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The Crystal Structure of Beyerol Monoethylidene Iodoacetate

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The crystal structure of beyerol monoethylidene iodoacetate ($C_{24}H_{35}O_4I$), a derivative of the diterpene-triol beyerol, has been determined by two-dimensional Patterson and three-dimensional Fourier methods and refined to a final R index of 0·113. The unit cell is orthorhombic, space group $P2_12_12_1$ with $a = 7{\cdot}806$, $b = 11{\cdot}731$, $c = 25{\cdot}161$ Å. The iodine atoms form an approximately centrosymmetric array, but inverse overlap effects appear to be small. It is shown that systematic errors in the estimation of film factors can lead to large discrepancies in the final parameters. The molecular distortions are explained as being largely due to the fusion of the bridge system across the C ring and to intramolecular steric interactions.

Introduction

Beyerol, a diterpene triol with the empirical formula $C_{20}H_{32}O_3$, was extracted from the viscid shrub *Beyeria leschenaultii* (DC) Baill. var. *drummondii* (Muell. Arg.) Gruning in the Chemistry Department of the University of Western Australia (Jefferies, Rosich, White & Woods, 1962). The occurrence of a large quantity of a diterpene in a family so well known for its triterpenes prompted an extensive program of research by Jefferies and his co-workers. By the use of chemical and spectroscopic techniques the structure was established as that shown in Fig. 1. Since beyerol is of particular interest in the study of natural products, an X-ray structure analysis was undertaken as an independent confirmation of the structure obtained from chemical and spectroscopic evidence. An iodine derivative, beyerol monoethylidene iodoacetate, was prepared for this analysis.

Experimental

Crystal data

Beyerol monoethylidene iodoacetate ($C_{24}H_{35}O_4I$)
$a = 7{\cdot}806 \pm 5$, $b = 11{\cdot}731 \pm 6$, $c = 25{\cdot}161 \pm 9$ Å.
$U = 2304{\cdot}05$ Å^3
$Z = 4$; $D_m = 1{\cdot}49 \pm 0{\cdot}01$ g.cm^{-3} by flotation;
$D_x = 1{\cdot}483 \pm 0{\cdot}002$ g.cm^{-3}
Space group: $P2_12_12_1$;
Absent spectra: $h00$, h odd; $0k0$, k odd; $00l$, l odd.
$\mu = 113{\cdot}5$ cm^{-1} for Cu $K\alpha$ radiation.

Intensity data

Crystals suitable for X-ray data collection were supplied by R. Rosich, Chemistry Department, University of Western Australia. The crystals, which were stable at room temperature, were in the form of flat rectangular plates elongated in the a-axis direction. Two specimens with dimensions $0{\cdot}90 \times 0{\cdot}33 \times 0{\cdot}07$ and $0{\cdot}30 \times 0{\cdot}60 \times 0{\cdot}13$ mm^3 were selected for the collection of intensities on layers $h = 0$ to 6 and $k = 0$ to 6, respectively, using multi-film and exposure equi-inclination Weissenberg techniques. Examination of these films revealed a systematic variation in the reflexion intensities. Terms having the conditions

$$0kl,\ k = 2n + 1$$
$$\text{general},\ h + k/2 + l = 2n + 1$$

were consistently weaker than their neighbours. This variation is discussed in more detail below.

The intensities were estimated by visual comparison with a graduated scale. Reflexions too weak to be observed were given a value equal to the smallest measurable intensity and treated as described below. Film factors used in the initial solution and refinement were obtained by averaging the ratio of intensities of reflexions common to adjacent films. Later it became apparent that systematic errors had occurred in the film factor estimation. They were therefore redetermined and a new refinement was undertaken.

General absorption corrections (Busing & Levy, 1957) and Lorentz and polarization factors were applied to the data. The interlayer correlation scales were calculated by a comparison of reflexions common to both a- and b-axis blocks. The agreement index

$$R_c = 2\, \Sigma\, |F_a - F_b| / \Sigma\, |F_a + F_b|$$

was 0·15 for the observed terms.

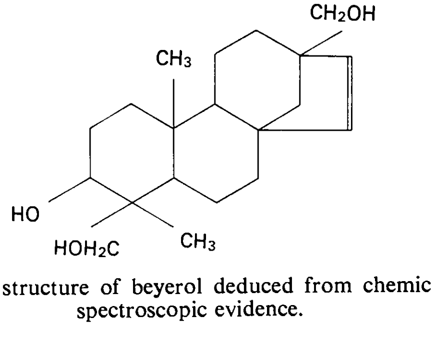

Fig. 1. The structure of beyerol deduced from chemical and spectroscopic evidence.

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Solution of the structure

Two-dimensional Patterson syntheses were evaluated for the [100] and [010] projections. Peaks corresponding to iodine–iodine vectors were readily identified, and the iodine atom was located at

$$x/a=0{\cdot}111,\ y/b=0{\cdot}125,\ z/c=0{\cdot}250\,.$$

These agree well with the final values $x/a=0{\cdot}1065$, $y/b=0{\cdot}1200$, $z/c=-0{\cdot}2516$, obtained from the least-squares refinement. The *c* axis has been reversed to give the correct absolute configuration. The systematic variation of intensities on the Weissenberg films is readily explained in terms of these coordinates since the iodine atom, which lies close to $(x, \frac{1}{8}, -\frac{1}{4})$, provides only a small contribution to the X-ray scattering for reflexions with the conditions described above.

The phases of all reflexions having a non-zero iodine contribution were used to calculate a three-dimensional Fourier synthesis with coefficients $|F_o|$. Since the heavy atoms form an approximately centrosymmetric array this synthesis contained false mirror planes at $z/c=\frac{1}{4}$ and $\frac{3}{4}$. In some similar cases (*e.g.* Duffield, Jefferies, Maslen & Rae, 1963) a slight displacement of the heavy atom from the pseudo mirror has been used to resolve the false symmetry. However, in the present analysis there was no evidence for a shift of the iodine atom from $z/c=\frac{1}{4}$. Thus all atomic peaks were exactly mirrored across this plane, producing the effect of two molecules per asymmetric unit interwoven with each other.

The method of structure solution adopted was to search for atomic peaks in tetrahedral configurations with separation distances approximately equal to the carbon–carbon single bond length (1·54 Å). Peaks not satisfying these conditions were considered to be the images of atoms lying on the opposite side of the false mirror. There were thirty-seven independent peaks with heights greater than 2 e.Å^{-3}, of which eight were less than 3 e.Å^{-3}. The region of the electron density maps near the iodine atoms contained strong diffraction ripple, making the tracing of the acetate chain difficult. The search for tetrahedrally situated peaks was therefore centred in the region of the synthesis away from the iodine, and fourteen atomic positions of the main beyerol skeleton were deduced. These atoms were arbitrarily assigned scattering factors of carbon and isotropic temperature factor coefficients $B=3{\cdot}5$ Å^2 for the evaluation of a set of structure factors. The scattering factor curves used in this and subsequent calculations for carbon and oxygen were those of Freeman (1959), and for iodine that by Thomas & Umeda (1957), corrected for the real part of the anomalous dispersion coefficient (*International Tables for X-ray Crystallography*, 1962), was employed.

In a second three-dimensional electron density synthesis, with phases based on this partial structure, the effect of the pseudo mirror was almost completely eliminated and the remaining ten atoms of the main beyerol skeleton were readily identified. A further three-dimensional difference synthesis was used to determine the positions of the four atoms of the acetate

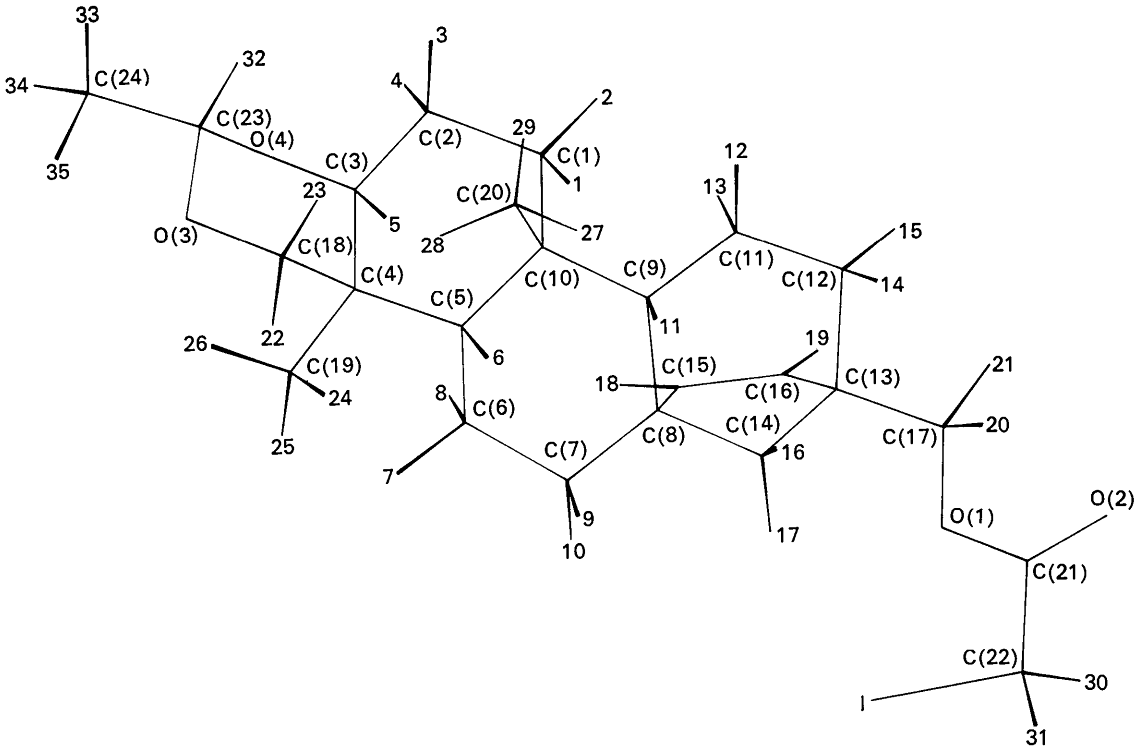

Fig. 2. Atom numbering.

chain. From chemical considerations atoms O(1), O(2), O(3) and O(4) were weighted as oxygen. The atom numbering is shown in Fig. 2. The structure factor residual, assuming a mean isotropic temperature coefficient $B=3{\cdot}5$ Å^2, for the proposed skeleton was 0·23.

The refinement

The structure was refined by least-squares methods with Mair's (1962) program for the IBM 1620 computer. This program, which makes use of the block diagonal approximation, allows positional, isotropic or anisotropic parameters to be varied. The function $\Sigma\, w(|F_o|-|F_c|)^2$ is minimized. Throughout the refinement unobserved terms with $|F_o|$ greater than $|F_c|$ were given zero weight, while those with $|F_o|$ less than $|F_c|$ were treated as observed reflexions. This is similar to the treatment of unobservably weak reflexions suggested by Vand & Dunning (1965). Reflexion weights were calculated according to the scheme

$$\omega=1/(1+[(|F_o|-b)/a]^2)\,,$$

the values of a and b being determined from plots of $(|F_o|-|F_c|)^2-1)$ *versus* $|F_o|$ (Mills & Rollett, 1960).

After a series of least-squares cycles, during which all positional parameters, anisotropic thermal parameters for the iodine atom and isotropic thermal parameters for the oxygen and carbon atoms were varied, the R index converged to 0·152 and no further significant shifts were indicated. Examination of the agreement between the observed and calculated structure factors for various intervals of $|F_o|$ showed that there were systematic errors in the data. In general, terms with $|F_o|$ less than 40 electrons were too large, while those with $|F_o|$ greater than 70 electrons were too small. Errors of this type are consistent with a systematic underestimation of the visually estimated film factors used in the initial data reduction. It was necessary, therefore, to redetermine the film factors by a method independent of visual estimation. This was accomplished by measuring the intensities of a number of reflexions on adjacent films with a microdensitometer. A mean film factor $R_0=2{\cdot}80\pm0{\cdot}10$ was determined for normal beam incidence. The appropriate angular corrections for oblique incidence were applied to the nonzero layer films (Grenville-Wells, 1955). The correlation R index (0·11 for the observed terms) indicated a marked improvement in the agreement of the a and b axis data after the application of new film factors.

The refinement was continued with the corrected data and after three cycles of least squares the residual decreased to 0·136. Anisotropic temperature factors were then introduced for all carbon and oxygen atoms and after three more rounds of refinement the R value decreased to 0·122.

Examination of the molecular formula of beyerol monoethylidene iodoacetate shows that each molecule contains thirty-five hydrogen atoms. Twenty six of these are sterically positioned and nine belong to methyl groups. The coordinates of the former atoms were calculated assuming a C–H distance of 1·08 Å. Examination of a difference synthesis, phased on the nonhydrogen atoms, showed that in twenty-two cases these calculated positions corresponded to positive areas of electron density with maxima varying between 0·1 and 0·8 e.Å^{-3}. The three planes in which the methyl hydrogen atoms were expected to lie were extracted from the difference synthesis and a possible orientation was deduced for each group. The hydrogen atom numbering is shown in Fig. 2 while their atomic coordinates are listed in Table 1. The structure factor residual, including all hydrogen atoms with isotropic temperature factor coefficients $B=6{\cdot}0$ Å^2, decreased by 0·005 to 0·117.

Table 1. *Hydrogen atom coordinates*

	x/a	y/b	z/c
H(1)	−0·768	−0·197	−0·025
H(2)	−0·910	−0·164	−0·076
H(3)	−1·009	−0·348	−0·032
H(4)	−0·945	−0·378	−0·097
H(5)	−0·719	−0·402	−0·001
H(6)	−0·484	−0·294	−0·049
H(7)	−0·297	−0·397	−0·115
H(8)	−0·424	−0·339	−0·165
H(9)	−0·213	−0·201	−0·082
H(10)	−0·172	−0·208	−0·150
H(11)	−0·539	−0·109	−0·057
H(12)	−0·790	−0·012	−0·088
H(13)	−0·741	−0·033	−0·152
H(14)	−0·589	0·141	−0·077
H(15)	−0·678	0·162	−0·141
H(16)	−0·322	0·022	−0·071
H(17)	−0·181	0·014	−0·125
H(18)	−0·431	−0·150	−0·221
H(19)	−0·479	0·071	−0·235
H(20)	−0·347	0·253	−0·109
H(21)	−0·447	0·262	−0·171
H(22)	−0·548	−0·532	−0·151
H(23)	−0·758	−0·477	−0·151
H(24)	−0·429	−0·478	−0·010
H(25)	−0·367	−0·525	−0·073
H(26)	−0·519	−0·601	−0·036
H(27)	−0·692	−0·192	−0·188
H(28)	−0·700	−0·350	−0·167
H(29)	−0·875	−0·245	−0·154
H(30)	0·085	0·352	−0·247
H(31)	0·153	0·303	−0·186
H(32)	−0·985	−0·562	−0·098
H(33)	−1·055	−0·724	−0·034
H(34)	−0·953	−0·787	−0·087
H(35)	−0·833	−0·763	−0·028

After three more cycles of least squares the average shift in atomic positions was 0·004 Å and none of the parameter shifts were significant when compared with their e.s.d.'s. The structure was therefore considered to be refined to the limit of accuracy of the data. The final structure factor residuals were 0·113 when all terms were included and 0·107 for the observed terms only. The observed and calculated structure factors are listed in Table 2. Examination of the agreement between $\Sigma\,|F_o|$ and $\Sigma\,|F_c|$ for ranges of $|F_o|$ showed that there were no large systematic differences between the observed and calculated values, indicating that the ef-

Table 2. *Observed and calculated structure factors*

H	K	L	FO	FC	AO	BO
0	0	6	254.2	214.4	-254.2	0.0
		8	161.1	124.0	161.1	0.0
		10	122.6	104.5	-122.6	0.0
		12	73.4	62.1	73.4	0.0
		14	137.8	129.9	-137.8	0.0
		16	106.4	100.8	106.4	0.0
		18	69.2	67.9	-69.2	0.0
		20	53.4	55.3	53.4	0.0
		22	61.8	56.8	-61.8	0.0
		24	33.6	29.9	33.6	0.0
		26	18.4	18.0	-18.4	0.0
		28	20.4	20.0	20.4	0.0
		30	13.9	12.2	-13.9	0.0
	1	3	53.0	36.3	0.0	-53.0
		4	130.0	106.3	0.0	130.0
		5	132.0	100.6	0.0	132.0
		6	142.0	119.0	0.0	142.0
		7	11.0	9.2	0.0	-11.0
		8	23.3	22.3	0.0	23.3
		9	10.7	11.9	0.0	-10.7
		10	4.2U	2.0	0.0	4.2
		11	9.1	9.3	0.0	9.1
		12	22.6	21.6	0.0	-22.6
		13	12.9	15.5	0.0	-12.9
		14	26.2	27.8	0.0	26.2
		15	8.4	8.1	0.0	8.4
		16	6.8U	6.9	0.0	-6.8
		17	16.2	17.5	0.0	-16.2
		18	4.9U	7.1	0.0	4.9
		19	4.9U	7.6	0.0	4.9
		20	16.8	16.5	0.0	-16.8
	2	0	8.1	11.3	-8.1	0.0
		1	110.9	145.5	110.9	0.0
		2	44.6	45.8	44.6	0.0
		3	158.5	172.8	-158.5	0.0
		4	34.0	31.5	34.0	0.0
		5	149.7	149.2	149.7	0.0
		6	18.8	19.9	-18.8	0.0
		7	144.2	140.6	-144.2	0.0
		8	54.0	48.3	54.0	0.0
		9	167.5	176.7	167.5	0.0
		10	4.2U	7.3	4.2	0.0
		11	173.3	172.5	-173.3	0.0
		12	35.9	34.5	-35.9	0.0
		13	96.7	91.1	96.7	0.0
		14	23.9	23.5	-23.9	0.0
		15	73.4	77.4	-73.4	0.0
		16	8.4U	12.1	8.4	0.0
		17	63.1	71.9	63.1	0.0
		18	24.3	23.3	-24.3	0.0
		19	53.4	56.8	-53.4	0.0
		20	4.9U	3.5	-4.9	0.0
		21	40.4	42.2	40.4	0.0
		22	5.2U	4.8	-5.2	0.0
		23	36.9	43.4	-36.9	0.0
		24	4.5U	6.2	4.5	0.0
		25	30.7	32.0	30.7	0.0
		26	8.4	9.7	8.4	0.0
		27	15.2	17.0	-15.2	0.0
		28	3.6U	1.4	3.6	0.0
		29	20.7	20.7	20.7	0.0
		30	2.9U	.9	-2.9	0.0
		31	13.6	14.4	-13.6	0.0
	3	2	22.0	19.3	0.0	-22.0
		3	13.9	10.8	0.0	-13.9
		4	22.0	20.2	0.0	22.0
		5	64.7	58.4	0.0	-64.7
		6	16.2	11.5	0.0	-16.2
		7	37.5	34.0	0.0	37.5
		8	85.7	76.8	0.0	85.7
		9	18.4	12.0	0.0	18.4
		10	9.7	6.1	0.0	9.7
		11	18.4	16.9	0.0	16.4
		12	15.2	12.9	0.0	-15.2
		13	18.8	21.3	0.0	-18.8
		14	15.5	13.5	0.0	15.5
		15	10.4	9.7	0.0	10.4
		16	5.5U	.8	0.0	5.5
		17	14.6	13.1	0.0	-14.6
		18	4.9U	0.0	4.9	0.0
		19	16.2	15.0	0.0	16.2
		20	5.2U	6.7	0.0	-5.2
		21	16.8	19.5	0.0	-16.8
	4	0	84.1	116.5	-84.1	0.0
		1	8.4	10.9	8.4	0.0
		2	127.4	158.9	127.4	0.0
		3	40.4	43.0	-40.4	0.0
		4	122.9	135.5	-122.9	0.0
		5	46.6	48.2	46.6	0.0
		6	149.1	162.5	149.1	0.0
		7	36.9	36.6	-36.9	0.0
		8	114.8	126.0	-114.8	0.0
		9	3.6U	3.8	3.6	0.0
		10	83.8	83.4	83.8	0.0
		11	8.7U	2.9	-8.7	0.0
		12	98.0	111.6	-98.0	0.0
		13	11.3	13.3	-11.3	0.0
		14	68.2	77.5	68.2	0.0
		15	6.1U	9.9	-6.1	0.0
		16	62.7	69.9	-62.7	0.0
		17	5.8U	1.3	5.8	0.0
		18	63.1	72.4	63.1	0.0
		19	5.2U	5.3	-5.2	0.0
		20	42.7	49.0	-42.7	0.0
		21	11.6	12.8	11.6	0.0
		22	21.0	24.3	21.0	0.0
		23	5.2U	4.4	-5.2	0.0
		24	23.6	25.7	-23.6	0.0
		25	4.2U	4.4	-4.2	0.0
		26	20.4	27.5	20.4	0.0
		27	3.6U	1.4	-3.6	0.0
		28	16.5	19.4	-16.5	0.0
		29	2.9U	4.0	2.9	0.0
		30	9.7	11.5	9.7	0.0
	5	1	16.2	18.8	0.0	16.2
		2	16.5	16.3	0.0	-16.5
		3	10.7	12.8	0.0	10.7
		4	6.5	1.3	0.0	-6.5
		5	16.2	15.0	0.0	16.2
		6	3.6U	6.3	0.0	-3.6
		7	7.8	7.0	0.0	7.8
		8	22.0	24.0	0.0	22.0
		9	4.2U	4.8	0.0	-4.2
		10	15.9	13.7	0.0	15.9
		11	20.4	18.5	0.0	-20.4
		12	5.2U	4.3	0.0	-5.2
		13	5.8U	7.8	0.0	-5.8
		14	19.4	21.3	0.0	-19.4
		15	6.8U	9.7	0.0	6.8
		16	20.4	23.4	0.0	20.4
	6	0	34.0	44.9	-34.0	0.0
		1	76.7	96.6	-76.7	0.0
		2	22.0	21.8	22.0	0.0
		3	89.3	107.6	89.3	0.0
		4	17.5	21.7	-17.5	0.0
		5	117.4	131.8	-117.4	0.0
		6	4.2U	5.7	4.2	0.0
		7	83.8	96.3	83.8	0.0
		8	4.2U	1.7	4.2	0.0
		9	110.0	116.4	-110.0	0.0
		10	24.9	25.3	24.9	0.0
		11	57.2	63.3	57.2	0.0
		12	23.3	24.0	-23.3	0.0
		13	49.5	55.8	-49.5	0.0
		14	6.5U	5.2	6.5	0.0
		15	55.3	67.0	55.3	0.0
		16	7.4U	2.8	-7.4	0.0
		17	45.3	46.1	-45.3	0.0
		18	12.9	13.0	12.9	0.0
		19	28.5	29.8	28.5	0.0
		20	5.5U	8.1	-5.5	0.0
		21	27.2	38.8	-27.2	0.0
		22	5.2U	6.1	5.2	0.0
		23	22.0	26.7	22.0	0.0
		24	3.9U	3.7	3.9	0.0
		25	30.4	21.3	-30.4	0.0
	7	2	28.1	24.0	0.0	28.1
		3	7.1	6.0	0.0	-7.1
		4	9.4	7.4	0.0	-9.4
		5	33.6	34.9	0.0	33.6
		6	24.9	26.2	0.0	-24.9
		7	4.5U	2.6	0.0	4.5
		8	12.9	15.0	0.0	12.9
		9	4.9U	5.0	0.0	4.9
		10	12.9	14.4	0.0	-12.9
	8	0	91.5	96.3	91.5	0.0
		1	3.9U	3.2	-3.9	0.0
		2	63.7	71.8	-63.7	0.0
		3	25.2	24.1	25.2	0.0
		4	38.8	43.3	38.8	0.0
0	8	5	4.9U	2.6	4.9	0.0
		6	82.1	91.8	-82.1	0.0
		7	4.9U	13.1	4.9	0.0
		8	77.6	81.3	77.6	0.0
		9	46.6	50.8	-46.6	0.0
		10	48.8	46.6	-48.8	0.0
		11	16.2	17.3	16.2	0.0
		12	45.0	47.6	45.0	0.0
		13	22.6	21.9	-22.6	0.0
		14	46.3	53.4	-46.3	0.0
		15	7.1U	5.8	7.1	0.0
		16	42.0	44.5	42.0	0.0
		17	6.8U	1.3	6.8	0.0
		18	15.2	15.3	-15.2	0.0
		19	5.8U	6.7	5.8	0.0
		20	33.0	37.1	33.0	0.0
		21	4.9U	2.3	-4.9	0.0
		22	24.3	30.8	-24.3	0.0
		23	4.2U	5.8	4.2	0.0
		24	12.0	15.0	12.0	0.0
	9	2	34.6	35.7	0.0	-34.6
		3	13.3	11.8	0.0	13.3
		4	25.6	26.5	0.0	-25.6
		5	5.2U	.5	0.0	-5.2
		6	31.7	35.2	0.0	31.7
		7	5.2U	6.7	0.0	-5.2
		8	8.7U	11.8	0.0	-8.7
		9	15.2	13.9	0.0	15.2
		10	3.2U	7.7	0.0	-3.2
	10	0	40.1	46.9	40.1	0.0
		1	24.3	25.1	24.3	0.0
		2	29.8	34.0	-29.8	0.0
		3	79.9	86.8	-79.9	0.0
		4	5.2U	11.5	-5.2	0.0
		5	34.0	39.5	34.0	0.0
		6	11.0	11.8	-11.0	0.0
		7	28.5	24.8	-28.5	0.0
		8	20.7	25.4	20.7	0.0
		9	37.2	38.8	37.2	0.0
		10	6.1U	1.7	-6.1	0.0
		11	50.1	50.3	-50.1	0.0
		12	6.1U	1.6	6.1	0.0
		13	36.9	39.2	36.9	0.0
		14	6.8U	8.7	-6.8	0.0
		15	20.4	25.4	-20.4	0.0
		16	14.6	15.7	14.6	0.0
		17	25.6	29.3	25.6	0.0
		18	5.2U	5.2	-5.2	0.0
		19	23.0	23.3	-23.0	0.0
		20	4.2U	3.5	4.2	0.0
		21	17.5	19.1	17.5	0.0
		22	3.6U	.1	-3.6	0.0
		23	12.0	14.6	-12.0	0.0
	11	1	15.5	19.1	0.0	15.5
	12	0	38.5	40.5	-38.5	0.0
		1	10.4	9.3	10.4	0.0
		2	31.1	32.2	31.1	0.0
		3	16.2	16.9	-16.2	0.0
		4	34.0	34.6	-34.0	0.0
		5	4.9U	7.5	4.9	0.0
		6	26.5	27.7	26.5	0.0
		7	16.2	15.2	-16.2	0.0
		8	20.4	22.7	-20.4	0.0
		9	5.5U	9.5	5.5	0.0
		10	19.4	19.9	19.4	0.0
		11	5.8U	2.9	-5.8	0.0
		12	19.1	20.2	-19.1	0.0
		13	5.5U	8.7	5.5	0.0
		14	17.5	18.9	17.5	0.0
		15	4.9U	5.0	-4.9	0.0
		16	12.0	15.5	-12.0	0.0
		17	3.2U	2.2	3.2	0.0
		18	13.9	15.7	13.9	0.0
	14	0	15.9	13.0	-15.9	0.0
		1	16.5	16.0	-16.5	0.0
		2	4.2U	4.6	4.2	0.0
		3	13.6	13.2	13.6	0.0
		4	4.9U	.2	4.9	0.0
		5	17.8	20.0	-17.8	0.0
		6	4.5U	9.5	4.5	0.0
		7	12.6	13.6	12.6	0.0
		8	10.7	11.2	-10.7	0.0
		9	13.3	11.6	-13.3	0.0
1	0	1	55.6	63.2	0.0	-55.6
		2	46.3	49.6	46.3	0.0
		3	192.4	244.7	0.0	192.4
		4	164.6	182.1	164.6	0.0
		5	188.9	236.9	0.0	-188.9
		6	17.8	14.5	17.8	0.0
		7	53.7	47.7	0.0	53.7
		8	9.4	7.5	-9.4	0.0
		9	107.4	96.1	0.0	-107.4
		10	5.8U	4.5	-5.8	0.0
		11	147.5	128.3	0.0	147.5
		12	6.1U	7.7	6.1	0.0
		13	88.3	82.5	0.0	-88.3
		14	31.1	29.3	31.1	0.0
		15	62.4	58.8	0.0	62.4
		16	20.4	12.0	-20.4	0.0
		17	61.5	54.9	0.0	-61.5
		18	22.3	20.2	-22.3	0.0
		19	41.7	33.6	0.0	41.7
		20	25.2	20.1	25.2	0.0
		21	38.2	37.9	0.0	-38.2
		22	6.5U	4.7	-6.5	0.0
		23	30.7	31.3	0.0	30.7
		24	6.5U	.9	6.5	0.0
		25	26.5	21.6	0.0	-26.5
		26	12.9	12.3	-12.9	0.0
		27	24.9	24.4	0.0	24.9
		28	5.2U	3.2	-5.2	0.0
		29	14.6	13.5	0.0	-14.6
		30	4.2U	.2	-4.2	0.0
		31	10.0	11.5	0.0	10.0
	1	0	32.0	26.5	0.0	-32.0
		1	52.4	60.0	-45.5	25.9
		2	134.5	150.5	63.4	-118.6
		3	102.8	98.6	73.8	-71.6
		4	104.8	100.5	-3.0	104.7
		5	88.1	90.1	-25.3	84.4
		6	99.3	81.8	28.5	-84.6
		7	167.2	145.3	16.9	-166.3
		8	75.1	67.4	-40.5	63.0
		9	122.3	98.5	-41.4	115.0
		10	47.5	41.2	-13.0	-45.7
		11	18.1	14.1	4.7	-17.5
		12	73.1	69.1	31.2	66.1
		13	39.8	35.6	15.1	36.8
		14	43.0	39.4	-6.5	-42.5
		15	46.6	43.5	3.7	-46.4
		16	37.2	39.6	5.5	36.7
		17	42.0	38.8	-3.4	41.9
		18	22.0	20.8	-3.1	-21.8
		19	23.6	20.6	11.6	-20.5
		20	35.6	34.7	-1.4	35.5
		21	16.2	15.5	-11.9	10.9
		22	21.7	19.5	-12.2	-17.9
		23	25.2	27.7	16.6	-19.0
		24	16.2	15.7	9.2	13.3
		25	15.5	16.7	-3.1	15.2
		26	16.2	15.9	-.9	-16.1
	2	0	71.2	91.6	0.0	71.2
		1	66.6	67.3	18.2	63.9
		2	98.7	136.1	18.9	-96.8
		3	22.0	19.5	-8.0	20.5
		4	109.0	140.9	-4.1	108.9
		5	51.7	44.2	-46.5	22.7
		6	105.8	119.4	-20.8	-103.7
		7	48.5	41.4	17.0	45.4
		8	118.0	116.7	30.1	114.1
		9	36.7	36.2	24.2	-26.9
		10	102.5	99.9	27.1	-98.9
		11	8.4U	10.3	1.8	8.2
		12	75.0	80.8	16.4	73.2
		13	41.4	38.7	15.1	-38.5
		14	82.8	92.3	-3.6	-82.7
		15	32.7	31.0	-29.3	-14.5
		16	64.4	64.5	9.6	63.6
		17	4.9	5.6	4.6	1.6
		18	42.0	37.4	4.8	-41.8
		19	4.9U	6.8	.5	4.8
		20	49.5	48.2	-10.2	48.4
		21	4.9U	5.6	2.2	4.3
		22	30.1	30.8	-14.3	-26.5
		23	5.2U	10.1	-5.1	1.1
		24	23.3	21.3	0.0	23.3
		25	4.9U	3.6	-4.1	-2.6
		26	28.1	27.2	-.9	-28.1
		27	3.9U	4.3	-1.2	3.7
		28	14.6	15.0	2.3	14.4
1	2	29	3.2U	5.0	3.2	-.8
		30	8.4	7.5	-1.2	-8.3
	3	0	60.2	73.4	0.0	-60.2
		1	96.7	116.1	22.9	94.0
		2	51.7	59.9	-13.3	50.0
		3	43.3	46.7	3.6	-43.2
		4	78.6	85.6	13.7	-77.4
		5	38.5	41.2	1.6	38.4
		6	53.4	54.2	-10.7	52.3
		7	76.7	72.5	-19.2	-74.2
		8	69.5	59.0	11.9	-68.5
		9	61.8	60.2	-9.8	61.0
		10	55.3	47.5	-35.8	42.1
		11	65.0	60.2	-29.0	-58.2
		12	30.7	24.9	24.5	-18.5
		13	73.1	67.5	7.1	72.7
		14	39.1	37.8	0.0	39.1
		15	43.0	36.9	6.1	-42.6
		16	45.0	43.3	23.4	-38.4
		17	29.8	29.0	9.5	28.2
		18	33.3	36.6	-2.8	33.2
		19	23.0	18.2	7.0	-21.9
		20	18.1	16.4	2.6	-17.9
		21	26.8	27.4	5.7	26.2
		22	24.6	25.6	-10.8	22.1
		23	19.4	16.1	-1.7	-19.3
		24	18.1	15.2	5.3	-17.3
		25	12.9	9.9	-5.3	11.8
		26	13.6	10.7	-10.8	8.2
	4	0	37.5	34.9	0.0	37.5
		1	79.6	101.8	-8.4	79.4
		2	27.5	30.8	3.5	-27.3
		3	98.6	114.0	10.3	-98.1
		4	32.7	31.8	-31.1	10.0
		5	108.3	120.2	-7.3	108.1
		6	32.7	30.0	23.2	-23.0
		7	74.4	88.2	5.1	-74.2
		8	24.3	22.0	20.7	12.7
		9	82.1	83.9	25.1	78.2
		10	6.5U	15.2	4.6	-4.6
		11	78.6	84.3	-9.3	-78.0
		12	18.4	15.4	-18.4	0.0
		13	64.4	64.1	4.0	64.2
		14	9.1U	3.2	4.0	-8.1
		15	61.8	64.8	-3.4	-61.7
		16	8.1U	8.6	4.4	6.8
		17	44.3	49.4	-1.1	44.3
		18	7.4U	9.2	6.9	-2.8
		19	38.5	39.0	-7.1	-37.8
		20	7.8U	9.1	-4.8	6.1
		21	37.2	36.4	1.4	37.2
		22	7.8U	5.6	1.8	7.5
		23	30.7	32.0	-7.1	-29.9
		24	6.1U	5.8	-1.8	5.9
		25	19.1	17.9	5.6	18.2
		26	5.5U	4.7	4.0	-3.7
		27	12.9	12.7	-7.3	-10.7
		28	4.9U	7.0	-4.2	-2.4
		29	12.9	13.7	-.9	12.9
	5	0	63.1	73.2	0.0	-63.1
		1	78.3	92.1	39.3	-67.7
		2	82.5	96.3	-4.6	82.3
		3	21.7	26.4	-18.0	12.0
		4	49.5	55.3	19.9	-45.3
		5	38.2	37.6	-26.2	-27.8
		6	38.8	37.6	23.8	30.6
		7	62.4	62.4	1.1	62.4
		8	54.0	55.4	5.0	-53.8
		9	35.9	34.3	-1.8	-35.9
		10	47.9	44.0	-4.3	47.7
		11	50.1	45.4	-7.6	49.6
		12	43.0	39.5	2.6	-42.9
		13	37.2	35.9	12.1	-35.2
		14	44.6	40.1	2.6	44.5
		15	32.3	31.4	-7.4	31.5
		16	33.3	30.1	-1.5	-33.3
		17	23.6	18.7	17.2	-16.2
		18	20.4	18.8	.5	20.4
		19	26.2	27.0	-21.4	15.1
		20	19.4	17.5	9.0	-17.2
		21	22.3	23.0	12.5	-18.5
		22	18.1	18.2	-1.1	18.1
		23	14.9	15.7	0.0	14.9
		24	16.2	16.1	-1.0	-16.1
		25	5.5U	8.3	4.1	-3.6
		26	11.0	11.7	-6.2	9.1
	6	0	112.2	124.7	0.0	-112.2
		1	19.4	23.9	13.0	14.4
		2	66.6	80.9	-10.7	65.8
		3	18.1	18.8	-17.5	-4.6
		4	88.6	96.4	-23.6	-85.4
		5	46.6	43.3	27.9	37.3
		6	84.1	84.5	-4.3	84.0
		7	27.2	22.0	19.5	-18.9
		8	55.0	59.8	-5.3	-54.7
		9	12.0	12.9	-7.6	9.2
		10	60.5	60.6	7.8	60.0
		11	7.8U	11.9	-4.4	-6.4
		12	51.4	50.9	-9.7	-50.5
		13	8.1U	13.2	-7.1	3.9
		14	43.7	40.3	4.3	43.5
		15	9.4U	13.7	7.7	-5.3
		16	41.7	37.3	1.9	-41.7
		17	12.9U	4.6	5.7	11.6
		18	40.8	42.2	8.8	39.8
		19	9.1U	4.5	-2.1	-8.8
		20	28.5	33.1	-11.4	-26.1
		21	7.8U	7.7	-7.6	1.8
		22	25.6	25.2	8.9	24.0
		23	7.1U	10.2	1.3	-7.0
		24	19.7	15.2	3.6	-19.4
		25	8.7	8.6	-5.3	6.9
		26	17.1	16.6	4.5	16.5
	7	0	51.4	52.7	0.0	51.4
		1	41.7	50.4	8.5	-40.8
		2	38.2	38.2	0.0	-38.2
		3	33.0	38.4	-11.3	31.0
		4	36.9	39.1	-1.7	36.8
		5	46.9	52.2	14.3	-44.6
		6	6.5U	8.9	-2.0	-6.2
		7	55.6	50.3	1.3	55.6
		8	26.2	20.8	-4.4	25.8
		9	28.1	26.9	8.6	-26.8
		10	43.3	41.5	17.5	-39.6
		11	44.0	39.0	-16.3	40.8
		12	28.5	26.6	-11.0	26.2
		13	31.4	26.5	-4.9	-31.0
		14	33.3	28.8	23.6	-23.5
		15	36.9	32.4	-5.6	36.4
		16	11.0U	10.3	-7.7	7.9
		17	34.0	25.7	-4.1	-33.7
		18	23.9	25.2	10.9	-21.3
		19	20.7	17.1	-2.9	20.5
		20	13.6	12.3	-9.6	9.6
		21	14.6	15.5	8.9	-11.5
		22	7.1U	6.3	2.2	-6.8
		23	12.9	13.0	0.0	12.9
		24	16.5	15.1	-9.2	13.7
		25	10.7	9.0	1.5	-10.6
	8	0	5.5U	5.1	0.0	-5.5
		1	49.5	53.4	3.7	-49.3
		2	26.8	30.9	21.1	16.5
		3	55.0	57.9	-7.1	54.5
		4	14.8	14.9	-3.1	-14.5
		5	59.2	60.7	-2.9	-59.1
		6	26.5	26.6	-25.1	8.7
		7	48.5	52.7	20.2	44.1
		8	22.3	20.6	-10.2	-19.9
		9	43.7	40.0	17.3	-40.1
		10	9.7U	11.5	-9.3	-2.6
		11	66.3	62.3	3.3	66.2
		12	22.6	18.6	7.1	-21.5
		13	48.5	43.0	-33.2	-35.3
		14	21.0	22.0	-2.2	20.9
		15	33.0	25.5	12.7	30.4
		16	11.0U	7.2	-7.7	-7.9
		17	38.8	40.4	-2.0	-38.8
		18	8.7U	14.9	-.5	8.7
		19	26.8	22.9	-2.7	26.7
		20	7.1U	10.1	6.7	-2.4
		21	19.4	21.2	-9.9	-16.7
		22	6.5U	6.3	6.2	1.7
		23	19.1	19.0	6.5	18.0
		24	4.9U	4.4	3.0	-3.8
		25	13.3	12.6	4.0	-12.6
	9	0	33.3	35.0	0.0	33.3
		1	33.3	29.5	-25.9	20.9
		2	21.0	22.7	-9.9	-18.6
		3	40.1	33.9	27.7	-29.0
		4	46.3	53.0	1.6	46.2
1	9	5	27.5	27.7	18.3	20.8
		6	35.9	39.3	-10.9	-34.2
		7	19.4	14.5	15.6	-11.5
		8	15.8	14.0	5.3	14.6
		9	33.6	30.0	-24.8	22.7
		10	28.1	24.1	14.4	-24.2
		11	22.6	17.6	4.7	-22.1
		12	30.7	22.8	-7.1	29.9
		13	25.2	22.8	-11.5	22.5
		14	34.6	31.5	15.0	-31.2
		15	6.5U	8.9	1.2	-6.4
		16	17.8	12.4	-8.6	15.6
		17	9.4U	13.4	-4.4	8.3
		18	18.4	17.6	-1.3	-18.4
		19	16.2	17.3	6.1	-15.0
		20	15.2	17.5	0.0	15.2
		21	6.1U	6.2	-4.1	4.6
		22	15.5	12.0	5.7	-14.4
	10	0	46.9	48.6	0.0	46.9
		1	28.5	21.5	28.0	-13.7
		2	31.4	36.9	-18.9	-25.0
		3	29.1	29.2	-.7	29.1
		4	24.3	17.9	9.7	22.4
		5	26.8	23.1	-14.0	-22.9
		6	45.6	44.1	-8.9	-44.7
		7	7.8U	10.4	-4.9	6.0
		8	52.7	46.7	-11.8	51.4
		9	7.8U	8.4	5.1	5.9
		10	32.7	31.0	-7.5	-31.8
		11	8.7U	16.3	1.7	8.6
		12	35.9	29.4	3.4	35.7
		13	9.7U	12.1	-3.2	-9.1
		14	32.7	28.0	-2.5	-32.6
		15	9.4U	6.5	-8.7	3.5
		16	22.3	20.3	6.3	21.4
		17	7.8U	8.2	2.5	-7.4
		18	17.5	18.1	-6.1	-16.4
		19	6.1U	3.4	3.9	4.8
		20	18.1	15.2	7.5	16.5
	11	0	7.8U	5.6	0.0	-7.8
		1	19.7	22.8	1.8	19.6
		2	19.7	16.3	0.0	19.7
		3	15.8	12.9	11.3	-10.6
		4	13.3	10.5	-.5	-13.2
		5	28.8	25.2	0.0	28.8
		6	15.9	15.3	0.0	15.9
		7	31.7	27.8	-1.9	-31.6
		8	7.4U	9.2	.7	-7.4
		9	30.7	24.1	-3.0	30.6
		10	8.4U	10.7	-4.0	7.4
		11	24.3	18.2	3.0	-24.1
		12	9.1U	12.9	2.9	-8.6
		13	21.7	13.2	-10.8	18.8
		14	8.7U	4.0	-4.2	7.7
		15	16.8	10.9	.8	-16.8
		16	7.1U	10.9	3.7	-6.1
		17	11.3	13.2	-6.5	9.3
	12	0	12.6	7.9	0.0	12.6
		1	32.7	31.9	5.8	32.2
		2	12.6	8.3	1.6	-12.5
		3	24.9	22.8	-3.2	-24.7
		4	20.1	15.2	-11.0	16.7
		5	24.3	22.3	-1.7	24.2
		6	8.1U	8.1	0.0	-8.1
		7	22.0	17.2	-2.0	-21.9
		8	8.1U	8.9	2.3	7.8
		9	21.0	20.2	3.5	20.7
		10	7.8U	12.9	-2.6	-7.3
		11	13.9	15.2	-6.4	-12.3
		12	8.1U	5.0	-4.7	6.6
		13	16.5	15.9	5.5	15.6
		14	7.4U	7.0	-2.4	-7.0
		15	13.9	12.9	-3.2	-13.5
		16	5.8U	5.1	0.0	5.8
		17	11.6	13.1	4.4	10.8
	13	0	12.6	10.7	0.0	-12.6
		1	7.4U	6.1	3.8	-6.4
		2	17.5	18.2	-3.0	17.2
		3	7.4U	7.8	-.9	7.4
		4	16.2	14.9	8.0	-15.4
		5	7.1U	5.7	1.6	-6.9
		6	16.5	10.1	-8.8	13.9
		7	7.1U	10.0	-1.4	7.0
		8	14.9	10.7	2.3	-14.7
	14	0	14.6	11.7	0.0	-14.6
		1	6.8U	4.5	6.8	.7
		2	15.9	13.9	-3.5	15.5
2	0	0	17.1	15.7	-17.1	0.0
		1	55.6	57.0	0.0	55.6
		2	39.8	41.8	-39.8	0.0
		3	41.4	42.2	0.0	41.4
		4	102.2	100.8	102.2	0.0
		5	22.0	18.7	0.0	22.0
		6	78.9	71.8	-78.9	0.0
		7	15.9	16.1	0.0	15.9
		8	14.2	13.3	-14.2	0.0
		9	57.2	46.7	0.0	-57.2
		10	45.0	39.9	-45.0	0.0
		11	68.9	58.7	0.0	-68.9
		12	47.2	36.1	47.2	0.0
		13	5.2U	1.7	0.0	5.2
		14	17.8	12.0	17.8	0.0
		15	41.1	40.4	0.0	41.1
		16	17.5	13.9	17.5	0.0
		17	18.1	17.7	0.0	-18.1
		18	34.0	29.5	-34.0	0.0
		19	3.2U	.3	0.0	-3.2
		20	23.9	19.1	23.9	0.0
		21	19.7	11.8	0.0	-19.7
	1	0	96.4	97.5	-96.4	0.0
		1	142.3	154.3	141.7	12.6
		2	97.0	97.9	96.5	-9.7
		3	148.4	151.6	-148.2	8.7
		4	121.3	122.9	-116.3	34.3
		5	50.8	55.9	50.8	-.8
		6	138.7	129.8	137.8	-16.1
		7	112.2	100.1	-111.3	14.3
		8	118.0	100.9	-117.9	-5.6
		9	77.9	70.9	76.5	-14.8
		10	88.3	82.8	88.1	-5.5
		11	87.6	86.7	-82.5	-29.4
		12	99.6	95.7	-95.8	-27.4
		13	54.3	47.7	54.2	3.2
		14	57.6	51.7	57.2	6.8
		15	59.5	57.4	-59.3	5.2
		16	15.1	20.0	-13.5	-12.1
		17	67.3	69.4	66.9	7.3
		18	42.7	43.6	41.8	12.5
		19	47.2	47.0	-45.6	12.3
		20	42.4	43.1	-42.1	5.1
		21	33.6	32.3	31.3	-12.4
		22	25.2	26.6	25.2	-1.6
		23	23.8	23.8	-23.6	-.5
		24	19.1	16.7	-18.1	0.0
		25	17.8	19.0	17.7	1.3
		26	15.5	16.6	15.0	4.1
		27	12.6	9.6	-12.0	3.9
		28	14.2	18.3	-14.1	2.1
		29	10.0	10.6	9.9	-1.8
		30	9.7	11.0	8.5	2.0
	2	0	23.9	26.8	23.9	0.0
		1	57.2	60.1	57.1	-4.1
		2	29.1	30.7	-29.0	2.3
		3	8.4	7.8	-6.0	4.8
		4	23.9	19.4	-12.7	-20.3
		5	48.2	52.8	22.7	42.5
		6	37.2	34.2	26.8	-26.1
		7	58.9	60.7	-58.9	0.0
		8	24.9	21.8	-22.1	11.4
		9	21.0	17.4	18.0	-10.9
		10	13.9	10.0	-13.6	-2.9
		11	43.0	37.3	-9.8	41.9
		12	22.0	22.3	14.5	16.5
		13	43.1	33.7	29.1	-32.1
		14	17.8	20.1	-7.0	-17.7
		15	18.8	20.0	-12.8	-13.7
		16	12.6	10.2	11.9	4.2
		17	30.4	27.2	22.5	-20.5
		18	26.2	25.7	0.0	-26.2
		19	15.2	11.1	-15.1	1.7
		20	18.1	15.2	12.7	12.9
		21	15.9	16.7	15.4	3.8
		22	12.6	9.7	-4.1	11.9
	3	0	82.8	109.6	-82.8	0.0
		1	62.7	77.8	-55.8	-28.7
		2	60.2	81.3	60.1	-.8
		3	87.3	110.2	85.0	20.1
		4	97.7	123.7	-97.3	8.6
		5	77.0	92.4	-76.4	9.4
		6	97.7	109.2	94.3	-25.4
2	3	7	62.4	61.4	57.6	23.9
		8	66.3	70.5	-65.2	-12.1
		9	87.6	86.7	-85.5	-19.1
		10	91.5	92.0	91.3	6.0
		11	64.7	57.8	64.2	-7.7
		12	98.3	88.8	-97.2	14.4
		13	71.5	64.3	-71.4	-2.1
		14	56.3	48.2	55.9	-6.3
		15	38.8	34.9	38.2	6.7
		16	46.6	47.6	-44.4	-14.2
		17	39.1	40.1	-37.3	-11.8
		18	50.8	53.2	50.2	-7.8
		19	46.6	47.1	46.4	-3.3
		20	32.7	28.7	-30.2	12.4
		21	29.8	25.4	-29.6	3.0
		22	33.0	32.2	32.8	3.5
		23	20.4	20.5	17.9	9.7
		24	22.0	20.7	-22.0	-1.2
		25	18.4	15.2	-18.3	2.4
		26	14.9	14.1	14.6	-2.7
		27	13.3	14.0	12.3	4.8
		28	12.6	14.2	-12.4	2.5
		29	10.0	9.9	-9.9	-1.6
		30	6.1	7.7	5.8	1.9
	4	0	64.7	65.2	-64.7	0.0
		1	18.1	18.8	17.5	4.8
		2	32.0	28.8	24.2	-21.0
		3	48.8	47.5	-45.9	16.7
		4	36.9	30.9	24.8	-27.3
		5	27.3	23.7	-9.7	20.1
		6	27.5	27.5	25.2	-10.9
		7	25.6	21.6	4.2	-25.2
		8	48.8	48.5	-48.8	2.6
		9	16.5	17.1	11.1	12.2
		10	33.0	33.8	29.7	-14.4
		11	6.1U	8.0	-5.4	-3.0
		12	31.1	30.0	-30.7	4.8
		13	4.5U	4.4	4.5	.5
		14	19.1	19.0	18.6	-4.3
		15	21.7	18.0	0.0	-21.7
		16	18.8	17.3	-18.7	-1.6
		17	9.7	5.9	9.3	2.7
		18	14.9	13.8	8.5	-12.2
		19	6.5U	3.6	4.8	4.3
		20	6.5U	8.7	0.0	6.5
		21	6.5U	10.7	3.5	5.5
		22	13.9	14.0	11.8	-7.4
		23	5.5U	11.0	.3	-5.5
		24	12.0	13.6	-4.4	11.1
	5	0	13.3	14.2	13.3	0.0
		1	108.7	116.0	-99.2	44.2
		2	124.2	117.4	-94.8	80.2
		3	109.3	111.1	107.5	-19.6
		4	72.8	72.5	71.4	14.2
		5	62.1	70.9	-60.3	-14.6
		6	53.0	55.5	-52.8	-5.4
		7	56.9	62.4	54.5	-16.4
		8	59.2	61.1	58.7	-7.4
		9	82.5	82.5	-82.5	0.0
		10	52.4	49.7	-51.9	6.9
		11	66.9	60.1	66.9	0.0
		12	60.5	59.7	57.8	17.9
		13	61.8	56.6	-61.5	-5.2
		14	41.4	40.2	-38.8	-14.4
		15	49.2	52.1	48.9	-5.3
		16	42.7	34.4	41.0	-11.9
		17	40.4	37.5	-40.4	0.0
		18	30.4	29.7	-29.8	-5.8
		19	31.7	33.8	30.0	10.1
		20	24.3	25.1	24.0	3.3
		21	20.4	19.8	-20.1	3.2
		22	16.8	13.3	-16.8	-.9
		23	14.9	14.0	14.8	-1.9
		24	18.1	18.7	17.6	4.1
		25	18.4	19.7	-18.4	1.5
		26	12.9	13.9	-11.6	-5.8
		27	14.9	17.1	14.9	0.0
		28	9.4	10.6	7.7	5.4
		29	7.8	10.3	-7.7	1.1
	6	0	4.2U	5.7	-4.2	0.0
		1	36.2	35.6	-36.1	-2.7
		2	28.8	24.1	28.4	4.9
		3	28.5	29.1	28.4	2.4
		4	25.6	21.2	8.3	-24.2
		5	23.9	22.8	-23.9	.9
		6	33.0	34.0	10.0	-31.4
		7	14.9	12.6	5.7	-13.8
		8	30.1	27.0	-27.6	-11.9
		9	24.3	23.7	-14.0	19.8
		10	20.4	20.1	-3.3	20.1
		11	21.3	19.6	20.2	-6.8
		12	6.8U	5.1	-.8	-6.7
		13	16.2	12.7	-15.4	4.8
		14	13.3	9.9	6.5	-11.6
		15	22.6	23.0	14.5	-17.4
		16	20.4	15.0	-20.4	-.8
		17	18.1	17.1	1.4	18.1
	7	0	54.0	61.4	54.0	0.0
		1	37.5	41.8	37.5	-1.9
		2	60.8	72.1	-60.1	-9.2
		3	47.5	53.7	-47.3	-4.4
		4	48.8	57.3	48.3	7.0
		5	40.4	41.3	39.9	6.3
		6	60.8	68.2	-60.7	3.3
		7	43.3	48.3	-42.2	-9.8
		8	57.6	63.0	55.2	16.4
		9	40.8	45.5	39.5	9.9
		10	50.8	56.7	-50.7	2.9
		11	22.6	19.1	-22.5	-2.7
		12	48.2	54.9	48.0	3.8
		13	46.6	40.1	44.8	-12.7
		14	40.8	36.9	-40.8	0.0
		15	32.0	29.6	-31.8	-4.0
		16	36.2	33.4	36.2	-2.1
		17	13.9	13.6	12.9	6.3
		18	22.0	25.1	-21.6	-3.9
		19	16.8	14.5	-16.8	0.0
		20	31.1	28.7	30.6	-5.4
		21	12.6	14.7	9.9	7.8
		22	16.8	16.7	-16.6	-2.7
		23	14.2	16.9	-13.7	-3.9
		24	14.6	15.3	14.2	-3.3
		25	12.3	14.6	12.2	1.6
		26	12.9	15.0	-12.9	1.1
		27	8.7	9.7	-8.7	-1.1
	8	0	5.2U	2.1	5.2	0.0
		1	5.2U	2.1	2.7	-4.4
		2	20.4	21.0	-3.4	20.1
		3	9.1	9.0	5.5	7.2
		4	36.2	33.4	36.0	-3.7
		5	5.2U	8.7	-5.2	-.3
		6	5.8U	4.6	-5.7	-1.3
		7	21.3	19.1	16.4	-13.6
		8	17.8	18.5	6.2	-16.7
		9	22.3	25.9	-12.7	-18.4
		10	25.6	27.1	-23.3	10.5
		11	6.8U	11.5	5.4	4.1
		12	12.6	14.4	2.9	-12.3
		13	6.8U	9.4	-1.1	6.7
		14	14.9	14.3	-12.1	-8.7
		15	20.4U	18.8	10.2	17.6
		16	18.4	15.3	6.6	-17.2
		17	7.8U	3.2	-7.5	-2.0
		18	26.2	27.4	-10.3	24.1
	9	1	48.8	52.4	48.8	-1.7
		2	33.0	32.2	32.7	4.1
		3	45.3	54.8	-45.1	-3.6
		4	32.7	29.3	-31.9	6.9
		5	33.0	36.4	32.0	8.0
		6	21.7	22.5	17.7	12.5
		7	34.0	33.2	-33.5	-5.5
		8	24.9	22.6	-23.6	8.0
		9	62.7	63.7	61.9	-10.5
		10	13.6	16.6	9.4	9.8
		11	32.0	31.3	-31.3	6.7
		12	12.9	13.6	-12.4	-3.6
		13	23.3	20.3	23.1	2.7
		14	32.7	34.2	32.4	-4.0
		15	34.9	32.1	-34.9	0.0
		16	24.3	24.7	-22.4	-9.3
		17	32.3	32.1	32.3	.8
		18	17.1	14.9	16.6	4.2
		19	21.0	20.6	-21.0	-.7
		20	13.6	12.5	-13.5	1.7
		21	12.3	13.3	12.0	2.7
		22	10.0	11.8	10.0	0.0
		23	12.0	14.1	-11.9	-1.6
		24	8.7	9.8	-7.3	-4.8
	10	0	11.3	12.9	11.3	0.0
		1	13.6	13.1	13.2	-3.1
2	10	2	5.8U	5.6	-2.8	5.1
		3	6.5U	6.2	-6.2	-1.9
		4	15.9	14.7	15.8	-1.2
		5	18.1	15.7	8.1	-16.2
		6	6.5U	10.3	-4.3	-4.8
		7	15.2	15.4	-11.7	9.7
		8	14.2	13.0	5.1	-13.3
		9	6.8U	8.8	4.4	-5.2
		10	14.2	12.3	-14.0	-2.5
		11	.1U	5.0	6.9	1.6
		12	18.4	14.9	7.2	17.0
		13	7.4U	8.2	5.6	4.9
		14	7.8U	4.1	-7.7	.9
		15	18.8	19.9	-13.1	13.4
	11	0	31.7	32.3	-31.7	0.0
		1	12.3	14.0	-12.2	-1.3
		2	24.9	28.0	24.9	.8
		3	16.2	15.3	15.8	3.6
		4	36.2	37.0	-36.1	3.4
		5	14.2	15.9	-14.2	-1.1
		6	37.8	37.0	37.8	1.4
		7	22.3	22.1	22.1	-2.7
		8	25.2	25.5	-25.1	-2.9
		9	12.0	11.8	-11.8	2.2
		10	30.4	27.7	30.3	2.5
		11	17.5	16.6	17.3	-2.6
		12	27.5	26.3	-26.6	7.0
		13	7.1U	8.7	-7.0	-1.4
		14	19.1	19.4	17.8	6.8
		15	13.9	13.6	12.8	5.4
		16	12.6	12.3	-12.2	-3.0
		17	12.3	12.0	-12.3	.4
		18	12.9	12.5	12.8	-1.5
		19	3.9U	3.7	3.7	1.3
		20	12.6	16.4	-12.3	-2.7
	13	0	11.6	10.7	11.6	0.0
		1	18.4	20.7	-18.3	1.9
		2	14.2	11.4	-12.3	7.2
		3	22.0	21.8	22.0	-.9
		4	5.8U	8.6	4.7	3.4
		5	20.1	17.5	-20.0	-1.6
		6	6.1U	7.4	-5.8	-2.0
		7	18.1	18.9	18.0	2.0
		8	13.9	14.7	13.2	-4.4
		9	13.3	16.8	-13.0	-2.4
		10	5.8	7.9	-5.7	1.3
		11	13.3	14.0	13.0	2.7
		12	4.5	5.8	2.0	4.1
		13	9.1	11.3	-9.0	-1.4
3	0	1	93.7	96.5	0.0	93.7
		2	12.3	11.9	-12.3	0.0
		3	94.8	100.0	0.0	-94.8
		4	89.6	75.9	89.6	0.0
		5	110.3	123.1	0.0	110.3
		6	5.8U	3.8	-5.8	0.0
		7	65.3	57.4	0.0	65.3
		8	60.5	51.6	-60.5	0.0
		9	9.4	11.3	0.0	9.4
		10	33.0	27.0	-33.0	0.0
		11	70.8	64.1	0.0	-70.8
		12	6.5U	5.1	6.5	0.0
		13	55.3	46.9	0.0	55.3
		14	6.8U	1.5	-6.8	0.0
		15	24.9	19.6	0.0	-24.9
		16	6.8U	9.9	6.8	0.0
		17	41.4	36.1	0.0	41.4
		18	3.2U	1.7	-3.2	0.0
		19	46.9	39.2	0.0	-46.9
		20	20.7	20.6	20.7	0.0
		21	14.9	11.8	0.0	14.9
		22	16.5	14.3	-16.5	0.0
		23	8.7U	10.7	0.0	-8.7
		24	12.9	11.4	12.9	0.0
		25	15.9	13.8	0.0	15.9
		26	11.6	9.9	-11.6	0.0
		27	12.3	8.6	0.0	-12.3
	1	0	61.1	74.3	0.0	61.1
		1	99.9	107.8	35.7	93.3
		2	59.2	65.4	-17.2	-56.6
		3	112.2	111.5	13.6	-111.4
		4	93.5	93.3	44.2	82.4
		5	81.2	81.3	3.9	81.1
		6	96.1	91.0	0.0	-96.1
		7	43.0	45.8	2.8	-42.9
		8	111.6	106.1	-5.8	111.4
		9	80.5	80.6	.9	80.5
		10	64.0	61.5	-2.3	-64.0
		11	70.5	63.4	-13.5	-69.2
		12	58.9	62.1	-32.5	49.1
		13	41.4	39.9	-17.9	37.3
		14	84.1	82.3	8.8	-83.6
		15	50.1	47.6	-9.7	-49.2
		16	36.5	31.8	8.5	35.5
		17	39.5	39.8	-1.2	39.4
		18	22.6	19.4	-9.2	-20.7
		19	23.6	20.4	-.7	-23.6
		20	34.3	32.8	-1.0	34.3
		21	17.1	16.6	-1.2	17.1
		22	22.3	21.7	5.7	-21.6
		23	23.3	25.0	-3.1	-23.1
		24	20.4	19.4	3.5	20.1
		25	17.5	18.1	2.9	17.2
		26	14.9	15.1	-1.0	-14.8
		27	8.4	10.9	2.3	-8.1
		28	10.4	13.7	1.6	10.2
	2	0	40.4	40.2	0.0	-40.4
		1	10.7	9.9	-5.2	-9.3
		2	57.2	60.6	-10.3	56.3
		3	11.6	11.1	-2.0	-11.5
		4	41.1	41.4	0.0	-41.1
		5	27.8	28.1	23.2	15.4
		6	60.8	68.2	-24.5	55.6
		7	21.7	18.0	5.0	21.1
		8	56.0	60.9	9.6	-55.1
		9	27.5	24.5	7.8	26.4
		10	47.2	44.4	-15.5	44.6
		11	30.4	27.6	-27.7	12.5
		12	47.9	40.0	2.6	-47.8
		13	22.6	20.7	22.3	3.7
		14	47.9	39.3	10.4	46.7
		15	21.7	18.8	-18.8	10.7
		16	26.5	24.6	3.4	-26.3
		17	15.2	11.7	-4.9	-14.4
		18	16.2	13.9	1.5	16.1
		19	13.6	14.8	-5.4	-12.4
		20	23.9	24.3	12.9	-20.1
		21	12.3	9.8	12.2	1.4
		22	12.0	10.0	-6.2	10.2
		23	7.4U	7.0	-4.9	5.6
		24	13.6	14.3	-3.8	-13.0
		25	6.8U	7.7	6.7	-1.2
		26	12.0	12.8	-2.5	11.7
		27	3.6U	4.7	-3.1	-1.7
		28	7.4	6.5	1.7	-7.2
	3	0	69.9	79.7	0.0	-69.9
		1	71.2	86.7	12.2	70.1
		2	72.1	82.0	-3.0	72.1
		3	81.5	99.1	14.9	-80.1
		4	41.7	43.2	-19.7	-36.8
		5	67.3	74.7	2.1	67.2
		6	65.3	64.5	-28.9	58.6
		7	71.2	73.7	9.1	-70.6
		8	76.7	72.7	-11.8	-75.7
		9	82.8	77.6	0.0	82.8
		10	27.2	26.5	3.8	26.9
		11	43.3	39.9	-6.8	-42.8
		12	58.2	47.1	22.6	-53.6
		13	58.2	53.9	-13.3	56.6
		14	61.8	53.2	2.3	61.7
		15	66.6	59.5	-24.4	-62.0
		16	48.8	44.7	-22.5	-43.3
		17	50.1	51.3	14.1	48.1
		18	43.3	31.5	-3.3	43.2
		19	37.2	34.0	5.8	-36.7
		20	26.2	24.8	0.0	-26.2
		21	18.8	15.0	-8.3	16.8
		22	23.9	23.2	1.8	23.9
		23	24.6	27.6	-1.5	-24.5
		24	13.6	13.0	2.9	-13.3
		25	15.9	15.4	-1.8	15.7
		26	14.6	11.1	5.8	13.4
	4	0	33.6	26.4	0.0	33.6
		1	64.4	68.1	1.5	-64.3
		2	18.1	17.8	-1.5	18.0
		3	33.3	37.0	13.5	30.5
		4	17.5	17.8	-12.7	12.0
		5	33.3	36.2	16.6	-28.9
		6	23.0	18.8	-21.8	-7.3
		7	70.8	71.2	-14.8	69.3
		8	16.2	18.0	-3.4	-15.8

Table 2 (*cont.*)

H	K	L	FO	FC	AO	BO
3	4	9	34.0	30.7	-9.7	-33.5
		10	32.0	29.9	31.7	4.3
		11	26.8	25.3	1.5	26.8
		12	15.5	14.1	-7.8	14.5
		13	34.3	30.8	5.4	-33.9
		14	9.7U	10.7	2.1	-9.5
		15	37.2	32.3	-14.1	34.4
		16	8.4U	12.6	-7.2	-4.4
		17	26.8	21.2	-7.0	-25.7
		18	17.8	14.6	17.8	3.0
		19	14.9	15.7	-7.1	13.1
		20	7.4U	12.9	-6.7	-3.7
		21	21.7	22.2	15.1	-15.5
		22	6.5U	3.5	5.5	3.7
		23	12.9	15.2	-6.2	11.4
	5	0	59.2	60.1	0.0	-59.2
		1	40.4	45.5	3.8	-40.3
		2	51.4	65.7	-9.0	50.6
		3	68.2	71.7	9.5	67.6
		4	77.9	87.0	-12.5	-76.9
		5	54.0	44.1	-27.3	-46.6
		6	80.9	88.2	-5.3	80.7
		7	53.0	49.5	5.0	52.7
		8	66.3	68.1	-1.7	-66.3
		9	44.0	42.5	14.3	-41.6
		10	49.2	46.8	.9	49.1
		11	40.4	36.8	6.3	39.9
		12	59.8	56.7	-16.8	-57.4
		13	32.7	25.2	-9.4	-31.3
		14	47.5	53.0	-9.0	46.7
		15	26.2	25.6	-8.1	24.9
		16	23.6	18.1	2.9	-23.4
		17	40.8	40.0	-10.3	-39.4
		18	23.6	19.4	9.5	21.6
		19	22.6	23.2	11.8	19.3
		20	27.2	31.0	0.0	-27.2
		21	14.6	13.3	3.5	-14.1
		22	23.0	22.6	-1.3	22.9
		23	12.6	15.5	-3.0	12.3
		24	13.9	14.7	-.6	-13.9
		25	11.0	11.2	-.7	-11.0
		26	12.6	14.5	1.6	12.5
		27	8.7	7.6	5.8	6.5
		28	7.1	9.8	1.4	-7.0
	6	0	25.9	30.9	0.0	25.9
		1	14.9	12.3	13.3	-6.7
		2	18.1	21.5	5.9	-17.1
		3	9.4	8.1	-7.6	-5.4
		4	49.8	49.2	-14.9	47.5
		5	15.9	11.5	-12.0	10.4
		6	31.4	33.5	7.5	-30.5
		7	23.6	19.4	23.0	5.3
		8	39.5	34.7	7.2	38.8
		9	7.1U	10.3	4.9	-5.2
		10	45.6	42.3	6.2	-45.2
		11	16.8	14.0	-13.4	-10.2
		12	28.5	25.1	-11.8	25.9
		13	21.3	17.2	-20.8	4.7
		14	21.7	21.3	13.6	-16.9
		15	10.7U	8.1	.8	10.6
		16	20.1	17.6	-10.8	16.9
		17	9.4U	4.1	0.0	-9.4
		18	27.5	22.0	6.8	-26.6
		19	13.9	12.2	10.7	-8.8
		20	19.1	19.1	-10.8	15.7
		21	12.0	9.0	-12.0	-.6
		22	16.7	16.9	8.8	-13.6
	7	0	38.5	41.1	0.0	38.5
		1	61.8	71.2	5.2	-61.5
		2	34.6	33.4	.8	-34.6
		3	51.7	55.0	1.7	51.7
		4	23.6	25.6	-.9	23.6
		5	61.8	61.5	-1.1	-61.8
		6	42.4	39.9	-12.4	-40.5
		7	35.9	42.0	-9.5	34.6
		8	27.5	30.5	-5.4	27.0
		9	42.0	33.8	-14.6	-39.4
		10	32.0	26.5	-9.7	-30.5
		11	55.6	51.2	4.1	55.5
		12	33.3	29.1	-2.2	33.2
		13	33.3	30.6	2.4	-33.2
		14	19.4	15.8	0.0	-19.4
		15	35.6	34.0	2.1	35.5
		16	17.8	15.2	5.6	16.9
		17	38.2	37.8	10.0	-36.8
		18	14.6	13.8	-2.9	-14.2
		19	22.6	20.5	3.4	22.4
		20	14.2	14.5	0.0	14.2
		21	19.1	20.5	-4.9	-18.4
		22	12.3	11.0	-4.4	-11.5
		23	17.8	19.1	2.1	17.7
		24	9.4	6.6	5.5	7.6
		25	10.0	12.2	-1.2	-10.0
	8	0	6.5U	3.2	0.0	-6.5
		1	18.8	20.0	-9.7	16.0
		2	6.5U	5.5	-.5	6.4
		3	36.2	38.0	-2.8	-36.1
		4	6.5U	7.0	0.0	6.5
		5	42.7	35.3	7.7	42.0
		6	7.1U	7.4	6.2	3.5
		7	18.4	22.1	10.4	-15.2
		8	7.4U	8.1	5.3	5.2
		9	23.0	20.1	-1.5	22.9
		10	8.1U	3.6	-3.1	-7.5
		11	34.3	37.8	12.8	-31.8
		12	8.7U	8.4	8.3	-2.7
		13	18.8	24.3	-17.9	5.7
		14	9.7U	13.0	-7.7	-5.9
		15	17.8	16.1	14.1	-10.8
		16	10.0U	6.3	5.5	-8.4
		17	21.3	19.1	-6.3	20.4
		18	9.1U	7.5	-5.5	6.0
		19	14.6	12.6	-.5	-14.5
	9	0	45.9	46.7	0.0	45.9
		1	20.4	19.9	4.8	19.8
		2	35.9	39.8	2.7	-35.8
		3	26.8	25.2	-16.1	-21.5
		4	30.7	33.1	-6.7	30.0
		5	7.4U	13.9	-5.5	5.0
		6	50.1	48.4	-7.8	-49.5
		7	22.3	18.6	3.6	-22.0
		8	38.2	38.6	0.0	38.2
		9	30.1	27.2	15.3	25.9
		10	25.2	20.6	-3.6	-25.0
		11	24.9	21.0	-2.4	-24.8
		12	41.4	36.3	2.0	41.4
		13	9.7U	16.7	-3.3	9.1
		14	41.1	37.5	-7.9	-40.3
		15	10.0U	6.6	3.5	-9.4
		16	26.2	20.1	3.3	26.0
		17	13.9	13.2	6.7	12.2
		18	14.6	15.2	4.4	-13.9
		19	6.8U	9.6	0.0	-6.8
		20	16.8	20.7	1.7	16.8
		21	5.2U	8.9	.9	5.1
		22	12.3	15.4	-3.6	-11.8
	10	0	21.3	22.9	0.0	-21.3
		1	7.8U	.9	-4.5	-6.3
		2	23.9	24.6	1.6	23.9
		3	7.8U	8.7	-2.9	-7.2
		4	7.4U	9.6	4.9	-5.6
		5	7.4U	7.5	7.2	2.1
		6	16.2	18.9	-7.3	14.4
		7	13.6	14.3	-11.0	7.9
		8	31.7	30.4	-3.9	-31.4
		9	18.6	16.4	2.5	-18.3
		10	8.4U	7.5	-2.7	8.0
		11	15.2	12.4	12.0	-9.3
		12	8.7U	16.3	8.1	-3.2
		13	9.1U	5.7	6.0	6.8
		14	9.4U	18.5	-1.4	9.3
		15	3.2U	3.0	-2.5	2.1
		16	15.5	13.7	0.0	-15.5
		17	3.6U	3.8	-3.5	.4
	11	0	7.4U	10.8	0.0	-7.4
		1	28.5	27.8	3.4	28.3
		2	12.9	13.3	-4.1	12.3
		3	29.1	29.1	-2.2	-29.0
		4	7.4U	6.5	1.1	-7.4
		5	30.7	29.2	-3.1	30.6
		6	7.8U	10.5	-5.1	5.9
		7	31.4	30.8	-9.6	-29.9
		8	11.0	12.0	-1.7	-10.9
		9	23.6	23.9	-2.2	23.5
		10	8.4U	10.8	5.9	6.3
		11	25.9	25.1	1.6	-25.8
		12	17.1	16.9	-5.3	-16.4
		13	19.1	15.5	5.6	18.2
		14	13.6	10.7	8.4	10.7
3	11	15	14.6	13.0	.8	-14.5
		16	5.8U	3.6	-5.7	-1.3
		17	16.8	20.8	3.2	16.5
	12	0	7.4U	1.9	0.0	7.4
		1	12.6	14.1	0.0	-12.6
		2	7.1U	6.1	-7.1	0.0
		3	14.6	12.8	0.0	14.6
	13	0	19.1	18.1	0.0	-19.1
		1	6.5U	.7	-6.5	0.0
		2	17.8	18.1	1.1	17.8
		3	13.6	14.9	-.7	13.6
		4	16.8	18.5	[illegible]	-16.8
		5	15.5	11.1	-7.9	-13.4
		6	18.4	18.0	0.0	18.4
		7	7.1U	3.9	5.4	-4.6
		8	16.8	13.2	-.9	-16.8
		9	6.8U	6.8	2.9	-6.1
		10	12.6	11.8	0.0	12.6
		11	5.2U	6.6	2.1	4.7
		12	13.6	13.8	1.4	-13.5
4	0	0	122.3	145.2	-122.3	0.0
		1	12.9	11.8	0.0	12.9
		2	92.8	103.0	92.8	0.0
		3	61.5	57.7	0.0	-61.5
		4	69.9	69.6	-69.9	0.0
		5	44.3	35.7	0.0	44.3
		6	88.6	91.1	88.6	0.0
		7	7.1U	1.6	0.0	-7.1
		8	86.0	85.0	-86.0	0.0
		9	15.5	14.8	0.0	-15.5
		10	82.1	75.6	82.1	0.0
		11	8.4U	13.2	0.0	8.4
		12	79.9	82.2	-79.9	0.0
		13	24.3	20.0	0.0	-24.3
		14	62.4	43.6	62.4	0.0
		15	26.2	16.6	0.0	26.2
		16	79.9	86.2	-79.9	0.0
		17	9.7U	1.0	0.0	9.7
		18	57.9	48.8	57.9	0.0
		19	9.1U	10.4	0.0	9.1
		20	29.4	25.3	-29.4	0.0
		21	8.1U	.1	0.0	8.1
		22	33.3	31.2	33.3	0.0
		23	7.8U	6.0	0.0	7.8
		24	21.7	17.3	-21.7	0.0
		25	6.8U	6.8	0.0	-6.8
		26	19.7	18.6	19.7	0.0
		27	4.9U	2.9	0.0	4.9
		28	14.9	13.6	-14.9	0.0
	1	0	67.3	70.3	-67.3	0.0
		1	39.8	41.8	39.0	-9.0
		2	35.3	36.8	34.6	6.7
		3	59.2	54.9	-57.9	12.2
		4	28.5	28.4	-28.3	-2.8
		5	34.0	35.2	29.2	-17.4
		6	45.9	47.5	42.9	-16.4
		7	12.0	13.7	-7.9	-9.0
		8	14.6	12.6	-9.6	10.9
		9	33.3	37.5	27.5	18.8
		10	22.6	20.3	21.1	8.3
		11	25.2	26.2	-24.3	-6.9
		12	27.5	26.5	-25.1	11.2
		13	27.2	28.3	26.6	-5.4
		14	21.0	16.1	19.9	-6.9
		15	10.0U	11.8	-10.0	.8
		16	20.4	16.7	-19.0	-7.3
		17	27.8	28.1	24.6	12.9
		18	20.7	21.1	10.2	-18.0
		19	22.0	21.0	-21.9	-2.2
	2	0	3.6U	6.8	-3.6	0.0
		1	93.5	101.5	-93.4	3.1
		2	15.5	11.8	-4.0	-15.0
		3	75.0	82.1	74.9	-3.4
		4	4.2U	7.0	2.5	3.3
		5	73.4	80.2	-72.7	-10.4
		6	15.9	12.7	13.2	-8.8
		7	99.9	98.3	99.9	2.9
		8	28.5	28.7	-10.4	26.5
		9	78.3	82.4	-78.3	0.0
		10	5.2U	9.8	.3	-5.2
		11	74.1	70.6	73.8	-6.1
		12	5.5U	11.1	-5.5	0.0
		13	57.9	52.2	-57.6	-6.0
		14	5.8U	2.3	-5.8	-.5
		15	62.7	60.5	57.8	24.5
		16	6.5U	9.4	-2.7	5.9
		17	39.1	37.6	-38.5	-7.1
		18	5.8U	7.2	2.3	-5.3
		19	29.8	27.0	29.5	-4.0
		20	12.3	13.5	10.1	6.9
		21	33.3	38.1	-32.7	6.2
		22	4.9U	5.1	3.9	-2.8
		23	19.4	21.7	19.4	0.0
		24	4.5U	6.4	-1.4	4.3
		25	15.5	17.6	-15.3	2.6
		26	3.9U	6.3	-.7	-3.8
		27	11.6	14.1	11.6	-1.1
	3	0	31.7	34.4	-31.7	0.0
		1	16.8	15.5	-16.0	5.7
		2	43.7	45.3	41.9	-12.3
		3	33.3	33.9	21.9	-25.1
		4	27.5	23.1	-27.4	-2.1
		5	8.4U	14.5	-8.0	2.5
		6	39.8	40.4	36.8	15.1
		7	26.2	22.3	25.0	-7.9
		8	38.5	39.4	-38.3	4.1
		9	30.1	21.6	-29.8	4.1
		10	23.3	21.9	23.3	.7
		11	33.0	25.0	32.9	-1.6
		12	38.8	29.8	-38.3	-6.4
		13	28.8	25.5	-25.6	13.1
		14	32.0	28.9	27.1	-17.0
		15	21.7	18.3	21.6	-1.6
	4	0	81.5	75.9	81.5	0.0
		1	8.1U	2.4	-2.1	7.8
		2	78.9	82.1	-78.0	-11.8
		3	17.8	15.9	17.6	-2.4
		4	69.2	70.9	68.6	9.5
		5	8.4U	10.7	-8.4	-.8
		6	73.7	72.4	-73.7	0.0
		7	18.1	15.2	14.6	-10.7
		8	58.5	66.5	58.4	-3.2
		9	22.0	23.8	19.0	11.1
		10	72.8	78.8	-72.4	6.9
		11	10.7U	11.6	10.6	-.9
		12	53.0	53.1	53.0	1.3
		13	12.0U	7.3	-11.9	-1.2
		14	42.7	43.9	-40.8	12.6
		15	12.6U	19.8	-2.8	-12.3
		16	41.1	51.3	39.9	9.9
		17	12.0U	7.9	-7.9	9.0
		18	27.2	36.3	-24.1	-12.5
		19	10.7U	6.7	8.6	6.3
		20	20.1	23.8	20.0	1.0
		21	9.1U	8.2	-6.3	6.5
		22	18.1	22.0	-18.1	1.1
		23	8.4U	1.7	-8.0	2.6
		24	18.4	21.0	18.3	2.5
		25	5.8U	4.2	-1.1	5.7
		26	8.7	13.9	-8.3	-2.7
	5	0	16.5	16.9	16.5	0.0
		1	33.0	37.3	-28.7	-16.2
		2	22.0	21.5	-14.9	-16.2
		3	29.8	34.2	29.1	6.1
		4	15.5	12.8	11.5	10.4
		5	35.3	34.0	-35.2	-2.4
		6	26.2	25.2	-12.9	22.8
		7	33.6	30.0	27.4	-19.5
		8	28.5	29.3	28.5	0.0
		9	56.3	55.5	-56.3	0.0
		10	22.0	22.3	6.1	-21.1
		11	35.3	33.5	32.6	13.5
		12	25.9	26.8	15.4	-20.8
		13	20.7	16.3	4.9	20.1
		14	40.8	38.5	-27.9	29.7
		15	18.1	17.7	17.6	4.0
		16	9.1U	8.3	-4.3	-8.0
		17	23.0	19.7	-22.9	-1.6
	6	0	11.0U	15.7	11.0	0.0
		1	67.3	47.0	67.2	3.9
		2	11.0U	4.3	-11.0	.9
		3	75.4	69.4	-74.5	11.1
		4	11.3U	19.0	1.5	-11.2
		5	74.4	67.3	74.4	0.0
		6	26.5	21.5	-21.0	16.1
		7	52.4	50.1	-52.3	-3.2
		8	13.3U	7.4	4.4	12.5
		10	14.9U	3.6	3.0	-14.9
		11	31.7	33.1	-25.0	-14.8
4	6	12	15.5U	13.3	11.2	10.7
		13	42.0	47.8	42.0	1.3
		14	16.8U	1.7	-3.4	16.5
		15	40.8	39.4	-40.6	-2.8
		16	15.5U	3.1	15.1	-3.7
		17	27.5	25.5	26.7	6.6
		18	12.9U	13.5	-8.7	9.5
		19	24.6	32.7	-24.4	-3.3
		20	7.4U	6.4	3.6	-6.5
		21	18.1	25.0	18.1	1.0
		22	6.1U	2.9	1.8	5.9
		23	11.6	17.3	-11.6	-1.2
		24	5.2U	5.7	0.0	-5.2
		25	8.1	12.2	7.8	2.3
	7	1	6.8U	2.7	-4.4	-5.2
		2	24.3	22.2	-24.2	2.1
		4	28.5	28.1	28.4	-.6
		5	10.4	14.2	9.1	-4.9
		6	22.3	26.0	-22.1	3.0
	8	0	56.0	41.5	-56.0	0.0
		1	7.1U	13.3	2.5	6.6
		2	43.0	39.7	42.8	-4.3
		3	23.0	10.5	-20.5	10.4
		4	28.5	45.9	-27.9	-5.4
		5	8.1U	6.2	1.8	-7.9
		6	54.3	53.1	51.8	16.5
		7	8.1U	9.7	-8.1	.3
		8	53.0	44.5	-52.4	-8.3
		9	25.9	17.5	25.9	-1.0
		10	35.6	37.7	35.2	5.2
		11	10.0U	2.8	-9.5	-3.1
		12	38.2	32.2	-38.1	-.7
		13	10.4U	11.1	8.4	-6.0
		14	41.4	30.1	41.1	4.8
		15	11.0U	1.1	2.6	10.8
		16	32.3	26.3	-32.3	1.5
		17	8.7U	5.1	1.4	-8.6
		18	17.1	22.4	17.1	1.3
		19	7.4U	3.4	-6.4	3.8
		20	17.1	17.1	-16.5	-4.7
		21	5.8U	2.9	-.5	-5.8
		22	11.6	12.7	10.5	5.0
	9	0	8.1U	5.2	8.1	0.0
		1	8.1U	10.6	6.9	4.2
		2	16.5	14.5	5.6	15.5
		3	32.3	33.0	-32.2	-2.6
		4	11.6	9.2	-10.4	5.1
		5	8.1U	9.4	7.8	-2.0
		6	13.6	13.3	1.6	-13.5
		8	10.4U	7.6	3.1	9.9
	10	0	30.1	16.6	-30.1	0.0
		1	18.1	29.2	-18.1	1.3
		2	24.6	16.0	23.7	-6.5
		3	54.7	34.3	54.7	0.0
		4	8.1U	4.4	6.2	5.2
		5	29.1	36.6	-28.1	7.7
		6	8.7U	9.1	-.8	8.7
		7	22.3	24.1	22.2	2.0
		8	8.7U	9.2	-8.6	-1.6
		9	30.1	25.3	-28.4	-9.9
		10	9.4U	13.8	2.0	-9.2
		11	36.2	26.0	36.2	.8
		12	10.0U	5.1	-8.6	5.2
		13	29.8	22.9	-29.7	-1.5
		14	9.4U	4.8	3.3	8.8
		15	18.8	19.3	18.5	3.0
		16	7.1U	4.4	-3.4	6.2
		17	15.2	13.5	-13.2	-7.6
		18	5.2U	5.7	5.2	0.0
		19	12.3	16.4	12.3	-1.0
	11	1	5.2U	5.5	4.1	-3.1
	12	0	27.8	23.3	27.8	0.0
		1	7.8U	4.6	-5.4	5.5
		2	22.6	20.0	-20.9	-8.6
		3	7.8U	6.5	7.8	0.0
		4	23.0	21.5	22.7	-3.3
		5	8.1U	3.2	-4.6	-6.7
		6	20.4	16.8	-20.2	2.2
		7	5.5U	6.8	2.9	4.7
		8	18.1	13.4	18.0	1.9
		9	8.1U	10.8	-8.0	-.9
		10	15.9	17.9	-15.1	-4.8
		11	7.1U	1.4	-2.3	-6.8
		12	13.9	17.4	13.7	2.3
5	0	1	71.5	78.6	0.0	71.5
		2	8.1U	6.7	8.1	0.0
		3	63.7	75.0	0.0	-63.7
		4	12.6U	10.7	-12.6	0.0
		5	84.4	88.1	0.0	84.4
		6	16.2	13.9	-16.2	0.0
		7	93.1	91.8	0.0	-93.1
		8	4.5U	1.5	4.5	0.0
		9	77.0	66.9	0.0	77.0
		10	13.9	11.6	-13.9	0.0
		11	66.9	55.8	0.0	-66.9
		12	4.9U	2.9	-4.9	0.0
		13	66.0	53.9	0.0	66.0
		14	16.5	14.3	16.5	0.0
		15	64.0	50.3	0.0	-64.0
		16	4.9U	2.3	-4.9	0.0
		17	34.0	27.4	0.0	34.0
		18	9.7	10.0	-9.7	0.0
		19	32.0	26.5	0.0	-32.0
		20	4.5U	2.7	4.5	0.0
		21	33.0	31.3	0.0	33.0
		22	4.2U	6.1	-4.2	0.0
		23	25.2	25.6	0.0	-25.2
		24	3.6U	5.9	3.6	0.0
		25	16.5	17.5	0.0	16.5
		26	3.2U	1.4	3.2	0.0
		27	10.0	9.9	0.0	-10.0
	1	0	14.9	14.5	0.0	-14.9
		1	8.4	9.5	8.4	0.0
		2	24.6	29.7	1.3	24.5
		3	13.3	14.9	-10.7	7.9
		4	16.2	16.7	-14.4	-7.3
		5	16.2	16.0	2.5	-16.0
		6	13.6	8.4	.6	13.6
		7	15.2	13.8	-7.2	13.4
		8	12.6	7.1	9.7	-8.0
		9	19.1	17.4	-.9	-19.1
		10	4.9U	6.2	-.3	-4.8
		11	18.1	14.4	-6.4	16.9
		12	7.4U	7.5	.8	-7.4
		13	19.4	15.0	12.0	-15.2
		14	16.2	14.4	10.4	12.4
		15	4.9U	4.4	-4.8	-.4
		16	17.5	14.3	-14.9	-9.1
		17	9.7	11.2	2.7	-9.3
		18	12.6	8.8	8.4	9.4
		19	12.9	11.8	-5.7	11.6
		20	12.6	11.4	-.7	-12.6
		21	15.5	13.8	15.4	2.2
	2	0	57.2	71.3	0.0	-57.2
		1	8.7	9.7	-8.6	1.5
		2	73.1	85.8	-23.7	69.1
		3	7.1	5.6	-6.9	-1.8
		4	72.1	90.8	10.0	-71.4
		5	3.2U	4.3	.8	3.1
		6	72.4	72.8	-11.0	71.6
		7	9.7	10.2	-3.2	-9.2
		8	61.8	61.6	-8.4	-61.2
		9	14.9	12.8	9.2	11.7
		10	71.2	59.8	0.0	71.2
		11	5.8U	6.0	-2.0	-5.5
		12	62.7	54.9	3.4	-62.6
		13	5.5U	4.9	3.9	3.9
		14	49.8	47.2	0.0	49.8
		15	10.4	10.7	3.0	-10.4
		16	47.9	41.4	-6.4	-47.4
		17	4.9U	2.5	4.8	-.8
		18	36.9	33.7	1.9	36.8
		19	9.7	5.1	5.0	8.3
		20	31.4	31.3	0.0	-31.4
		21	4.2U	7.5	4.2	.6
		22	19.1	21.2	1.8	19.0
		23	3.9U	3.7	-3.8	-.7
		24	13.9	15.3	2.4	-13.7
		25	3.2U	3.1	-3.1	.8
		26	16.5	18.4	-4.0	16.0
	3	0	30.4	35.4	0.0	30.4
		1	30.7	32.6	-22.0	-21.5
		2	9.4	10.1	-9.1	-2.1
		3	8.4	10.5	6.3	-5.6
		4	12.9	11.8	-9.0	9.3
		5	21.3	21.3	11.0	-18.3
		6	32.3	29.8	13.2	-29.5
		7	13.6	14.5	12.5	5.4
		8	22.3	21.4	-2.1	22.2
5	3	9	16.5	18.0	-3.8	-16.0
		10	17.8	15.4	15.6	-8.1
		11	15.5	10.4	-15.5	.5
		12	20.7	14.9	-20.5	2.6
		13	6.1U	1.4	-6.0	-1.5
		14	14.2	12.9	1.8	-14.1
		15	5.5U	6.7	5.0	2.2
		16	11.6	10.2	.4	11.6
	4	0	10.7	12.1	0.0	-10.7
		1	45.3	48.3	2.7	-45.2
		2	30.4	32.5	-12.9	27.5
		3	64.4	78.2	-16.8	62.1
		4	24.6	23.3	-21.8	-11.3
		5	79.6	90.6	-14.9	-78.2
		6	16.2	12.9	11.6	-11.3
		7	44.6	50.8	4.2	44.4
		8	21.0	19.5	13.5	-16.1
		9	44.0	42.5	.9	-44.0
		10	16.2	10.3	-14.3	-7.5
		11	72.8	75.4	12.5	71.7
		12	24.6	20.7	-24.5	2.0
		13	56.3	50.6	12.1	-54.9
		14	21.0	16.9	10.3	18.3
		15	31.4	26.4	1.9	31.3
		16	9.7U	9.3	5.3	-8.1
		17	32.7	34.3	-.6	-32.7
		18	5.2U	5.7	2.5	4.5
		19	25.9	27.1	1.4	25.8
		20	4.5U	1.6	0.0	-4.5
		21	22.0	22.2	0.0	-22.0
		22	3.9U	2.4	-3.6	1.4
		23	13.9	15.2	-.7	13.9
		24	3.2U	2.5	-2.0	-2.6
		25	11.0	13.4	.6	-11.0
	5	0	3.6U	1.4	0.0	3.6
		1	22.6	21.9	-15.0	17.0
		2	9.4	6.5	3.1	-8.9
		3	22.0	17.2	18.4	-12.0
		4	15.5	15.1	-12.5	9.2
		5	32.0	30.9	29.0	13.6
		6	27.8	26.1	-22.1	16.9
		7	32.3	33.2	-13.0	-29.6
		8	4.9U	3.6	.7	4.8
		9	31.7	29.0	-31.2	-5.6
		10	25.2	25.5	14.8	-20.4
		11	22.6	20.2	16.4	-15.6
		12	9.4U	13.4	8.8	3.2
		13	6.8U	9.4	-1.9	6.6
		14	7.1U	9.5	3.8	-6.0
		15	6.1U	7.7	4.4	-4.3
		16	22.0	9.1	-18.1	12.5
	6	1	20.1	23.6	-20.0	1.5
		2	61.1	63.6	0.0	-61.1
		3	28.8	27.8	6.4	28.1
		4	45.6	47.7	1.6	45.6
		5	21.0	18.6	18.2	-10.5
		6	48.2	44.8	-5.7	-47.8
		7	20.4	18.6	-17.9	9.7
		8	44.3	42.3	-9.1	43.4
		9	11.0	10.1	-5.7	-9.4
		10	42.0	38.2	-6.7	-41.5
		11	14.2	13.2	3.2	13.9
		12	34.6	29.8	3.7	34.4
		13	18.4	14.8	11.1	-14.7
		14	41.1	35.2	4.7	-40.8
		15	12.9	13.6	12.8	1.6
		16	34.3	35.8	4.1	34.0
		17	5.5U	4.3	-3.8	-3.9
		18	25.9	25.7	4.1	-25.5
		19	4.2U	3.7	-.8	4.1
		20	20.1	20.1	-2.8	19.9
		21	3.9U	2.7	0.0	-3.9
		22	13.3	15.0	.7	-13.2
		23	2.9U	2.9	.3	2.9
		24	10.7	15.0	0.0	10.7
	7	0	3.2U	1.7	0.0	3.2
		1	4.5U	3.5	4.4	1.0
		2	13.6	13.3	.4	13.6
		3	18.1	17.4	15.6	-9.3
		4	16.2	15.9	12.1	-10.7
		5	12.0	12.0	-11.6	2.9
		7	5.2U	5.2	0.0	-5.2
		8	15.2	13.9	.7	-15.2
		10	16.5	15.4	-12.3	11.0
		11	17.5	15.5	-4.5	-16.9
		12	21.0	20.7	8.7	-19.1
	8	0	8.7	7.9	0.0	8.7
		1	45.0	46.1	-4.3	44.7
		2	12.9	12.8	-4.1	-12.3
		3	30.4	26.5	-4.8	-30.0
		4	16.2	13.2	-2.8	15.9
		5	35.6	40.2	.9	35.6
		6	10.4	10.7	-2.3	-10.1
		7	36.2	34.7	0.0	-36.2
		8	5.5U	11.8	1.7	5.4
		9	35.3	35.9	-6.5	34.6
		10	5.8U	10.2	-1.2	-5.7
		11	34.0	31.3	7.7	-33.1
		12	6.5U	5.6	.7	6.4
		13	33.3	28.5	4.6	33.0
		14	6.5U	8.1	.8	-6.4
		15	28.1	27.7	0.0	-28.1
		16	5.2U	8.6	.7	5.1
		17	17.1	18.2	1.0	17.1
		18	4.2	4.4	-.4	-4.2
		19	11.6	13.8	1.2	-11.6
		20	3.2U	4.5	2.0	2.5
		21	12.3	14.5	1.4	12.2
	9	0	4.9U	4.9	0.0	-4.9
		1	20.4	22.9	12.1	-16.4
		2	4.9U	3.3	-1.8	4.7
		3	17.5	16.9	-4.0	17.0
	10	0	25.2	28.2	0.0	-25.2
		1	4.9U	8.8	-2.0	4.4
		2	24.6	26.2	2.7	24.4
		3	4.9U	8.8	.5	-4.8
		4	22.0	25.2	-2.1	-21.9
		5	16.2	17.2	3.7	15.7
		6	21.3	24.4	3.8	21.0
		7	10.4	12.4	-5.1	-9.0
		8	21.3	23.1	-1.5	-21.3
		9	5.5U	6.2	2.7	4.8
		10	25.6	26.3	0.0	25.6
		11	5.8U	6.0	4.0	-4.2
		12	21.3	19.5	0.0	-21.3
		13	5.2U	5.7	-1.8	4.9
		14	13.9	13.4	1.8	13.8
		15	3.9U	3.7	-.4	-3.9
		16	16.8	16.5	2.0	-16.7
		17	6.5	7.5	-3.4	5.5
		18	12.3	13.5	1.3	12.2
	12	0	4.9U	1.7	0.0	-4.9
		1	12.6	16.4	-2.1	-12.4
		2	11.0	9.6	-2.4	10.7
		3	16.2	20.2	0.0	16.2
		4	9.1	10.2	4.0	-8.1
		5	14.2	13.9	4.8	-13.4
		6	4.5U	6.6	0.0	4.5
		7	16.8	14.2	1.0	16.8
		8	9.1	7.6	.5	-9.0
		9	14.9	17.0	-1.0	-14.8
		10	2.9U	3.5	[illegible]	2.8
		11	11.6	12.2	2.2	11.4
6	0	0	53.4	48.4	-53.4	0.0
		1	8.4U	1.8	0.0	-8.4
		2	59.5	47.4	59.5	0.0
		3	6.8U	6.6	0.0	6.8
		4	45.0	38.0	-45.0	0.0
		5	16.8	10.6	0.0	16.8
		6	47.5	39.2	47.5	0.0
		7	15.9	11.3	0.0	-15.9
		8	35.6	30.4	-35.6	0.0
		9	4.9U	.6	0.0	4.9
		10	36.5	30.9	36.5	0.0
		11	10.0	10.1	0.0	-10.0
		12	34.3	26.8	-34.3	0.0
		13	4.9U	5.9	0.0	-4.9
		14	18.8	16.2	18.8	0.0
		15	3.2U	4.0	0.0	3.2
		16	23.6	17.8	-23.6	0.0
		18	20.4	21.2	20.4	0.0
		19	4.5U	2.3	0.0	4.5
		20	18.1	20.3	-18.1	0.0
		21	3.9U	1.5	0.0	3.9
		22	6.1	9.7	6.1	0.0
		0	27.2	29.7	27.2	0.0
		1	33.0	29.8	-32.4	6.1
		2	24.3	30.7	-24.0	3.4
6	1	3	31.7	34.8	30.0	-10.2
		4	35.3	34.9	34.7	-6.5
		5	39.5	38.2	-37.9	11.1
		6	33.3	31.5	-33.3	-1.9
		7	36.9	26.7	35.2	11.0
		8	34.0	27.8	32.2	10.9
		9	37.2	36.4	-36.4	-7.7
		10	32.7	27.3	-32.6	-.7
		11	34.3	32.4	34.2	-2.5
		12	31.1	27.9	29.0	11.1
		13	23.9	19.7	-23.0	6.6
		14	25.2	23.6	-23.7	-8.5
		15	21.7	20.6	20.4	-7.2
		16	21.0	21.3	18.2	10.5
		17	15.9	15.4	-15.5	3.3
		18	15.5	16.1	-14.8	-4.8
		19	14.6	15.5	12.9	-6.9
		20	13.3	14.5	13.1	-1.9
		21	6.8	8.1	-6.0	3.2
		22	11.0	13.0	-11.0	-.7
		23	6.8	8.0	6.8	-.7
	2	0	5.8	5.6	-5.8	0.0
		1	35.9	36.7	-34.6	9.6
		2	6.1	8.2	5.9	1.8
		3	28.8	35.1	28.3	-3.6
		4	6.1	7.5	-4.4	4.3
		5	34.6	42.4	-34.6	0.0
		6	4.5	4.9	4.3	-1.3
		7	31.4	26.4	31.2	-3.2
		8	5.5U	9.1	4.4	-3.3
		9	40.8	40.9	-40.3	-6.0
		10	6.1U	4.2	5.3	3.0
		11	36.2	33.2	35.9	4.6
		12	12.3	12.5	-12.3	-.4
		13	22.6	17.6	-22.6	-1.9
		14	5.5U	3.7	1.7	5.2
		15	29.1	20.1	28.4	-6.2
		16	5.2U	3.2	-4.2	3.0
		17	16.8	22.5	-16.7	1.7
		18	4.5U	6.1	4.5	0.0
		19	13.3	15.3	13.2	-.6
		20	3.9U	5.6	-3.6	-1.4
		21	11.6	11.8	-11.6	.8
		22	3.6U	1.7	-3.6	0.0
		23	9.7	11.9	9.7	0.0
	3	0	29.4	37.4	29.4	0.0
		1	27.8	29.9	25.6	11.0
		2	27.5	32.9	-27.2	3.9
		3	39.6	54.8	-39.2	6.9
		4	34.6	38.4	33.9	-6.9
		5	25.2	22.2	24.9	4.3
		6	32.3	34.9	-30.9	9.6
		7	23.9	26.7	-16.2	-17.6
		8	22.3	17.5	20.5	8.9
		9	26.8	26.0	25.6	8.0
		10	27.2	21.9	-27.2	0.0
		11	28.1	20.3	-27.7	-5.0
		12	29.1	29.3	28.1	-7.6
		13	27.2	22.5	26.6	-5.6
		14	23.3	17.4	-23.3	1.0
		15	16.2	15.6	-15.7	-3.8
		16	12.0	11.5	11.9	1.5
		17	13.3	17.6	12.3	4.9
		18	14.2	16.3	-14.1	2.2
		19	12.9	17.7	-11.6	-5.8
		20	9.7	10.1	9.4	-2.3
		21	10.7	13.8	10.0	3.8
		22	10.0	11.2	-9.8	1.9
	4	0	52.4	63.5	52.4	0.0
		1	22.6	28.0	-16.3	15.7
		2	34.0	38.0	-22.3	25.7
		3	3.9U	5.0	3.4	-1.9
		4	13.3	11.9	12.4	4.8
		5	12.3	13.3	-7.2	-10.0
		6	37.8	40.9	-37.7	2.8
		7	14.6	11.8	1.7	-14.5
		8	41.4	41.9	40.6	-8.1
		9	18.1	15.2	-17.2	4.8
		10	22.0	21.4	-22.0	1.1
		11	6.8U	2.8	4.9	-4.7
		12	21.3	16.2	21.0	-3.6
		13	12.0	8.6	-9.2	-7.7
		14	25.6	26.7	-25.5	-1.7
		15	9.7	9.3	3.3	9.1
		16	19.7	22.0	19.7	1.5
		17	4.9U	3.3	-4.3	-2.3
		18	11.0	11.8	-9.5	5.5
		19	4.2U	4.4	3.1	2.8
		20	9.7	12.5	9.0	-3.6
		21	3.6U	1.1	2.5	2.5
		22	8.1	10.1	-8.0	-1.3
	5	0	18.8	21.4	-18.8	0.0
		1	21.0	26.4	20.8	2.8
		2	35.9	40.0	32.3	-15.7
		3	15.2	15.9	-15.1	1.4
		4	25.9	28.7	-24.3	8.8
		5	20.4	21.5	19.5	5.7
		6	21.0	19.2	18.2	10.6
		7	37.5	36.4	-36.9	6.8
		8	28.1	25.2	-27.6	-5.6
		9	31.4	29.5	31.3	-2.7
		10	18.8	17.1	17.7	6.3
		11	21.0	18.5	-21.0	-1.5
		12	22.6	17.9	-20.0	-10.7
		13	26.8	17.0	26.8	-1.2
		14	22.6	19.3	22.0	5.3
		15	18.4	15.0	-17.2	-6.6
		16	14.2	13.1	-13.7	-3.8
		17	15.5	17.0	15.1	-3.7
		18	8.7	10.8	6.8	5.5
		19	9.4	10.9	-9.0	-2.6
		20	12.0	13.7	-11.3	-4.1
		21	6.1	7.0	5.1	-3.4
		22	7.8	10.4	7.8	-.4
		23	9.1	10.1	-8.9	1.7
	6	0	23.3	28.0	23.3	0.0
		1	25.2	26.4	24.5	-6.1
		2	22.0	21.2	-11.1	-19.0
		3	33.6	36.5	-33.6	0.0
		4	4.5U	2.3	0.0	4.5
		5	17.5	19.0	17.1	3.7
		6	8.7	8.4	-8.4	2.5
		7	20.7	18.9	-19.8	6.0
		8	17.5	14.4	15.1	8.8
		9	23.3	20.4	23.1	-3.1
		10	10.7	9.7	-10.4	-2.6
		11	37.8	26.2	-37.7	3.4
		12	6.8U	4.4	6.8	-.6
		13	23.0	13.6	21.5	-8.2
		14	12.6	8.6	-12.4	2.4
		15	17.8	14.8	-17.8	0.0
		16	4.9U	6.6	4.6	1.5
		17	14.9	14.1	14.7	-2.1
		18	4.2U	5.3	-3.7	-2.0
		19	7.8	9.2	-6.5	4.3
		20	3.6U	3.1	3.2	1.6
		21	6.5	8.3	6.2	-1.9
	7	0	27.5	33.3	-27.5	0.0
		1	16.8	15.5	-14.9	7.7
		2	18.8	20.1	18.6	2.5
		3	18.4	19.6	17.8	4.6
		4	19.4	18.2	-19.4	1.2
		5	16.8	17.1	-14.9	-7.8
		6	27.8	27.9	27.2	5.7
		7	21.7	21.3	20.4	7.2
		8	18.1	14.3	-18.1	1.1
		9	23.6	23.0	-23.4	-2.9
		10	17.5	13.2	16.4	-5.9
		11	20.4	16.7	20.2	-2.7
		12	17.1	14.2	-16.2	-5.7
		13	19.7	14.5	-18.2	-7.7
		14	16.2	13.8	14.9	6.2
		15	15.5	14.2	14.2	6.3
		16	14.9	15.5	-14.9	0.0
		17	11.3	11.6	-10.8	-3.4
		18	10.4	11.9	10.1	-2.4
		19	6.8	9.0	6.6	1.7
		20	7.8	9.8	-7.7	-1.3
		21	7.1	7.7	-4.8	-5.3
	8		17.8	17.5	-17.8	0.0
		1	4.9U	6.5	4.4	-2.1
		2	19.4	18.8	19.4	.8
		3	12.3	11.3	-12.0	2.6
		4	18.4	19.9	-17.0	-7.0
		5	9.1	11.2	9.0	-1.2
		6	14.6	14.7	14.3	2.5
		7	16.5	13.9	-16.3	2.5
		8	19.4	15.2	-19.2	2.9
6	8	9	10.0	8.6	9.8	2.2
		10	21.0	16.8	20.8	-3.3
		11	13.3	12.0	-12.9	-3.2
		12	23.0	18.6	-22.0	6.6
		13	10.4	8.5	10.4	0.0
		14	14.2	12.4	13.7	-3.6
		15	4.5U	4.4	-4.1	-1.9
		16	8.7	8.4	-8.1	3.3
		17	3.6U	2.0	2.8	2.1
		18	6.8	7.9	6.5	-2.0
	9	0	15.5	12.1	15.5	0.0
		1	20.7	17.0	-20.6	1.8
		2	16.2	15.0	-16.1	-1.8
		3	17.5	19.4	17.4	1.4
		4	18.4	15.3	18.4	1.1
		5	19.2	14.4	-18.7	-4.0
		6	21.7	15.9	-20.7	-6.4
		7	17.8	13.3	16.5	6.6
		8	19.1	14.5	18.3	5.6
		9	18.4	16.5	-18.4	-1.2
		10	15.5	9.6	-15.5	-.6
		11	16.2	11.5	14.6	-6.9
		12	14.9	13.1	14.9	.7
		13	13.9	9.7	-13.3	3.9
		14	8.4	8.9	-6.0	-5.9
		15	9.4	9.9	8.8	3.3
		16	7.4	7.2	5.9	4.6
		17	5.2	7.0	-5.1	-1.1
	10	0	11.6	9.6	-11.6	0.0
		1	13.6	12.8	-13.6	0.0
		2	11.6	10.3	10.4	5.3
		3	14.6	11.1	14.5	-1.4
		4	9.7	8.8	-9.7	-.9
		5	17.1	14.5	-16.6	4.2
		6	13.3	11.5	12.0	-5.7
		7	15.2	11.1	15.2	-1.0
		8	14.9	13.1	-13.7	-5.9
		9	11.3	8.7	-8.6	7.4
		10	5.5U	4.2	4.9	2.4
		11	12.9	10.5	11.7	-5.5
		12	8.1	7.8	-6.4	4.9
		13	8.7	9.7	-7.8	-3.9
	11	0	12.3	9.5	12.3	0.0
		1	13.3	12.1	13.1	2.2
		2	14.6	12.4	-12.1	8.1
		3	4.5U	7.0	-4.0	-2.1
		4	9.1	9.5	9.1	0.0
		5	9.7	9.4	9.2	-3.1
		6	10.4	10.0	-10.2	-1.8
		7	13.9	13.2	-13.9	.9
		8	10.4	9.4	10.0	2.8
		9	6.5	6.8	6.1	2.3
		10	8.1	8.8	-7.7	-2.3
		11	6.5	7.5	-6.5	0.0
	12	0	9.1	7.1	9.1	0.0
		1	7.1	7.0	-7.0	-1.3
		2	7.4	7.0	-6.6	3.4
		3	9.7	11.0	9.6	1.2
		4	7.4	6.1	7.4	-1.0
7	1	0	23.3	25.5	0.0	-23.3
		1	39.5	40.2	7.2	-38.8
		2	36.8	41.5	0.0	36.8
		3	17.8	21.7	-9.1	15.3
		4	28.5	33.1	6.2	-27.8
		5	23.6	24.9	-.5	-23.6
		6	25.6	23.8	.7	25.5
		7	34.3	36.9	-2.9	34.2
		8	32.3	35.2	-2.9	-32.2
		9	20.7	21.5	8.3	-20.0
		10	21.0	18.7	1.8	21.0
		11	20.7	19.3	-3.7	20.4
		12	20.7	22.9	-1.8	-20.6
		13	24.3	22.6	-3.5	-24.0
		14	22.3	22.1	1.8	22.2
		15	20.1	22.4	1.6	20.0
		16	16.5	16.8	-1.2	-16.5
		17	14.9	19.7	3.4	-14.5
		18	13.9	16.2	2.1	13.8
	2	0	13.6	11.6	0.0	-13.6
	3	0	31.7	33.3	0.0	31.7
		1	33.6	34.6	2.5	-33.5
		2	29.8	26.6	7.2	-28.9
		3	35.3	38.4	-2.9	35.1
		4	27.8	25.2	0.0	27.8
		5	25.6	23.5	-1.4	-25.5
		6	25.6	26.4	2.0	-25.5
		7	30.7	31.0	0.0	30.7
		8	19.7	19.5	5.0	19.1
		9	25.9	26.2	-2.9	-25.7
		10	23.3	20.4	4.6	-22.8
		11	23.0	20.2	3.7	22.7
		12	22.6	23.5	-7.7	21.3
		13	19.4	19.1	-4.1	-19.0
		14	19.4	19.5	3.7	-19.0
	5	0	15.2	14.4	0.0	15.2
		1	21.7	23.5	-1.2	21.6
		2	21.7	22.1	-2.9	-21.5
		3	18.8	19.1	1.6	-18.7
		4	28.8	34.2	2.3	28.7
		5	15.9	19.3	-8.5	14.9
		6	24.6	30.5	4.5	-24.2
		7	18.8	19.0	3.8	-18.4
		8	24.6	26.6	2.8	24.4
		9	19.1	20.6	4.4	18.6
		10	21.7	23.9	0.0	-21.7
		11	19.4	17.1	-4.5	-18.9
		12	18.8	18.5	1.1	18.7
8	0	0	15.5	13.0	15.5	0.0
		1	8.7U	4.2	0.0	-8.7
		2	15.5	13.8	-15.5	0.0
		3	8.7U	6.1	0.0	8.7
		4	23.3	19.4	23.3	0.0
		5	8.4U	9.9	0.0	8.4
		6	21.7	18.1	-21.7	0.0
		7	9.1U	6.7	0.0	-9.1
		8	23.0	17.9	23.0	0.0
		9	8.7U	.2	0.0	-8.7
		10	25.6	23.2	-25.6	0.0
		11	8.4U	2.2	0.0	-8.4
		12	16.5	14.5	16.5	0.0
	1	0	8.4U	6.5	8.4	0.0
		1	19.4	21.3	-19.4	-.8
		2	21.7	24.2	-18.1	11.9
		3	17.5	16.8	17.1	3.6
		4	21.3	21.2	21.1	3.1
	2	0	5.5U	5.0	-5.5	0.0
		1	20.1	19.9	19.3	5.3
		2	5.5U	6.6	5.2	-1.7
		3	18.4	16.1	-17.7	5.2
		4	5.2U	8.5	3.2	-4.1
		5	21.3	21.5	21.2	-2.5
		6	5.8U	4.8	-5.8	-.4
		7	16.2	16.5	-15.4	-4.8
		8	5.5U	8.1	-5.0	-2.2
		9	15.2	15.1	15.2	.6
		10	5.2U	5.9	-2.9	4.3
		11	13.6	13.3	-13.5	-.9
		12	4.9U	5.4	4.2	-2.4
		13	12.9	12.1	12.9	.5
		14	4.5U	3.2	4.5	-.7
		15	11.6	11.6	-11.6	-1.2
	4	0	23.0	25.6	-23.0	0.0
9	0	1	20.1	19.6	0.0	-20.1
		2	7.8U	3.4	7.8	0.0
		3	22.6	21.1	0.0	22.6
		4	7.8U	5.8	-7.8	0.0
		5	22.0	23.3	0.0	-22.0
		6	7.4U	.4	7.4	0.0
		7	18.8	17.8	0.0	18.8
		8	6.8U	.1	6.8	0.0
		9	13.3	11.2	0.0	-13.3
		10	6.5U	.3	-6.5	0.0
		11	13.3	11.0	0.0	13.3
		12	4.9U	1.2	-4.9	0.0
		13	12.9	14.4	0.0	-12.9
	2	0	16.8	19.4	0.0	16.8
		1	4.9U	6.6	-2.2	-4.3
		2	16.8	17.9	0.0	-16.8
		3	4.5U	1.2	3.9	2.4
		4	16.2	19.6	-.6	16.2
		5	4.5U	4.1	.9	4.4
		6	13.9	16.2	.4	-13.9
		7	4.2U	2.3	4.0	-1.2
		8	13.9	19.8	-1.1	13.9
		9	3.9U	4.2	-1.9	-3.4
		10	15.9	16.8	2.4	-15.7
		11	3.6U	1.5	3.1	-1.8
		12	7.8	10.4	.4	7.8

fect of film factor errors had been completely eliminated. A composite electron density synthesis of the molecular skeleton is shown in Fig. 3.

Absolute configuration

Twelve sets of Bijvoet pairs having significantly different intensities were recorded. Correct indices were assigned according to the method of Peerdeman & Bijvoet (1956) and structure factors were evaluated, calculating the real and imaginary parts separately. In ten of the twelve cases the observed and calculated inequalities were in agreement (Table 3), thus establishing the absolute configuration as that shown in Fig. 3. This confirms the configuration predicted by Jefferies, Rosich & White (1963) from chemical and spectroscopic evidence.

Table 3. *Anomalous dispersion inequalities*

Index	A	B	Calculated inequality ($F^2 = A^2 + B^2$)	Observed inequality
6,7,1	12·70	2·53	$\bar{F}^2 > F^2$	8
6,7,$\bar{1}$	12·90	12·27		13
6,6,2	11·40	17·32	$\bar{F}^2 < F^2$	16
6,6,$\bar{2}$	11·50	10·64		12
2,2,6	23·67	28·46	$\bar{F}^2 < F^2$	15
2,2,$\bar{6}$	21·15	26·92		10
3,9,6	4·16	47·72	$\bar{F}^2 > F^2$	16
3,9,$\bar{6}$	15·53	46·90		19
2,2,11	7·92	33·45	$\bar{F}^2 > F^2$	11
2,2,$\bar{1}\bar{1}$	9·18	34·27		15
2,1,13	54·94	18·93	$\bar{F}^2 < F^2$	10
2,1,$\bar{1}\bar{3}$	52·08	8·09		13
3,1,13	31·56	45·31	$\bar{F}^2 < F^2$	16
3,1,$\bar{1}\bar{3}$	10·56	45·71		13
2,1,16	10·44	23·75	$\bar{F}^2 < F^2$	9
2,1,$\bar{1}\bar{6}$	12·44	3·11		4
2,2,17	18·43	9·43	$\bar{F}^2 > F^2$	8
2,2,$\bar{1}\bar{7}$	19·87	15·31		12
3,1,18	2·94	24·28	$\bar{F}^2 > F^2$	10
3,1,$\bar{1}\bar{8}$	14·40	24·50		12
2,1,20	43·40	3·40	$\bar{F}^2 > F^2$	8
2,1,$\bar{2}\bar{0}$	45·34	13·26		5
2,3,21	29·06	3·44	$\bar{F}^2 > F^2$	5
2,3,$\bar{2}\bar{1}$	30·84	9·60		10

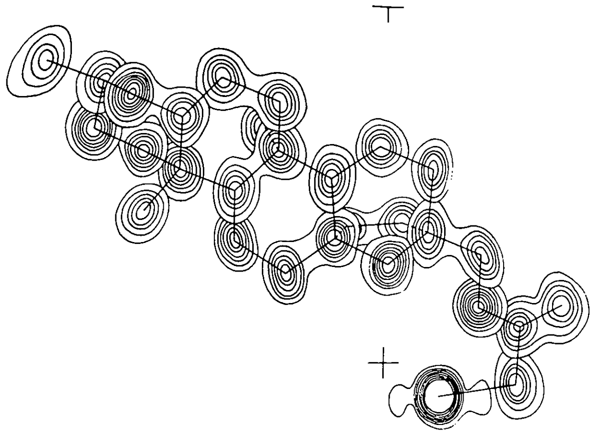

Fig. 3. A composite electron density synthesis viewed along the c axis. Contours are in intervals of 1 e.Å^{-3} for the carbon and oxygen atoms and 5 e.Å^{-3} for the iodine atom. Contours below 1 e.Å^{-3} and ten contours of the iodine peak have been omitted.

Discussion

Accuracy

The final parameters, with standard deviations estimated from the diagonal elements of the inverse to the normal equations matrix, are listed in Tables 4 and 5. The average standard deviation in the atomic coordinates of the carbon and oxygen atoms is 0·01 Å and the mean e.s.d. in the carbon–carbon bonds is 0·027 Å.

Table 4. *Atomic coordinates and (in parentheses) their e.s.d.'s*

	x/a	y/b	z/c
I	0·1065 (0·0001)	0·12000 (0·00005)	−0·25158 (0·00003)
C(1)	−0·8138 (0·0015)	−0·22844 (0·00094)	−0·06413 (0·00042)
C(2)	−0·8962 (0·0016)	−0·35313 (0·00096)	−0·05984 (0·00048)
C(3)	−0·7658 (0·0015)	−0·43593 (0·00091)	−0·03794 (0·00041)
C(4)	−0·6132 (0·0013)	−0·44296 (0·00081)	−0·07392 (0·00041)
C(5)	−0·5362 (0·0012)	−0·32357 (0·00082)	−0·08644 (0·00039)
C(6)	−0·3793 (0·0014)	−0·32331 (0·00079)	−0·12529 (0·00044)
C(7)	−0·2794 (0·0013)	−0·21070 (0·00090)	−0·12133 (0·00045)
C(8)	−0·3894 (0·0013)	−0·10887 (0·00066)	−0·13023 (0·00038)
C(9)	−0·5756 (0·0013)	−0·11596 (0·00080)	−0·09931 (0·00036)
C(10)	−0·6633 (0·0013)	−0·23114 (0·00080)	−0·10454 (0·00035)
C(11)	−0·6815 (0·0014)	−0·01549 (0·00077)	−0·11347 (0·00047)
C(12)	−0·6000 (0·0019)	0·10178 (0·00076)	−0·11618 (0·00052)
C(13)	−0·4164 (0·0014)	0·09140 (0·00076)	−0·14387 (0·00045)
C(14)	−0·3079 (0·0014)	0·00708 (0·00083)	−0·11548 (0·00037)
C(15)	−0·4264 (0·0014)	−0·08400 (0·00093)	−0·18938 (0·00047)
C(16)	−0·4431 (0·0015)	0·03003 (0·00099)	−0·19744 (0·00041)
C(17)	−0·3496 (0·0018)	0·20987 (0·00100)	−0·14907 (0·00046)
C(18)	−0·6603 (0·0014)	−0·52026 (0·00078)	−0·12533 (0·00043)
C(19)	−0·4676 (0·0014)	−0·51600 (0·00096)	−0·04685 (0·00049)
C(20)	−0·7351 (0·0015)	−0·25895 (0·00099)	−0·16186 (0·00043)
C(21)	−0·1209 (0·0015)	0·29769 (0·00086)	−0·19600 (0·00045)
C(22)	0·0624 (0·0017)	0·28845 (0·00087)	−0·21838 (0·00048)
C(23)	−0·8810 (0·0016)	−0·60659 (0·00069)	−0·07565 (0·00042)
C(24)	−0·9384 (0·0027)	−0·72896 (0·00126)	−0·05633 (0·00059)

Table 4 (*cont.*)

	x/a	y/b	z/c
O(1)	−0·1784	0·20519	−0·17518
	(0·0011)	(0·00066)	(0·00034)
O(2)	−0·1912	0·38713	−0·19476
	(0·0017)	(0·00075)	(0·00045)
O(3)	−0·7269	−0·62672	−0·10495
	(0·0012)	(0·00067)	(0·00029)
O(4)	−0·8413	−0·54616	−0·02791
	(0·0011)	(0·00059)	(0·00031)

The effect of systematic film factor errors is clearly illustrated in Table 6, which lists difference in atomic positions of the two refinements, the final isotropic thermal parameters of the initial refinement, the isotropic temperature factors before anisotropy was applied in the second refinement and the difference between these temperature factors. The average of the thermal parameter differences is 1·0 Å^2. In all cases except one the initial refinement gave lower values than those predicted from the corrected data, indicating that the film factor errors had been partly compensated for by an overall temperature factor change. The differences in atomic positions provide even stronger evidence of the erroneous results that can be obtained with incorrect film scales. The average difference between the two sets is 0·06 Å while the largest discrepancies are 0·14 Å and 0·13 Å for C(7) and C(24), respectively.

The effect of systematic film factor errors is probably not widely appreciated and is often not readily detected even when two sets of data are collected about

Table 6. *Comparison of the results obtained from the initial film factors* (I) *and the corrected film factors* (II)

	δP*	$B_{\rm I}$*	$B_{\rm II}$*	$B_{\rm II}-B_{\rm I}$
C(1)	0·03 Å	3·4 Å^2	4·2 Å^2	0·8
C(2)	0·08	3·4	4·8	1·4
C(3)	0·03	3·7	4·3	0·6
C(4)	0·06	3·0	3·8	0·8
C(5)	0·05	3·1	3·4	0·3
C(6)	0·02	2·9	3·8	0·9
C(7)	0·14	4·3	4·1	−0·2
C(8)	0·04	2·8	3·7	0·9
C(9)	0·04	2·8	3·8	1·0
C(10)	0·05	1·9	3·4	1·4
C(11)	0·05	2·9	4·7	1·8
C(12)	0·06	4·7	4·8	0·1
C(13)	0·07	2·4	4·0	1·6
C(14)	0·08	3·4	3·8	0·4
C(15)	0·02	3·0	4·8	1·8
C(16)	0·02	3·0	4·3	1·3
C(17)	0·13	4·6	4·9	0·3
C(18)	0·04	2·9	4·6	1·7
C(19)	0·12	2·9	4·3	1·4
C(20)	0·12	4·0	4·4	0·4
C(21)	0·06	4·1	4·6	0·5
C(22)	0·04	3·7	4·6	0·9
C(23)	0·08	3·6	5·0	1·4
C(24)	0·13	6·0	7·6	1·6
O(1)	0·05	5·2	5·8	0·6
O(2)	0·08	6·4	8·6	2·2
O(3)	0·06	4·5	5·4	0·9
O(4)	0·04	4·0	4·6	0·6
I	0·01			

* $B_{\rm I}$ and $B_{\rm II}$ are the isotropic thermal parameter coefficients determined from the uncorrected and corrected film factors, respectively, and δP is the difference in the atomic positions of the two refinements.

Table 5. *Anisotropic thermal parameters**

	b_{11}	b_{22}	b_{33}	b_{23}	b_{13}	b_{12}
I	0·01950 (11)	0·00849 (4)	0·00205 (1)	0·00193 (5)	0·00119 (9)	0·00523 (14)
C(1)	0·0150	0·0077	0·0018	0·0009	0·0010	−0·0010
C(2)	0·0195	0·0081	0·0022	0·0014	0·0043	0·0101
C(3)	0·0201	0·0065	0·0015	−0·0009	0·0022	−0·0036
C(4)	0·0108	0·0064	0·0019	−0·0011	0·0002	0·0024
C(5)	0·0098	0·0063	0·0015	0·0013	0·0018	−0·0048
C(6)	0·0150	0·0054	0·0022	−0·0011	0·0069	0·0067
C(7)	0·0130	0·0062	0·0026	0·0003	00·041	0·0027
C(8)	0·0158	0·0039	0·0017	−0·0006	0·0004	0·0001
C(9)	0·0149	0·0059	0·0013	0·0004	0·0036	0·0025
C(10)	0·0167	0·0053	0·0013	−0·0000	0·0034	0·0069
C(11)	0·0128	0·0043	0·0025	0·0022	0·0032	0·0044
C(12)	0·0273	0·0035	0·0025	0·0007	0·0020	−0·0016
C(13)	0·0164	0·0046	0·0021	0·0005	0·0008	0·0041
C(14)	0·0165	0·0063	0·0012	−0·0015	0·0016	−0·0076
C(15)	0·0151	0·0083	0·0020	−0·0020	−0·0003	−0·0017
C(16)	0·0180	0·0105	0·0013	0·0024	0·0008	0·0023
C(17)	0·0261	0·0083	0·0021	0·0008	0·0069	0·0058
C(18)	0·0173	0·0050	0·0020	−0·0006	0·0034	−0·0056
C(19)	0·0132	0·0073	0·0023	0·0029	0·0002	−0·0034
C(20)	0·0140	0·0096	0·0020	0·0006	−0·0054	−0·0022
C(21)	0·0163	0·0068	0·0023	0·0017	0·0013	−0·0012
C(22)	0·0251	0·0057	0·0022	−0·0028	0·0059	0·0044
C(23)	0·0210	0·0036	0·0020	−0·0002	0·0006	−0·0071
C(24)	0·0436	0·0109	0·0026	0·0013	0·0016	−0·0206
O(1)	0·0174	0·0081	0·0032	0·0014	0·0071	0·0001
O(2)	0·0373	0·0110	0·0040	0·0042	0·0102	0·0176
O(3)	0·0231	0·0076	0·0020	0·0000	0·0025	−0·0011
O(4)	0·0251	0·0058	0·0020	0·0009	0·0021	−0·0066

* The temperature factors are expressed in the form $\exp\{-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{23}kl+b_{13}hl+b_{12}hk)\}$.

The standard deviations for the iodine thermal parameters are given in parenthesis. The mean standard deviations for the carbon and oxygen parameters are 0·0022, 0·0008, 0·0002, 0·0007, 0·0011 and 0·0022 for b_{11}, b_{22}, b_{33}, b_{13} and b_{12} respectively.

different axes and correlated. In general it appears to be more reliable to determine the average zero angle film factor for intra-pack films by a method independent of the visual estimation, applying the appropriate angular correction for the higher layers. If the exposure times between different packs are adjusted so that the weakest film on one pack is approximately the same intensity as the strongest film on the next the inter-pack scales are made close to unity and can then be obtained reliably from the visually measured data.

Pseudosymmetry

The iodine atoms, which are displaced by only 0·035 Å from the planes $z/c=\frac{1}{4}$ and $\frac{3}{4}$, form an approximately centrosymmetrie array and may be considered to lie in special positions in the super-symmetrical space group *Pbnm* with the origin at $(\frac{1}{4}, 0, 0)$ relative to the non-centrosymmetric space group $P2_12_12_1$. Where a partial centre of symmetry of this type exists, the refinement of the structure may be affected by inverse overlap (Srinivasan, 1961; Rae & Maslen, 1963). This becomes important when there is interaction between pairs of atoms related by inversion through the approximate centre so that the shifts predicted by difference synthesis, diagonal or block-diagonal least-squares refinement are unreliable. When the interaction is strong, even full-matrix least-squares refinement leads to incorrect results (Geller, 1961). The analysis of inverse overlap can be simplified by considering all atoms as being in the supersymmetrical space group. When atomic separations are calculated using this symmetry, inversely overlapped atoms have contact distances less than the resolution of the Fourier synthesis (approximately 0·6 Å).

The iodine atom is almost exactly overlapped with its own image, the separation being 0·07 Å. In this case only the *z* coordinate is affected since the overlap in the *x* and *y* directions is exact. The error introduced in the I–C(22) distance is probably small as this bond lies nearly perpendicular to the *c* axis, and so has only a small component in the *z* direction. Two other pairs of atoms have contact distances which may result in inverse overlap interaction. There are C(9) and C(23) which are 0·70 Å apart in the centric space group, and C(15) and O(2) which have a separation of 1·04 Å. All these atoms have physically sensible thermal parameters, but two bonds associated with C(9) (C(8)–C(9), 1·65 Å; C(9)–C(11), 1·48 Å) differ significantly from the standard carbon–carbon single-bond distance of 1·54 Å. These differences may also be explained in terms of the rather large molecular distortions described below. However, it is difficult to establish the true nature of the deviations without evaluating the correlation matrix (Geller, 1961), which unfortunately was beyond the scope of the computing facilities available.

Molecular geometry

The final bond lengths and angles are shown in Figs. 4 and 5 and are listed, with their e.s.d.'s, in Tables 7 and 8. There are several large and significant deviations from the tetrahedral configuration and from the standard carbon–carbon single-bond distance of 1·54 Å. It is interesting to note that three of the four longest carbon–carbon bonds are associated with fully substituted carbon atoms. A similar correlation between bond length and degree of substitution has been observed in the analysis of methyl melaleucate iodoacetate (Hall & Maslen, 1965). None of the four C–O bonds associated with the ethylidene group differs significantly from their mean value of 1·44 Å. The two C–O–C angles (110° and 113°) are close to those found for carbon and oxygen in similar environments, *e.g.* in

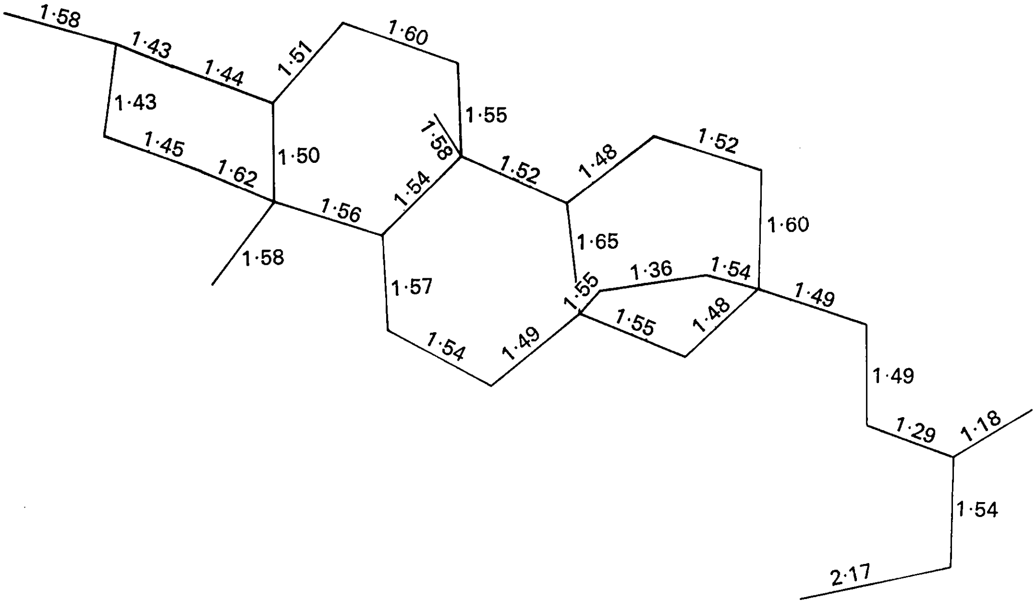

Fig. 4. Bond lengths.

trioxymethylene (Kimura & Aoki, 1951). The C(15)–C(16) distance (1·36 Å) is not significantly different from that found in *cis*-but-2-ene (Brockway & Cross, 1936) and the bond lengths and angles of the iodoacetate group are normal.

Table 7. *Bond lengths and (in parentheses) their e.s.d.'s*

C(1)—C(2)	1·60 (0·030) Å
C(1)—C(10)	1·55 (0·028)
C(2)—C(3)	1·51 (0·030)
C(3)—C(4)	1·50 (0·028)
C(4)—C(5)	1·56 (0·025)
C(4)—C(18)	1·62 (0·027)
C(4)—C(19)	1·58 (0·027)
C(5)—C(6)	1·57 (0·027)
C(5)—C(10)	1·54 (0·025)
C(6)—C(7)	1·54 (0·027)
C(7)—C(8)	1·49 (0·025)
C(8)—C(9)	1·65 (0·027)
C(8)—C(14)	1·55 (0·024)
C(8)—C(15)	1·55 (0·028)
C(9)—C(10)	1·52 (0·025)
C(9)—C(11)	1·48 (0·026)
C(10)-C(20)	1·58 (0·026)
C(11)-C(12)	1·52 (0·026)
C(12)-C(13)	1·60 (0·033)
C(13)-C(14)	1·48 (0·027)
C(13)-C(16)	1·54 (0·029)
C(13)-C(17)	1·49 (0·028)
C(15)-C(16)	1·36 (0·030)
C(21)-C(22)	1·54 (0·033)
C(23)-C(24)	1·58 (0·033)
O(1) -C(17)	1·49 (0·031)
O(1) -C(21)	1·29 (0·025)
O(2) -C(21)	1·18 (0·027)
O(3) -C(18)	1·45 (0·023)
O(3) -C(23)	1·43 (0·027)
O(4) -C(3)	1·44 (0·024)
O(4) -C(23)	1·43 (0·024)
I——C(22)	2·17 (0·020)

Table 8. *Bond angles and (in parentheses) their e.s.d.'s*

C(1)—C(2)—C(3)	109·9°(1·7°)
C(1)—C(10)—C(5)	107·9 (1·4)
C(1)—C(10)-C(9)	105·4 (1·4)
C(1)—C(10)-C(20)	109·5 (1·6)
C(2)—C(1)—C(10)	109·2 (1·6)
C(2)—C(3)—C(4)	110·5 (1·6)
C(2)—C(3)—O(4)	111·4 (1·8)
C(3)—C(4)—C(5)	112·4 (1·5)
C(3)—C(4)—C(18)	109·4 (1·5)
C(3)—C(4)—C(19)	110·0 (1·6)
C(3)—O(4) -C(23)	112·6 (1·4)
C(4)—C(5)—C(6)	115·5 (1·4)
C(4)—C(5)—C(10)	116·4 (1·5)
C(4)—C(18)-O(3)	106·3 (1·5)
C(4)—C(3)—O(4)	112·5 (1·6)
C(5)—C(6)—C(7)	111·0 (1·5)
C(5)—C(4)—C(18)	115·4 (1·5)
C(5)—C(4)—C(19)	107·3 (1·5)
C(5)—C(10)-C(9)	108·1 (1·5)
C(5)—C(10)-C(20)	110·6 (1·5)
C(6)—C(5)—C(10)	108·5 (1·4)
C(6)—C(7)—C(8)	112·8 (1·6)
C(7)—C(8)—C(9)	113·4 (1·4)
C(7)—C(8)—C(14)	115·6 (1·6)
C(7)—C(8)—C(15)	113·9 (1·5)
C(8)—C(9)—C(10)	113·5 (1·4)
C(8)—C(9)—C(11)	109·8 (1·4)
C(8)—C(14)-C(13)	103·6 (1·5)
C(8)—C(15)-C(16)	110·3 (1·7)
C(9)—C(8)—C(14)	107·0 (1·3)
C(9)—C(8)—C(15)	107·4 (1·5)
C(9)—C(10)-C(20)	115·0 (1·5)
C(9)—C(11)-C(12)	119·9 (1·8)
C(10)-C(9)—C(11)	115·8 (1·6)
C(11)-C(12)-C(13)	109·1 (1·5)
C(12)-C(13)-C(14)	110·7 (1·6)
C(12)-C(13)-C(16)	107·1 (1·7)
C(12)-C(13)-C(17)	106·3 (1·6)
C(13)-C(16)-C(15)	108·4 (1·7)
C(13)-C(17)-O(1)	108·6 (1·7)

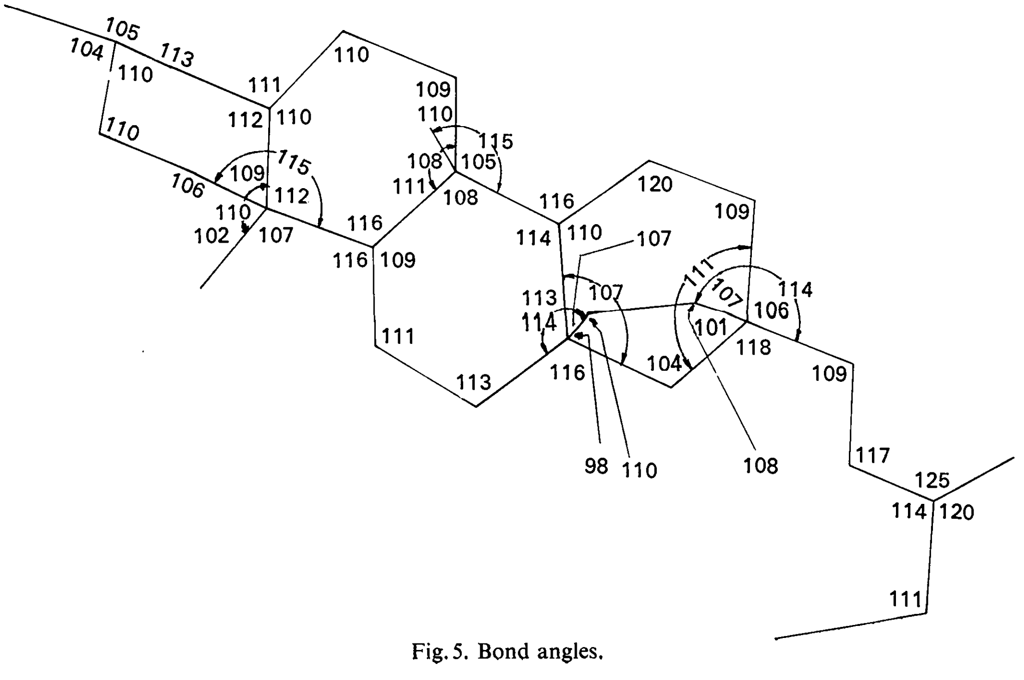

Fig. 5. Bond angles.

Table 8 (*cont.*)

C(14)–C(8)—C(15)	98·2 (1·3)
C(14)–C(13)–C(16)	100·8 (1·5)
C(14)–C(13)–C(17)	117·6 (1·8)
C(16)–C(13)–C(17)	113·9 (1·7)
C(17)–O(1) –C(21)	117·4 (1·7)
C(18)–C(4)—C(19)	101·7 (1·4)
C(18)–O(3) –C(23)	110·0 (1·4)
C(22)–C(21)–O(1)	114·4 (1·8)
C(22)–C(21)–O(2)	120·2 (2·0)
C(24)–C(23)–O(3)	104·3 (1·7)
C(24)–C(23)–O(4)	104·7 (1·6)
O(1) –C(21)–O(2)	125·2 (2·2)
O(3) –C(23)–O(4)	109·5 (1·7)
I———C(21)–C(22)	110·6 (1·3)

The molecular distortions may be explained in terms of intramolecular strains arising from

(*a*) the fusion of the olefinic bridge across the *C* ring,

(*b*) the steric interaction of the C(19) methyl group with neighbouring atoms,

(*c*) the steric interaction of the C(20) methyl group with neighbouring atoms, and

(*d*) the steric interaction of the hydrogen atoms at C(1) and C(11).

The fusion of the double bond bridge system between C(15) and C(16) results in large distortions in the *C* ring. There is a severe buckling across the C(11)–C(14) diameter and the distance C(8)–C(13) is reduced to 2·38 Å from the theoretical value of 2·51 Å in an unstrained system, while C(9)–C(12) is extended to 2·60 Å. The planes containing C(8)–C(13)–C(14) and C(6)–C(7)–C(8), normally parallel, are displaced by 25° with respect to each other and the general planes of the *B* and *C* rings, C(5)–C(6)–C(8)–C(9) and C(8)–C(9)–C(12)–C(13), are rotated by 6° from the parallel configuration. As might be expected, the compressive force between C(8) and C(13) causes a twisting of the bridge group and C(15) and C(16) are displaced by 0·13 Å with respect to each other perpendicular to the bridge plane. The twisting is further induced by the steric interaction of C(15) and its associated hydrogen with the C(20) methyl group, the separation being 3·24 Å.

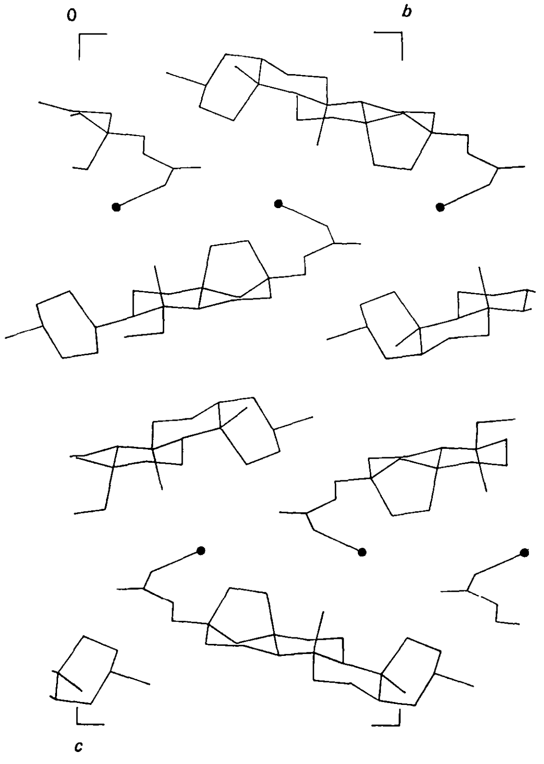

Fig. 6. Molecular packing viewed along the *a* axis.

The steric interaction of the methyl groups at C(19) and C(20) with their neighbouring atoms and the hindrance of the hydrogen atoms at C(1) and C(11) causes a general bowing of the molecule about the C(5)–C(10) bond. The major source of strain appears to be associated with C(20), which has nine intramolecular non-hydrogen contacts less than 3·25 Å (Table 9), while the methyl group at C(19) is oriented for minimum hindrance with H(5), H(6) and H(7). It is clear that the hydrogen atoms play an important role in the molecular distortions but in general the accuracy of their positions does not permit a detailed study of the hydrogen contacts in the structure.

Table 9. *Intramolecular contacts less than 3·25 Å for* C(20)

C(1) ······C(20)	2·56 Å
C(2) ······C(20)	3·01
C(4) ······C(20)	3·24
C(5) ······C(20)	2·57
C(6) ······C(20)	3·02
C(9) ······C(20)	2·62
C(11)······C(20)	3·13
C(15)······C(20)	3·24
C(18)······C(20)	3·25

Table 10. *Intermolecular* I–*X and X–X contacts less than* 4·0 Å *and* 3·70 Å, *respectively, where X refers to carbon or oxygen atoms*

The numbers I···X in parenthesis refer to the following equivalent positions:

I	x, y, z
II	$1+x, y, z$
III	$x, 1+y, z$
IV	$1+x, 1+y, z$
V	$1+x, y, 1+z$
VI	$1+x, 1+y, 1+z$
VII	$1-x, \frac{1}{2}+y, \frac{1}{2}-z$
VIII	$\frac{3}{2}+x, -(\frac{1}{2}+y), 1-z$

I(VII) ······C(6)(VI)	3·82 Å
I(VII) ······C(7)(VI)	3·99
I(I)·········C(16)(II)	3·92
I(VII) ······C(21)(V)	4·00
I(VII) ······O(2)(V)	3·12
C(12)(I)·····C(24)(III)	3·63
C(12)(I)·····O(3)(III)	3·35
C(14)(V) ····O(4)(VIII)	3·65
C(17)(I)·····O(3)(III)	3·69
C(22)(I)·····O(3)(IV)	3·44
C(24)(IV) ···O(1)(I)	3·65

Packing

Fig. 6 shows the packing of beyerol monoethylidene iodoacetate viewed down the *a* axis. The molecules are stacked in pairs of parallel layers at 20° and 160° to the *c* axis. The end of the molecule containing the iodine atom is tightly packed, as are the three methyl groups. There are five intermolecular contacts less than 4·0 Å between the iodine and the other non-hydrogen atoms and six less than 3·70 Å between the carbon and oxygen atoms (Table 10). It is interesting to note that the closest nonbonded approach, O(2)···I (3·12 Å), is about 0·4 Å less than the sum of the van der Waals radii for iodine and oxygen. This is apparently due to the reduction of the iodine radius (Pauling, 1960) in the C(22)–I direction, the angle C(22)–I···O(2) being 175·5°.

The contact C(22)···O(3) may arise from an intermolecular C–H···O hydrogen bond (Sutor, 1960) although the evidence is inconclusive since the distance (3·44 Å) is rather long for a bond of this type. However, the hydrogen atom points towards O(3), being displaced from the C···O direction by only 19°, and C(22) is attached to the electronegative iodine atom which may enhance the possibility of hydrogen bond formation.

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The Crystal Structure of the Intermolecular Complex 9-Ethyladenine: 1-Methyl-5-bromouracil

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The crystal structure of a 1:1 complex of 9-ethyladenine with 1-methyl-5-bromouracil has been determined from three-dimensional X-ray diffraction data. The unit cell is triclinic and contains two base pairs. Two hydrogen bonds are found between the adenine and uracil derivatives involving uracil O(2) and N(3) and adenine N(6) and N(7). Pairs adjacent to each other are linked into infinite, flat, ribbon-like structures perpendicular to **a*** by another set of hydrogen bonds, between uracil O(4) and adenine N(6). There is an additional short nearest neighbor interaction between the bromine atom and the uracil O(2). The crystal is disordered and approximately 6% of the uracil residues have a different orientation with an alternative hydrogen bonding to adenine.

Introduction

The specificity of the hydrogen bonding between purine and pyrimidine bases in the nucleic acids is believed to underlie the stability of transmission and expression of genetic information. Deoxyribonucleic acid (DNA) is a double stranded polynucleotide structure in which the strands are believed to be held together through hydrogen bonds between the purines and pyrimidines (Watson & Crick, 1953). DNA replication, the manufacture of ribonucleic acid (RNA) and the synthesis of proteins are all believed to take place through the ordered and sequential interaction of purine and pyrim-

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