THE DETERMINATION OF THE CRYSTAL STRUCTURE OF ACETYLTRIPHENYLGERMANE BY X-RAY DIFFRACTION

by

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B.Sc., University of British Columbia, 1965

A THESIS SUBMITTED IN PARTIAL FULFILMENT OF

THE REQUIREMENTS FOR THE DEGREE OF

MASTER OF SCIENCE

in the Department

of

Chemistry

We accept this thesis as conforming to the required standard.

THE UNIVERSITY OF BRITISH COLUMBIA

July, 1967

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ABSTRACT

Acetyltriphenylgermane, $(C_6H_5)_3GeCOCH_3$, crystallizes in the monoclinic system with $\underline{a}$ = 15.30, $\underline{b}$ = 14.53, $\underline{c}$ = 7.68 Å, and β = 94.8°. The space group is $P2_1/c$ and there are four molecules per unit cell, thus each molecule forms an asymmetric unit in the cell.

The intensities of 2537 reflections were measured by means of a scintillation counter using CuK_α radiation. The structure was determined by heavy atom Patterson and Fourier synthesis and refinement was by least-squares methods. The final discrepancy, $\underline{R}$, for 1834 observed reflections is 0.075.

The compound was found to be tetrahedral about the germanium atom, with only small deviations caused by the spreading of the phenyl rings. The phenyl rings are planar with a mean C-C bond distance of 1.383 Å, mean C-C-C bond angle of 120.0°, and a mean C-H bond distance of 1.09 Å. Intermolecular interaction causes one ring to deviate from a symmetric propeller orientation.

Two Ge-C bond distances were found: $Ge-C_{phenyl}$ distance of 1.945 Å and $Ge-C_{acetyl}$ distance of 2.011 Å. The longer Ge-C bond is attributed to contribution from a resonance structure in which there is no formal bond between germanium and the carbonyl carbon, resulting in a partial negative charge on the oxygen and a partial positive charge on the germanium. This is supported by the electronegativity difference between carbon and germanium. The C=O bond distance is 1.20 Å.

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ACKNOWLEDGMENTS

I would like to express my appreciation for the guidance and encouragement given to me by Dr. J. Trotter during the progress of this work.

I am also indebted to Dr. K. Yates for the crystal samples of the α-silyl and α-germyl ketones which he has provided.

INTRODUCTION

Investigations of the spectral activity of the α-silyl and α-germyl ketones (1-4) have shown these compounds to differ markedly from their carbon analogues. The ultraviolet spectra of benzoylsilanes are characterized by absorption at about 403-417 mμ, ascribed to a n-π^* transition of the carbonyl group, involving interaction with the 3d-orbitals of the silicon atom. Acetylsilanes have absorption about 360-370 mμ, while carbon analogues absorb at 80-100 mμ shorter wavelength than the corresponding silicon compound. At the same time, the infrared carbonyl stretching vibration is at a very low frequency: 1618 cm^{-1} (6.18μ) for benzoyl- and 1645 cm^{-1} (6.08μ) for acetylsilanes, while the carbon analogues absorb at about 1686 cm^{-1} (5.93μ) and 1715 cm^{-1} (5.83μ) respectively. For α-germyl ketones, the shift in frequency is only slightly lower. The positions of these absorption bands are relatively insensitive to the groups attached to silicon or germanium.

The first attempt to explain the abnormal spectral character of the α-silyl and α-germyl ketones was made by Brook et al (2) who attributed the large infrared shift in α-silyl ketones to the interaction between lone pair electrons on the carbonyl oxygen and vacant 3d-orbitals on the silicon (β-π bonding). This dπ-pπ bonding would distort and stretch the carbonyl group by transfer of electron density towards the silicon atom, resulting in a lowered force constant and thus a shift in the carbonyl stretching vibration to longer

wavelengths.

West and Harnish (5) similarly interpreted the ultraviolet absorption spectra, using d-orbitals on the silicon, but in terms of resonance interaction between the silicon atom and the π-orbitals of the carbonyl group, as shown in fig.1.

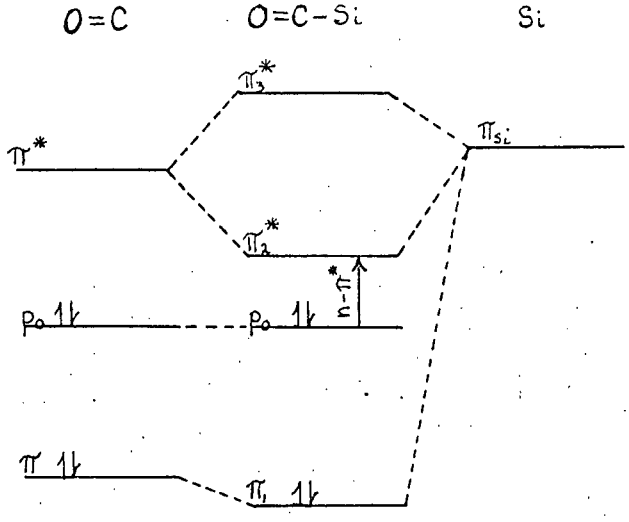
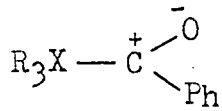


Fig. 1. Perturbation of the energy levels of carbonyl by silicon. Transition $(n-\pi^*)$ results from transition $s_o^2\pi^2p_o^2 - s_o^2\pi^2p_o\pi^*$, where π^* is the antibonding π level.

More recently, Brook, Kivisikk, and LeGrow (6), studying the spectral properties of p-substituted benzoyltriphenylsilanes, concluded that the low infrared carbonyl stretching frequency in benzoylsilanes was a result of significant single-bond character in the carbonyl group caused by the inductive release of electrons by the adjacent silicon atom. In support of this, Yates and Agolini (4) showed the order of base strength to be $R_3SiCOPh \geq R_3GeCOPh > R_3CCOPh$, and Brook and Pierce (7) showed that β- but not γ-silyl ketones absorb at lower frequency than their carbon

analogues. Thus, in the ground state, α-silyl and α-germyl ketones must have a significant negative charge associated with the carbonyl oxygen atom, which is consistent with contribution from a structure of the type



To our knowledge, no crystallographic studies had been done on compounds of this type, and a literature survey produced no X-C or C=O bond lengths for them. It was felt that, in such an investigation, if accurate bond lengths could be obtained, evidence for or against participation of the d-orbitals of the silicon or germanium in the bonding would be found in a study of the bond lengths. The compound chosen was acetyltriphenylgermane, which has a carbonyl stretching frequency at 1669 cm^{-1} and peaks at 352, 365, and 380 $m\mu$ in the ultraviolet spectrum (8).

EXPERIMENTAL

Crystals of acetyltriphenylgermane are white needles elongated along c. The density was measured by floatation in aqueous potassium iodide and the unit cell dimensions and space group were determined from rotation, Weissenberg, and precession films, and on the G. E. Spectrogoniometer.

Crystal Data (λ,CuKα = 1.5418 Å; λ,MoKα = 0.7107 Å)

Acetyltriphenylgermane, $(C_6H_5)_3GeCOCH_3$; mol. wt. 346.9, m. pt. 121.5 - 123.0°.

Monoclinic, a = 15.30 ± 0.02, b = 14.53 ± 0.02, c = 7.68 ± 0.02, β = 94.8 ± 0.3°.

Volume of unit cell = 1704 Å^3.

D_x (Z = 4) = 1.35 g. cm.$^{-3}$.

D_m = 1.36 g. cm.$^{-3}$.

Absorption coefficient for CuKα X-rays, λ = 1.5418 Å, μ = 26.4 cm.$^{-1}$.

Absorption coefficient for MoKα X-rays, λ = 0.7107 Å, μ = 19.0 cm.$^{-1}$.

Absent reflections: h0ℓ when ℓ is odd

0k0 when k is odd.

Space group: $P2_1/c$ (C_{2h}^5).

Total number of electrons per unit cell: F(000) = 712.

The intensities of the reflections were measured on a General Electric Spectrogoniometer, with Single Crystal Orienter, scintillation counter, approximately monochromatic CuKα radiation being obtained by use of a nickel filter

and pulse height analyzer. All 2537 reflections in the range $0 < 2\theta \leq 120^{\circ}$ (corresponding to a minimum interplanar spacing d = 0.89 Å) were examined, and 1834 (72%) had an intensity above background. The 703 unobserved reflections were included in the latter stages of the structure analysis with $|F_o| = \sqrt{0.4}\ F_{threshold}$. All intensities were corrected for background (approximately a function of θ only). The crystal used for recording the intensities had dimensions 0.2 x 0.25 x 0.4 mm and was mounted with c^* parallel to the ϕ axis of the goniostat. No absorption corrections were applied. Lorentz and polarization corrections were applied and structure amplitudes derived.

STRUCTURE ANALYSIS

The position of the germanium atom was determined from a three-dimensional Patterson synthesis as (0.7375, 0.5271, 0.3146). Structure factors were calculated for all the reflections using the scattering factors for Ge (corrected for anomalous dispersion) from the International Tables (9) and a temperature factor, B, of 3.0 $Å^2$, (R = 0.34). A three-dimensional Fourier series was summed with the signs of the structure amplitudes based on the germanium atom contribution. Peaks corresponding to all of the atoms (except hydrogens) appeared on the electron density map. The oxygen atom was distinguishable from the methyl carbon by both peak height and bond distance. The structure factors for all 22 atoms were calculated (R = 0.24), setting

$\underline{B}$ = 3.0 Å^2 for all atoms and using the C and O scattering factors from the International Tables (9).

The positional and isotropic thermal parameters and an overall scale factor were refined by block diagonal least-squares methods. The function minimized was $\Sigma \underline{w}(\underline{F_o}-\underline{F_c})^2$, with $\sqrt{\underline{w}} = 0$ for unobserved reflections, $\sqrt{\underline{w}} = 1$ when $|\underline{F_o}| \leq 15$, and $\sqrt{\underline{w}} = 15/\underline{F_o}$ when $|\underline{F_o}| > 15$. Several cycles of least-squares refinement reduced $\underline{R}$ to 0.087. A comparison of the calculated and observed structure factors showed twenty-five reflections, including the following strong reflections (311, 402, 212), had serious disagreement. Of these, eleven were corrected by comparison with films and the rest, all very weak reflections, were removed from the least-squares refinement. Following several more least-squares cycles, a $(\underline{F_o}-\underline{F_c})$ difference synthesis was computed to locate the hydrogen atoms. All fifteen phenyl hydrogens were located, but one of these, H(26), gave a C-H bond distance of 0.67 Å and so was placed at its theoretical position. Attempts to locate the methyl hydrogens were unsuccessful. Further refinement, including the hydrogen atoms at fixed positions and with $\underline{B}$ = 6.5 Å^2, reduced $\underline{R}$ to 0.073.

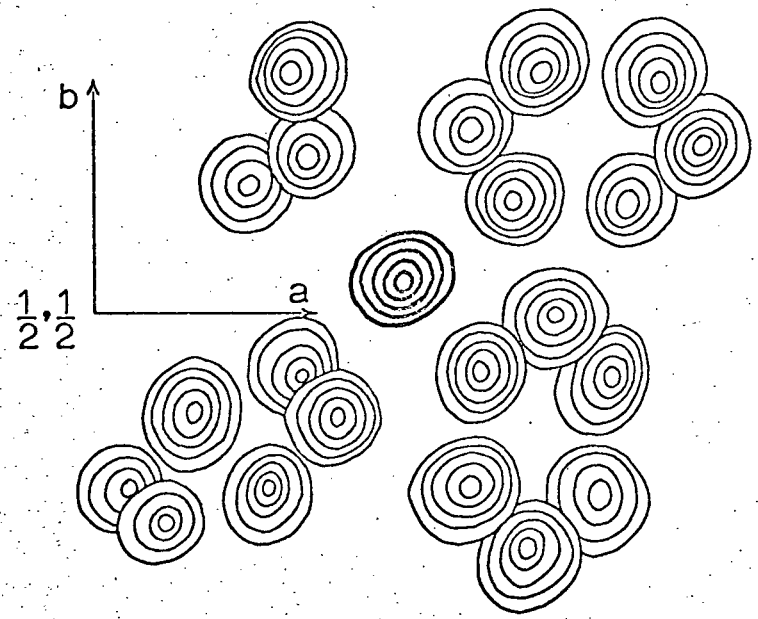
At this stage, an analysis of the values of $(\underline{F_o}-\underline{F_c})$ suggested a more appropriate weighting scheme:

$$\sqrt{\underline{w}} = \frac{1}{\left\{1 + \left[\frac{F_o - 17}{12}\right]^2\right\}^{1/2}}$$

The unobserved reflections were also included, with

$|F_o| = \sqrt{0.4}\ F_{threshold}$ and were given a weight $\sqrt{w} = 0.62$. The average $w(F_o - F_c)^2$ was now approximately constant over all values of F_o taken at intervals of 5. Refining all 37 atoms with the new weighting scheme changed R to 0.077. Ge, O, C(3), C(4), C(5), C(11), and C(17) were then refined for three cycles with anisotropic temperature factors, the hydrogens being fixed in their best position (peak position or first or second refinement position) according to bond length after the first cycle, and the remaining carbon atoms being fixed in position after the second cycle, reducing R to 0.073. A final structure factor calculation, including the 14 reflections that were removed from the refinement, gave $R = 0.075$.

The final measured and calculated structure factors are listed in Table VI (Appendix I). A final three-dimensional Fourier series was summed and superimposed sections of the resulting electron-density distribution are shown in Figure 2, together with a drawing of the structure giving the atom numbering used in the analysis. A final difference map showed maximum fluctuations of $\pm$ 0.5eÅ^{-3}.



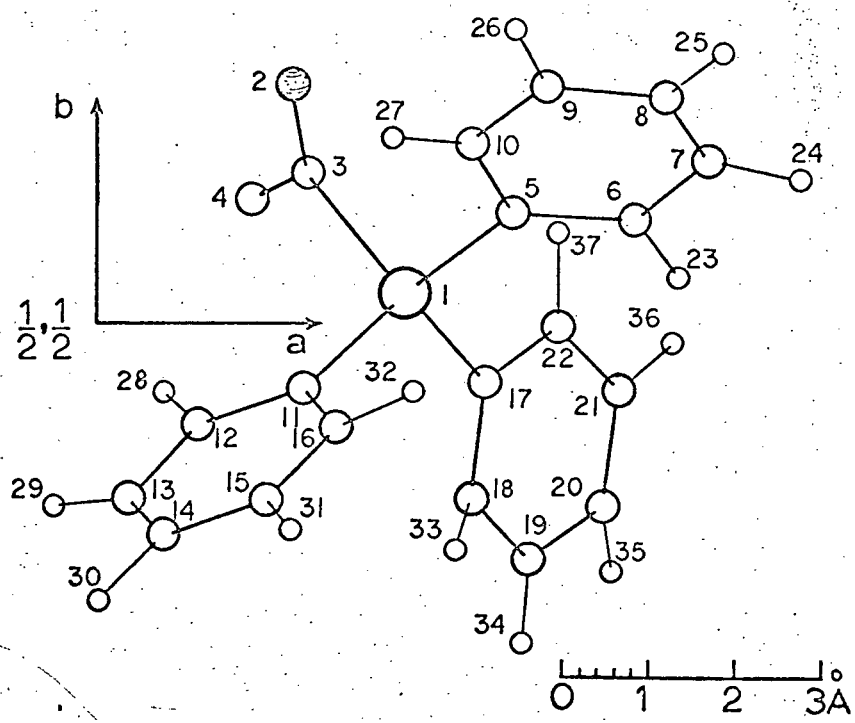


Figure 2. (a) Electron-density projection along the c axis. Contours are at intervals of 1 e. Å^{-3}, starting at 2 e. Å^{-3} for carbon, and of 10 e. Å^{-3} starting at 10 e. Å^{-3} for Ge.

(b) Perspective drawing of the structure giving the numbering used.

COORDINATES AND MOLECULAR DIMENSIONS

The final positional parameters and their standard deviations are given in Table I. $\underline{x}$, $\underline{y}$, and $\underline{z}$ are fractional coordinates referred to the monoclinic crystal axes; $\sigma(x)$, $\sigma(y)$, and $\sigma(z)$ are the standard deviations of the coordinates (in Å) computed from the least-squares residuals. The positions of the hydrogen atoms are least accurately determined and are not considered further. Table II gives the final thermal parameters, where $\underline{U}_{ij}$ are the components of the vibration tensors, written in matrix form, and referred to the axes $\underline{a}^*$, $\underline{b}^*$, and $\underline{c}^*$. The equations of the mean planes of the three phenyl rings are given in Table III, along with the planes through C(3)-Ge-C(phenyl) and the interplanar angles. Bond distances and valency angles together with their standard deviations are listed in Table IV, and Table V lists all the crystallographically independent intermolecular distances shorter than 3.8 Å. Two important distances involving the C(11)-C(16) rings are also listed. Figure 3 illustrates the packing of the molecules.

Table I

Final positional parameters (fractional)
And standard deviations (Å).

Atom	x	y	z	σ(x)	σ(y)	σ(z)
Ge(1)	0.7354	0.5264	0.3163	0.0015	0.0015	0.0015
O(2)	0.6499	0.6951	0.2546	0.011	0.012	0.012
C(3)	0.6615	0.6227	0.1862	0.014	0.015	0.015
CH_3(4)	0.6200	0.6011	0.0052	0.023	0.023	0.021
C(5)	0.8176	0.5900	0.4806	0.013	0.013	0.013
6	0.9082	0.5855	0.4723	0.015	0.016	0.015
7	0.9629	0.6324	0.5891	0.017	0.019	0.018
8	0.9307	0.6852	0.7191	0.018	0.020	0.019
9	0.8419	0.6933	0.7268	0.016	0.017	0.016
10	0.7854	0.6451	0.6095	0.016	0.017	0.017
11	0.6584	0.4484	0.4411	0.015	0.014	0.014
12	0.5776	0.4199	0.3651	0.019	0.020	0.019
13	0.5260	0.3600	0.4554	0.021	0.022	0.021
14	0.5520	0.3306	0.6208	0.019	0.020	0.020
15	0.6315	0.3596	0.6976	0.021	0.022	0.021
16	0.6845	0.4177	0.6072	0.018	0.019	0.018
17	0.7961	0.4539	0.1501	0.015	0.014	0.014
18	0.7867	0.3602	0.1383	0.017	0.018	0.017
19	0.8311	0.3108	0.0183	0.020	0.021	0.020
20	0.8855	0.3539	-0.0853	0.020	0.021	0.020
21	0.8959	0.4478	-0.0778	0.020	0.020	0.020
22	0.8508	0.4983	0.0384	0.017	0.017	0.017
H(23)	0.942	0.538	0.392			
24	1.034	0.617	0.595			
25	0.974	0.720	0.816			
26	0.816	0.738	0.828			
27	0.724	0.652	0.626			
28	0.553	0.444	0.225			
29	0.467	0.354	0.417			
30	0.502	0.277	0.699			
31	0.649	0.335	0.857			
32	0.742	0.446	0.683			
33	0.775	0.317	0.250			
34	0.825	0.242	0.011			
35	0.892	0.300	-0.183			
36	0.940	0.485	-0.148			
37	0.850	0.575	0.042			

$\sigma(x) = \sigma(y) = \sigma(z) = 0.24$

Table II

Final thermal parameters and standard deviations (U_{ij} in $Å^2 \times 10^2$; B in $Å^2$).

Atom	B	U_{11}	U_{12}	U_{13}	U_{22}	U_{23}	U_{33}	Mean $\sigma(U)$
Ge(1)	3.54	4.57	-0.19	0.15	4.29	-0.10	4.55	0.07
O(2)	5.33	5.81	0.74	-1.37	6.21	-0.53	8.14	0.60
C(3)	4.15	4.27	0.14	0.54	5.45	0.66	6.32	0.71
CH_3(4)	7.26	10.45	2.08	-2.77	9.88	0.69	7.41	1.19
C(5)	3.46	4.86	-0.39	0.31	3.45	0.21	4.74	0.61
C(11)	3.93	5.51	-0.41	0.48	4.71	-0.72	4.74	0.67
C(17)	3.78	5.25	-0.31	-0.28	5.02	-0.36	4.31	0.66

Atom	B	$\sigma(B)$
C(6)	4.24	0.28
7	5.33	0.35
8	5.61	0.37
9	4.80	0.31
10	4.59	0.30
12	5.78	0.37
13	6.52	0.43
14	5.91	0.39
15	6.47	0.42
16	5.27	0.35
18	4.96	0.32
19	6.23	0.41
20	6.36	0.42
21	6.00	0.40
22	4.61	0.31

Table III

Equations of mean planes and angles between planes.

Equations of mean planes, in the form $\ell X' + mY' + nZ' + p = 0$, where X', Y', Z' are coordinates in Å referred to orthogonal axes a, b, c^*.

Plane	Atoms	ℓ	m	n	p	Maximum Displacement (Å)
1	1,5-10	-0.022	-0.788	0.615	4.779	0.016
2	1,11-16	0.465	-0.799	-0.380	1.913	0.021
3	1,17-22	-0.716	0.117	-0.689	8.668	0.016
4	1,3,5	-0.720	-0.045	0.693	6.620	0.0
5	1,3,11	-0.056	-0.606	-0.793	7.175	0.0
6	1,3,17	-0.764	-0.638	-0.094	13.550	0.0

Angles between planes.

Planes	Angle
1 - 4	61.5°
2 - 5	40.6
3 - 6	57.5
4 - 5	118.8°
4 - 6	120.9
5 - 6	120.3

Table IV

Bond distances (Å) and angles (degrees) with standard deviations.

Germanium-Carbon bond lengths

		σ			σ
Ge-C(3)	2.011	0.015	C(3)-Ge-C(5)	107.4°	0.6
			C(3)-Ge-C(11)	108.2	0.6
Ge-C(5)	1.940	0.014	C(3)-Ge-C(17)	109.2	0.6
Ge-C(11)	1.945	0.014	C(5)-Ge-C(11)	110.1	0.6
Ge-C(17)	1.950	0.014	C(5)-Ge-C(17)	111.4	0.6
			C(11)-Ge-C(17)	110.5	0.6
mean Ge-C_{phenyl}	1.945 ± 0.008 Å				

Phenyl rings

C(5) - C(6)	1.40	C(10)-C(5)-C(6)	118.1°
C(6) - C(7)	1.36	C(5)-C(6)-C(7)	120.4
C(7) - C(8)	1.38	C(6)-C(7)-C(8)	121.2
C(8) - C(9)	1.37	C(7)-C(8)-C(9)	119.6
C(9) - C(10)	1.39	C(8)-C(9)-C(10)	119.7
C(10) - C(5)	1.40	C(9)-C(10)-C(5)	120.9
C(11) - C(12)	1.39	C(16)-C(11)-C(12)	118.2
C(12) - C(13)	1.40	C(11)-C(12)-C(13)	119.9
C(13) - C(14)	1.37	C(12)-C(13)-C(14)	121.6
C(14) - C(15)	1.37	C(13)-C(14)-C(15)	118.8
C(15) - C(16)	1.40	C(14)-C(15)-C(16)	120.2
C(16) - C(11)	1.38	C(15)-C(16)-C(11)	121.4
C(17) - C(18)	1.37	C(22)-C(17)-C(18)	118.7
C(18) - C(19)	1.39	C(17)-C(18)-C(19)	120.2
C(19) - C(20)	1.35	C(18)-C(19)-C(20)	120.6
C(20) - C(21)	1.38	C(19)-C(20)-C(21)	120.7
C(21) - C(22)	1.38	C(20)-C(21)-C(22)	119.4
C(22) - C(17)	1.41	C(21)-C(22)-C(17)	120.4
mean $C_{ar.}$-$C_{ar.}$	1.38_3 ± 0.006 Å	mean C-C-C-	120.0 ± 0.4°
mean C-H	1.09 ± 0.06 Å		

C(3) - CH_3(4) 1.51 ± 0.03 Å

C(3) - O(2) 1.20 ± 0.02 Å

Table V

Shorter Intermolecular Distances

(All crystallographically independent distances ≤ 3.8 Å between molecule 1 at $\underline{x}$, $\underline{y}$, $\underline{z}$ and neighbouring molecules are listed as well as two distances involving interaction of C(11)-C(16) rings.)

Atom (of molecule 1)	to Atom of	Molecule #	Distance (Å)
O(2)	C(14)	2	3.33
O(2)	C(10)	6	3.36
O(2)	C(9)	6	3.38
O(2)	CH_3(4)	3	3.58
C(21)	C(21)	7	3.64
O(2)	C(13)	2	3.72
C(5)	C(9)	6	3.74
C(6)	C(6)	4	3.75
C(3)	C(14)	2	3.76
C(6)	C(7)	4	3.78
C(13)	C(14)	5	3.82
C(12)	C(13)	2	3.88

Molecule 1	at	x	y	z
2	at	1-x	1-y	1-z
3	at	x	$1\frac{1}{2}$-y	$\frac{1}{2}$+z
4	at	2-x	1-y	1-z
5	at	x	$\frac{1}{2}$-y	$-\frac{1}{2}$+z
6	at	x	$1\frac{1}{2}$-y	$-\frac{1}{2}$+z
7	at	2-x	1-y	-z

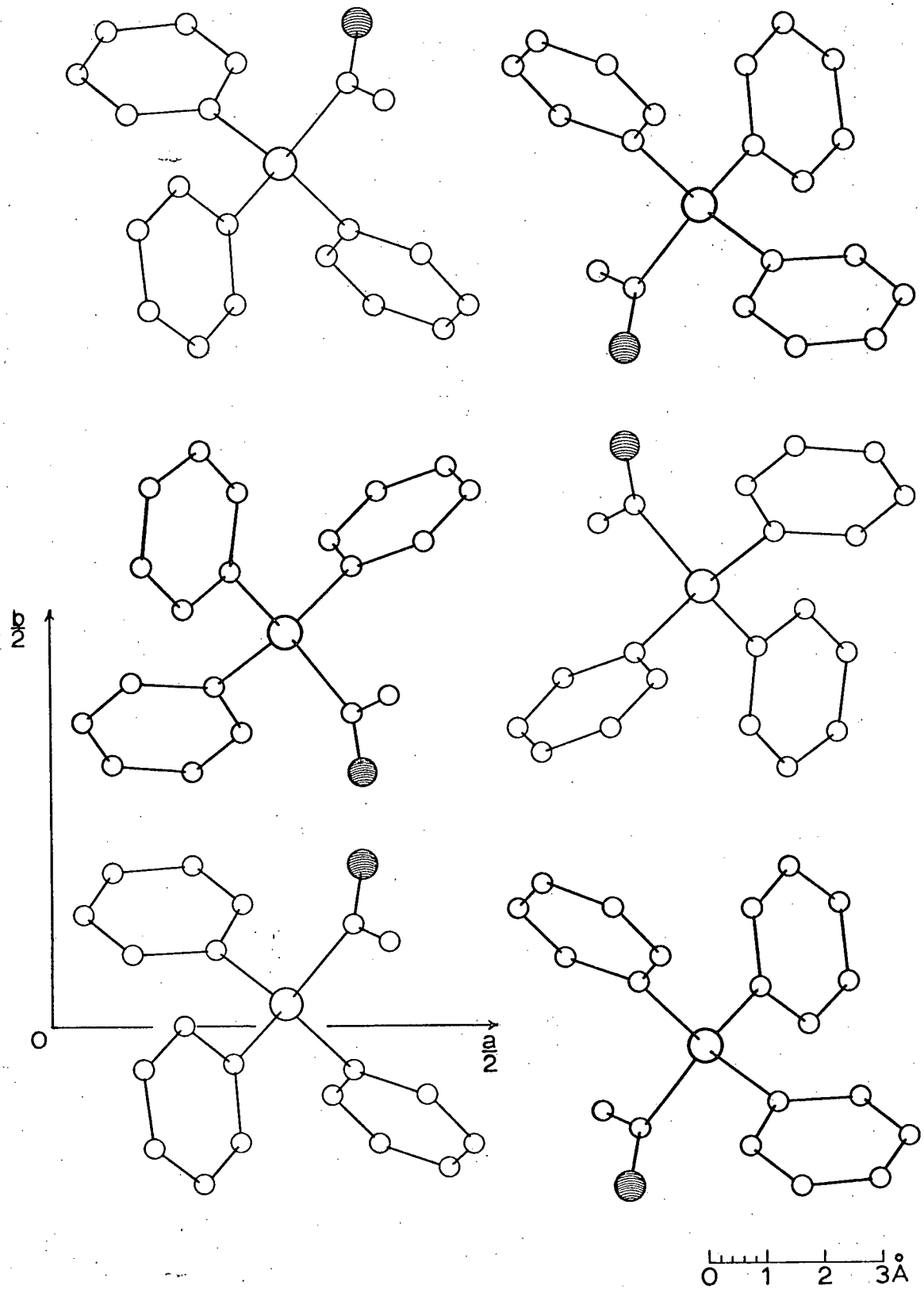


Figure 3. View of the structure along c, illustrating the packing of the molecules. Heavier lined molecules are closer to the viewer.

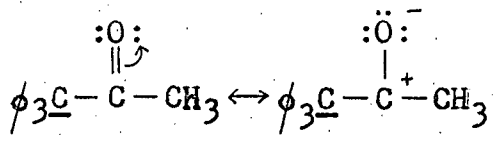
DISCUSSION

The analysis has shown acetyltriphenylgermane to be tetrahedral about the germanium atom corresponding to sp^3 hybridization on the germanium, as was expected. Distortion from this tetrahedral shape caused by the spreading of the phenyl rings is very small, the average C_{acetyl}-Ge-C_{phenyl} angle being 108.3°, and the average C_{phenyl}-Ge-C_{phenyl} angle being 110.7°. The angles between the C(3), Ge, C_{phenyl} planes are 118.8, 120.9, and 120.3°.

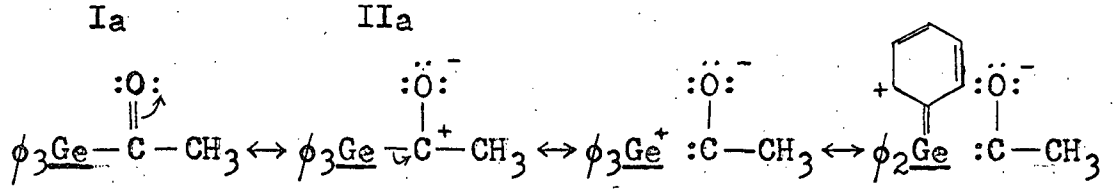
The three phenyl rings are planar (maximum deviation from ring plane is 0.021 Å) with a mean C-C bond distance of 1.383 ± 0.006 Å and a mean C-C-C angle of 120.0 ± 0.4°. The mean C-H bond distance is 1.09 ± 0.06 Å. The rings are oriented in a propeller fashion about germanium with angles between the ring planes and the C(3), Ge, C_{phenyl} planes of 61.5, 40.6, and 57.5°. The smaller interplanar angle of the ring containing C(11)-C(16) appears to be caused by intermolecular interaction between this ring and symmetry related C(11)-C(16) rings. Increasing this angle to 60° would cause severe carbon-carbon interactions (shortening of the C(12)-C(13) and C(13)-C(14) intermolecular distances in Table V).

The germanium-carbon bonds are not all equivalent. The mean Ge-C_{phenyl} bond distance is 1.945 ± 0.008 Å which agrees with the bond distance found in CH_3GeH_3 by microwave spectroscopy of 1.9453 ± 0.0005 Å (10). The Ge-C_{acetyl} bond length is significantly (4σ) longer at 2.011 ± 0.015 Å. A

bonding scheme responsible for the lengthening of this Ge-C bond can be deduced by comparing the resonance structures available to the germanium compound with those of the corresponding carbon analogue. When the α-substituent



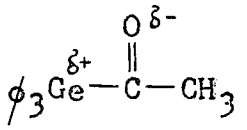
Ia IIa



Ib IIb IIIb IVb

(underlined) is carbon, Ia, the difference in the electronegativities of the carbon and oxygen in the carbonyl group result in contribution from the resonance structure IIa. When the α-substituent is germanium, Ib, the electronegativity difference in the carbonyl group is still present, and contribution from IIb would be expected. However, the α-germanium atom is more electropositive than the carbonyl carbon and the positive charge is more likely to reside on the germanium than on the carbon. Contribution from the resulting resonance structure, IIIb, with no formal bond between the germanium and carbon atoms, explains the long Ge-C bond length. Further dissipation of the positive charge to the ortho and para carbons of the phenyl rings is also possible, IVb. It is not possible, however, to determine whether this occurs, since the resultant shortening of the $Ge\text{-}C_{phenyl}$ bonds would be too small to be noticed. The final structure is thus probably derived from Ib with significant

contribution from IIIb, ie.,



This explains the negative charge found on the carbonyl oxygen by Yates and Agolini (4) and gives a normal C=O bond length (experimentally 1.20±0.02 Å). No evidence for participation of the germanium d-orbitals was found.

The results of the spectral studies on the α-silyl and α-germyl ketones (1-3) and the basicity studies of Yates and Agolini (4) suggest that the amount of negative charge on the carbonyl oxygen increases in the order C < Ge < Si, so that if the inductive effect is solely responsible for the charge distribution, it is expected that the electronegativities would be in the reverse order, ie., C > Ge > Si. The electronegativities determined by Allred and Rochow (11) support this as shown in Table VI, in which the trend in the carbonyl

Table VI. Comparison of the carbonyl stretching frequencies and the electronegativity of the α-substituent.

Compound	C=O stretching freq. (cm^{-1})	Electronegativity
$\phi_3\underline{C}COCH_3$	1721 (2)	2.50
$\phi_3\underline{Ge}COCH_3$	1669 (8)	2.02
$\phi_3\underline{Si}COCH_3$	1645 (2)	1.74

stretching frequency is closely paralleled by that of the electronegativities. While these electronegativities are strictly only those of the isolated atom, since the environment of the α-substituent is identical in each compound their

relative values should be correct.

These trends suggest that the $Si\text{-}C_{acetyl}$ bond in the analogous silicon compound should be relatively longer than the corresponding bond in the germanium compound and a structure analysis of acetyltriphenylsilane would be useful in supporting the bonding scheme which has been proposed for the α-germanium ketone.

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APPENDIX I

Table VII

Observed and Calculated

Structure Factors

(* indicates a reflection which was not included in the least-squares refinement. Negative F_o values indicate an unobserved reflection.)

Table VII

h	k	l	F_o	F_c
1	0	0	1.8	2.1
2	0	0	145.4	-148.1
3	0	0	5.5	-10.2
4	0	0	7.9	-6.4
5	0	0	22.8	-19.9
6	0	0	26.7	-24.5
7	0	0	9.6	-7.4
8	0	0	24.8	24.6
9	0	0	20.5	-19.6
10	0	0	45.0	-45.4
11	0	0	45.9	45.6
12	0	0	15.8	21.3
13	0	0	42.0	-40.6
14	0	0	9.2	-4.7
15	0	0	26.1	24.1
16	0	0	9.1	-8.5
17	0	0	22.0	-20.4
0	2	0	119.0	115.6
1	2	0	4.2	2.0
2	2	0	121.5	-118.8
3	2	0	30.4	30.4
4	2	0	69.7	72.0
5	2	0	49.0	-46.5
6	2	0	75.2	-79.7
7	2	0	49.5	50.5
8	2	0	44.6	43.9
9	2	0	30.9	-33.1
10	2	0	13.5	-14.1
11	2	0	34.0	31.4
12	2	0	22.5	18.1
13	2	0	36.4	-33.6
14	2	0	10.4	-10.5
15	2	0	25.5	25.3
16	2	0	-2.3	1.9
17	2	0	21.7	-20.3
0	4	0	47.2	-42.3
1	4	0	24.5	25.9
2	4	0	86.2	-84.4
3	4	0	-1.2	0.4
4	4	0	59.0	62.4
5	4	0	42.8	-41.0
6	4	0	47.0	-44.2
7	4	0	60.2	59.4
8	4	0	39.3	40.9
9	4	0	35.9	-46.8
10	4	0	31.7	-31.1
11	4	0	27.3	27.0
12	4	0	22.8	22.2
13	4	0	19.1	-18.9
14	4	0	-2.2	-1.6
15	4	0	19.2	19.1
16	4	0	-2.3	2.9
0	6	0	74.5	71.5
1	6	0	6.5	4.4
2	6	0	35.1	-38.6
3	6	0	14.9	-12.7
4	6	0	44.9	42.8
5	6	0	12.1	-11.9
6	6	0	22.5	-21.4
7	6	0	17.0	14.9
8	6	0	32.5	32.4
9	6	0	22.0	-19.8
10	6	0	37.9	-35.4
11	6	0	16.9	14.5
12	6	0	-2.2	-1.2
13	6	0	7.9	-7.9
14	6	0	-2.5	4.8
15	6	0	15.1	11.9
0	8	0	9.1	-5.9
1	8	0	-1.7	-1.7
2	8	0	10.3	-10.5
3	8	0	7.2	4.8
4	8	0	34.8	32.8
5	8	0	-1.8	1.4
6	8	0	9.6	-10.1
7	8	0	-2.0	6.3
8	8	0	23.2	22.3
9	8	0	10.8	-7.9
10	8	0	-2.2	-5.2
11	8	0	-2.2	-3.9
12	8	0	-2.2	-6.9
13	8	0	-2.4	-4.0
14	8	0	-2.3	-2.5
0	10	0	-2.0	-5.4
1	10	0	6.9	4.9
2	10	0	-2.0	3.5
3	10	0	-2.0	0.4
4	10	0	22.1	-21.0
5	10	0	-2.1	1.8
6	10	0	13.0	13.1
7	10	0	6.9	8.9
8	10	0	-2.2	-5.8
9	10	0	15.8	-13.7
10	10	0	-2.2	-7.7
11	10	0	-2.9	1.3
12	10	0	11.8	11.6
13	10	0	-2.2	6.7
0	12	0	18.3	-17.9
1	12	0	-2.2	2.4
2	12	0	20.9	19.4
3	12	0	15.8	-15.3
4	12	0	16.4	-15.3
5	12	0	-2.2	4.5
6	12	0	-2.2	3.0
7	12	0	-2.2	5.0
8	12	0	11.6	-12.5
9	12	0	-2.4	2.2
10	12	0	13.3	8.5
11	12	0	-2.2	-5.1
0	14	0	15.8	-12.1
1	14	0	-2.2	2.8
2	14	0	16.8	17.4
3	14	0	7.8	-7.9
4	14	0	14.5	-15.3
5	14	0	8.6	7.2
6	14	0	12.4	12.8
7	14	0	-2.3	-8.1
8	14	0	-2.2	-7.4
0	16	0	11.5	-13.2
1	16	0	-2.2	2.2
2	16	0	18.1	17.0
3	16	0	-2.1	-1.0
0	1	1	68.3	73.7
1	1	1	152.6	-154.4
-1	1	1	71.5	75.4
2	1	1	27.3	27.7
-2	1	1	60.2	-60.7
3	1	1	152.8	149.5
-3	1	1	63.3	-59.7
4	1	1	76.8	70.3
-4	1	1	79.4	75.8
5	1	1	86.8	-85.7
-5	1	1	38.7	38.6
6	1	1	5.4	0.0
-6	1	1	48.3	-48.8
7	1	1	51.7	50.2
-7	1	1	36.6	-37.6
8	1	1	36.5	-33.2
-8	1	1	24.0	24.0
9	1	1	45.3	-45.2
-9	1	1	17.9	18.0
10	1	1	19.2	16.5
-10	1	1	48.2	-46.1
11	1	1	52.5	46.5
-11	1	1	9.5	-8.3
12	1	1	23.3	-22.8
-12	1	1	52.0	51.2
13	1	1	28.7	-27.3
-13	1	1	-2.5	-4.7
14	1	1	25.3	25.8
-14	1	1	44.4	-42.1
15	1	1	-2.5	5.6
-15	1	1	13.0	10.8
16	1	1	21.2	-19.4
-16	1	1	21.6	22.1
-17	1	1	-2.2	-6.3
0	3	1	5.9	2.8
1	3	1	111.4	-113.3
-1	3	1	98.7	99.6
2	3	1	96.6	-93.7
-2	3	1	39.3	-40.2
3	3	1	80.2	82.8
-3	3	1	6.5	-5.0
4	3	1	6.0	-6.9
-4	3	1	7.5	9.8
5	3	1	94.7	-89.2
-5	3	1	62.8	64.3
6	3	1	13.3	14.1
-6	3	1	53.8	-53.7
7	3	1	51.7	54.4
-7	3	1	26.7	-30.0
8	3	1	26.2	-28.4
-8	3	1	67.5	69.2
9	3	1	35.3	-38.3
-9	3	1	17.7	17.7
10	3	1	25.4	29.8
-10	3	1	44.3	-45.2
11	3	1	31.4	30.8
-11	3	1	-2.3	-2.2
12	3	1	9.2	-7.1
-12	3	1	41.1	37.4
13	3	1	17.7	-19.8
-13	3	1	14.2	-12.7
14	3	1	14.1	10.7
-14	3	1	21.7	-20.6
15	3	1	16.2	14.2
-15	3	1	-2.5	2.6
16	3	1	14.6	-15.3
-16	3	1	22.6	20.4
0	5	1	25.7	-25.7
1	5	1	87.0	-84.7
-1	5	1	13.3	16.4
2	5	1	23.3	20.6
-2	5	1	47.0	-49.1
3	5	1	104.9	100.9
-3	5	1	32.1	-35.6
4	5	1	10.3	-8.3
-4	5	1	56.9	59.7
5	5	1	33.3	-30.0
-5	5	1	14.0	14.8
6	5	1	19.1	-17.5
-6	5	1	46.5	-44.6
7	5	1	33.2	33.6
-7	5	1	32.8	-32.1
8	5	1	9.3	10.7
-8	5	1	41.6	43.3
9	5	1	35.2	-35.3
-9	5	1	29.2	27.4
10	5	1	7.4	8.3
-10	5	1	33.1	-29.8
11	5	1	17.1	15.2
-11	5	1	-2.2	1.6
12	5	1	8.7	-25.2
-12	5	1	21.6	19.5
13	5	1	12.8	-11.8
-13	5	1	-2.2	-2.5
14	5	1	15.6	16.4
-14	5	1	14.7	-14.5
15	5	1	13.8	12.3
-15	5	1	-2.4	5.5
16	5	1	7.5	-7.1
-16	5	1	12.1	11.0
0	7	1	-1.5	-4.4
1	7	1	27.8	-26.4
-1	7	1	10.9	9.5
2	7	1	7.1	-6.4
-2	7	1	19.2	20.1
3	7	1	40.8	37.7
-3	7	1	36.6	-36.5
4	7	1	25.5	24.2
-4	7	1	45.4	46.7
5	7	1	11.8	-14.0
-5	7	1	25.1	24.4
6	7	1	11.7	9.7
-6	7	1	33.1	-35.9
7	7	1	13.3	10.4
-7	7	1	12.8	-12.1
8	7	1	-2.0	-4.0
-8	7	1	26.7	27.4
9	7	1	18.9	-18.1
-9	7	1	-2.1	-2.7
10	7	1	8.5	7.5
-10	7	1	17.8	-16.2
11	7	1	12.2	13.7
-11	7	1	-2.2	-3.8
12	7	1	10.6	-8.3
-12	7	1	-2.2	-6.8
13	7	1	11.0	-10.6
-13	7	1	-2.2	5.4
14	7	1	-2.3	3.1
-14	7	1	11.4	-8.7
15	7	1	-2.2	4.7
-15	7	1	-2.2	0.3
0	9	1	7.7	-6.2
1	9	1	7.1	7.1
-1	9	1	26.7	25.8
2	9	1	-1.9	0.0
-2	9	1	-1.5	-2.7
3	9	1	15.9	-13.3
-3	9	1	5.5	-4.3
4	9	1	-1.9	1.7
-4	9	1	13.5	13.6
5	9	1	-2.0	-2.9
-5	9	1	-2.0	1.0
6	9	1	-2.1	-0.2
-6	9	1	14.3	-16.2
7	9	1	-2.1	2.8
-7	9	1	-2.1	-4.2
8	9	1	-2.2	1.3
-8	9	1	-2.2	-2.2
9	9	1	7.8	-6.0
-9	9	1	-2.2	1.9
10	9	1	11.7	10.8
-10	9	1	9.4	8.9
11	9	1	-2.2	8.7
-11	9	1	7.9	-2.8
12	9	1	-2.4	-2.4
-12	9	1	-2.5	-0.7
13	9	1	-2.3	-5.9
-13	9	1	-2.4	-1.4
14	9	1	-2.1	-3.8
-14	9	1	-2.2	-4.4
0	11	1	-2.1	-0.2
1	11	1	19.7	20.3
-1	11	1	8.1	-6.1
2	11	1	-2.1	1.3
-2	11	1	-2.1	-0.8
3	11	1	21.4	-22.5
-3	11	1	7.5	7.4
4	11	1	-2.2	-3.2
-4	11	1	7.5	-8.1
5	11	1	5.8	8.5
-5	11	1	10.8	-11.5
6	11	1	12.1	-11.6
-6	11	1	-2.2	-0.5
7	11	1	-2.2	-1.6
-7	11	1	7.0	-6.4
8	11	1	7.9	-7.8
-8	11	1	11.6	-11.4
9	11	1	-2.2	7.5
-9	11	1	7.5	10.0
10	11	1	-2.4	7.0
-10	11	1	17.5	16.7
11	11	1	-2.3	-0.7
-11	11	1	7.5	7.4
12	11	1	-2.2	1.1
-12	11	1	-2.2	0.2
0	13	1	-2.2	1.7
1	13	1	20.7	20.6
-1	13	1	21.2	-23.6
2	13	1	11.8	-8.6
-2	13	1	18.7	17.7
3	13	1	24.5	-22.9
-3	13	1	16.2	14.6
4	13	1	-2.2	5.2
-4	13	1	15.6	-15.1
5	13	1	10.5	11.8
-5	13	1	-2.2	-1.8
6	13	1	-2.2	1.1
-6	13	1	-2.2	7.1
7	13	1	13.8	-13.9
-7	13	1	-2.5	0.4
8	13	1	9.1	-8.8
-8	13	1	10.7	-8.6
9	13	1	13.3	13.2
-9	13	1	-2.3	-3.3
10	13	1	-2.1	2.1
-10	13	1	11.4	11.8
0	15	1	10.0	-9.4
1	15	1	15.5	13.8
-1	15	1	16.7	-17.6
2	15	1	12.4	11.6
-2	15	1	7.4	8.1
3	15	1	13.8	-11.9
-3	15	1	18.9	18.9
4	15	1	-2.3	1.4
-4	15	1	10.5	-8.8
5	15	1	15.6	16.7
-5	15	1	12.3	-10.9
6	15	1	-2.1	-2.9
-6	15	1	10.3	10.0
0	0	2	21.4	-21.5
1	0	2	20.6	18.8
-1	0	2	47.9	47.9
2	0	2	81.0	81.9
-2	0	2	71.6	72.7
3	0	2	66.7	-55.1
-3	0	2	85.4	-90.1
4	0	2	94.9	-111.3
-4	0	2	15.0	-14.6
5	0	2	27.4	-25.6
-5	0	2	60.9	60.8
6	0	2	111.0	104.9
-6	0	2	20.3	-19.9
7	0	2	68.2	64.2
-7	0	2	91.1	-86.5
8	0	2	64.0	-64.6
-8	0	2	-1.9	1.5
9	0	2	-1.9	-7.4
-9	0	2	52.8	51.7
10	0	2	73.3	70.1
-10	0	2	-2.2	-0.9
11	0	2	-2.1	-0.7
-11	0	2	45.2	-41.9
12	0	2	47.6	-45.6
-12	0	2	24.2	24.7
13	0	2	-2.2	1.6
-13	0	2	46.1	44.6
14	0	2	17.2	14.9
-14	0	2	33.2	-31.8
15	0	2	15.6	-13.9
-15	0	2	22.5	-25.4
16	0	2	9.8	-6.8
-16	0	2	-2.3	4.4
-17	0	2	12.5	13.1
0	2	2	11.4	8.0
1	2	2	57.5	-51.7
-1	2	2	85.5	94.4
2	2	2	73.3	69.8
-2	2	2	36.6	36.1
3	2	2	31.0	29.7
-3	2	2	25.8	-12.7
4	2	2	117.5	-114.8
-4	2	2	72.7	-71.3
5	2	2	41.8	-51.1
-5	2	2	73.4	73.3
6	2	2	64.8	80.6
-6	2	2	27.3	27.1
7	2	2	-1.7	3.0
-7	2	2	79.9	-80.8
8	2	2	47.5	-46.8
-8	2	2	-1.9	-0.6
9	2	2	-1.5	1.3
-9	2	2	50.8	51.2
10	2	2	37.9	34.2
-10	2	2	20.6	-20.0
11	2	2	6.8	3.3
-11	2	2	42.3	-42.9
12	2	2	32.9	-30.0
-12	2	2	25.5	25.2
13	2	2	8.7	8.9
-13	2	2	29.3	30.1
14	2	2	25.7	24.5
-14	2	2	8.5	-8.4
15	2	2	13.5	-11.7
-15	2	2	16.5	-17.2
16	2	2	14.5	-15.2
-16	2	2	-2.3	6.4
0	4	2	64.5	-69.5
1	4	2	75.5	-75.5
-1	4	2	74.8	80.9
2	4	2	57.5	54.6
-2	4	2	6.8	-3.4
3	4	2	61.4	55.4
-3	4	2	59.1	-56.3
4	4	2	83.4	-77.5
-4	4	2	23.5	-23.0
5	4	2	31.1	-28.8
-5	4	2	67.3	64.7
6	4	2	30.0	31.1
-6	4	2	42.0	44.0
7	4	2	-1.8	4.1
-7	4	2	28.7	-29.8
8	4	2	30.8	-29.7
-8	4	2	8.2	-8.0
9	4	2	-2.0	0.8
-9	4	2	43.6	43.5
10	4	2	12.5	16.2
-10	4	2	9.2	-7.4
11	4	2	6.5	-10.7
-11	4	2	33.6	-34.0
12	4	2	14.6	-21.4
-12	4	2	14.1	13.2
13	4	2	17.7	12.3
-13	4	2	17.8	18.8
14	4	2	23.2	22.2
-14	4	2	-2.5	-4.1
15	4	2	-2.3	-7.3
-15	4	2	12.0	-10.9
-16	4	2	11.7	10.0
0	6	2	57.6	-54.4
1	6	2	10.0	-14.0
-1	6	2	7.6	7.9
2	6	2	41.5	43.3
-2	6	2	19.0	19.6
3	6	2	16.4	16.2
-3	6	2	62.4	-65.9
4	6	2	38.5	-37.5
-4	6	2	27.6	31.4
5	6	2	-1.8	-0.9
-5	6	2	20.6	18.8
6	6	2	43.3	40.0
-6	6	2	-1.8	1.7
7	6	2	28.4	25.2
-7	6	2	9.9	-10.5
8	6	2	24.4	-22.3
-8	6	2	-2.0	4.6
9	6	2	-2.1	-1.7
-9	6	2	26.6	27.6
10	6	2	17.6	17.6
-10	6	2	9.0	-8.3
11	6	2	18.0	-16.4
-11	6	2	24.8	-24.1
12	6	2	17.3	-15.9
-12	6	2	-2.2	-2.0
13	6	2	-2.5	1.6
-13	6	2	21.1	18.5
14	6	2	13.3	14.2
-14	6	2	-2.4	-7.1
15	6	2	-2.1	0.3
-15	6	2	12.0	-11.6
0	8	2	-1.8	3.7
1	8	2	6.4	6.1
-1	8	2	5.6	4.4
2	8	2	14.6	12.3
-2	8	2	20.1	19.4
3	8	2	6.6	7.1
-3	8	2	20.2	-23.9
4	8	2	-1.9	-4.8
-4	8	2	9.3	-10.4
5	8	2	9.3	-8.6
-5	8	2	17.9	19.2
6	8	2	23.0	22.5
-6	8	2	6.3	-7.6
7	8	2	-2.1	0.8
-7	8	2	10.3	-6.5
8	8	2	11.9	-10.1
-8	8	2	-2.1	5.6
9	8	2	-2.2	-3.3
-9	8	2	-2.2	-1.7
10	8	2	136.9	7.7
-10	8	2	14.6	-15.3
11	8	2	7.0	-4.8
-11	8	2	8.7	-8.3
12	8	2	-2.4	-6.7
-12	8	2	-2.2	-5.1
13	8	2	-2.3	4.6
-13	8	2	7.6	8.5
14	8	2	7.5	7.4
-14	8	2	-2.3	5.0
0	10	2	-2.0	-0.1
1	10	2	-2.1	3.3
-1	10	2	-2.0	5.2
2	10	2	10.3	-9.3
-2	10	2	7.9	-7.9
3	10	2	-2.1	-1.6
-3	10	2	19.2	-18.2
4	10	2	19.0	17.5
-4	10	2	9.5	-12.1
5	10	2	-2.2	-0.6
-5	10	2	18.6	19.4
6	10	2	19.0	-20.5
-6	10	2	14.4	13.7
7	10	2	-2.2	3.7
-7	10	2	-2.2	9.2
8	10	2	-2.2	3.5
-8	10	2	7.5	-5.6
9	10	2	-2.2	-3.2
-9	10	2	14.2	-15.3
10	10	2	-2.5	3.0
-10	10	2	10.5	8.9
11	10	2	-2.4	-2.2
-11	10	2	11.6	10.1
12	10	2	-2.2	-1.5
-12	10	2	-2.3	-2.0
-13	10	2	-2.2	-4.0
0	12	2	23.1	23.0
1	12	2	10.6	8.7
-1	12	2	-2.2	-5.1
2	12	2	23.4	-20.5
-2	12	2	8.6	-11.3
3	12	2	11.7	-9.4
-3	12	2	-2.2	6.3
4	12	2	9.3	9.0
-4	12	2	-2.2	-7.2
5	12	2	-2.2	3.2
-5	12	2	9.9	-8.1
6	12	2	-2.2	-15.5
-6	12	2	12.6	13.5
7	12	2	-2.2	-2.3
-7	12	2	11.5	9.7
8	12	2	9.3	7.5
-8	12	2	-2.5	-2.9
9	12	2	-2.3	1.6
-9	12	2	10.7	-12.3
10	12	2	9.2	-8.6
-10	12	2	-2.3	3.3
-11	12	2	12.8	11.1
0	14	2	16.1	16.3
1	14	2	20.2	18.0
-1	14	2	14.0	-12.8
2	14	2	11.6	-11.7
-2	14	2	7.8	-7.8
3	14	2	17.1	-15.9
-3	14	2	17.8	16.5
4	14	2	16.8	15.7
-4	14	2	-2.4	4.3
5	14	2	-2.3	0.2
-5	14	2	16.8	-16.6
6	14	2	10.7	-9.4
-6	14	2	8.2	-6.8
7	14	2	-2.2	-0.6
-7	14	2	12.8	13.1
-8	14	2	-2.1	-0.6
0	1	3	79.4	-80.2
1	1	3	49.3	43.3
-1	1	3	4.7	2.1
2	1	3	51.9	52.9
-2	1	3	68.9	69.6
3	1	3	50.9	-54.4
-3	1	3	5.5	-3.8
4	1	3	16.8	-17.5
-4	1	3	83.4	-83.0
5	1	3	29.8	50.6
-5	1	3	6.7	-3.0
6	1	3	44.0	40.9
-6	1	3	84.1	80.6
7	1	3	79.2	-72.5
-7	1	3	41.7	-41.1
8	1	3	41.1	-41.9
-8	1	3	54.2	-53.2
9	1	3	55.1	55.1
-9	1	3	38.2	37.2
10	1	3	34.4	37.1
-10	1	3	34.9	34.9
11	1	3	21.4	-21.8
-11	1	3	26.8	-27.8
12	1	3	-2.2	0.0
-12	1	3	26.5	-26.2
13	1	3	21.2	18.9
-13	1	3	15.4	14.6
14	1	3	-2.4	-2.3
-14	1	3	11.1	10.6
15	1	3	20.6	-19.1
-15	1	3	-2.4	-7.6
-16	1	3	8.7	-8.6
0	3	3	47.8	-44.8
1	3	3	6.8	5.7
-1	3	3	5.0	3.7
2	3	3	78.5	75.8
-2	3	3	49.6	50.1
3	3	3	35.8	-33.5
-3	3	3	4.7	4.1
4	3	3	63.2	-60.5
-4	3	3	63.7	-62.0
5	3	3	60.6	61.1
-5	3	3	15.8	13.5
6	3	3	29.5	25.4
-6	3	3	54.2	55.4
7	3	3	52.2	-51.1
-7	3	3	16.3	-14.9
8	3	3	16.7	-17.0
-8	3	3	55.3	-58.4
9	3	3	5.4	21.5
-9	3	3	25.0	24.4
10	3	3	-2.2	-3.3
-10	3	3	45.5	45.8
11	3	3	18.7	-21.5
-11	3	3	13.3	-14.9
12	3	3	13.7	-14.3
-12	3	3	18.1	-15.6
13	3	3	26.3	27.7
-13	3	3	13.2	16.0
14	3	3	-2.4	4.6
-14	3	3	10.3	8.9
15	3	3	20.0	-20.4
-15	3	3	15.5	-17.1
-16	3	3	-2.2	-2.6
0	5	3	72.6	-72.3
1	5	3	8.8	-5.8
-1	5	3	27.3	-27.7
2	5	3	15.6	20.8
-2	5	3	75.8	81.7
3	5	3	6.5	4.7

Table VII - cont.

Continued:-

h	k	l	F_o	F_c
-3	5	3	24.8	24.1
4	5	3	32.5	-31.4
-4	5	3	28.4	-29.8
5	5	3	38.6	34.9
-5	5	3	9.2	7.3
6	5	3	14.5	15.5
-6	5	3	13.0	16.5
7	5	3	34.5	-32.1
-7	5	3	6.1	0.1
8	5	3	20.8	-20.0
-8	5	3	7.8	-5.3
9	5	3	28.5	26.5
-9	5	3	13.2	16.5
10	5	3	12.1	12.5
-10	5	3	28.9	28.6
11	5	3	27.4	-25.2
-11	5	3	23.3	-23.9
12	5	3	-2.2	-1.0
-12	5	3	29.3	-32.8
13	5	3	15.7	15.0
-13	5	3	14.9	12.7
14	5	3	-2.3	-2.0
-14	5	3	11.5	12.3
-15	5	3	12.4	-11.9
0	7	3	24.0	-25.1
1	7	3	-1.8	1.0
-1	7	3	22.1	-22.2
2	7	3	37.6	39.1
-2	7	3	11.4	12.1
3	7	3	-1.9	-3.2
-3	7	3	-1.8	-0.4
4	7	3	15.6	-14.4
-4	7	3	10.7	-11.4
5	7	3	19.5	19.6
-5	7	3	10.5	-8.6
6	7	3	18.2	15.7
-6	7	3	11.9	11.9
7	7	3	11.7	-9.5
-7	7	3	-2.1	-3.3
8	7	3	7.7	-6.3
-8	7	3	18.5	-20.1
9	7	3	11.1	9.3
-9	7	3	13.9	12.5
10	7	3	8.7	7.9
-10	7	3	7.1	6.5
11	7	3	18.5	-16.8
-11	7	3	14.2	-12.1
12	7	3	-2.4	2.7
-12	7	3	9.3	-9.5
13	7	3	8.8	9.0
-13	7	3	-2.4	5.5
-14	7	3	-2.3	6.2
0	9	3	-2.0	-2.7
1	9	3	-2.1	-1.5
-1	9	3	-2.0	-0.5
2	9	3	-2.1	-1.3
-2	9	3	14.8	16.2
3	9	3	-2.1	-3.5
-3	9	3	-2.0	6.2
4	9	3	6.7	6.2
-4	9	3	13.1	-10.2
5	9	3	-2.2	-4.0
-5	9	3	-2.1	-0.9
6	9	3	8.5	8.7
-6	9	3	-2.1	-7.8
7	9	3	-2.2	4.9
-7	9	3	-2.2	-5.6
8	9	3	7.9	-7.7
-8	9	3	-2.2	-5.8
9	9	3	-2.2	3.8
-9	9	3	-2.2	2.3
10	9	3	-2.4	0.5
-10	9	3	-2.2	0.4
11	9	3	-2.3	-3.0
-11	9	3	-2.5	5.6
12	9	3	-2.2	2.2
-12	9	3	-2.4	1.3
-13	9	3	-2.2	-1.4
0	11	3	-2.2	-4.2
1	11	3	-2.2	-2.1
-1	11	3	9.2	10.3
2	11	3	24.5	-25.2
-2	11	3	15.6	14.7
3	11	3	-2.2	0.7
-3	11	3	5.3	9.2
4	11	3	7.1	8.0
-4	11	3	8.5	7.4
5	11	3	12.7	-12.2
-5	11	3	-2.2	-1.4
6	11	3	-2.2	-6.5
-6	11	3	12.8	-13.1
7	11	3	10.4	8.8
-7	11	3	-2.2	-1.6
8	11	3	-2.4	-2.3
-8	11	3	12.9	15.3
9	11	3	-2.3	-5.1
-9	11	3	7.7	-8.5
10	11	3	-2.2	2.6
-10	11	3	-2.4	-0.7
-11	11	3	8.6	8.1
0	13	3	16.1	12.5
1	13	3	-2.2	0.4
-1	13	3	-2.2	7.1
2	13	3	-2.2	-7.1
-2	13	3	17.4	-15.3
3	13	3	-2.5	2.4
-3	13	3	-2.2	-1.1
4	13	3	7.6	9.1
-4	13	3	14.1	13.8
5	13	3	9.2	-9.8
-5	13	3	-2.4	-4.5
6	13	3	8.9	-8.4
-6	13	3	14.1	-12.9
7	13	3	9.3	10.5
-7	13	3	-2.3	1.6
-8	13	3	8.6	9.3
0	15	3	10.4	12.2
1	15	3	11.9	-9.5
-1	15	3	-2.2	-0.7
2	15	3	13.5	-12.1
-2	15	3	10.8	-11.8
-3	15	3	-2.1	3.2
0	0	4	-1.6	-1.4
1	0	4	42.3	45.2
-1	0	4	31.9	-32.9
2	0	4	6.3	-5.7
-2	0	4	20.1	18.8
3	0	4	81.2	-75.9
-3	0	4	82.7	76.7
4	0	4	30.1	-30.6
-4	0	4	51.1	-50.6
5	0	4	60.5	58.3
-5	0	4	70.8	-71.1
6	0	4	-1.9	-3.7
-6	0	4	61.7	58.9
7	0	4	41.5	-43.5
-7	0	4	31.1	30.6
8	0	4	66.5	62.8
-8	0	4	54.9	-56.1
9	0	4	9.6	10.2
-9	0	4	52.5	-53.6
10	0	4	35.1	-33.7
-10	0	4	17.0	13.8
11	0	4	-2.2	-4.5
-11	0	4	29.1	30.3
12	0	4	28.7	27.9
-12	0	4	-2.5	-4.4
13	0	4	12.5	10.6
-13	0	4	-2.5	2.4
14	0	4	14.5	-14.8
-14	0	4	13.4	14.3
-15	0	4	-2.3	1.7
0	2	4	24.6	-24.0
1	2	4	55.6	56.5
-1	2	4	53.3	-54.7
2	2	4	6.0	4.4
-2	2	4	21.0	21.0
3	2	4	63.2	-62.0
-3	2	4	46.1	47.2
4	2	4	19.1	17.9
-4	2	4	15.4	-16.4
* 5	2	4	16.8	47.7
-5	2	4	49.0	-48.3
6	2	4	33.1	-35.5
-6	2	4	32.8	31.2
7	2	4	27.8	-32.1
-7	2	4	42.7	40.9
8	2	4	40.8	40.0
-8	2	4	41.4	-39.7
9	2	4	31.6	30.7
-9	2	4	30.4	-27.2
10	2	4	23.7	-23.2
-10	2	4	32.1	33.5
11	2	4	18.8	-19.9
-11	2	4	18.0	18.6
12	2	4	11.0	10.2
-12	2	4	18.6	-20.0
13	2	4	7.5	10.5
-13	2	4	-2.5	-1.9
14	2	4	16.6	-16.7
-14	2	4	15.8	15.6
-15	2	4	-2.3	0.8
0	4	4	11.0	10.1
1	4	4	67.3	65.3
-1	4	4	57.1	-57.3
2	4	4	8.0	-8.1
-2	4	4	-1.7	5.8
3	4	4	40.1	-40.1
-3	4	4	30.5	32.0
4	4	4	16.4	15.9
-4	4	4	10.0	-11.8
5	4	4	35.5	27.3
-5	4	4	17.6	-17.7
6	4	4	21.5	-21.0
-6	4	4	29.2	30.9
7	4	4	27.4	-25.0
-7	4	4	30.9	32.3
8	4	4	11.9	9.1
* -8	4	4	-2.1	-20.9
9	4	4	36.7	33.3
-9	4	4	16.4	-15.2
* 10	4	4	8.7	-25.6
-10	4	4	24.7	24.0
* 11	4	4	10.6	-24.5
-11	4	4	-2.2	3.5
12	4	4	13.5	14.1
-12	4	4	22.7	-23.2
13	4	4	8.1	9.1
-13	4	4	-2.5	-6.7
-14	4	4	20.4	20.3
-15	4	4	-2.2	-0.6
0	6	4	-1.5	-4.0
1	6	4	30.8	30.1
-1	6	4	37.7	-38.4
2	6	4	8.1	6.4
-2	6	4	-1.9	-1.5
3	6	4	22.1	-20.0
-3	6	4	35.8	35.9
4	6	4	-2.0	-2.3
-4	6	4	17.1	-16.2
5	6	4	12.3	13.0
-5	6	4	22.6	-22.9
6	6	4	-2.1	-0.3
-6	6	4	20.7	21.2
7	6	4	8.5	-9.0
-7	6	4	22.6	22.9
8	6	4	7.5	9.3
-8	6	4	12.4	-15.1
9	6	4	11.2	9.3
-9	6	4	14.0	-16.3
10	6	4	17.9	-17.0
-10	6	4	10.0	7.8
11	6	4	16.4	-15.7
-11	6	4	-2.2	2.5
12	6	4	17.6	17.6
-12	6	4	8.8	-9.7
13	6	4	8.3	7.0
-13	6	4	-2.4	-3.6
-14	6	4	12.1	11.5
0	8	4	11.9	-12.3
1	8	4	-2.1	5.2
-1	8	4	29.4	-27.0
2	8	4	18.3	18.8
-2	8	4	8.7	-7.2
3	8	4	-2.1	-7.5
-3	8	4	8.7	4.9
4	8	4	-2.2	5.5
-4	8	4	-2.1	-3.6
5	8	4	7.8	7.9
-5	8	4	9.5	-12.6
6	8	4	-2.2	-4.9
-6	8	4	-2.2	-0.8
7	8	4	-2.2	0.9
-7	8	4	12.2	14.0
8	8	4	7.9	7.1
-8	8	4	8.7	-8.2
9	8	4	-2.2	5.4
-9	8	4	-2.2	-0.9
10	8	4	-2.4	-0.2
-10	8	4	-2.2	8.3
11	8	4	-2.3	-5.7
-11	8	4	-2.4	3.3
-12	8	4	-2.3	-5.8
-13	8	4	-2.2	-0.5
0	10	4	27.5	24.8
1	10	4	14.1	13.9
-1	10	4	-2.2	3.7
2	10	4	14.1	-11.2
-2	10	4	-2.2	-6.8
3	10	4	-2.2	-4.1
-3	10	4	16.7	-16.7
4	10	4	7.1	-7.5
-4	10	4	-2.2	-4.3
5	10	4	-2.2	-0.2
-5	10	4	17.5	17.5
6	10	4	-2.2	3.8
-6	10	4	-2.2	4.4
7	10	4	-2.5	-6.6
-7	10	4	9.8	-7.4
8	10	4	9.3	-8.3
-8	10	4	-2.2	3.9
9	10	4	-2.3	3.0
-9	10	4	-2.4	-1.8
10	10	4	-2.1	4.5
-10	10	4	-2.3	-2.8
-11	10	4	-2.2	1.0
0	12	4	-2.2	3.8
1	12	4	-2.2	5.8
-1	12	4	16.4	13.7
2	12	4	-2.2	-5.9
-2	12	4	-2.2	-0.9
3	12	4	-2.4	3.5
-3	12	4	18.0	-15.5
4	12	4	-2.4	-2.8
-4	12	4	-2.5	5.0
5	12	4	12.4	-10.9
-5	12	4	16.4	17.9
6	12	4	-2.3	2.9
-6	12	4	-2.4	-4.8
7	12	4	-2.2	4.9
-7	12	4	13.3	-13.0
-8	12	4	8.7	9.3
-9	12	4	-2.1	-0.1
0	14	4	-2.2	-2.5
1	14	4	15.9	-12.9
-1	14	4	9.5	10.3
2	14	4	-2.2	5.2
-2	14	4	-2.2	-3.4
3	14	4	12.5	11.0
-3	14	4	11.9	-11.6
-4	14	4	-2.1	4.5
0	1	5	41.1	39.6
1	1	5	35.9	30.4
-1	1	5	11.9	-12.7
2	1	5	43.5	-41.6
-2	1	5	42.6	-43.6
* 3	1	5	13.6	-29.4
-3	1	5	28.3	28.0
4	1	5	33.8	37.2
-4	1	5	25.6	31.4
5	1	5	8.1	7.1
-5	1	5	58.1	-55.9
6	1	5	44.3	-41.6
-6	1	5	36.2	-37.0
7	1	5	-2.2	42.4
* -7	1	5	-2.4	40.5
8	1	5	36.5	37.0
-8	1	5	18.7	16.6
9	1	5	18.8	-18.4
-9	1	5	29.2	-28.5
10	1	5	17.3	-14.8
-10	1	5	-2.5	-4.0
11	1	5	24.4	24.3
* -11	1	5	-2.5	30.4
12	1	5	18.6	18.9
-12	1	5	-2.5	-1.7
13	1	5	17.5	-15.8
-13	1	5	18.7	-17.4
-14	1	5	-2.3	5.1
0	3	5	42.2	40.8
1	3	5	12.7	14.3
-1	3	5	26.7	-27.2
2	3	5	56.9	-52.8
-2	3	5	22.7	-22.0
3	3	5	9.0	-9.1
-3	3	5	33.1	32.6
4	3	5	47.4	43.3
-4	3	5	43.3	43.3
5	3	5	14.2	11.3
-5	3	5	35.1	-33.9
6	3	5	33.5	-32.9
-6	3	5	19.8	-18.4
7	3	5	-2.2	5.1
-7	3	5	31.8	31.7
8	3	5	8.7	16.9
-8	3	5	13.0	12.5
9	3	5	-2.2	-4.8
-9	3	5	22.3	-21.0
10	3	5	14.0	-23.7
-10	3	5	-2.5	-0.1
11	3	5	12.6	13.1
-11	3	5	17.7	16.5
12	3	5	18.5	18.1
-12	3	5	-2.5	-6.9
-13	3	5	18.3	-20.6
-14	3	5	-2.2	1.4
0	5	5	30.9	32.1
1	5	5	-2.1	3.3
-1	5	5	19.9	-18.7
2	5	5	16.8	-16.5
-2	5	5	32.0	-32.6
3	5	5	-2.1	6.3
-3	5	5	38.6	39.1
4	5	5	28.4	26.7
-4	5	5	16.2	15.6
5	5	5	-2.2	5.8
-5	5	5	29.6	-30.2
6	5	5	27.5	-24.3
-6	5	5	10.3	-11.3
7	5	5	-2.2	-2.2
-7	5	5	23.6	21.0
8	5	5	19.7	21.0
-8	5	5	7.1	7.6
9	5	5	12.1	-11.6
-9	5	5	12.8	-12.6
10	5	5	23.0	-22.4
-10	5	5	-2.2	0.7
11	5	5	-2.1	5.1
-11	5	5	-2.2	5.4
12	5	5	7.5	8.3
-12	5	5	-2.4	0.8
-13	5	5	16.0	-14.8
0	7	5	-2.2	8.0
1	7	5	-2.2	1.3
-1	7	5	23.1	-22.6
2	7	5	17.9	-17.8
-2	7	5	9.0	-9.3
3	7	5	-2.2	-1.6
-3	7	5	20.7	19.4
4	7	5	18.9	20.7
-4	7	5	-2.2	-4.9
5	7	5	-2.2	-4.5
-5	7	5	7.7	-8.5
6	7	5	7.1	-7.2
-6	7	5	13.2	-13.8
7	7	5	-2.2	4.3
-7	7	5	12.3	13.5
8	7	5	-2.5	6.6
-8	7	5	12.3	14.2
9	7	5	-2.4	-3.3
-9	7	5	8.8	-8.0
10	7	5	-2.3	-4.5
-10	7	5	-2.5	-1.1
11	7	5	-2.1	0.8
-11	7	5	5.2	7.4
-12	7	5	-2.2	-5.9
0	9	5	-2.2	-1.3
1	9	5	-2.2	-4.5
-1	9	5	-2.2	-2.3
2	9	5	18.4	-13.6
-2	9	5	11.7	7.8
3	9	5	-2.2	-5.8
-3	9	5	-2.2	-2.4
4	9	5	13.2	11.9
-4	9	5	-2.2	1.6
5	9	5	-2.2	3.5
-5	9	5	-2.2	1.8
6	9	5	-2.4	-2.7
-6	9	5	-2.2	-0.8
7	9	5	-2.4	3.1
-7	9	5	-2.2	0.4
8	9	5	-2.3	-3.9
-8	9	5	-2.4	0.2
9	9	5	-2.2	3.8
-9	9	5	-2.4	-4.2
-10	9	5	-2.3	-1.0
-11	9	5	-2.1	5.8
0	11	5	-2.5	-3.5
1	11	5	-2.5	-3.8
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2	11	5	-2.4	-2.9
-2	11	5	13.5	12.6
3	11	5	-2.4	2.4
-3	11	5	-2.5	-5.1
4	11	5	-2.4	0.5
-4	11	5	-2.4	-5.1
5	11	5	-2.3	3.7
-5	11	5	-2.4	4.7
6	11	5	-2.2	3.8
-6	11	5	7.4	6.6
7	11	5	6.6	-6.1
-7	11	5	9.6	-9.3
-8	11	5	-2.2	-6.4
0	13	5	9.1	-9.1
1	13	5	-2.1	-6.7
-1	13	5	8.4	8.6
2	13	5	-2.1	3.2
-2	13	5	12.8	14.9
-3	13	5	-2.1	-6.0
0	0	6	31.3	30.0
1	0	6	40.5	-38.6
-1	0	6	22.5	24.4
2	0	6	35.9	-32.9
-2	0	6	47.6	-45.1
3	0	6	36.3	30.4
-3	0	6	33.9	-33.0
4	0	6	23.5	22.7
-4	0	6	42.2	37.3
5	0	6	25.7	-26.5
-5	0	6	32.8	30.0
6	0	6	17.1	-15.7
-6	0	6	32.7	-31.9
7	0	6	21.1	22.0
-7	0	6	-2.5	3.3
8	0	6	16.5	17.4
-8	0	6	-2.5	8.1
9	0	6	22.7	-23.5
-9	0	6	19.4	-16.3
10	0	6	-2.3	2.9
-10	0	6	18.4	-15.0
11	0	6	14.5	14.3
-11	0	6	20.4	23.0
-12	0	6	22.4	23.0
-13	0	6	6.9	-8.3
0	2	6	37.2	37.7
1	2	6	33.1	-30.4
-1	2	6	25.2	26.3
2	2	6	34.3	-30.3
-2	2	6	33.9	-32.6
3	2	6	28.5	26.6
-3	2	6	17.4	-17.4
4	2	6	14.0	11.4
-4	2	6	42.3	40.8
* 5	2	6	8.7	-19.2
-5	2	6	7.8	7.2
6	2	6	9.4	-14.3
-6	2	6	27.8	-27.6
* 7	2	6	5.4	20.1
-7	2	6	-2.5	0.2
8	2	6	-2.2	7.5
-8	2	6	21.0	22.0
9	2	6	18.3	-18.9
-9	2	6	9.7	-10.3
10	2	6	-2.3	1.8
-10	2	6	22.7	-25.2
11	2	6	18.5	18.7
-11	2	6	7.6	7.3
-12	2	6	17.8	16.8
-13	2	6	-2.1	-5.4
0	4	6	21.9	21.7
1	4	6	6.9	-5.9
-1	4	6	14.2	15.7
2	4	6	-2.2	-4.9
-2	4	6	36.2	-34.1
3	4	6	15.7	15.7
-3	4	6	12.1	-11.3
4	4	6	14.5	14.4
-4	4	6	41.6	41.3
5	4	6	21.8	-19.4
-5	4	6	-2.2	-0.5
6	4	6	15.8	-13.4
-6	4	6	25.1	-24.3
7	4	6	29.5	27.2
-7	4	6	-2.2	-0.4
8	4	6	-2.4	2.3
-8	4	6	22.4	22.0
9	4	6	17.7	-17.6
-9	4	6	-2.2	-3.1
10	4	6	-2.2	0.3
-10	4	6	13.5	-15.7
-11	4	6	-2.3	-1.2
-12	4	6	12.6	11.7
0	6	6	-2.2	5.4
1	6	6	8.7	-6.7
-1	6	6	-2.2	0.1
2	6	6	-2.2	-3.8
-2	6	6	25.8	-26.8
3	6	6	20.0	17.8
-3	6	6	-2.2	-5.3
4	6	6	19.8	18.8
-4	6	6	11.8	11.2
5	6	6	24.8	-26.2
-5	6	6	10.0	10.6
6	6	6	-2.5	-5.2
-6	6	6	13.3	-12.9
7	6	6	17.0	17.1
-7	6	6	-2.2	0.3
8	6	6	-2.3	4.6
-8	6	6	10.4	11.6
9	6	6	10.4	-10.7
-9	6	6	-2.4	-0.4
-10	6	6	9.0	-6.3
-11	6	6	-2.2	4.3
0	8	6	10.0	9.8
1	8	6	-2.2	-5.5
-1	8	6	-2.2	-4.5
2	8	6	13.5	-12.5
-2	8	6	-2.2	-2.9
3	8	6	12.5	12.2
-3	8	6	-2.2	2.6
4	8	6	-2.4	1.4
-4	8	6	-2.2	-5.3
5	8	6	16.0	-15.6
-5	8	6	6.5	4.4
6	8	6	-2.3	0.1
-6	8	6	-2.5	-0.3
7	8	6	-2.2	2.4
-7	8	6	-2.4	-3.6
8	8	6	-2.1	0.6
-8	8	6	5.8	9.4
-9	8	6	-2.2	-0.1
-10	8	6	8.9	-9.0
0	10	6	-2.4	2.6
1	10	6	12.4	10.1
-1	10	6	-2.4	-5.6
2	10	6	8.2	5.4
-2	10	6	-2.4	0.7
3	10	6	-2.3	-3.3
-3	10	6	-2.4	0.6
4	10	6	7.8	-7.6
-4	10	6	-2.3	0.3
5	10	6	-2.1	-0.2
-5	10	6	-2.3	-1.9
-6	10	6	-2.2	-0.2
-7	10	6	-2.2	-2.7
0	1	7	5.4	-11.9
1	1	7	42.3	-39.3
-1	1	7	46.8	44.1
2	1	7	10.0	9.6
-2	1	7	12.8	11.5
* 3	1	7	-2.2	18.3
-3	1	7	32.0	-30.2
4	1	7	10.5	-15.9
-4	1	7	-2.5	1.5
5	1	7	20.8	-21.4
-5	1	7	15.3	16.7
6	1	7	12.0	13.2
-6	1	7	15.7	-14.5
7	1	7	16.5	15.5
-7	1	7	5.5	-8.2
8	1	7	12.6	-13.6
-8	1	7	7.7	7.5
-9	1	7	17.2	16.2
-10	1	7	8.8	-8.4
-11	1	7	8.5	-10.6
0	3	7	-2.2	-0.4
1	3	7	19.3	-18.7
-1	3	7	27.5	27.8
2	3	7	14.5	13.8
-2	3	7	-2.2	0.4
3	3	7	20.1	20.4
-3	3	7	26.0	-26.7
4	3	7	14.0	-16.6
-4	3	7	-2.2	5.2
5	3	7	12.1	-9.6
-5	3	7	16.5	17.3
6	3	7	-2.4	12.7
-6	3	7	-2.2	-6.4
7	3	7	13.5	13.6
-7	3	7	20.6	-22.6
8	3	7	14.0	-12.9
-8	3	7	12.0	10.9
-9	3	7	11.6	10.0
-10	3	7	-2.2	-11.7
0	5	7	10.5	-9.3
1	5	7	18.0	-16.3
-1	5	7	10.5	9.6
2	5	7	-2.5	3.6
-2	5	7	-2.2	6.4
3	5	7	21.1	19.1
-3	5	7	12.4	-12.8
4	5	7	-2.4	0.4
-4	5	7	-2.2	-1.9
5	5	7	12.2	-12.6

Table VII - cont.

Continued:-

h	k	l	F_o	F_c
-5	5	7	15.1	16.1
6	5	7	10.7	11.2
-6	5	7	8.6	-9.1
7	5	7	8.3	9.2
-7	5	7	13.5	-14.9
-8	5	7	16.7	17.0
-9	5	7	13.9	14.7
0	7	7	-2.4	-2.8
1	7	7	7.5	-8.7
-1	7	7	10.1	8.7
2	7	7	-2.3	1.8
-2	7	7	-2.4	-2.5
3	7	7	-2.3	7.2
-3	7	7	7.6	-7.4
4	7	7	-2.2	-4.3
-4	7	7	-2.4	-3.2
5	7	7	-2.2	-9.1
-5	7	7	7.4	7.9
-6	7	7	-2.3	0.3
-7	7	7	-2.2	-5.3
0	9	7	-2.2	2.6
1	9	7	-2.2	-1.3
-1	9	7	-2.2	1.8
2	9	7	-2.1	-4.4
-2	9	7	-2.2	-2.8
-3	9	7	-2.2	-0.8
-4	9	7	-2.1	1.0
0	0	8	17.5	-16.6
1	0	8	-2.3	-3.9
-1	0	8	-2.4	7.1
2	0	8	21.3	18.8
-2	0	8	13.6	15.6
3	0	8	8.8	-10.4
-3	0	8	13.0	-11.4
4	0	8	15.7	-20.7
-4	0	8	5.8	-10.1
5	0	8	10.0	8.4
-5	0	8	22.5	22.6
-6	0	8	14.3	12.0
-7	0	8	8.5	-8.2
0	2	8	21.5	-22.8
1	2	8	-2.3	0.6
-1	2	8	-7.4	3.3
2	2	8	25.5	23.9
-2	2	8	12.4	15.7
3	2	8	-2.2	-2.4
-3	2	8	9.1	-9.6
4	2	8	18.1	-17.4
-4	2	8	11.6	-11.1
-5	2	8	12.5	12.4
-6	2	8	11.7	9.3
-7	2	8	-2.2	-11.7
0	4	8	17.5	-17.6
1	4	8	-2.2	2.0
-1	4	8	-2.3	-0.9
2	4	8	18.3	19.2
-2	4	8	13.0	13.8
3	4	8	-2.1	2.7
-3	4	8	-2.3	-5.2
-4	4	8	11.7	-12.2
-5	4	8	6.5	5.5
-6	4	8	9.5	10.1
1	1	0	29.8	-30.4
2	1	0	12.2	-7.2
3	1	0	13.3	10.9
4	1	0	61.7	-62.4
5	1	0	8.3	4.9
6	1	0	44.6	-39.2
7	1	0	-1.4	0.6
8	1	0	14.3	-12.5
9	1	0	11.8	-11.8
10	1	0	14.7	13.4
11	1	0	29.1	20.0
12	1	0	11.0	-7.5
13	1	0	8.4	-3.3
14	1	0	6.5	6.9
15	1	0	7.7	-5.9
16	1	0	-2.4	-4.5
17	1	0	-2.1	2.6
1	3	0	17.8	-15.8
2	3	0	26.7	-28.6
3	3	0	53.1	51.9
4	3	0	9.0	-9.0
5	3	0	42.0	-39.9
6	3	0	-1.4	3.5
7	3	0	29.0	30.4
8	3	0	37.7	-36.9
9	3	0	18.4	-17.8
10	3	0	37.4	35.4
11	3	0	11.3	9.4
12	3	0	22.2	-19.6
13	3	0	11.2	-11.7
14	3	0	8.7	8.4
15	3	0	-2.5	6.3
16	3	0	10.9	-10.2
1	5	0	38.8	-35.3
2	5	0	-1.3	-0.0
3	5	0	48.8	50.6
4	5	0	7.0	7.6
5	5	0	55.4	-54.4
6	5	0	51.9	47.0
7	5	0	52.2	49.1
8	5	0	32.1	-32.6
9	5	0	35.1	-33.9
10	5	0	46.3	44.2
11	5	0	5.6	7.6
12	5	0	20.5	-21.6
13	5	0	7.1	-7.6
14	5	0	11.1	11.0
15	5	0	-2.4	7.7
16	5	0	12.5	-11.1
1	7	0	40.9	-42.0
2	7	0	21.0	21.5
3	7	0	66.3	67.0
4	7	0	38.2	-37.2
5	7	0	57.4	-56.4
6	7	0	31.0	32.4
7	7	0	45.2	44.0
8	7	0	40.5	-40.2
9	7	0	30.1	-31.2
10	7	0	31.7	29.6
11	7	0	20.1	22.7
12	7	0	12.2	-13.9
13	7	0	-2.2	-3.9
14	7	0	18.5	17.8
15	7	0	-2.2	-0.4
1	9	0	34.7	-36.7
2	9	0	27.6	25.5
3	9	0	65.1	68.4
4	9	0	20.9	-21.9
5	9	0	59.9	-60.0
6	9	0	29.9	31.4
7	9	0	26.9	27.9
8	9	0	30.1	-41.8
9	9	0	22.6	-20.5
10	9	0	9.3	9.9
11	9	0	17.6	16.6
12	9	0	17.4	-17.5
13	9	0	-2.3	-8.6
14	9	0	18.8	18.1
1	11	0	57.5	-58.7
2	11	0	24.4	22.4
3	11	0	29.3	28.8
4	11	0	21.2	-20.2
5	11	0	25.0	-25.6
6	11	0	20.6	19.2
7	11	0	18.6	20.7
8	11	0	14.1	-14.1
9	11	0	23.6	-22.6
11	11	0	17.9	16.2
12	11	0	19.2	-19.7
1	13	0	33.1	-36.0
2	13	0	-2.2	-1.3
3	13	0	25.0	22.8
4	13	0	-2.2	-6.5
5	13	0	16.5	-17.3
6	13	0	-2.2	8.0
7	13	0	19.7	20.9
8	13	0	-2.4	-6.0
9	13	0	7.2	-8.3
10	13	0	17.7	17.8
1	15	0	15.6	-16.7
2	15	0	-2.4	-4.9
3	15	0	16.6	16.7
4	15	0	-2.3	0.5
5	15	0	11.2	-11.6
6	15	0	-2.2	2.8
0	2	1	25.5	-31.5
1	2	1	6.1	8.3
-1	2	1	94.5	104.5
2	2	1	125.0	-118.1
-2	2	1	173.3	186.0
3	2	1	33.1	-33.1
-3	2	1	101.1	-104.2
4	2	1	37.0	33.8
-4	2	1	29.4	27.5
5	2	1	32.1	30.8
-5	2	1	73.0	69.3
6	2	1	16.4	-16.1
-6	2	1	17.1	17.1
7	2	1	8.5	5.8
-7	2	1	26.3	-27.7
8	2	1	35.6	-34.5
-8	2	1	25.8	-27.8
9	2	1	12.5	11.5
-9	2	1	15.8	-12.5
10	2	1	22.6	23.1
-10	2	1	13.6	11.9
11	2	1	33.5	-31.5
-11	2	1	16.1	-15.5
12	2	1	24.6	-22.1
-12	2	1	-2.4	4.0
13	2	1	12.8	12.0
-13	2	1	13.0	16.8
14	2	1	10.0	9.4
-14	2	1	-2.5	6.6
15	2	1	-2.4	-5.7
-15	2	1	-2.5	-6.6
16	2	1	-2.3	-3.2
-16	2	1	-2.4	-2.6
-17	2	1	-2.1	0.1
0	4	1	56.1	-52.5
1	4	1	56.4	-59.0
-1	4	1	60.2	-58.4
2	4	1	24.5	28.8
-2	4	1	85.0	87.4
3	4	1	18.7	17.8
-3	4	1	5.2	-0.8
4	4	1	58.0	-56.6
-4	4	1	59.5	-61.9
5	4	1	-1.4	-4.1
-5	4	1	75.6	79.6
6	4	1	61.3	60.5
-6	4	1	24.1	22.1
7	4	1	9.1	-10.4
-7	4	1	50.8	-50.1
8	4	1	16.0	-15.9
-8	4	1	21.5	-19.9
9	4	1	37.1	36.5
-9	4	1	40.1	42.2
10	4	1	28.5	28.3
-10	4	1	11.8	-10.0
11	4	1	12.2	-15.8
-11	4	1	8.8	-10.3
12	4	1	23.8	-28.3
-12	4	1	-2.5	3.3
13	4	1	-2.2	0.4
-13	4	1	11.9	8.3
14	4	1	12.1	11.8
-14	4	1	-2.5	3.5
15	4	1	5.2	-7.8
-15	4	1	17.3	-14.9
16	4	1	6.5	-6.5
-16	4	1	-2.3	4.7
0	6	1	53.7	-51.8
1	6	1	18.0	-20.3
-1	6	1	35.7	35.7
2	6	1	57.1	59.1
-2	6	1	48.5	46.4
3	6	1	-1.5	-7.7
-3	6	1	34.8	-32.2
4	6	1	70.6	-68.9
-4	6	1	68.0	-68.6
5	6	1	14.0	13.4
-5	6	1	36.4	38.2
6	6	1	68.1	65.4
-6	6	1	27.3	28.3
7	6	1	6.5	-4.9
-7	6	1	41.6	-41.1
8	6	1	46.8	-46.3
-8	6	1	23.5	-23.0
9	6	1	12.1	10.4
-9	6	1	33.2	32.8
10	6	1	42.1	40.3
-10	6	1	8.8	-7.2
11	6	1	17.1	-16.4
-11	6	1	25.2	-29.2
12	6	1	12.7	-13.4
-12	6	1	-2.2	2.9
13	6	1	16.4	15.8
-13	6	1	28.5	28.0
14	6	1	13.1	10.4
-14	6	1	-2.5	-0.6
15	6	1	10.1	-10.1
-15	6	1	14.7	-14.2
-16	6	1	-2.1	5.7
0	8	1	46.6	-48.0
1	8	1	26.6	-26.7
-1	8	1	44.4	43.2
2	8	1	41.0	43.5
-2	8	1	32.0	33.1
3	8	1	16.5	13.8
-3	8	1	42.4	-40.7
4	8	1	48.2	-49.1
-4	8	1	25.2	-27.2
5	8	1	-1.5	3.0
-5	8	1	45.3	45.8
6	8	1	49.6	50.6
-6	8	1	42.5	43.6
7	8	1	16.7	-16.3
-7	8	1	60.6	-63.6
8	8	1	48.6	-47.2
-8	8	1	18.7	-20.0
9	8	1	23.1	21.7
-9	8	1	35.8	40.1
10	8	1	19.9	20.9
-10	8	1	24.1	24.5
11	8	1	27.4	-26.8
-11	8	1	27.7	-26.5
12	8	1	16.4	-15.7
-12	8	1	10.6	-8.0
13	8	1	21.2	20.4
-13	8	1	15.0	16.3
14	8	1	15.9	14.6
-14	8	1	-2.3	-2.2
0	10	1	44.5	-46.7
1	10	1	15.0	-14.6
-1	10	1	24.1	25.3
2	10	1	53.7	53.7
-2	10	1	31.1	30.6
3	10	1	-2.0	4.9
-3	10	1	36.8	-35.1
4	10	1	36.8	-36.3
-4	10	1	22.2	-24.4
5	10	1	-2.1	-4.6
-5	10	1	45.5	44.5
6	10	1	41.0	40.7
-6	10	1	25.5	24.1
7	10	1	11.0	-10.1
-7	10	1	30.6	-31.8
8	10	1	35.2	-35.8
-8	10	1	11.7	-11.1
9	10	1	17.3	15.0
-9	10	1	31.6	32.7
10	10	1	15.2	17.0
-10	10	1	19.4	19.9
11	10	1	16.3	-15.2
-11	10	1	24.2	-22.3
12	10	1	20.4	-19.3
-12	10	1	9.2	-9.9
13	10	1	17.7	17.9
-13	10	1	16.5	15.2
0	12	1	35.3	-35.1
1	12	1	-2.2	-4.3
-1	12	1	24.5	23.2
2	12	1	38.0	40.3
-2	12	1	33.3	30.2
3	12	1	-2.2	1.3
-3	12	1	22.4	-23.4
4	12	1	36.5	-35.5
-4	12	1	25.3	-29.3
5	12	1	-2.2	0.4
-5	12	1	10.5	12.0
6	12	1	30.2	27.9
-6	12	1	9.5	10.8
7	12	1	-2.2	-6.9
-7	12	1	10.5	-9.6
8	12	1	22.1	-23.7
-8	12	1	6.9	-6.0
9	12	1	-2.4	1.3
-9	12	1	15.0	14.7
10	12	1	21.5	21.6
-10	12	1	-2.4	-1.3
11	12	1	-2.1	-3.0
-11	12	1	22.7	-21.9
0	14	1	22.2	-20.9
1	14	1	15.7	-14.0
-1	14	1	7.0	6.4
2	14	1	18.2	18.6
-2	14	1	16.3	16.9
3	14	1	11.1	10.2
-3	14	1	-2.2	-6.4
4	14	1	23.4	-23.2
-4	14	1	13.5	-14.9
5	14	1	-2.4	3.5
-5	14	1	7.7	7.1
6	14	1	16.5	15.5
-6	14	1	9.2	10.6
7	14	1	10.1	-5.7
-7	14	1	15.0	-13.9
8	14	1	-2.2	-6.1
-8	14	1	-2.2	-6.7
0	16	1	8.4	-8.5
1	16	1	-2.2	-6.1
-1	16	1	9.6	8.5
2	16	1	7.5	8.7
-2	16	1	10.1	11.2
0	1	2	11.2	11.1
1	1	2	70.7	64.9
-1	1	2	23.5	-17.3
2	1	2	350.4	40.9
-2	1	2	20.3	20.2
3	1	2	9.7	6.0
-3	1	2	-1.3	0.6
4	1	2	-1.3	-2.6
-4	1	2	34.1	-35.9
5	1	2	27.5	-26.6
-5	1	2	8.6	10.7
6	1	2	16.7	-14.5
-6	1	2	23.8	20.7
7	1	2	14.4	12.3
-7	1	2	24.3	-23.8
8	1	2	-1.7	-2.0
-8	1	2	6.7	3.3
9	1	2	20.5	20.2
-9	1	2	11.2	-8.5
10	1	2	7.0	-5.5
-10	1	2	7.7	8.4
11	1	2	35.4	-30.3
-11	1	2	-2.3	7.2
12	1	2	-2.2	4.0
-12	1	2	-2.4	-0.4
13	1	2	-2.2	2.2
-13	1	2	7.5	-7.4
14	1	2	9.1	-6.6
-14	1	2	8.5	6.9
15	1	2	-2.4	3.1
-15	1	2	-2.5	-4.2
16	1	2	-2.2	-3.1
-16	1	2	-2.3	-5.5
0	3	2	12.1	-11.6
1	3	2	22.3	-18.8
-1	3	2	10.6	5.7
2	3	2	39.5	37.4
-2	3	2	90.3	94.8
3	3	2	45.2	-45.3
-3	3	2	43.8	41.7
4	3	2	5.0	-7.4
-4	3	2	75.0	-70.8
5	3	2	43.9	40.5
-5	3	2	20.4	-19.4
6	3	2	24.2	-21.9
-6	3	2	56.1	54.1
7	3	2	22.6	-23.5
-7	3	2	12.0	12.7
8	3	2	-1.8	-2.6
-8	3	2	10.1	-12.1
9	3	2	28.5	35.1
-9	3	2	-2.1	2.0
10	3	2	-2.1	4.1
-10	3	2	-2.2	-3.1
11	3	2	20.0	-20.6
-11	3	2	9.5	-8.6
12	3	2	-2.2	4.6
-12	3	2	-2.5	-6.9
13	3	2	-2.2	5.4
-13	3	2	-2.5	-2.4
14	3	2	11.7	-11.4
-14	3	2	16.8	16.1
15	3	2	10.4	-9.0
-15	3	2	5.5	-8.1
16	3	2	-2.1	2.7
-16	3	2	12.0	-12.3
0	5	2	61.7	-63.6
1	5	2	13.8	17.7
-1	5	2	62.0	-58.0
2	5	2	25.7	24.9
-2	5	2	74.5	75.6
3	5	2	52.8	-46.4
-3	5	2	34.3	35.4
4	5	2	27.9	-29.3
-4	5	2	76.8	-78.6
5	5	2	42.8	41.5
-5	5	2	5.1	-4.7
6	5	2	13.9	13.7
-6	5	2	22.1	25.6
7	5	2	37.8	-38.4
-7	5	2	18.8	16.3
8	5	2	-2.0	2.1
-8	5	2	36.4	-36.6
9	5	2	40.6	39.9
-9	5	2	-2.0	1.9
10	5	2	-2.1	-3.0
-10	5	2	17.6	17.9
11	5	2	20.4	-18.4
-11	5	2	-2.2	-2.2
12	5	2	13.8	12.6
-12	5	2	20.6	-17.7
13	5	2	15.3	16.4
-13	5	2	12.8	14.1
14	5	2	-2.4	-4.8
-14	5	2	17.4	16.2
15	5	2	15.7	-15.0
-15	5	2	13.5	-11.9
-16	5	2	8.4	-8.2
0	7	2	51.3	-49.4
1	7	2	86.7	85.7
-1	7	2	55.7	-54.7
2	7	2	43.1	40.9
-2	7	2	34.5	34.5
3	7	2	22.8	-24.3
-3	7	2	-1.7	9.4
4	7	2	32.9	-31.2
-4	7	2	58.5	-64.5
5	7	2	16.7	17.8
-5	7	2	11.7	-12.6
6	7	2	21.0	21.7
-6	7	2	35.4	40.1
7	7	2	43.2	-42.7
-7	7	2	-2.0	-2.2
8	7	2	-2.1	0.6
-8	7	2	37.5	-36.6
9	7	2	37.6	35.3
-9	7	2	-2.1	1.1
10	7	2	11.1	-10.7
-10	7	2	44.8	47.6
11	7	2	35.0	-13.0
-11	7	2	-2.2	-1.5
12	7	2	14.0	14.6
-12	7	2	27.5	-24.2
13	7	2	26.1	24.0
-13	7	2	12.5	10.1
14	7	2	7.9	-6.8
-14	7	2	12.4	12.3
-15	7	2	11.5	-12.4
0	9	2	28.3	-28.4
1	9	2	36.1	37.2
-1	9	2	17.9	-20.7
2	9	2	37.1	38.1
-2	9	2	41.3	41.1
3	9	2	34.7	-34.5
-3	9	2	28.5	27.1
4	9	2	23.5	-25.4
-4	9	2	35.1	-40.2
5	9	2	37.2	36.4
-5	9	2	31.0	-33.2
6	9	2	9.5	9.1
-6	9	2	57.5	60.3
7	9	2	44.9	-44.5
-7	9	2	9.0	7.7
8	9	2	7.0	-7.4
-8	9	2	33.6	-32.4
9	9	2	20.6	28.9
-9	9	2	14.1	14.0
10	9	2	-2.2	-3.7
-10	9	2	29.5	29.2
11	9	2	19.4	-19.2
-11	9	2	13.6	-13.9
12	9	2	-2.3	8.2
-12	9	2	23.5	-24.6
13	9	2	24.5	22.4
-13	9	2	-2.3	2.0
-14	9	2	11.2	11.0
0	11	2	26.4	-27.6
1	11	2	36.1	34.5
-1	11	2	35.2	-33.4
2	11	2	28.3	24.1
-2	11	2	32.3	32.8
3	11	2	26.7	-26.2
-3	11	2	22.7	20.3
4	11	2	14.8	-15.7
-4	11	2	35.6	-32.8
5	11	2	24.8	24.2
-5	11	2	-2.2	-4.7
6	11	2	14.1	14.7
-6	11	2	33.1	33.8
7	11	2	27.3	-25.5
-7	11	2	-2.2	-1.1
8	11	2	-2.2	-6.7
-8	11	2	27.3	-30.1
9	11	2	23.5	24.6
-9	11	2	-2.2	0.8
10	11	2	-2.4	-5.2
-10	11	2	20.4	20.8
11	11	2	22.2	-23.0
-11	11	2	-2.3	0.5
-12	11	2	16.5	-16.9
0	13	2	25.0	-27.2
1	13	2	15.0	12.4
-1	13	2	10.6	-9.7
2	13	2	12.8	12.8
-2	13	2	15.8	16.8
3	13	2	24.8	-24.4
-3	13	2	5.3	11.3
4	13	2	5.2	-8.5
-4	13	2	15.6	-19.3
5	13	2	28.6	30.0
-5	13	2	-2.2	-5.7
6	13	2	-2.4	5.1
-6	13	2	17.5	16.3
7	13	2	15.7	-20.7
-7	13	2	-2.4	2.5
8	13	2	-2.3	2.9
-8	13	2	22.2	-21.1
9	13	2	14.3	13.7
-9	13	2	-2.7	-3.3
0	15	2	12.1	-12.0
1	15	2	-2.3	1.2
-1	15	2	-2.3	-0.2
2	15	2	-2.3	6.5
-2	15	2	14.5	13.8
3	15	2	20.1	-19.6
-3	15	2	-2.3	3.3
4	15	2	-2.7	-3.5
-4	15	2	7.1	-6.0
5	15	2	18.6	19.3
-5	15	2	-2.2	-3.0
0	2	3	24.0	21.1
1	2	3	13.0	-8.4
-1	2	3	53.2	-50.0
2	2	3	12.6	-13.7
-2	2	3	21.8	-20.3
3	2	3	11.7	-12.9
-3	2	3	71.1	67.8
4	2	3	31.3	27.1
-4	2	3	26.2	27.3
5	2	3	37.1	55.2
-5	2	3	5.0	-5.4
6	2	3	12.7	16.0
-6	2	3	9.3	9.3
7	2	3	34.5	-38.8
-7	2	3	-2.0	0.4
8	2	3	13.2	14.1
-8	2	3	-2.1	3.7
9	2	3	16.7	15.6
-9	2	3	12.0	-17.4
10	2	3	21.3	-20.4
-10	2	3	-2.7	-3.3
11	2	3	-2.2	4.3
-11	2	3	7.6	-7.7
12	2	3	7.1	-3.4
-12	2	3	-2.5	-2.4
13	2	3	17.2	-15.8
-13	2	3	-2.5	-4.6
14	2	3	-2.4	-3.1
-14	2	3	16.6	15.4
15	2	3	-2.2	6.3
-15	2	3	-2.4	1.4
-16	2	3	13.6	-14.5
0	4	3	-1.5	3.8
1	4	3	36.5	37.2
-1	4	3	37.6	-37.4
2	4	3	24.3	-23.3
-2	4	3	17.5	17.0
3	4	3	51.7	-54.5
-3	4	3	41.6	40.9
4	4	3	18.7	20.5
-4	4	3	12.0	10.4
5	4	3	22.5	25.6
-5	4	3	22.6	-23.5
6	4	3	25.2	-27.4
-6	4	3	-1.8	-5.4
7	4	3	-1.5	-2.3
-7	4	3	42.2	40.2
8	4	3	23.4	21.3
-8	4	3	16.8	-19.6
9	4	3	13.8	12.6
-9	4	3	36.5	-38.3
10	4	3	18.4	-28.7
-10	4	3	-2.1	5.6
11	4	3	-2.2	-4.2
-11	4	3	10.4	11.4
12	4	3	12.8	20.3
-12	4	3	12.5	-12.4

Table VII - cont.

Continued:-

h	k	l	F_o	F_c
13	4	3	-2.5	-1.5
-13	4	3	-2.5	-4.8
14	4	3	10.4	-11.5
-14	4	3	17.4	16.7
15	4	3	-2.1	3.0
-15	4	3	11.0	10.8
-16	4	3	11.1	-11.0
0	6	3	-1.7	2.4
1	6	3	38.4	39.7
-1	6	3	80.4	-77.5
2	6	3	43.1	-42.1
-2	6	3	12.0	-13.0
3	6	3	27.1	-26.0
-3	6	3	57.2	59.9
4	6	3	28.7	27.3
-4	6	3	26.5	-27.9
5	6	3	18.0	19.3
-5	6	3	37.3	-36.3
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3	9	6	7.6	7.0
-3	9	6	22.7	-23.2
4	9	6	20.3	-20.9
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5	9	6	-2.3	-2.9
-5	9	6	18.3	18.1
6	9	6	24.1	22.2
-6	9	6	-2.4	-3.3
-7	9	6	23.0	-22.8
-8	9	6	-2.2	0.3
0	11	6	12.2	-10.1
1	11	6	13.1	-11.3
-1	11	6	18.0	16.2
2	11	6	16.1	15.0
-2	11	6	-2.2	5.5
3	11	6	12.5	11.9
-3	11	6	-2.2	-19.9
-4	11	6	-2.2	-7.3
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0	2	7	13.7	-13.8
1	2	7	-2.2	-6.9
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2	2	7	12.2	10.2
-2	2	7	11.2	11.7
3	2	7	-2.2	6.0
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4	2	7	-2.2	-2.7
-4	2	7	12.3	-12.0
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6	2	7	-2.4	3.9
-6	2	7	14.1	16.0
7	2	7	8.2	-6.2
-7	2	7	-2.5	5.2
8	2	7	-2.2	2.4
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0	4	7	19.7	-19.4
1	4	7	-2.2	1.2
-1	4	7	-2.2	1.9
2	4	7	7.0	7.0
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3	4	7	-2.2	-4.4
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4	4	7	12.2	-10.9
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0	6	7	11.0	-10.8
1	6	7	8.6	5.0
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3	6	7	-2.4	-3.1
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6	6	7	12.8	12.0
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4	8	7	14.2	-14.7
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-5	8	7	-2.2	2.0
-6	8	7	15.7	19.0
2	3	8	-2.2	-0.2
0	1	8	-2.4	-8.1
1	1	8	-2.3	-0.5
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2	1	8	-2.3	2.1
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-4	1	8	-2.3	0.2
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-6	1	8	-2.2	4.0
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0	3	8	-2.3	-5.4
1	3	8	-2.3	3.1
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1	5	8	12.8	13.4
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2	5	8	-2.1	1.0
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-3	5	8	13.9	15.2
-4	5	8	-2.2	-3.6
-5	5	8	17.1	-11.5