.5	23.3	10.6
		23	8.9U	3.6	-2.2	8.6
		24	18.8	22.7	18.8	0.0
		25	9.2U	12.0	-8.6	3.1
	4	0	48.7	38.0	48.7	0.0
		1	58.6	53.7	6.3	-58.2
		2	52.8	45.2	52.5	-5.4
		3	43.2	38.3	-33.8	-26.9
		4	27.4	22.2	-2.3	-27.3
		5	20.2	17.4	-5.3	19.5
		6	44.9	40.0	-26.1	-36.5
		7	42.7	40.7	11.3	41.2
		8	23.0	25.1	-21.9	6.9
		9	46.5	49.2	-6.5	46.0
		10	53.0	56.3	-42.3	31.9
		11	5.7U	3.3	4.8	3.1
		12	36.9	31.6	-9.5	35.6
		13	15.0U	9.9	-14.4	-4.1
		14	26.8	22.8	15.7	21.7
		15	30.0	33.7	8.1	-28.9
		16	28.8	29.1	28.5	4.0
		17	11.7	15.6	5.2	-10.5
		18	34.0	33.6	14.8	-30.6
		19	12.8	14.2	-5.0	-11.4
		20	17.0	16.6	-2.4	-16.8
		21	16.7	17.3	4.7	16.0
		22	8.3U	3.7	-3.7	-7.4
		23	16.2	20.2	0.0	16.2
		24	13.4	14.7	-12.2	5.5
		25	11.4	9.6	-5.3	10.1
	5	0	28.5	20.7	28.5	0.0
		1	64.6	59.1	61.8	18.9
		2	23.9	16.6	9.3	-22.0
		3	89.0	80.5	83.1	31.8
		4	49.2	48.3	-21.8	44.1
		5	54.7	49.3	49.2	-23.9
		6	19.4	20.6	11.0	16.0
		7	24.8	21.7	11.5	-22.0
		8	12.8	10.3	-12.7	-1.6
		9	30.6	30.4	-23.0	-20.1
		10	21.1	20.2	-20.5	5.0
		11	62.0	67.1	-61.6	6.9
		12	5.2U	4.7	-5.1	.9
		13	46.7	50.6	-45.1	11.9
		14	29.1	34.1	26.7	4.5
		15	10.9U	9.1	9.4	-5.4
		16	33.0	32.5	11.9	-30.7
		17	33.7	35.5	29.7	15.8
		18	12.8	8.7	-12.5	2.8
		19	23.3	27.4	23.0	3.9
		20	5.7U	3.6	4.7	3.2
		21	19.1	21.7	16.7	-9.2
		22	5.7U	3.2	-5.6	1.1
		23	5.7U	6.0	4.8	-3.1
		24	5.7U	7.9	-4.8	3.0
		25	14.8	15.2	-13.2	-6.7
		26	5.4U	4.9	-5.2	-1.7
		27	13.4	17.5	-12.6	-4.6
	6	0	28.5	26.8	-28.5	0.0
		1	50.3	47.4	-20.4	-46.0
		2	45.7	44.4	0.0	45.7
		3	31.3	31.9	-30.9	5.2
		4	55.4	53.7	-5.1	55.2
		5	38.9	37.1	-30.4	24.3
		6	45.7	47.2	-15.8	42.9
		7	26.8	25.9	-11.6	24.1
		8	27.1	23.8	26.7	-4.4
		9	29.1	30.2	-15.3	24.8
		10	34.5	37.5	3.0	-34.4
		11	24.8	24.3	23.7	7.4
		12	20.9	22.2	11.3	-17.6
		13	34.0	39.1	18.5	-26.5
		14	16.2	21.4	-6.6	-14.8
		15	24.5	26.0	11.1	-21.8
		16	5.7U	3.1	4.5	-3.5
		17	5.7U	3.1	2.6	-5.1
		18	11.8U	11.9	6.6	9.6
		19	14.1	13.6	-13.5	3.9
		20	20.9	27.0	-5.2	20.2
		21	9.9	9.1	-5.1	8.5
		22	11.1	15.1	6.0	9.4
		23	13.4	13.4	-8.4	10.5
	7	0	52.4	49.1	52.4	0.0
		1	16.5	16.3	-3.7	16.1
		2	21.7	18.8	14.8	-15.8
		3	14.5	14.1	-9.9	10.6
		4	17.0	14.4	4.0	-16.5
		5	13.4	14.6	-13.0	3.2
		6	36.6	38.7	-24.6	-27.1
		7	14.1	15.9	-5.5	-13.0
		8	40.5	42.7	-39.9	7.0
		9	23.9	24.5	8.2	-22.4
		10	25.4	27.5	-23.7	9.0
		11	16.5	15.9	8.9	-13.9
4	7	12	20.2	17.4	13.2	15.3
		13	16.2	17.3	10.9	12.0
		14	29.7	33.5	29.1	5.9
		15	5.7U	7.0	4.8	3.1
		16	30.0	35.0	29.7	-4.4
		17	12.3	11.0	-6.5	10.4
		18	11.7	9.9	11.3	-3.0
		19	9.4	8.4	-9.3	1.6
		20	13.8	14.3	-8.6	-10.8
		21	7.6	6.0	-7.4	1.6
		22	18.0	20.8	-17.9	-2.0
		23	8.5	8.6	-4.4	-7.2
		24	12.3	16.0	-12.1	2.3
	8	0	24.8	29.2	-24.8	0.0
		1	27.4	20.0	4.8	27.0
		2	29.7	29.0	-20.9	21.1
		3	14.8	14.1	12.2	8.3
		4	29.7	27.0	-3.6	29.5
		5	9.7U	11.3	9.6	-1.6
		6	26.5	26.3	22.8	13.5
		7	15.1	16.1	7.1	-13.3
		8	11.1	12.0	10.7	-2.9
		9	13.1	12.5	6.6	-11.3
		10	25.9	24.0	11.9	-23.0
		11	9.4	9.8	4.3	-8.3
		12	15.9	16.6	11.6	-10.9
		13	11.7	9.1	-11.4	2.6
		14	8.5	7.8	-6.4	-5.6
		15	10.8	9.0	-2.5	10.5
		16	12.3	14.2	-11.2	5.1
		17	9.9	13.3	.8	9.9
		18	8.8	14.5	-6.3	6.2
		19	6.0U	4.6	-6.0	0.0
		20	13.6	13.6	0.0	13.6
	9	0	6.0U	3.5	-6.0	0.0
		1	18.2	22.4	-15.2	-10.0
		2	7.7U	9.2	7.3	2.3
		3	30.0	32.7	-28.2	-10.2
		4	14.1	17.7	-1.3	-14.0
		5	30.0	34.1	-29.7	4.0
		6	7.4U	12.9	-4.0	-6.2
		7	14.8	17.3	-3.0	14.5
		8	9.1	9.3	-9.1	0.0
		9	19.1	19.7	15.8	10.7
		10	6.8U	8.2	-4.9	4.8
		11	28.8	32.9	28.8	1.1
		12	9.5U	11.3	2.1	9.2
		13	16.7	29.0	16.7	-.4
		14	14.1	15.3	5.6	12.9
		15	10.8	11.4	0.0	-10.8
		16	8.0U	5.6	7.6	2.3
		17	18.9	18.4	-14.8	-5.8
		18	9.1	10.9	5.1	-7.5
		19	12.0	14.8	-12.0	-.4
		20	7.9	11.1	-.9	-7.8
		21	9.6	11.1	-9.6	.4
	10	0	5.7U	10.6	5.7	0.0
		1	18.2	24.7	3.7	17.8
		2	13.6	16.4	6.6	-11.9
		3	18.0	24.8	16.1	8.1
		4	9.7U	12.9	2.5	-9.4
		5	24.2	24.8	21.6	-10.9
		6	8.6U	12.2	-1.3	-8.5
		7	20.6	23.3	6.7	-19.5
		8	5.7U	7.9	-5.3	2.2
		9	22.3	26.4	-16.4	-15.1
		10	8.9U	11.8	-7.5	4.7
		11	14.5	15.5	-13.7	-4.6
		12	5.2U	6.8	.2	5.1
		13	9.9	8.6	-6.9	7.0
		14	5.2U	6.1	-.6	5.1
		15	15.9	18.7	-1.0	15.9
		16	5.2U	1.8	-3.1	-4.1
		17	10.8	12.3	7.8	7.4
		18	4.8U	10.4	0.0	-4.8
		19	4.5U	3.9	4.4	-.9
		20	4.5U	4.0	1.5	-4.2
		21	9.1	12.6	6.8	-6.0
5	0	1	13.8	17.1	0.0	-13.8
		2	22.2	23.8	-22.2	0.0
		3	27.2	31.3	0.0	-27.2
		4	38.8	46.9	-38.8	0.0
		5	40.3	45.3	0.0	-40.3
		6	15.7	15.7	-15.7	0.0
		7	9.9U	17.6	0.0	-9.9
		8	22.8	20.1	22.8	0.0
		9	4.0U	1.6	0.0	4.0
		10	40.0	47.0	40.0	0.0
		11	24.4	23.0	0.0	24.4
		12	23.9	25.8	23.9	0.0
		13	34.0	41.5	0.0	34.0
		14	5.2U	8.3	5.2	0.0
		15	18.7	20.3	0.0	18.7
		16	19.5	18.4	-19.5	0.0
		17	6.1U	8.1	0.0	-6.1
		18	12.1U	20.5	-12.1	0.0
		19	21.5	26.8	0.0	-21.5
		20	27.4	29.2	-27.4	0.0
		21	10.4	11.1	0.0	-10.4
		22	6.4U	.2	6.4	0.0
		23	6.7U	.7	0.0	-6.7
		24	11.6	9.9	11.6	0.0
		25	11.6	11.8	0.0	11.6
		26	12.2	12.8	12.2	0.0
	1	0	28.7	34.4	0.0	28.7
		1	23.5	27.3	-20.8	-10.9
		2	32.3	33.2	23.6	22.1
		3	19.5	20.6	-18.6	-5.7
		4	25.9	25.0	25.9	0.0
		5	9.2U	10.6	9.0	-1.9
		6	29.6	28.7	15.2	-25.4
		7	29.5	31.0	29.5	-1.4
		8	21.2	23.7	-.7	-21.2
		9	37.2	36.2	33.2	16.8
		10	17.1	14.2	-15.1	-8.0
		11	18.0	19.8	7.8	16.2
		12	21.1	22.0	-20.8	3.7
		13	11.3U	11.6	-6.0	8.0
		14	23.9	22.7	-12.7	20.2
		15	18.4	19.6	-18.2	-2.8
		16	11.6U	17.2	5.8	10.1
		17	24.9	30.6	-14.1	-20.5
		19	11.6U	16.3	-7.5	-8.9
		20	14.4	15.4	4.9	-13.5
		21	6.7U	4.9	3.9	-5.4
		22	20.4	23.3	7.9	-18.8
		23	6.7U	7.9	6.6	-.9
		24	6.7U	10.4	0.0	-6.7
		25	13.8	14.5	11.1	8.2
	2	0	62.0	65.2	0.0	-62.0
		1	40.6	33.9	-40.1	-6.3
		2	47.1	42.6	-3.0	-47.0
		3	11.4U	10.4	-8.8	-7.3
		4	12.9U	10.3	-8.7	9.6
		5	12.9U	14.6	12.9	1.2

Table 4 (*cont.*)

H	K	L	FO	FC	AO	BO
5	2	6	43.1	37.9	-12.1	41.4
		7	37.2	35.7	37.0	3.3
		8	47.6	45.8	-7.8	46.9
		9	36.7	38.6	36.4	-4.8
		10	32.0	30.2	10.0	30.4
		11	18.2	14.5	-13.4	12.3
		12	11.1U	12.2	7.3	8.4
		13	24.7	21.2	-24.7	0.0
		14	23.1	20.9	6.7	-22.1
		15	30.7	30.5	-30.2	5.7
		16	28.1	27.8	-5.4	-27.6
		17	11.3	12.1	-11.3	0.0
		18	18.2	16.8	2.6	-18.0
		19	11.9	9.9	6.3	-10.1
		20	12.2	12.3	-5.2	-11.1
		21	13.6	15.0	11.2	-7.7
		22	11.9	8.5	0.0	11.9
		23	14.4	14.9	14.3	-1.8
		24	15.1	17.5	1.8	15.0
	3	0	11.6	7.1	0.0	11.6
		1	50.4	33.3	35.9	-35.4
		2	28.2	22.7	25.7	11.5
		3	70.1	52.0	17.9	-67.8
		4	34.6	28.8	34.4	-3.3
		5	40.8	33.7	-7.4	-40.1
		6	25.3	22.1	19.2	16.5
		7	25.0	24.2	-22.2	-11.4
		8	12.2	13.0	11.2	-4.9
		9	20.7	22.4	-10.4	7.3
		10	28.8	29.0	-26.0	-12.3
		11	27.9	26.1	-8.5	26.6
		12	34.2	38.7	-33.8	-5.4
		13	13.6	12.9	-11.9	6.6
		14	29.9	29.5	-28.7	-8.5
		15	19.2	23.2	19.0	-2.9
		16	13.1	13.5	8.0	-10.4
		17	16.2	15.1	11.0	-11.8
		18	19.7	21.0	19.7	-1.0
		19	15.9	18.4	11.7	-10.7
		20	17.7	20.3	14.7	9.9
		21	6.4U	1.5	2.8	-5.7
		22	14.4	15.1	12.6	6.9
		23	10.4	9.5	-8.1	6.5
		24	6.1U	6.4	4.2	4.4
		25	13.1	14.5	-8.0	10.3
	4	0	8.0	5.7	0.0	-8.0
		1	47.8	31.6	-35.6	31.9
		2	42.7	32.1	42.1	6.9
		3	58.9	53.2	-6.1	58.6
		4	51.3	41.9	51.3	0.0
		5	60.0	56.3	27.1	53.5
		6	40.2	36.3	35.8	18.2
		7	24.0	23.9	3.1	23.8
		8	11.3	10.7	-6.1	-9.5
		9	49.2	47.2	27.9	-40.5
		10	19.7	17.8	-14.3	-13.5
		11	34.0	37.9	7.8	-33.1
		12	28.4	29.7	-22.4	-17.5
		13	34.6	38.8	-16.7	-30.3
		14	22.6	25.4	-20.2	10.1
		15	20.0	20.4	-17.6	-9.5
		16	16.5	17.3	15.5	5.7
		17	14.4	15.2	-7.8	12.1
		18	18.5	20.1	18.3	-2.8
		19	18.5	19.6	0.0	18.5
		20	10.1	11.3	6.8	5.0
		21	20.7	25.9	8.5	18.9
		22	6.4U	2.0	-4.4	-4.6
		23	6.9U	4.8	6.3	2.8
		24	9.5	10.8	-9.5	.8
	5	0	36.0	28.5	0.0	-36.0
		1	18.0	14.7	17.1	-5.5
		2	46.0	37.0	-37.7	-26.3
		3	31.9	23.9	-20.4	-24.5
		4	41.0	33.9	-22.5	-34.2
		5	14.7	11.3	4.8	13.9
		6	39.6	32.8	-6.7	39.0
		7	10.5U	5.4	-8.0	6.8
		8	45.5	40.1	2.5	45.4
		9	20.7	21.3	-10.2	-18.0
		10	14.7	15.9	13.6	-5.4
		11	13.4	15.0	-10.9	7.8
		12	15.3	16.3	14.7	4.0
		13	11.0	10.4	7.9	7.6
		14	21.2	24.3	20.9	-3.7
		15	21.8	22.1	21.8	-1.1
		16	18.5	20.0	-12.8	-13.4
		17	10.4	9.5	9.4	4.4
		18	7.9U	6.4	-7.5	-2.2
		19	7.9U	6.5	6.8	4.0
		20	13.8	14.7	-13.1	4.3
		21	6.4U	4.2	-5.6	2.9
		22	16.8	19.5	-10.3	13.3
	6	0	19.2	18.5	0.0	19.2
		1	47.8	39.9	41.5	23.7
		2	13.4	11.4	8.3	10.5
		3	10.4	10.7	10.4	0.0
		4	25.5	23.0	19.0	17.0
		5	11.6	7.6	-9.5	6.6
		6	34.2	32.6	29.7	-16.9
		7	20.0	18.4	-18.0	8.8
		8	41.1	45.2	-23.0	-34.0
		9	16.5	18.2	-14.0	8.6
		10	27.9	24.2	-26.0	-10.0
		11	11.9	12.2	-9.2	-7.5
		12	11.9	9.5	-11.9	.9
		13	15.6	15.2	-1.4	-15.5
		14	20.0	21.4	-15.2	12.9
		15	11.3	11.4	11.3	-.9
		16	17.1	20.1	7.7	15.3
		17	6.4U	3.7	3.1	5.5
		18	15.9	16.0	11.9	10.5
		19	6.4U	4.2	-5.1	3.8
		20	11.3	12.9	11.3	-.6
		21	11.3	10.6	-8.6	7.3
	7	0	10.1	10.3	0.0	-10.1
		1	22.6	20.4	-11.6	19.4
		2	34.0	32.2	-33.8	3.4
		3	32.2	27.4	7.0	31.4
		4	30.9	27.6	-30.5	-5.0
		5	28.8	27.0	9.5	27.2
		6	20.0	20.8	-16.2	11.7
		7	6.9U	4.3	3.4	6.0
		8	16.8	14.8	13.3	10.2
		9	12.4	10.8	6.2	-10.8
		10	18.0	18.6	17.9	-1.5
		11	28.4	25.6	7.2	-27.5
		12	16.2	15.9	15.8	3.3
		13	19.5	19.2	-7.5	-18.0
		14	17.1	16.3	13.7	-10.2
		15	10.1	10.2	-10.1	.3
		16	11.9	10.1	-1.2	-11.8
		17	14.7	15.6	-9.1	11.5
		18	11.6	12.0	-11.5	-1.7
		19	14.1	16.5	.8	14.1
5	7	20	11.0	9.6	-10.9	1.5
		21	5.8U	5.0	1.4	5.6
		22	9.3	10.6	-8.5	3.7
	8	0	9.3	8.2	0.0	9.3
		1	29.9	26.8	20.4	-21.8
		2	14.4	14.3	-11.9	8.0
		3	24.7	28.4	-2.4	-24.6
		4	15.6	14.7	-13.9	7.1
		5	32.2	35.6	-16.0	-28.0
		6	11.0	7.6	-10.8	-2.3
		7	19.5	21.9	-16.1	-11.0
		8	11.0	12.3	-4.7	-10.0
		9	15.9	13.5	-11.4	11.0
		10	12.2	12.6	6.2	-10.5
		11	25.5	29.3	3.2	25.3
		12	6.7U	7.6	4.5	-4.9
		13	23.8	23.2	17.1	16.6
		14	6.7U	2.4	6.2	2.3
		15	16.8	16.7	15.4	6.7
		16	10.1	8.4	-5.7	8.3
		17	11.0	12.0	9.7	-5.2
		18	6.1U	3.6	-5.6	2.3
		19	10.7	11.6	-2.1	-10.5
		20	5.8U	3.1	-1.6	5.6
		21	10.4	11.7	-6.0	-8.5
		22	4.9U	3.9	-3.4	-3.5
		23	9.5	9.0	-9.3	-2.1
	9	0	12.4	11.3	0.0	12.4
		1	20.3	26.0	-19.0	7.1
		2	8.9	9.0	4.2	7.8
		3	12.4	11.2	-3.7	11.8
		4	8.6	10.5	8.1	2.9
		5	12.4	12.8	9.7	7.7
		6	15.3	19.1	10.2	-11.4
		7	12.7	14.0	12.7	.6
		8	16.2	19.1	1.2	-16.1
		9	16.2	21.0	15.0	-6.1
		10	6.9U	10.3	-4.8	-5.0
		11	15.9	16.5	7.0	-14.3
		12	9.5	12.9	-8.8	3.5
		13	7.8	8.3	-5.6	-5.4
		14	10.7	13.0	-4.9	9.5
		15	11.0	13.3	-10.9	-1.1
		16	11.0	15.7	-4.8	9.9
		17	10.1	13.3	-8.5	5.5
		18	6.9U	7.0	5.9	3.7
		19	6.8	6.3	-6.5	2.0
	10	0	17.1	20.5	0.0	-17.1
		1	6.4U	3.9	-1.8	-6.1
		2	13.6	17.0	-6.1	-12.1
		3	6.1U	7.3	-3.2	-5.1
		4	13.8	14.6	-13.3	-3.5
		5	6.1U	6.5	3.3	-5.1
		6	12.7	13.7	-3.4	12.2
		7	5.8U	6.2	5.6	-1.4
		8	12.7	17.4	3.4	12.2
		9	5.8U	1.5	5.4	2.0
		10	16.8	21.2	10.0	13.5
		11	5.2U	6.6	-4.1	3.2
		12	13.6	12.5	13.5	1.7
		13	5.2U	4.4	-4.6	2.5
		14	8.0	8.3	5.4	-5.8
		15	4.9U	3.5	1.0	-4.8
		16	13.4	16.3	-4.7	-12.6
		17	4.6U	3.3	-3.3	-3.2
		18	12.2	14.0	-10.5	-6.1
		19	4.3U	6.4	-3.9	1.8
		20	6.8	10.2	-6.4	2.2
		21	3.7U	7.9	3.6	1.0
		22	6.8	6.5	-3.0	6.1
6	0	0	39.1	44.7	-39.1	0.0
		1	13.8	18.9	0.0	13.8
		2	5.3	3.9	-5.3	0.0
		3	5.6	7.5	0.0	-5.6
		4	7.6	7.7	7.6	0.0
		5	4.5	3.8	0.0	-4.5
		6	12.0	10.6	12.0	0.0
		7	5.3	6.9	0.0	5.3
		8	23.6	21.9	23.6	0.0
		9	6.0U	2.3	0.0	-6.0
		10	17.9	17.8	17.9	0.0
		11	13.4	13.4	0.0	-13.4
		12	6.8U	2.2	-6.8	0.0
		13	7.1U	.1	0.0	7.1
		14	23.3	22.9	-23.3	0.0
		15	14.4	10.4	0.0	14.4
		16	9.9	11.9	-9.9	0.0
		17	9.9	4.8	0.0	-9.9
		18	12.8	16.0	-12.8	0.0
		19	15.6	16.8	0.0	-15.6
		20	8.6U	4.6	-8.6	0.0
		21	8.6U	2.7	0.0	-8.6
		22	14.4	12.2	14.4	0.0
	1	0	4.2U	.6	4.2	0.0
		1	20.6	22.9	-9.6	-18.2
		2	36.1	43.4	-4.7	-35.8
		3	13.5	16.6	-3.7	-13.0
		4	32.6	34.5	-6.3	-32.0
		5	14.5	16.5	-14.3	2.5
		6	23.3	24.5	7.8	-21.9
		7	27.8	26.8	0.0	27.8
		8	6.3U	.8	-4.7	4.2
		9	22.0	24.1	6.3	21.1
		10	10.2U	26.7	-.8	10.2
		11	10.3U	11.2	9.3	4.4
		12	28.3	31.3	-12.3	25.5
		13	7.7U	1.0	7.1	3.1
		14	15.3	16.9	4.2	14.7
		15	11.6U	16.4	-4.3	-10.8
		16	13.3	13.7	10.7	-7.9
		17	19.0	20.3	-9.8	-16.3
		18	10.2	8.5	6.5	-7.9
		19	8.6U	1.2	-7.7	4.0
		20	17.9	17.1	8.4	-15.8
	2	0	8.2U	5.3	-8.2	0.0
		1	14.0U	7.6	13.3	4.1
		2	14.0U	11.9	-.4	-13.9
		3	36.7	27.8	36.4	-4.5
		4	25.4	20.2	-.9	-25.4
		5	42.1	37.0	40.9	-9.8
		6	11.4U	8.0	-4.1	-10.6
		7	23.3	19.3	11.1	-20.5
		8	13.2U	6.5	11.0	7.3
		9	28.8	25.8	-28.4	4.7
		10	8.2U	4.1	0.0	8.2
		11	31.4	29.2	-30.7	6.7
		12	10.9U	9.0	4.7	9.8
		13	25.2	22.0	-23.6	8.7
		14	10.8	7.0	-8.2	-7.0
		15	17.9	16.6	-12.3	13.0
		16	6.8U	5.1	-7.3	4.2
		17	17.3	17.1	14.8	9.0
		18	8.6U	3.5	2.0	-8.4
		19	16.7	20.9	16.7	0.0
6	3	0	10.8	7.7	-10.8	0.0
		1	38.8	21.7	7.7	-38.0
		2	33.0	22.9	3.1	32.9
		3	29.7	23.4	-1.7	-29.6
		4	28.3	26.0	-2.9	28.1
		5	24.4	17.0	-12.2	21.1
		6	20.2	16.5	12.7	15.7
		7	34.1	27.5	-4.4	33.8
		8	13.4	12.7	11.2	7.4
		9	35.4	32.2	10.9	33.7
		10	14.7	14.7	6.9	-13.0
		11	8.0U	6.6	-2.9	7.4
		12	22.0	21.1	-7.6	-20.6
		13	8.8	7.8	8.5	-2.4
		14	22.4	24.8	-19.9	-10.2
		15	22.4	23.1	3.5	-22.1
		16	14.1	14.1	-13.7	-3.4
		17	19.1	20.3	-5.6	-18.2
		18	8.1	7.5	-.8	8.1
		19	8.2U	6.4	-.7	-8.2
		20	17.0	16.8	11.7	12.3
	4	0	61.2	35.3	61.2	0.0
		1	22.0	14.4	0.0	-22.0
		2	22.4	15.5	19.0	-11.9
		3	23.0	11.4	22.2	-6.0
		4	15.9	11.0	-14.9	-5.5
		5	24.4	17.9	6.8	23.4
		6	25.6	18.2	-25.3	4.1
		7	9.8U	10.9	-6.0	7.3
		8	36.5	32.9	-26.6	25.0
		9	13.1	12.1	2.7	12.8
		10	23.6	23.3	-17.4	16.0
		11	11.7	8.5	-8.7	-7.8
		12	8.0U	6.7	2.1	-7.7
		13	20.2	19.4	-4.5	-19.7
		14	22.3	22.3	22.2	1.3
		15	8.2U	2.7	4.6	-6.8
		16	22.3	24.0	20.7	-8.4
		17	8.2U	3.2	8.2	0.0
		18	11.3	12.8	10.1	-4.9
	5	0	13.4	8.0	-13.4	0.0
		1	18.5	16.9	-7.3	17.0
		2	25.1	20.6	-11.2	22.5
		3	19.6	11.5	9.0	17.4
		4	38.0	29.1	-18.8	33.0
		5	23.0	19.4	-22.0	-6.8
		6	31.6	27.9	2.1	31.5
		7	31.2	27.8	-11.4	-29.0
		8	23.6	22.7	21.3	-10.1
		9	20.8	14.1	2.6	-20.6
		10	20.5	24.7	-.6	-20.5
		11	20.9U	16.4	-18.4	9.9
		12	21.4	18.3	11.1	-18.3
		13	8.2U	2.4	1.5	8.1
		14	12.3	12.4	4.5	-11.4
		15	15.6	14.1	13.7	7.3
		16	7.6	4.9	-4.0	6.5
		17	13.6	11.6	11.9	6.6
		18	9.4	9.5	0.0	9.4
		19	8.8	9.0	7.6	4.5
		20	10.5	15.6	-2.9	10.1
	6	0	26.2	21.0	26.2	0.0
		1	26.5	21.5	-14.5	-22.2
		2	17.6	15.7	2.4	-17.4
		3	20.2	19.2	-19.0	-6.9
		4	9.9	8.6	8.2	-5.5
		5	23.9	21.1	-15.4	18.2
		6	20.5	18.1	-16.3	-12.4
		7	8.0U	2.0	0.0	8.0
		8	18.8	16.2	-18.5	3.2
		9	23.0	21.0	5.0	22.4
		10	10.2	4.4	0.0	-10.2
		11	21.4	21.2	20.3	6.6
		12	9.7U	6.9	4.2	8.8
		13	25.6	27.5	23.1	-11.0
		14	14.1	12.8	8.9	10.9
		15	13.6	13.8	2.9	-13.3
		16	26.5	9.4	21.0	16.1
		17	10.2	12.2	-9.3	-4.2
		18	7.7U	1.3	7.6	.9
		19	14.4	12.2	-14.3	1.6
	7	0	14.4	12.8	14.4	0.0
		1	27.6	23.4	8.6	26.2
		2	14.7	11.5	14.3	-3.5
		3	27.3	26.7	23.6	13.8
		4	17.3	18.8	-12.0	-12.4
		5	24.4	25.6	20.0	-14.0
		6	14.1	12.4	-12.4	-6.7
		7	24.4	25.6	11.2	-21.7
		8	11.3	8.0	-10.4	4.3
		9	15.6	15.6	0.0	-15.6
		10	12.5	11.1	.7	12.5
		11	15.3	14.5	-13.5	-7.2
		12	10.2	11.0	5.2	8.7
		13	12.8	12.3	-7.8	10.2
		14	10.8	10.0	9.6	4.9
		15	16.7	14.7	-4.0	16.2
		16	7.7U	4.2	7.5	1.7
		17	11.7	12.7	-2.2	11.5
		18	8.8	8.6	2.4	-8.5
		19	7.6	5.1	4.5	6.1
	8	0	11.7	12.8	-11.7	0.0
		1	8.2U	1.7	0.0	-8.2
		2	12.3	10.8	-9.0	8.3
		3	11.7	10.4	-11.1	3.7
		4	17.9	16.9	-.9	17.9
		5	13.4	14.9	-13.4	.8
		6	17.6	20.0	10.5	14.1
		7	9.7U	2.0	-9.4	-2.6
		8	15.9	16.6	14.4	6.7
		9	7.7U	1.3	3.0	7.0
		10	9.9	11.8	7.0	-7.0
		11	9.6	9.1	9.5	1.5
		12	9.9	10.9	-1.6	-9.8
		13	8.8	7.1	8.7	1.2
		14	8.8	10.0	-6.6	-5.8
		15	8.5	7.6	8.5	.6
		16	8.1	11.6	-8.1	.4
		17	9.1	6.9	-5.9	-6.9
	9	0	12.3	12.4	12.3	0.0
		1	7.7U	4.2	-4.6	-6.2
		2	12.8	17.7	7.9	-10.1
		3	9.9	9.0	-9.1	3.8
		4	15.6	21.1	-1.0	-15.6
		5	11.0	9.8	-11.0	1.0
		6	15.6	18.7	-7.6	-13.6
		7	7.1U	4.4	-1.4	7.0
		8	10.8	10.9	-10.8	-.6
		9	8.8	5.1	8.0	3.6
		10	18.2	19.9	-7.3	16.7
		11	6.8U	5.1	5.2	4.4
		12	12.5	15.6	2.7	12.2
		13	9.1	4.3	5.7	-7.1
		14	8.5	11.7	4.0	7.5

Four more rounds of BDLS were calculated to refine the parameters of all the non-hydrogen atoms further, giving each anisotropic temperature factor coefficients. The hydrogen atoms were included in the computation of structure factors but excluded from the BDLS refinement. To ensure convergence, empirical relaxation factors of 0·8 and 0·6 were applied to the positional and thermal shifts respectively.

The R index for all observed reflexions stood at 0·101 for the last two rounds of BDLS refinement. Since this R value is comparable to the average standard deviation $\sigma(F_o)$ or 9·7% (*cf.* §2) and all parametric shifts were less than one-third of the estimated standard deviations, refinement of the structure was discontinued.

The final structure factors were listed in Table 4, and the final positional and thermal parameters for all non-hydrogen atoms together with their associated standard deviations are contained in Tables 1 and 2 respectively. All standard deviations were estimated from block-diagonal residues by a procedure similar to that described by Cruickshank (1949).

When the magnitudes and direction cosines of the principal axes of thermal motion for each non-hydrogen atom were computed with the use of the values of B_{ij} in Table 2, it was discovered that the largest thermal eigenvalue for atom C(3) had its axis parallel to the C(2)–C(3) bond. This was very surprising and errors in the parameters of C(3) were suspected, since the C(2)–C(3) bond was also unusually short. Structure factors were calculated, phased with all atoms except C(3) and its associated hydrogen atoms, and a difference synthesis was computed in the region containing C(3). A peak of height 3 e.Å^{-3} was observed at a site within 0·02 Å of the BDLS coordinates of C(3). There were no other peaks in the synthesis of height greater than the standard deviation of electron density distribution of 0·3 e.Å^{-3}. It was concluded that further refinement would not yield information which would resolve the anomaly, and the analysis was terminated.

4. Discussion

The method of anomalous dispersion phasing

There are two methods of utilizing the effect of anomalous dispersion in the determination of phases for non-centrosymmetric structures, one by way of the Fourier synthesis suggested by Ramachandran & Raman (1956) and the other by way of a difference Patterson synthesis (Okaya, Saito & Pepinsky, 1955; Okaya & Pepinsky, 1956, 1961). Ramachandran & Raman's method was adopted because of its simplicity in application; moreover, Bijvoet and his collaborators showed in 1963 that this method provides more details than the difference Patterson synthesis.

Table 6(*a*) lists the peak heights of non-hydrogen light atoms taken from the three-dimensional Fourier synthesis: (*A*) the direct anomalous dispersion phased with the use of the initial iodine coordinates; (*H*) the heavy atom phased by the initial iodine coordinates and (*HF*) the heavy atom phased by final iodine coordinates. The column *A*/*H* gives the ratios of the peak heights of an atom in (*A*) to that of the corresponding one in (*H*). The average peak ratio is 1·5. It is obvious that the peaks in (*A*) are decidedly sharper than those in (*H*), showing the general superiority of the direct method.

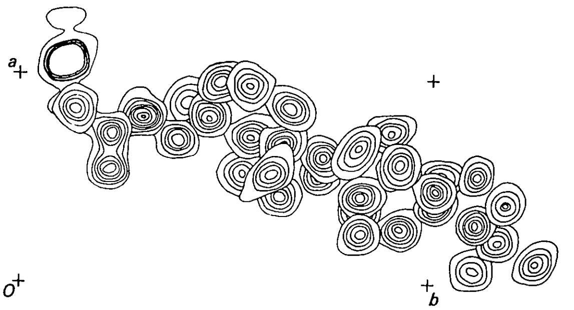

Fig. 2. Summary of the final Fourier synthesis. The contours are at 1 e.Å^{-3} intervals, beginning at 1 e.Å^{-3} for all atoms except iodine, which has the first contour at 1 e.Å^{-3} and the others at arbitrary intervals.

From the point of view of structure determination it is often important that the number of spurious peaks in the synthesis should be small. Table 6(*b*) gives an analysis of the background details. From a comparison of column (*A*) and column (*H*) one cannot but conclude in favour of the direct method.

It is appropriate to mention that the Fourier synthesis computed from structure factors phased by the final iodine coordinates with the use of the fully treated

Table 5. *Thermal eigenvalues*

Atom	*i*	B_i(Å^2)	$D1_i$	$D2_i$	$D3_i$	U_i(Å)
C(1)	1	5·79	−0·314	0·821	−0·475	0·270
	2	4·33	−0·531	−0·567	−0·629	0·234
	3	2·08	0·786	−0·054	−0·614	0·162
C(2)	1	6·98	−0·524	−0·790	0·316	0·297
	2	8·06	0·584	−0·063	0·809	0·319
	3	2·45	−0·619	0·608	0·495	0·176
C(3)	1	1·98	0·921	−0·253	−0·294	0·158
	2	11·79	0·088	−0·602	0·793	0·386
	3	4·40	−0·378	−0·756	−0·532	0·236
C(4)	1	4·20	−0·787	0·571	−0·231	0·230
	2	5·13	−0·435	−0·251	0·864	0·254
	3	2·89	0·435	0·781	0·446	0·191
C(5)	1	3·82	−0·892	0·442	0·085	0·219
	2	4·40	0·426	0·890	−0·156	0·236
	3	3·15	0·145	0·103	0·983	0·199
C(6)	1	5·02	0·748	−0·497	−0·437	0·252
	2	6·15	0·556	0·112	0·823	0·279
	3	3·34	0·360	0·859	−0·361	0·205
C(7)	1	4·15	0·598	−0·598	−0·533	0·229
	2	7·67	0·704	0·076	0·705	0·311
	3	2·42	0·381	0·797	−0·467	0·175
C(8)	1	1·75	0·885	−0·462	0·034	0·148
	2	5·76	0·158	0·370	0·915	0·270
	3	3·14	−0·435	−0·805	0·401	0·199
C(9)	1	5·41	−0·067	0·971	0·227	0·261
	2	4·17	−0·701	0·115	−0·702	0·229
	3	2·64	0·709	0·206	−0·674	0·182
C(10)	1	3·61	−0·647	−0·131	−0·750	0·213
	2	6·92	−0·264	0·962	0·059	0·296
	3	1·98	0·714	0·236	−0·658	0·158
C(11)	1	12·50	0·975	0·003	0·217	0·397
	2	3·64	0·176	−0·599	−0·780	0·214
	3	2·92	0·127	0·800	−0·585	0·192

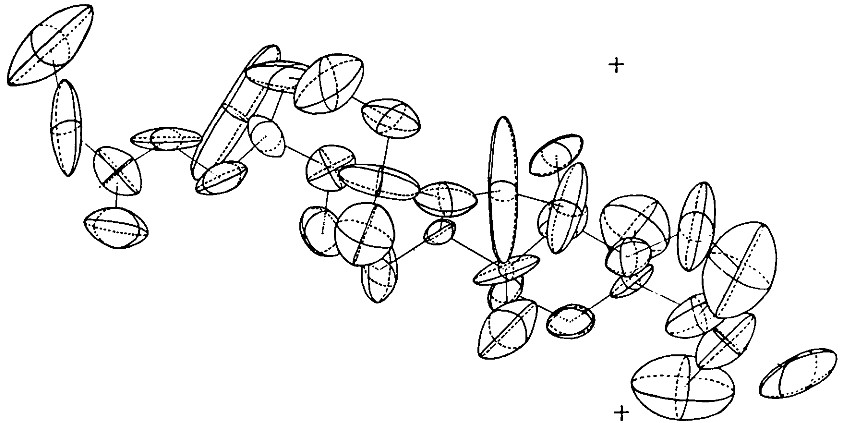

Fig. 3. The thermal ellipsoids.

Table 5 (*cont.*)

Atom	i	B_i(Å^2)	$D1_i$	$D2_i$	$D3_i$	U_i(Å)
C(12)	1	8·14	0·910	0·284	0·300	0·321
	2	3·19	0·121	0·509	−0·852	0·201
	3	2·86	−0·395	0·812	0·428	0·190
C(13)	1	3·77	−0·790	0·531	−0·303	0·218
	2	4·73	0·418	0·831	0·365	0·244
	3	3·51	−0·446	−0·161	0·879	0·210
C(14)	1	6·35	0·272	0·861	−0·429	0·283
	2	2·82	−0·365	−0·319	−0·873	0·188
	3	1·91	0·889	−0·395	−0·227	0·155
C(15)	1	3·35	−0·161	−0·761	0·627	0·205
	2	5·30	0·624	0·413	0·663	0·259
	3	2·60	−0·764	0·498	0·408	0·181
C(16)	1	2·22	0·982	−0·112	−0·147	0·167
	2	7·24	0·070	−0·512	0·856	0·302
	3	4·68	−0·171	−0·851	−0·495	0·243
C(17)	1	2·36	−0·484	−0·290	−0·825	0·172
	2	5·07	0·495	0·685	−0·532	0·253
	3	1·85	−0·720	0·667	0·187	0·153
C(18)	1	3·97	−0·304	−0·924	0·227	0·224
	2	5·57	0·592	0·003	0·805	0·265
	3	2·96	−0·745	0·379	0·547	0·193
C(19)	1	8·81	0·822	0·201	0·531	0·334
	2	4·38	0·468	0·291	−0·834	0·235
	3	2·89	−0·323	0·935	0·145	0·191
C(20)	1	5·70	0·540	−0·835	−0·103	0·268
	2	11·03	0·690	0·369	0·621	0·373
	3	2·32	0·480	0·407	−0·776	0·171
C(21)	1	3·79	−0·833	0·225	−0·504	0·219
	2	6·24	0·381	0·895	−0·230	0·281
	3	2·74	−0·400	0·384	0·831	0·186
C(22)	1	5·54	0·102	−0·027	−0·994	0·264
	2	6·32	0·684	0·726	0·050	0·282
	3	3·29	0·721	−0·686	0·093	0·204
C(23)	1	2·41	0·910	−0·412	−0·037	0·174
	2	7·55	0·227	0·575	−0·785	0·309
	3	4·31	−0·345	−0·706	−0·617	0·233
C(24)	1	3·02	0·527	−0·800	0·283	0·195
	2	13·01	0·843	0·533	−0·063	0·405
	3	6·05	0·100	−0·272	−0·956	0·276
C(25)	1	5·08	0·402	−0·915	0·016	0·253
	2	6·48	0·774	0·330	−0·539	0·286
	3	3·21	0·488	0·230	0·841	0·201
C(26)	1	2·39	0·858	−0·459	−0·227	0·173
	2	9·46	0·124	−0·242	0·962	0·346
	3	5·05	−0·496	−0·854	−0·150	0·252
C(27)	1	4·55	−0·395	−0·473	−0·787	0·240
	2	8·16	0·551	0·562	−0·615	0·321
	3	3·76	0·734	−0·677	0·038	0·218
C(28)	1	6·11	0·556	−0·817	−0·148	0·278
	2	7·30	0·574	0·507	−0·641	0·304
	3	3·80	0·600	0·271	0·752	0·219
C(29)	1	5·51	0·944	0·148	−0·293	0·264
	2	8·55	−0·110	0·983	0·142	0·329
	3	6·42	−0·309	0·102	−0·945	0·285
C(30)	1	5·64	−0·641	−0·475	−0·602	0·267
	2	10·72	0·292	0·573	−0·764	0·368
	3	2·57	−0·708	0·667	0·229	0·180
C(31)	1	2·59	−0·048	−0·101	0·993	0·181
	2	4·97	0·763	−0·645	−0·028	0·250
	3	3·46	−0·643	−0·757	−0·109	0·209
C(32)	1	8·26	0·965	−0·002	0·260	0·325
	2	3·37	−0·171	−0·758	0·628	0·206
	3	2·55	−0·195	0·651	0·733	0·179
I	1	5·53	−0·254	−0·462	−0·849	0·264
	2	11·25	0·571	0·636	−0·517	0·377
	3	3·91	0·780	−0·617	0·102	0·222
O(1)	1	1·93	0·996	0·053	0·060	0·156
	2	7·79	−0·004	0·783	−0·620	0·314
	3	4·44	0·081	−0·618	−0·781	0·237
O(2)	1	3·31	0·978	0·199	0·046	0·204
	2	9·20	0·040	−0·410	0·911	0·341
	3	5·95	0·200	−0·889	−0·409	0·274

data shows the least spurious details although the peak heights are low. In practice, however, it is not always possible to determine the coordinates of the heavy atom very precisely from the projection Patterson syntheses and it seems preferable that whenever there is an anomalous scatterer in the non-centrosymmetric structure and whenever the Bijvoet inequality (ΔI) is measurable Ramachandran & Raman's method should be used.

Description of the structure

This study confirms the stereochemical model and absolute configuration of davallic acid as proposed by Nakanishi *et al.* (1963).

Table 6(*a*). *Peak heights taken from the* three-dimensional Fourier synthesis

Atom	A (e.Å^{-3})	H(e.Å^{-3})	A/H	HF(e.Å^{-3})
C(1)	5·8	2·9	2·0	2·3
C(2)	3·5	3·2	1·09	2·1
C(3)	5·3	4·2	1·26	3·0
C(4)	5·3	2·6	2·04	1·9
C(5)	4·4	2·7	1·63	2·0
C(6)	3·6	2·6	1·38	2·4
C(7)	5·5	4·1	1·34	2·4
C(8)	4·6	3·3	1·39	2·0
C(9)	5·6	2·6	2·15	1·9
C(10)	5·3	4·6	1·15	3·2
C(11)	3·3	2·6	1·27	2·2
C(12)	3·8	3·2	1·19	2·2
C(13)	5·6	3·0	1·87	2·0
C(14)	4·9	3·9	1·26	2·6
C(15)	4·7	2·0	2·35	2·9
C(16)	4·2	3·0	1·40	2·1
C(17)	6·4	3·1	2·06	1·8
C(18)	4·8	2·5	1·92	2·5
C(19)	3·4	2·6	1·35	2·2
C(20)	3·6	2·7	1·33	2·6
C(21)	4·9	3·6	1·36	2·5
C(22)	4·2	2·3	1·83	1·6
C(23)	4·4	3·8	1·16	3·6
C(24)	4·0	2·9	1·38	1·9
C(25)	3·1	3·0	1·03	2·6
C(26)	4·9	3·7	1·32	2·6
C(27)	4·1	3·9	1·05	2·6
C(28)	5·0	2·4	2·08	1·4
C(29)	6·4	3·7	1·73	2·1
C(30)	2·6	2·3	1·13	1·9
C(31)	4·8	3·3	1·45	2·0
C(32)	5·0	2·2	2·27	1·8
O(1)	6·6	4·9	1·35	3·6
O(2)	5·3	3·6	1·47	3·1
Average ϱ	4·67	3·15	1·48	2·34
$\frac{3}{4}\bar{\rho}$	3·5	2·4		1·76
$\frac{1}{2}\bar{\rho}$	2·3	1·6		1·20

Table 6(*b*). *Analysis of background details: number of peaks*

		A	H	HF
True peaks	$\frac{3}{4}\varrho \geq \varrho > \frac{1}{2}\bar{\rho}$	4	4	2
	$\varrho \leq \frac{1}{2}\bar{\rho}$	0	0	0
Spurious peaks*	$\frac{3}{4}\varrho \geq \varrho > \frac{1}{2}\bar{\rho}$	4	13†	0
	$\varrho \leq \frac{1}{2}\bar{\rho}$	19	31	3

A Direct anomalous phased using initial iodine coordinates.
H Heavy atom phased using initial iodine coordinates.
HF Heavy atom phased using final iodine coordinates.
* Obvious heavy atom ripples *not* included.
† Three of these are larger than $\bar{\rho}$.

The molecular packing is illustrated in Figs. 4 and 5, with close intermolecular distances indicated. The molecules are held together in the unit cell principally by van der Waals forces. If an asymmetric unit is assigned to be (a, b, $\frac{1}{4}c$) the molecule lies approximately parallel to the diagonal of the unit. The ring system bows slightly from *A* to *E*. Rings *A* and *D* are in the form of chairs whilst ring *B* conforms to the boat configuration. The conformation of a chair in ring *A* followed by a boat in ring *B* is unusual and this configuration seems to have arisen from the co-planarity of the atoms C(8), C(9), C(10), C(11) and C(12), due to the double bond at C(9)–C(11). The equation of the least-squares plane through these atoms is

$$0{\cdot}9043x+0{\cdot}0826y+0{\cdot}4189z+1{\cdot}5770=0$$

where x, y and z are expressed in Å. The largest deviation from the plane for any atom in the group is 0·021 Å for C(9) which is well within the standard deviation, $\sigma(x, y, z)$, of the atomic parameters.

Another planar section of the molecule occurs at the carbonyl group. The equation of the least-squares plane for C(31), C(32), O(1) and O(2) is

$$-0{\cdot}0533x-0{\cdot}4549y+0{\cdot}8889z-5{\cdot}9571=0\ .$$

The largest deviation from planarity is 0·011 Å for C(31) which again is well within the standard deviation σ of the atomic coordinates.

Table 7. *Bond lengths*

	l	$\sigma(l)$
C(1)—C(2)	1·553 Å	0·034 Å
C(1)—C(10)	1·576	0·027
C(2)—C(3)	1·427	0·037
C(3)—C(4)	1·524	0·031
C(4)—C(5)	1·547	0·030
C(4)—C(23)	1·521	0·030
C(4)—C(24)	1·552	0·034
C(5)—C(6)	1·586	0·031
C(5)—C(10)	1·534	0·028
C(6)—C(7)	1·449	0·031
C(7)—C(8)	1·488	0·028
C(8)—C(14)	1·627	0·028
C(10)-C(25)	1·566	0·030
C(12)-C(13)	1·532	0·028
C(13)-C(14)	1·586	0·029
C(13)-C(18)	1·565	0·029
C(13)-C(26)	1·526	0·031
C(14)-C(15)	1·534	0·026
C(14)-C(27)	1·520	0·031
C(15)-C(16)	1·548	0·030
C(16)-C(17)	1·526	0·028
C(17)-C(18)	1·544	0·026
C(17)-C(21)	1·542	0·029
C(17)-C(28)	1·577	0·030
C(18)-C(19)	1·535	0·031
C(19)-C(20)	1·512	0·036
C(20)-C(21)	1·518	0·033
C(21)-C(22)	1·548	0·031
C(22)-C(29)	1·562	0·037
C(22)-C(30)	1·560	0·037
C(8)—C(9)	1·557	0·028
C(9)—C(10)	1·561	0·031
C(9)—C(11)	1·320	0·032
C(11)-C(12)	1·512	0·031
C(23)-O(1)	1·436	0·026
C(31)-C(32)	1·490	0·031
C(31)-O(1)	1·297	0·026
C(31)-O(2)	1·183	0·026
C(32)-I	2·127	0·025

Table 8. *Bond angles*

	θ	$\sigma(\theta)$
C(2)—C(1)—C(10)	112·5°	1·8°
C(1)—C(2)—C(3)	110·1	2·0
C(2)—C(3)—C(4)	121·6	2·0
C(3)—C(4)—C(5)	104·0	1·7
C(3)—C(4)—C(23)	111·2	1·8
C(3)—C(4)—C(24)	109·8	2·0
C(5)—C(4)—C(23)	115·5	1·7
C(5)—C(4)—C(24)	106·4	1·7
C(23)-C(4)—C(24)	109·6	1·9
C(4)—C(5)—C(6)	113·1	1·7
C(4)—C(5)—C(10)	117·3	1·6
C(6)—C(5)—C(10)	107·7	1·6
C(5)—C(6)—C(7)	115·3	1·8
C(6)—C(7)—C(8)	113·4	1·9
C(7)—C(8)—C(9)	111·3	1·7
C(7)—C(8)—C(14)	116·0	1·6
C(9) – C(8) – C(14)	108·2	1·5
C(8)—C(9)—C(10)	113·9	1·7
C(8)—C(9)—C(11)	123·3	2·0
C(10)-C(9)—C(11)	122·7	1·8
C(1)—C(10)—C(5)	110·0	1·6
C(1)—C(10)—C(9)	106·1	1·7
C(1)—C(10)—C(25)	106·2	1·5
C(5)—C(10)—C(9)	108·5	1·5
C(5)—C(10)—C(25)	118·5	1·8
C(9)—C(10)—C(25)	106·9	1·7
C(9)—C(11)—C(12)	125·2	2·1
C(11)-C(12)-C(13)	111·6	1·7
C(12)-C(13)-C(14)	106·9	1·6
C(12)-C(13)-C(18)	109·9	1·6
C(12)-C(13)-C(26)	108·6	1·9
C(14)-C(13)-C(18)	104·6	1·6
C(14)-C(13)-C(26)	113·1	1·7
C(18)-C(13)-C(26)	113·5	1·7
C(8)—C(14)-C(13)	107·0	1·4
C(8)—C(14)—C(15)	107·5	1·5
C(8)—C(14)-C(27)	106·5	1·6
C(13)-C(14)-C(15)	110·6	1·5
C(13)-C(14)-C(27)	115·8	1·7
C(15)-C(14)-C(27)	109·1	1·6
C(14)-C(15)-C(16)	111·2	1·7
C(15)-C(16)-C(17)	114·7	1·6
C(16)-C(17)-C(18)	106·2	1·6
C(16)-C(17)-C(21)	118·1	1·6
C(16)-C(17)-C(28)	109·7	1·7
C(18)-C(17)-C(21)	97·6	1·4
C(18)-C(17)-C(28)	116·8	1·6
C(21)-C(17)-C(28)	108·3	1·6
C(13)-C(18)-C(17)	118·5	1·6
C(13)-C(18)-C(19)	119·0	1·8
C(12)-C(18)-C(19)	104·2	1·6
C(18)-C(19)-C(20)	102·3	1·9
C(19)-C(20)-C(21)	108·0	1·9
C(17)-C(21)-C(20)	104·8	1·7
C(17)-C(21)-C(22)	119·5	1·7
C(20)-C(21)-C(22)	115·7	1·9
C(21)-C(22)-C(29)	115·5	2·1
C(21)-C(22)-C(30)	109·4	1·9
C(29)-C(22)-C(30)	109·7	2·0
C(4)—C(23)-O(1)	108·6	1·6
C(32)-C(31)-O(1)	113·2	1·8
C(32)-C(31)-O(2)	123·0	2·0
O(1) -C(31)-O(2)	123·8	2·0
C(23)-O(1) -C(31)	116·1	1·5
C(31)-C(32)-I	113·5	1·4

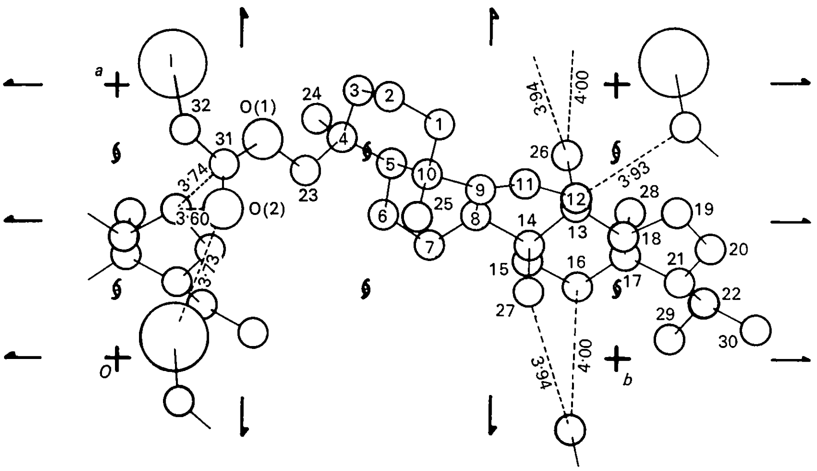

Fig. 4. Packing diagram, projecting down one-quarter of the *c* axis.

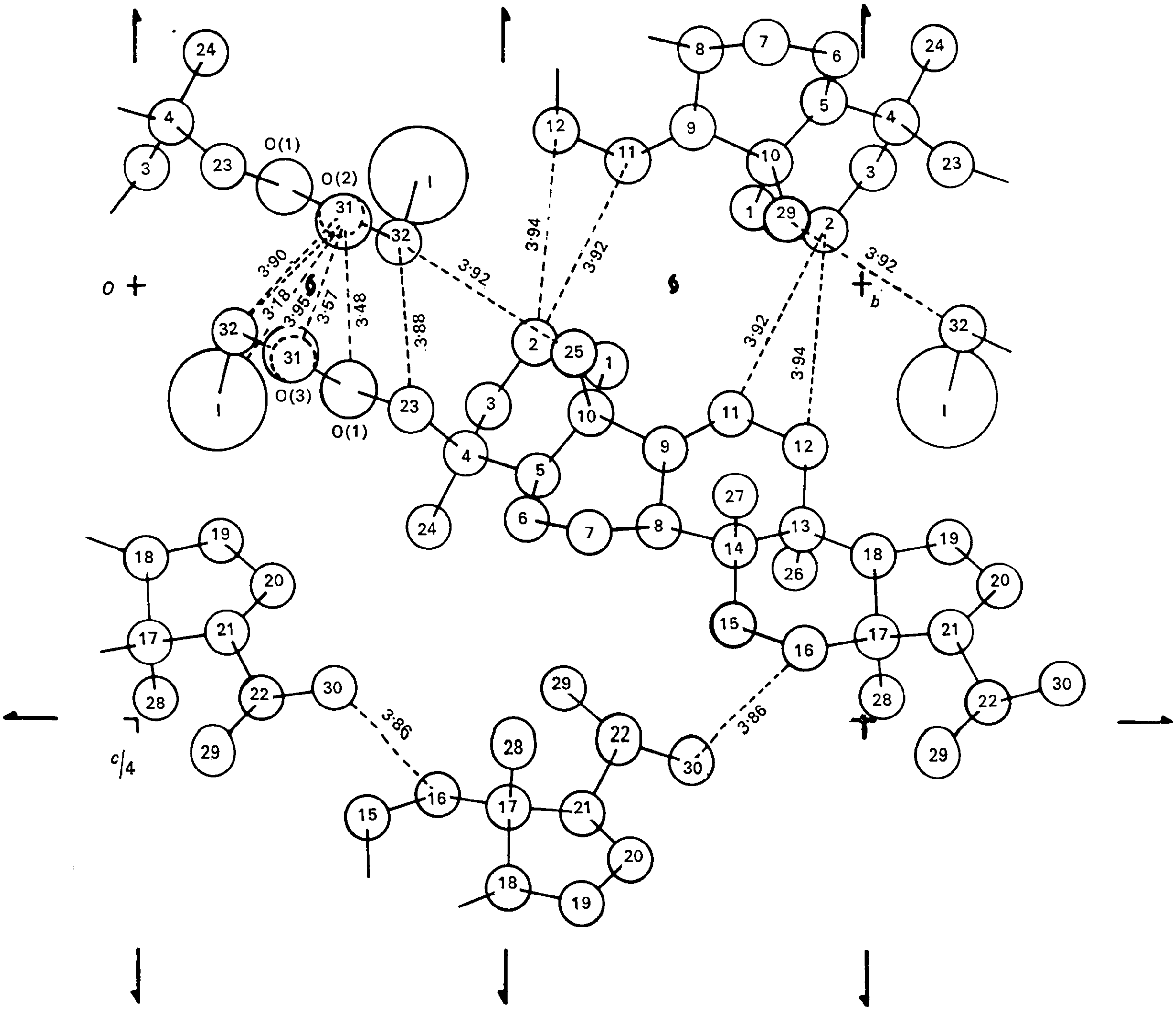

Fig. 5. Packing diagram, projecting down the *a* axis.

Bond lengths and bond angles

The bond lengths and bond angles for all non-hydrogen atoms calculated from the final atomic coordinates (Table 1) are listed in Tables 7 and 8, together with the associated standard deviations.

The bond lengths and bond angles in the iodoacetate chain are normal and compare well with those obtained by other workers (Fridrichsons & Mathieson, 1953; O'Connell, 1965; Arnott, Davie, Robertson, Sim & Watson, 1961; Hall & Maslen, 1965). More interesting are the sp^3-sp^3 single bonds of carbon atoms in the ring system. The mean value for 30 sp^3-sp^3 single C–C bonds is 1·54 Å, which compares very well with the C–C bond in diamond. However, there is considerable variation among the individual bonds, the largest being 1·627 Å for C(8)–C(14) and the shortest being 1·427 Å for C(2)–C(3). Many of the bond angles formed by pairs of sp^3-sp^3 bonds deviate from the tetrahedral value of 109°28′ by 3σ. The large variation in bond lengths and bond angles indicates that the structure is subject to considerable strain, the principal sources of which arise from the twisting of the five-membered *E* ring, from the repulsion of methyl groups at C(26) and C(28) and also from the constraint placed on C(8), C(9), C(11) and C(12) to lie in one plane due to the presence of the double bond at C(9)–C(11).

The interatomic distance between C(26) and C(28) is 2·95 Å, which is much less than the normal van der Waals separation for two methyl groups, assuming a van der Waals radius for a methyl carbon atom of 2·0 Å (Pauling, 1960). Repulsion between the two methyl groups is evident in that the angles C(18)–C(13)–C(28) (113·5°) and C(18)–C(17)–C(28) (116·8°) are much larger than normal.

The five membered ring *E* is strongly twisted and this is seen in the small bond angles: C(18)–C(17)–C(21), C(18)–C(19)–C(20), C(17)–C(18)–C(19) and C(17)–C(21)–C(20) are 97·6°, 102°, 104° and 104·8° respectively. The severe distortion at ring *E* is not unusual in structures of this type, *e.g.* methyl melaleucate iodoacetate (Hall & Maslen, 1965). The corresponding angles in that structure are 100°, 100°, 102° and 105°.

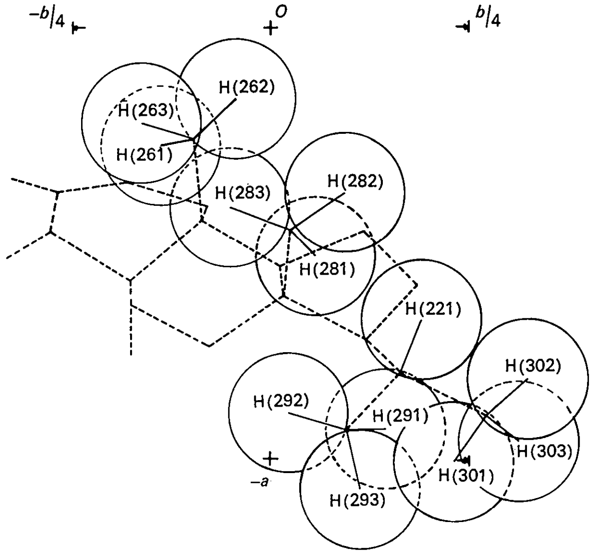

Fig. 6. The staggered conformation of methyl groups.

It is interesting to note that all the long bonds (greater by at least σ than 1·54 Å) are associated with one or more fully substituted carbon atoms, with the exception of C(5)–C(6) which is associated with C(5), a triply substituted carbon atom. Moreover, every fully substituted carbon atom other than C(4) has at least one long bond attached to it. The formation of long bonds to C(4) is not favoured since the angle C(4)–C(5)–C(10) is large and the strain seems better relieved by relaxing the C(5)–C(6) bond.

The effect of the degree of substitution on sp^3-sp^3 single bonds for carbon has also been observed in the structures of methyl melaleucate iodoacetate ($R=0{\cdot}079$; Hall & Maslen, 1965) and beyerol monoethylidine iodoacetate ($R=0{\cdot}107$; O'Connell, 1965). One should perhaps note, however, that each of the three structures contains an iodine atom and consequently the estimated standard deviation for all C–C bonds is fairly large ($\sigma\simeq0{\cdot}03$ Å). The data for the three structures were collected independently, and although the structures were refined by the same method one could still infer with some confidence that the anomalously long C–C bonds are real and are affected by the degree of substitution in the carbon atom. The effect can indeed be largely explained in terms of strong non-bonded interactions between atoms (Bartell, 1959, 1962). For every hydrogen atom that is substituted by a carbon atom which is normally bonded to some other atoms, the environment necessarily becomes more crowded and non-bonding repulsive forces become stronger, resulting in the lengthening of the C–C bond.

It is difficult to determine the precise nature of how the non-bonded atoms interact. An attempt was made to relate the bond lengths to the angular rotation from the ideal staggered conformation for the C–C bonds in all the three structures but no obvious relationship could be adduced. It seems probable that long range steric effects are at least in part responsible for the extension of these bonds, as shown by the fact that the extension of some of them is rather larger than that found in hexamethylethane (Bauer & Beach, 1942).

The hydrogen atom positions

The method of locating hydrogen atoms was described in §3 under *Location of hydrogen atoms*. Although the atomic sites of most of the hydrogen atoms appeared in the positive areas of the difference maps their coordinates were determined only approximately, since the 'peak heights' of the hydrogen atoms are not significantly larger than the standard deviation $\sigma(\varrho)$ which is equal to 0·3 e.Å^{-3}. It is the consistency of their appearance in a physically meaningful way that suggests that they are at least nearly correct. This is affirmed by the drop of 0·009 in the R index by the inclusion of hydrogen atoms in the structure factor evaluation, which is large considering the relatively low contribution of the hydrogen atoms in a heavy atom structure of this type.

The configurations of the hydrogen atoms belonging to the seven methyl groups are of particular interest. They appear rather unambiguously for the six methyl groups which are constrained to adopt a staggered conformation by close van der Waals contacts. An example of the staggered conformation is illustrated in Fig. 6 for the C(26) and C(28) methyl groups.

Thermal parameters

The magnitudes and the direction cosines of the principal axes of thermal vibration for non-hydrogen atoms evaluated from the values of B_{ij} contained in Table 2 are listed in Table 5. The direction cosines were computed with respect to the orthogonal cell axes. The last column of Table 5 gives the U_i values which are the root mean square amplitudes of vibration. Fig. 3 illustrates the thermal ellipsoids on an arbitrary scale.

In view of the large standard deviations for the thermal parameters no detailed discussion is warranted. All atoms with the exception of C(3), however, seem to execute physically sensible thermal vibrations and the molecule as a whole appears to vibrate more like a flexible chain than a rigid body. Generally, the thermal eigenvalues of the fully substituted carbon atoms in the ring system are smaller than those of the methyl carbon atoms.

Atom C(3) is the only atom that exhibits anomalous thermal behaviour. It is physically improbable for any atom to vibrate preferentially along one of its bonds, and it appears that the determination of its thermal parameters is in error. Lonsdale & Milledge (1961) have pointed out that the orientations of thermal ellipsoids are sensitive to any errors in the cross terms in the values of B_{ij} and it is possible that factors such as inaccuracies in the absorption corrections and the non-inclusion of the imaginary part of the scattering factors may have influenced the determination of the thermal parameters. However, it is difficult to see why only the parameters of one atom should be critically affected. No explanation has been found for this anomaly.

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