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The Crystal Structure of $(TiCl_4.CH_3COOC_2H_5)_2$

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The crystal structure of $(TiCl_4 . CH_3COOC_2H_5)_2$ has been determined from three-dimensional X-ray data. Crystals of this compound are monoclinic, space group $P2_1/a$, with 4 formula units of $TiCl_4 . CH_3COOC_2H_5$ in the unit cell. Cell dimensions are,

$$a = 13{\cdot}598,\ b = 9{\cdot}140,\ c = 9{\cdot}070\ \text{Å};\ \beta = 108°35'.$$

The atomic parameters were refined by the method of least squares. The structure is built up from dimeric molecules $(TiCl_4 . CH_3COOC_2H_5)_2$ with double chlorine bridges between the two titanium atoms of the dimer. The titanium atom is octahedrally coordinated by five chlorine atoms and the carbonyl oxygen atom of ethyl acetate. Changes in the configurations and dimensions from that of the free acceptor and donor molecules are briefly discussed.

Introduction

In the system $TiCl_4 - CH_3COOC_2H_5$, three compounds have been identified with the compositions $TiCl_4 . 2CH_3COOC_2H_5$, $TiCl_4 . CH_3COOC_2H_5$ and $2TiCl_4 . CH_3COOC_2H_5$ (Demarçay, 1873). Extensive physico-chemical studies of this system have been reported by Osipov and co-workers (Lysenko & Osipov, 1954*a*, *b*; Lysenko, Osipov & Feodosév, 1954; Lysenko, Osipov & Akopov 1956; Osipov & Lysenko, 1958; Kletenik & Osipov, 1961).

The present paper concerns the determination of the crystal structure of the 1:1 adduct. This compound sublimes when heated (Bradley, Hancock & Wardlaw, 1952) forming yellow, very hygroscopic crystals with m.p. 102·5°C (Lysenko, Osipov & Akopov, 1956).

Preparation of crystals

When titanium(IV) chloride and ethyl acetate are mixed at room temperature irreversible exothermic decomposition of the reactants occurs. This decomposition was minimized during the preparation of the 1:1 adduct by cooling titanium(IV) chloride with liquid nitrogen while adding an equivalent amount of ethyl acetate. The temperature was then allowed to rise to a few degrees above the melting point of the adduct. Rod-shaped crystals were obtained by very slow sublimation onto a glass rod placed a few millimetres above the surface of the melt. The crystals were transferred in a dry box to glass capillaries with a diameter of 0·4–0·6 mm and a wall thickness of 0·02–0·04 mm. The capillaries were sealed in the dry box using an electrically heated platinium wire.

Crystal data

The unit-cell dimensions and angle of the monoclinic crystals were determined from quartz-calibrated rotation and zero-layer Weissenberg photographs ($a = 4{\cdot}913$, $c = 5{\cdot}405$ Å for α-quartz, $\lambda(\text{Cu } K\alpha_1) = 1{\cdot}54433$ Å, $\lambda(\text{Cu } K\alpha_2) = 1{\cdot}54051$ Å, $\lambda(\text{Cu } K\beta)_1 = 1{\cdot}39217$ Å). A small crystal with the b axis parallel to the rod axis was selected, and was rotated about this axis. The following values of the parameters and their standard deviations were obtained:

$a = 13{\cdot}598$ Å	$\sigma(a) = 0{\cdot}005$ Å
$b = 9{\cdot}140$	$\sigma(b) = 0{\cdot}007$
$c = 9{\cdot}070$	$\sigma(c) = 0{\cdot}004$
$\beta = 108°35'$	$\sigma(\beta) = 2'$

The value for b is an average of twenty-eight estimations. The values for a, c, β and their standard deviations were calculated from twelve equations by the least-squares method.

The crystal used for the intensity measurements was 1·98 mm in length, and 0·40–0·53 mm in cross section. With the crystal rotating about the b axis, equi-inclination Weissenberg photographs for the 13 layers $0 \leq k \leq 12$ were recorded. The layers were recorded with Nb-filtered Mo $K\alpha$ radiation using four films interleaved with iron foils. The value 0·71069 Å was assumed for the wavelength of Mo $K\alpha$ radiation. No correction was made for absorption errors. A method described by Magnéli (1948) was applied to correlate intensities in the separate layer lines. 2571 independent intensities were estimated visually by comparison with an intensity scale*. 52 of these intensities were rejected during the refinement; of these 4 were too strong to be accurately estimated, and the rest were defective or coincided with streaks due to white radiation. The data were corrected for Lorentz and polarization effects.

Extinctions were observed for h odd in $h0l$ reflexions. Since no $0k0$ reflexions were recorded, the data suggest one of the three space groups $P2_1/a$, $P2/a$ and Pa.

On the basis of a unit cell containing four formula units $TiCl_4 . CH_3COOC_2H_5$, the density was calculated

* I am indebted to R. Strandberg for help with the measurement of the intensities.

to be 1·73 g.cm^{-3}. An ideal mixture formed between titanium(IV) chloride and ethyl acetate with a mole ratio 1:1 would have a density of 1·34 g.cm^{-3}. The density of the hygroscopic crystals could not be measured very easily and it was therefore assumed that the unit cell contained four formula units of $TiCl_4 . CH_3COOC_2H_5$. This was later confirmed by the structure determination.

Determination of the atomic positions

In the three-dimensional Patterson function $P(x, y, z)$ there was an obvious concentration of peaks in the section $P(x, \frac{1}{2}, z)$ as compared with the section $P(x, 0, z)$, indicating a translation by 0·5 along a twofold axis. Accordingly $P2_1/a$ was chosen as the most plausible space group. All atoms in the formula unit $TiCl_4 . CH_3COOC_2H_5$ were assumed to occupy general positions, 4(*e*), in this space group. Approximate parameters for the titanium and four chlorine atomic positions were derived by locating the corresponding vectors in the Patterson function. These parameters were used to determine the signs of the observed structure factors. Atomic scattering factors for the elements in this and the following calculations were obtained from *International Tables for X-ray Crystallography* (1962, p. 202 and 204). Programs devised by Liminga & Olovsson (1964) for the Swedish electronic computer FACIT EDB were employed in the calculation of structure factors and Fourier functions. An F_o synthesis was used to derive approximate parameters for the oxygen and carbon atoms. Using the atomic positions of the titanium and chlorine atoms, regions of an F_c synthesis were calculated in order to apply a back-shift correction to the parameters of these atoms. The parameters thus obtained for the titanium and chlorine atoms were used in calculating a Fourier synthesis. A 'difference' synthesis was computed to obtain more accurate parameters for the oxygen and carbon atoms. The Fourier coefficients for this calculation were of the form $F_o - F_h$ where F_o are the observed structure factors with signs calculated taking account of all the atomic positions in the structure and F_h are the structure factors calculated for the titanium and chlorine atoms only.

Refinement of the parameters

The atomic parameters were refined by the least-squares method. A program devised by Åsbrink & Brändén (1963) for the computer FACIT EDB was used. The parameters refined were atomic coordinates (H atoms excluded), individual isotropic temperature factors and thirteen scale factors, one for each layer-line. The weights, w, were calculated according to an equation suggested by Cruickshank, Pilling, Bujosa, Lovell & Truter (1961), $w = 1/(a + |F_o| + c|F_o|^2)$, final values for the constants being $a = 2{\cdot}0$ and $c = 0{\cdot}02$. Only observed reflexions were included in the refinement. At the end of each cycle a weight analysis was computed. The mean value of $w(|F_o| - |F_c|)^2$ was calculated at intervals of increasing $|F_o|$ and sin θ. The values of a and c were adjusted between the refinement cycles so that this mean value was as constant as possible at all intervals. The weight analysis for the last cycle of refinement is given in Table 1. The R value $\Sigma \, ||F_o| - |F_c|| / \Sigma \, |F_o|$ was 0·123 at this point and the shifts for all the parameters were less than one-tenth of their estimated standard deviations.

Table 1. *Final weight analysis*

sin θ interval	$\overline{\omega \Delta^2}$	Number of reflexions
0·00–0·30	1·01	548
0·30–0·37	1·21	559
0·37–0·43	1·20	447
0·43–0·47	1·03	385
0·47–0·51	0·69	287
0·51–0·54	0·60	148
0·54–0·57	0·52	88
0·57–0·59	0·35	36
0·59–0·62	0·40	17
0·62–0·64	0·51	4

$\|F_o\|$ interval	$\overline{\omega \Delta^2}$	Number of reflexions
0–5	1·15	721
5–10	1·12	745
10–15	1·00	371
15–20	0·84	222
20–25	0·82	144
25–30	0·73	90
30–35	0·57	69
35–40	0·45	47
40–45	0·36	30
45–105	0·59	80

A difference synthesis was calculated in which no spurious peaks were observed. As the difference synthesis suggested anisotropy in the individual temperature factors the refinement was continued with the program ORFLS devised by Busing, Martin & Levy (1962), modified by Brändén to accommodate more parameters. This program was first used to repeat the last cycle of isotropic refinement in order to compare the results obtained from the earlier block-diagonal matrix approximation with those from a full-matrix calculation. No significant deviations were found. During the following refinement of the atomic coordinates and the individual anisotropic temperature factors, the scale factors were kept constant and the same weights were used as in the last cycle of the isotropic refinement. After a few cycles all the shifts were less than the estimated standard deviations for corresponding parameters. The values for

$$R = \Sigma \, ||F_o| - |F_c|| / \Sigma \, |F_o|$$

and

$$R = [\Sigma \, w(|F_o| - |F_c|)^2 / \Sigma \, w|F_o|^2]^{\frac{1}{2}}$$

were 0·062 and 0·084, respectively.

The final atomic parameters are listed in Tables 2 and 3 together with their estimated standard deviations. Observed and calculated F values are collected in Table 4.

Description and discussion of the structure

The structure of one adduct molecule is shown in Fig. 1. The bond lengths and bond angles are given in Table 5 together with their standard deviations calculated with no correction for thermal motion by the program ORFFE devised by Busing, Martin & Levy (1964). Intramolecular, non-covalent distances less than 4·0 Å are listed in Table 6 and non-equivalent distances less than 4·0 Å between atoms in different molecules in Table 7. The packing of the molecules is shown in Fig. 2.

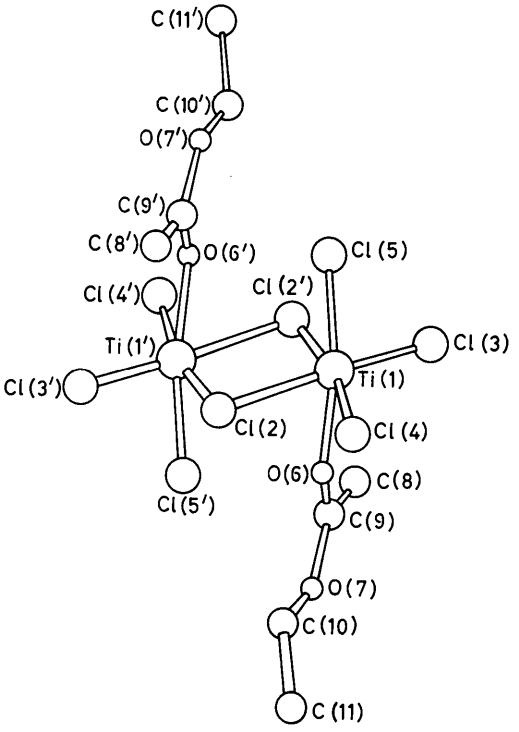

Fig. 1. The molecular structure of $(TiCl_4 . CH_3COOC_2H_5)_2$.

The carbonyl oxygen of the ethyl acetate molecule acts as the donor atom. This was suggested by Bystrov & Filimonov (1960), who found that the infrared spectrum of the titanium(IV) chloride – ethyl acetate adduct shows lower carbonyl C=O frequencies and higher acetyl–oxygen frequencies than the free ester. Several spectroscopic studies indicate that the carbonyl oxygen is the donor atom in different adducts with esters (Aubin & Rivest, 1958; Lappert, 1961; Zackrisson & Lindqvist, 1961; Rivet, Aubin & Rivest, 1961; Mori, Göhring, Cassimatis & Susz, 1962; Dembitskii & Sumarokova, 1962), carboxylic acids (Zackrisson & Lindqvist, 1961), acid anhydrides (Cooke, Susz & Herschmann, 1954), lactones (Paoloni & Marini-Bettòlo, 1959) and γ-pyrones (Cook, 1961). The only reported structure determination of such an adduct is an X-ray crystal structure analysis of a mercury(II) chloride 1:1 adduct with coumarin (Struchkov, Kitaigorodskii & Khotsyanova, 1953). In this adduct the carbonyl oxygen is again the donor atom.

The adduct of titanium(IV) chloride with ethyl acetate is a dimer $(TiCl_4 . CH_3COOC_2H_5)_2$ containing two Ti–Cl–Ti bridges. Such double chlorine bridges have previously been found in the adduct molecule $(TiCl_4 . POCl_3)_2$ (Brändén & Lindqvist, 1960), in which the oxygen atom functions as a donor atom. In both ad-

Table 2. *Final positional parameters (fractions of cell edges) and standard deviations* (Å) *from anisotropic least-squares refinement*

Atom	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
Ti(1)	0·0301	0·0007	0·1897	0·0006	0·0966	0·0007
Cl(2)	−0·1209	0·0009	0·0310	0·0008	−0·0415	0·0010
Cl(3)	0·1808	0·0013	0·3077	0·0012	0·1789	0·0015
Cl(4)	−0·0780	0·0014	0·3707	0·0011	0·0999	0·0015
Cl(5)	0·0366	0·0016	0·0925	0·0014	0·3252	0·0012
O(6)	0·0155	0·0034	0·2422	0·0028	−0·1268	0·0031
O(7)	−0·0070	0·0037	0·3075	0·0039	−0·3678	0·0035
C(8)	0·1586	0·0055	0·2173	0·0062	−0·2262	0·0063
C(9)	0·0508	0·0047	0·2561	0·0039	−0·2356	0·0045
C(10)	−0·1176	0·0057	0·3426	0·0078	−0·3855	0·0075
C(11)	−0·1539	0·0085	0·4527	0·0091	−0·5109	0·0077

Table 3. *Final anisotropic temperature coefficients in the expression* $\exp[-\beta_{11}h^2-\beta_{22}k^2-\beta_{33}l^2-2\beta_{12}hk-2\beta_{13}hl-2\beta_{23}kl]$ *and standard deviations* (10^{-3} Å^2)

Atom	β_{11}	$\sigma(\beta_{11})$	β_{22}	$\sigma(\beta_{22})$	β_{33}	$\sigma(\beta_{33})$	β_{12}	$\sigma(\beta_{12})$	β_{13}	$\sigma(\beta_{13})$	β_{23}	$\sigma(\beta_{23})$
Ti(1)	5·79	0·05	10·13	0·07	10·94	0·09	0·04	0·04	2·91	0·05	−0·75	0·05
Cl(2)	4·78	0·05	10·88	0·09	14·55	0·13	0·73	0·05	2·43	0·06	0·02	0·08
Cl(3)	6·75	0·08	15·57	0·14	20·49	0·22	−2·11	0·08	2·99	0·10	−2·82	0·13
Cl(4)	7·97	0·09	12·87	0·12	21·83	0·21	1·31	0·07	6·08	0·11	−2·34	0·11
Cl(5)	10·26	0·10	18·87	0·16	10·78	0·14	−0·74	0·10	3·99	0·09	0·13	0·11
O(6)	7·17	0·20	12·85	0·31	12·81	0·41	0·63	0·19	4·36	0·24	1·74	0·27
O(7)	7·07	0·23	21·46	0·54	13·93	0·47	0·13	0·27	4·06	0·26	3·83	0·39
C(8)	6·10	0·30	22·52	0·80	19·88	0·88	0·23	0·38	5·39	0·43	3·00	0·66
C(9)	6·41	0·26	13·14	0·42	12·73	0·55	−0·22	0·25	3·76	0·31	0·55	0·36
C(10)	5·80	0·31	28·66	1·08	25·80	1·10	1·15	0·47	4·90	0·48	9·60	0·92
C(11)	10·71	0·55	29·66	1·28	20·17	1·05	1·95	0·67	3·20	0·60	6·05	0·92

Table 4. *Observed and calculated structure factors*

$|F_o|$ for reflexions marked* are threshold values. Those marked ** were omitted from the least-squares refinement.

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
*	0	0	-11	4.7	1.2
	0	0	-10	7.6	7.7
	0	0	-9	16.8	16.3
	0	0	-8	6.5	6.2
	0	0	-7	32.2	30.7
	0	0	-6	5.5	5.8
	0	0	-5	56.3	53.8
	0	0	-4	73.4	78.9
**	0	0	-3	11.6	6.0
*	2	0	-11	4.6	0.0
	2	0	-10	11.4	11.6
	2	0	-9	25.8	26.2
	2	0	-8	23.3	21.8
	2	0	-7	21.9	19.3
	2	0	-6	3.1	3.3
	2	0	-5	80.7	90.4
	2	0	-4	62.4	64.8
**	2	0	-3	80.1	91.7
**	2	0	2	17.8	13.8
	2	0	3	17.0	14.7
	2	0	4	90.2	95.2
	2	0	5	62.5	63.9
	2	0	6	43.8	44.7
	2	0	7	41.3	41.7
**	2	0	8	3.9	4.7
	2	0	9	22.5	22.7
	2	0	10	6.4	5.6
	4	0	-13	7.3	8.1
	4	0	-12	4.8	6.3
	4	0	-11	4.5	5.7
	4	0	-10	19.0	19.3
	4	0	-9	18.5	17.3
	4	0	-8	9.7	9.3
*	4	0	-7	3.4	2.6
	4	0	-6	10.2	9.9
	4	0	-5	46.9	46.1
	4	0	-4	11.3	9.6
	4	0	-3	12.9	15.0
**	4	0	-2	113.8	131.3
**	4	0	-1	30.0	35.1
**	4	0	0	5.7	9.9
	4	0	1	7.7	6.4
	4	0	2	17.4	16.3
	4	0	3	16.1	15.2
	4	0	4	86.4	93.8
	4	0	5	37.7	35.3
*	4	0	6	3.6	3.6
*	4	0	7	3.9	1.2
	4	0	8	17.1	16.1
	4	0	9	17.8	18.2
	6	0	-13	10.2	10.5
	6	0	-12	4.8	4.6
*	6	0	-11	4.5	0.2
*	6	0	-10	4.2	0.8
	6	0	-9	29.1	27.4
	6	0	-8	40.1	35.8
	6	0	-7	10.3	8.7
	6	0	-6	10.1	9.5
	6	0	-5	32.0	29.7
*	6	0	-4	2.7	0.3
	6	0	-3	31.3	28.6
	6	0	-2	36.7	31.2
	6	0	-1	25.0	28.9
	6	0	0	59.1	57.7
	6	0	1	41.9	43.2
	6	0	2	26.4	24.3
	6	0	3	22.0	21.1
	6	0	4	17.5	16.0
	6	0	5	33.1	30.6
	6	0	6	30.5	30.0
*	6	0	7	4.1	1.3
	6	0	8	18.2	16.8
	6	0	9	11.5	12.7
	8	0	-13	7.3	8.4
*	8	0	-12	4.9	2.0
	8	0	-11	4.6	4.5
	8	0	-10	7.5	9.3
	8	0	-9	35.5	35.5
	8	0	-8	25.5	22.2
	8	0	-7	11.3	9.6
	8	0	-6	28.3	26.4
	8	0	-5	12.7	12.7
	8	0	-4	51.1	50.1
	8	0	-3	87.6	95.4
	8	0	-2	73.7	73.2
	8	0	-1	38.0	38.7
*	8	0	0	3.0	2.4
	8	0	1	34.6	32.6
	8	0	2	15.6	13.2
*	8	0	3	3.4	2.4
	8	0	4	20.4	18.9
	8	0	5	12.3	12.4
	8	0	6	5.9	6.2
*	8	0	7	4.4	2.7
	8	0	8	12.4	12.3
	10	0	-11	9.4	8.1
*	10	0	-10	4.4	3.0
	10	0	-9	21.4	20.5
	10	0	-8	20.3	19.0
	10	0	-7	9.2	8.9
	10	0	-6	5.1	5.3
	10	0	-5	39.7	37.4
	10	0	-4	50.5	50.3
	10	0	-3	55.6	56.9
	10	0	-2	29.2	27.4
	10	0	-1	36.8	33.1
*	10	0	0	3.4	1.3
	10	0	1	15.6	15.9
	10	0	2	6.3	5.9
	10	0	3	35.2	33.3
	10	0	4	39.9	37.0
	10	0	5	4.2	3.9
*	10	0	6	4.5	0.5
	12	0	-11	6.8	7.7
*	12	0	-10	4.6	0.0
	12	0	-9	9.8	10.2
*	12	0	-8	4.2	2.7
*	12	0	-7	4.0	0.4
	12	0	-6	7.8	7.2
	12	0	-5	8.4	7.7
*	12	0	-4	3.7	0.0
	12	0	-3	11.6	10.2
	12	0	-2	5.2	5.3
	12	0	-1	17.4	17.5
	12	0	0	15.6	14.2
	12	0	1	33.3	32.6
	12	0	2	25.6	24.3
	12	0	3	25.6	23.2
	12	0	4	4.4	5.9
	14	0	-9	6.5	7.3
*	14	0	-8	4.5	1.5
	14	0	-7	7.5	6.0
	14	0	-6	11.1	11.7
	14	0	-5	4.1	5.6
*	14	0	-4	4.1	1.9
	14	0	-3	8.1	7.6
	14	0	-2	5.7	5.1
	14	0	-1	17.4	15.6
	14	0	0	19.7	18.4
	14	0	1	6.1	4.8
	14	0	2	4.4	5.1
	16	0	-10	10.1	9.9
	16	0	-9	9.8	9.9
*	16	0	-8	4.7	3.1
*	16	0	-7	4.6	0.0
	16	0	-6	11.1	10.0
	16	0	-5	19.5	18.5
*	16	0	-4	4.4	2.7
	18	0	-10	7.5	7.8
*	18	0	-9	5.2	2.0
	18	0	-8	7.2	6.0
	18	0	-7	7.0	7.4
	18	0	-6	17.6	16.1
	18	0	-5	16.8	16.6
	20	0	-1	7.6	8.3
	20	0	0	5.4	6.4
	0	1	-13	7.5	7.9
	0	1	-12	5.0	5.5
*	0	1	-11	4.7	0.5
*	0	1	-10	4.4	3.5
	0	1	-9	26.1	25.5
	0	1	-8	25.0	22.6
*	0	1	-7	3.5	3.4
	0	1	-6	29.6	29.6
	0	1	-5	16.1	15.4
	0	1	-4	34.3	35.4
	0	1	-3	49.4	53.9
*	1	1	-12	4.9	2.1
	1	1	-11	6.6	6.3
*	1	1	-10	4.3	2.5
	1	1	-9	11.4	10.6
	1	1	-8	18.9	16.7
	1	1	-7	3.4	4.3
	1	1	-6	17.3	14.8
**	1	1	-5	2.8	5.2
	1	1	-4	51.3	55.2
**	1	1	-3	84.1	104.5
	1	1	2	17.9	18.0
	1	1	3	22.6	21.8
	1	1	4	30.4	32.5
	1	1	5	33.3	34.3
	1	1	6	5.6	5.8
	1	1	7	10.6	9.7
	1	1	8	15.8	13.9
	1	1	9	4.1	4.1
	1	1	10	4.5	5.9
	1	1	11	6.7	7.2
*	2	1	-10	4.3	1.4
	2	1	-9	25.4	24.9
	2	1	-8	19.8	19.2
	2	1	-7	11.2	10.1
	2	1	-6	37.9	36.7
	2	1	-5	9.2	8.8
	2	1	-4	57.3	65.4
**	2	1	-3	66.6	83.5
	2	1	2	36.2	34.2
	2	1	3	11.0	11.8
	2	1	4	59.1	62.7
	2	1	5	18.9	18.2
	2	1	6	14.9	14.0
	2	1	7	17.0	14.4
	2	1	8	25.2	24.8
	2	1	9	8.5	9.2
	2	1	10	4.5	4.9
	3	1	-12	8.4	7.6
*	3	1	-11	4.6	1.3
	3	1	-10	17.5	16.5
	3	1	-9	9.7	8.5
	3	1	-8	14.6	13.0
	3	1	-7	10.6	9.9
	3	1	-6	17.3	15.6
	3	1	-5	21.4	19.6
	3	1	-4	34.5	35.1
	3	1	-3	27.9	29.5
	3	1	-2	21.6	20.0
**	3	1	1	73.5	90.8
	3	1	2	63.6	69.0
	3	1	3	54.8	58.9
	3	1	4	56.9	61.0
	3	1	5	30.1	30.6
	3	1	6	8.4	8.8
	3	1	7	10.5	11.1
*	3	1	8	4.0	0.1
	3	1	9	8.7	9.3
*	4	1	-10	4.2	0.5
	4	1	-9	28.1	28.8
	4	1	-8	17.8	17.1
	4	1	-7	3.4	3.8
	4	1	-6	15.1	13.9
	4	1	-5	57.7	63.0
	4	1	-4	34.2	35.2
	4	1	-3	30.0	28.2
**	4	1	-2	18.5	12.2
	4	1	-1	26.5	23.6
	4	1	0	9.3	7.6
**	4	1	1	5.8	2.5
	4	1	2	22.8	21.7
	4	1	3	37.0	39.9
	4	1	4	20.5	19.4
	4	1	5	18.5	17.4
	4	1	6	14.7	13.8
	4	1	7	3.8	4.5
	4	1	8	4.1	3.8
*	4	1	9	4.4	1.9
	5	1	-13	8.9	8.2
	5	1	-12	4.8	5.6
*	5	1	-11	4.5	0.9
	5	1	-10	15.2	15.4
*	5	1	-9	3.9	0.6
	5	1	-8	20.3	18.8
	5	1	-7	8.9	8.8
	5	1	-6	35.4	36.6
	5	1	-5	61.5	68.2
	5	1	-4	18.0	16.2
**	5	1	-3	5.4	3.3
	5	1	-2	16.8	15.5
	5	1	-1	35.1	37.2
**	5	1	0	2.3	0.3
	5	1	1	51.1	56.1
	5	1	2	18.0	17.0
	5	1	3	10.4	10.0
	5	1	4	29.0	29.2
*	5	1	5	3.4	0.9
	5	1	6	6.4	7.0
	5	1	7	4.0	4.4
	5	1	8	15.9	14.2
	5	1	9	15.8	15.3
*	6	1	-11	4.5	3.7
	6	1	-10	13.4	12.7
	6	1	-9	24.7	23.7
	6	1	-8	7.4	7.4
	6	1	-7	28.6	28.9
	6	1	-6	15.5	14.1
	6	1	-5	33.3	32.9
	6	1	-4	17.7	16.5
	6	1	-3	11.2	9.4
	6	1	-2	16.9	14.6
	6	1	-1	37.9	39.2
	6	1	0	83.4	94.9
	6	1	1	33.6	37.5
	6	1	2	8.5	7.8
	6	1	3	17.4	15.6
	6	1	4	27.3	27.7
	6	1	5	14.7	15.2
*	6	1	6	3.8	2.6
*	6	1	7	4.1	1.6
*	6	1	8	4.4	2.3
	7	1	-10	4.3	6.1
	7	1	-9	8.9	9.8
	7	1	-8	25.6	25.5
	7	1	-7	10.5	10.6
	7	1	-6	40.8	41.0
	7	1	-5	37.3	37.1
	7	1	-4	7.0	6.7
*	7	1	-3	2.7	2.0
	7	1	-2	15.8	15.9
	7	1	-1	52.3	57.3
	7	1	0	28.2	28.8
	7	1	1	29.9	31.4
	7	1	2	34.7	35.5
	7	1	3	9.2	8.0
	7	1	4	7.8	8.1
	7	1	5	11.2	10.4
	7	1	6	8.9	8.0
	7	1	7	4.3	5.1
	7	1	8	7.9	8.1
	8	1	-12	6.9	8.5
	8	1	-11	6.5	5.9
	8	1	-10	9.6	9.9
	8	1	-9	21.8	20.3
	8	1	-8	3.8	2.7
	8	1	-7	9.4	7.5
	8	1	-6	19.0	18.3
	8	1	-5	60.1	64.0
	8	1	-4	36.8	39.5
	8	1	-3	14.3	12.5
	8	1	-2	12.5	13.7
	8	1	-1	78.0	86.1
	8	1	0	70.1	76.0
*	8	1	1	7.5	6.8
	8	1	2	16.8	16.2
	8	1	3	23.3	23.7
	8	1	4	14.2	14.7
	8	1	5	7.8	7.7
	8	1	6	12.4	12.0
	8	1	7	9.9	8.8
*	9	1	-10	4.3	2.8
	9	1	-9	10.9	10.9
*	9	1	-8	3.9	3.1
	9	1	-7	20.0	19.1
*	9	1	-6	3.5	2.9
	9	1	-5	6.6	5.6
	9	1	-4	30.1	30.2
*	9	1	-3	3.1	2.1
	9	1	-2	22.7	22.9
	9	1	-1	39.6	43.8
	9	1	0	18.7	18.0
	9	1	1	12.3	11.0
	9	1	2	15.4	14.4
	9	1	3	5.1	6.5
*	9	1	4	3.8	2.1
*	9	1	5	4.1	1.5
*	9	1	6	4.3	2.6
	9	1	7	6.5	6.7
	10	1	-10	14.0	12.5
	10	1	-9	21.3	20.3
	10	1	-8	4.0	4.5
	10	1	-7	5.3	5.1
	10	1	-6	30.5	31.8
	10	1	-5	62.1	66.8
	10	1	-4	12.5	11.8
	10	1	-3	22.7	22.7
	10	1	-2	9.2	8.7
	10	1	-1	23.5	24.9
	10	1	0	14.7	16.0
	10	1	1	17.0	17.1
	10	1	2	17.8	17.0
	10	1	3	10.8	11.1
	10	1	4	21.6	22.1
	10	1	5	17.0	17.6
	10	1	6	6.3	7.0
	11	1	-10	6.4	5.1
*	11	1	-9	4.3	2.8
	11	1	-8	11.5	11.4
	11	1	-7	22.0	20.5
	11	1	-6	7.5	7.4
	11	1	-5	20.4	19.8
	11	1	-4	24.8	25.8
*	11	1	-3	3.5	1.7
	11	1	-2	4.9	4.7
	11	1	-1	8.5	8.0
	11	1	0	25.2	27.7
	11	1	1	19.8	19.2
	11	1	2	8.6	8.8
	11	1	3	12.0	10.7
	11	1	4	7.3	7.0
*	11	1	5	4.4	3.8
	11	1	6	4.7	5.6
·	12	1	-10	11.2	10.7
*	12	1	-9	4.4	3.7
	12	1	-8	12.5	11.9
*	12	1	-7	4.0	3.0
	12	1	-6	6.7	6.6
	12	1	-5	22.9	23.3
	12	1	-4	9.7	10.2
	12	1	-3	15.5	14.5
*	12	1	-2	3.6	3.4
	12	1	-1	21.5	21.2
	12	1	0	22.3	21.1
	12	1	1	14.5	13.8
*	12	1	2	4.0	2.5
	12	1	3	13.3	12.5
	12	1	4	13.9	13.6
	13	1	-9	9.0	8.3
*	13	1	-8	4.3	1.8
*	13	1	-7	4.2	0.7
	13	1	-6	4.0	5.2
	13	1	-5	11.8	11.5
	13	1	-4	3.9	4.5
	13	1	-3	10.9	11.2
	13	1	-2	16.8	16.1
	13	1	-1	18.3	18.5
	13	1	0	24.2	22.7
	13	1	1	10.8	11.3
	13	1	2	8.5	7.9
	13	1	3	6.2	6.7
*	14	1	-7	4.3	2.0
	14	1	-6	4.2	4.4
	14	1	-5	10.9	10.5
*	14	1	-4	4.0	3.4
	14	1	-3	4.0	3.7
	14	1	-2	11.5	12.3
	14	1	-1	18.3	17.3
	14	1	0	4.2	4.8
	14	1	1	6.1	5.9
	15	1	-10	6.9	7.9
	15	1	-9	12.5	12.2
	15	1	-8	7.9	7.7
	15	1	-7	6.3	7.6
	15	1	-6	6.2	6.3
*	15	1	-5	4.3	0.3
	16	1	-8	4.7	5.6
*	16	1	-7	4.6	3.9
*	16	1	-6	4.5	3.0
*	16	1	-5	4.5	0.9
	16	1	-4	12.5	12.4
	16	1	-3	14.7	15.1
	16	1	-2	4.4	5.6
	17	1	-5	6.6	5.7
	17	1	-4	8.0	8.9
	17	1	-3	9.2	8.1
	17	1	-2	11.4	10.7
	18	1	-8	10.1	8.4
*	18	1	-7	4.9	3.0
*	18	1	-6	4.9	4.2
*	18	1	-5	4.8	3.7
	18	1	-4	4.8	4.7
*	18	1	-3	4.8	1.9
*	18	1	-2	4.9	3.2
	18	1	-1	7.0	5.8
*	0	2	-12	5.1	2.3
	0	2	-11	13.6	11.2
	0	2	-10	11.9	11.1
	0	2	-9	10.2	10.0
	0	2	-8	16.4	14.9
	0	2	-7	3.5	4.8
	0	2	-6	27.0	26.4
**	0	2	-5	5.0	4.3
	0	2	-4	56.3	60.6
	0	2	-3	69.8	80.6
**	0	2	-2	62.0	72.0
*	1	2	-10	4.4	1.2
	1	2	-9	17.4	17.8
	1	2	-8	26.3	25.2
	1	2	-7	4.9	5.7
	1	2	-6	7.8	6.5
*	1	2	-5	2.8	2.8
	1	2	-4	50.3	54.9
**	1	2	-3	12.4	8.9
**	1	2	-2	95.5	90.2
	1	2	2	52.7	58.3
	1	2	3	18.1	18.7
	1	2	4	20.8	19.4
	1	2	5	46.3	49.4
	1	2	6	19.6	19.7
	1	2	7	3.6	5.3
	1	2	8	11.8	11.1
*	1	2	9	4.2	0.2
	1	2	10	7.9	8.2
*	2	2	-10	4.4	4.6
**	2	2	-9	4.1	4.6
	2	2	-8	13.0	11.8
	2	2	-7	20.4	19.2
	2	2	-6	49.6	52.3
	2	2	-5	59.6	63.1
	2	2	-4	67.3	76.4
	2	2	-3	15.7	12.9
	2	2	-2	31.2	33.7
	2	2	1	34.9	38.1
	2	2	2	29.7	27.9
	2	2	3	13.2	11.6
*	2	2	4	2.8	0.8
*	2	2	5	3.1	2.0
	2	2	6	14.0	12.1
	2	2	7	6.4	5.2
	2	2	8	24.8	22.5
	2	2	9	15.0	14.6
	2	2	10	13.1	12.2
*	3	2	-11	4.7	3.5
	3	2	-10	8.7	7.0
	3	2	-9	23.9	24.0
	3	2	-8	16.7	14.7
	3	2	-7	22.2	22.1
	3	2	-6	10.4	9.4
	3	2	-5	31.2	30.1
	3	2	-4	70.2	83.6
	3	2	-3	26.7	27.5
	3	2	-2	30.7	30.0
**	3	2	-1	55.6	64.4
**	3	2	0	73.9	103.9
**	3	2	1	75.2	102.6
	3	2	2	12.4	14.4
	3	2	3	18.1	16.7
	3	2	4	19.3	19.1
	3	2	5	40.6	41.8
	3	2	6	6.1	5.4
*	3	2	7	3.8	2.5
	3	2	8	10.9	11.0
	3	2	9	4.4	4.0
	3	2	10	6.7	7.5
*	4	2	-11	4.6	4.2
	4	2	-10	4.3	5.1
	4	2	-9	7.0	7.2
*	4	2	-8	3.7	1.3
	4	2	-7	34.3	33.2
	4	2	-6	24.4	22.5
	4	2	-5	7.6	5.9
	4	2	-4	5.8	5.8
	4	2	-3	36.1	37.4
	4	2	-2	54.9	60.5
	4	2	-1	33.2	32.2
**	4	2	0	68.9	86.2
	4	2	1	71.4	87.5
	4	2	2	42.7	45.8
	4	2	3	18.0	17.5
	4	2	4	29.8	28.5
	4	2	5	21.2	22.0
**	4	2	6	3.6	4.7
	4	2	7	8.8	8.8
	4	2	8	10.4	9.2
	5	2	-14	5.5	5.7
*	5	2	-13	5.2	4.3
*	5	2	-12	4.9	3.2
*	5	2	-11	4.6	1.0
*	5	2	-10	4.3	3.1
	5	2	-9	20.9	20.3
	5	2	-8	8.4	7.4
*	5	2	-7	3.5	3.3
	5	2	-6	10.6	10.1
	5	2	-5	46.7	48.6
	5	2	-4	84.8	105.0
	5	2	-3	40.9	41.6
	5	2	-2	24.1	24.1
	5	2	-1	27.8	26.3
	5	2	0	71.9	89.4
	5	2	1	62.8	67.6
	5	2	2	15.3	14.8
	5	2	3	39.7	41.2
	5	2	4	11.2	10.1
	5	2	5	17.5	18.5
	5	2	6	3.8	4.3
	5	2	7	10.8	10.6
	5	2	8	15.1	14.5
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	6	2	-11	10.3	8.6
	6	2	-10	4.3	4.6
*	6	2	-9	4.0	3.0
	6	2	-8	3.8	2.5
*	6	2	-7	3.5	2.5
	6	2	-6	15.9	15.6
	6	2	-5	30.9	28.8
*	6	2	-4	2.8	2.0
	6	2	-3	30.8	30.4
	6	2	-2	39.9	42.1
	6	2	-1	41.9	48.4
	6	2	0	52.7	54.0
	6	2	1	14.6	13.4
	6	2	2	48.3	51.8
	6	2	3	42.1	44.0
	6	2	4	33.0	31.3
	6	2	5	11.5	11.1
	6	2	6	11.8	10.9
	6	2	7	4.2	4.6
*	6	2	8	4.5	2.1
	7	2	-14	5.5	5.6
*	7	2	-13	5.2	1.7
*	7	2	-12	4.9	0.8
	7	2	-11	6.6	6.3
	7	2	-10	7.6	7.0
	7	2	-9	23.1	22.3
	7	2	-8	7.6	7.9
	7	2	-7	9.4	9.5
	7	2	-6	6.7	5.2
	7	2	-5	29.6	27.4
	7	2	-4	23.9	22.7
*	7	2	-3	2.8	1.2
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	7	2	-1	10.9	11.5
	7	2	0	30.7	30.7
	7	2	1	26.6	26.1
	7	2	2	24.1	22.4
	7	2	3	38.6	40.3
*	7	2	4	3.6	1.3
	7	2	5	25.6	26.1
	7	2	6	7.1	7.4
	7	2	7	12.3	11.7
	8	2	-14	5.5	4.2
	8	2	-13	5.2	4.5
	8	2	-12	8.6	8.2
	8	2	-11	8.1	7.1
*	8	2	-10	4.4	4.4
*	8	2	-9	4.1	0.2
	8	2	-8	6.7	5.8
	8	2	-7	5.2	4.6
	8	2	-6	7.7	6.0
	8	2	-5	12.1	11.8
	8	2	-4	16.6	15.3
	8	2	-3	40.0	38.4
	8	2	-2	22.3	20.3
	8	2	-1	30.9	29.6
	8	2	0	28.6	26.8
	8	2	1	31.4	30.4
	8	2	2	25.9	24.8
	8	2	3	18.9	19.3
	8	2	4	23.0	22.0
	8	2	5	12.6	12.6
*	8	2	6	4.2	1.6
	8	2	7	6.4	6.3
	8	2	8	8.3	7.5
*	9	2	-11	4.7	0.9
	9	2	-10	11.8	11.3
	9	2	-9	5.9	6.8
	9	2	-8	6.9	5.7
	9	2	-7	5.3	4.2
	9	2	-6	10.0	9.1
	9	2	-5	3.4	4.1
	9	2	-4	10.3	8.6
*	9	2	-3	3.2	1.4
	9	2	-2	17.7	17.0
	9	2	-1	17.8	17.2
	9	2	0	22.8	23.5
*	9	2	1	3.3	3.9
	9	2	2	7.9	8.1
*	9	2	3	3.7	0.8
	9	2	4	19.2	19.0
	9	2	5	11.0	10.1
*	9	2	6	4.4	3.3
*	9	2	7	4.7	4.4
*	10	2	-11	4.8	1.7
	10	2	-10	6.4	5.5
	10	2	-9	12.8	12.1
	10	2	-8	21.4	19.7
	10	2	-7	26.1	25.8
*	10	2	-6	3.7	0.9
*	10	2	-5	3.5	3.2
	10	2	-4	14.1	12.2
	10	2	-3	5.8	3.6
	10	2	-2	7.5	7.3
	10	2	-1	18.7	17.9
*	10	2	0	3.4	1.5
**	10	2	1	3.6	3.9
*	10	2	2	3.7	2.2
	10	2	3	5.5	4.6
	10	2	4	7.1	5.6
*	10	2	5	4.3	3.2
	10	2	6	13.7	13.8
	10	2	7	12.8	12.5
	10	2	8	7.2	6.2
	11	2	-13	7.6	6.4
	11	2	-12	5.1	4.8
*	11	2	-11	4.8	2.3
	11	2	-10	4.6	6.4
	11	2	-9	6.2	5.7
	11	2	-8	13.2	12.1
	11	2	-7	4.0	2.9
	11	2	-6	7.6	7.2
	11	2	-5	15.2	13.1
	11	2	-4	6.2	7.2
	11	2	-3	14.2	13.6
	11	2	-2	10.0	9.7
	11	2	-1	15.1	13.4
	11	2	0	3.6	5.3
	11	2	1	21.3	22.4
	11	2	2	17.1	16.3
	11	2	3	4.1	3.4
	11	2	4	9.6	8.6
*	11	2	5	4.5	0.8
	12	2	-11	4.9	6.5
	12	2	-10	13.3	12.3
	12	2	-9	12.7	12.2
	12	2	-8	15.4	14.4
	12	2	-7	5.8	7.3
	12	2	-6	15.8	15.2
	12	2	-5	10.2	9.7
*	12	2	-4	3.8	0.2
	12	2	-3	12.9	11.2
	12	2	-2	14.0	12.8
	12	2	-1	21.4	20.9
	12	2	0	15.4	13.4
*	12	2	1	4.0	3.2
*	12	2	2	4.1	3.0
	12	2	3	6.1	6.9
	12	2	4	6.3	7.2
	12	2	5	4.7	6.3
	13	2	-10	6.8	5.7
	13	2	-9	4.6	4.4
	13	2	-8	13.9	14.1
	13	2	-7	18.5	17.8
	13	2	-6	22.9	22.1
	13	2	-5	13.3	14.3
	13	2	-4	10.5	8.9
	13	2	-3	19.2	19.2
	13	2	-2	13.6	12.9
	13	2	-1	16.9	15.2
	13	2	0	4.1	4.8
	13	2	1	4.2	4.7
*	13	2	2	4.3	1.4
*	13	2	3	4.5	2.1
	13	2	4	6.6	6.1
*	14	2	-8	4.5	1.9
	14	2	-7	6.2	6.7
	14	2	-6	14.2	14.0
	14	2	-5	15.7	15.5
	14	2	-4	19.4	19.5
	14	2	-3	22.6	21.5
	14	2	-2	5.9	6.0
*	14	2	-1	4.2	3.7
	14	2	0	6.0	6.4
	14	2	1	6.2	6.2
*	14	2	2	4.5	1.3
	15	2	-8	8.1	8.1
	15	2	-7	7.9	7.5
·	15	2	-6	10.9	10.3
*	15	2	-5	4.4	3.9
	15	2	-4	9.7	7.9
*	15	2	-3	4.3	4.5
	15	2	-2	11.5	9.7
	15	2	-1	15.9	16.0
	15	2	0	13.5	11.6
	15	2	1	4.6	4.7
*	15	2	2	4.7	2.3
	15	2	3	6.9	6.7
	16	2	-7	4.7	4.7
	16	2	-6	14.6	13.5
	16	2	-5	12.9	11.9
	16	2	-4	4.5	3.9
	16	2	-3	6.4	4.3
	16	2	-2	12.0	11.2
	16	2	-1	12.2	11.1
	16	2	0	8.1	7.3
	16	2	1	11.8	9.5
	16	2	2	4.9	5.7
*	17	2	-4	4.7	0.2
*	17	2	-3	4.7	1.9
	17	2	-2	8.2	8.2
	17	2	-1	4.8	5.1
*	17	2	0	4.9	0.1
*	17	2	1	5.0	2.6
	18	2	-4	4.9	4.2
	18	2	-3	4.9	6.0
	18	2	-2	7.0	7.3
*	18	2	-1	5.0	4.0
*	18	2	0	5.1	3.8
	18	2	1	5.2	5.4
*	0	3	-11	4.6	2.8
	0	3	-10	10.6	10.7
*	0	3	-9	4.0	1.4
	0	3	-8	12.9	13.3
*	0	3	-7	3.4	2.1
	0	3	-6	22.3	20.3
	0	3	-5	25.5	24.3
	0	3	-4	13.9	13.3
	0	3	-3	13.0	12.6
	0	3	-2	42.5	37.6
	1	3	-11	4.6	5.2
	1	3	-10	12.1	11.4
	1	3	-9	8.9	8.9
	1	3	-8	11.6	11.3
	1	3	-7	23.9	22.7
	1	3	-6	41.4	40.3
	1	3	-5	45.4	42.7
	1	3	-4	13.1	12.3
	1	3	-3	13.2	12.2
	1	3	-2	14.6	13.3
	1	3	2	4.6	4.1
	1	3	3	29.3	27.1
	1	3	4	27.1	24.6
	1	3	5	33.4	32.0
	1	3	6	5.5	6.0
	1	3	7	18.5	17.3
	1	3	8	14.7	14.4
	1	3	9	14.8	15.5
	1	3	10	8.8	8.6
	2	3	-10	11.2	10.7
*	2	3	-9	3.9	2.0
*	2	3	-8	3.6	0.7
*	2	3	-7	3.3	3.3
	2	3	-6	23.3	21.1
	2	3	-5	29.4	28.3
	2	3	-4	14.3	14.2
	2	3	-3	37.4	34.8
**	2	3	-2	7.0	8.3
**	2	3	1	4.1	5.0
	2	3	2	33.5	33.5
	2	3	3	16.6	16.9
*	2	3	4	2.7	2.2
	2	3	5	25.0	23.5
	2	3	6	11.4	10.1
	2	3	7	20.3	19.2
*	2	3	8	3.9	4.2
*	2	3	9	4.2	4.1
	2	3	10	6.3	6.8
*	3	3	-10	4.2	4.3
	3	3	-9	11.7	10.9
	3	3	-8	33.5	33.8
	3	3	-7	25.3	24.7
	3	3	-6	38.1	35.8
	3	3	-5	31.8	29.5
	3	3	-4	17.6	17.1
**	3	3	-3	6.1	2.6
	3	3	-2	62.7	65.6
**	3	3	-1	103.1	111.1
	3	3	0	83.0	82.3
	3	3	1	47.1	46.1
	3	3	2	32.7	31.0
	3	3	3	36.1	33.4
	3	3	4	23.6	23.4
*	3	3	5	3.1	2.3
	3	3	6	15.2	15.0
	3	3	7	12.2	13.1
	3	3	8	5.6	6.1
	3	3	9	9.6	9.5

Table 4 (*cont.*)

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	3	3	10	4.6	5.5
	4	3	-10	13.2	12.5
	4	3	-9	8.7	9.1
	4	3	-8	25.8	25.5
	4	3	-7	19.9	18.8
	4	3	-6	31.9	30.8
	4	3	-5	32.8	31.2
	4	3	-4	2.5	2.3
	4	3	-3	16.2	14.3
	4	3	-2	13.8	11.4
	4	3	-1	71.7	74.0
•	4	3	0	2.0	2.2
	4	3	1	20.3	19.8
	4	3	2	43.1	41.5
	4	3	3	14.0	13.7
	4	3	4	23.7	22.5
	4	3	5	4.6	4.8
	4	3	6	32.7	32.2
	4	3	7	13.7	13.8
•	4	3	8	4.1	3.1
	5	3	-10	5.9	6.0
•	5	3	-9	3.9	0.4
	5	3	-8	10.9	10.2
	5	3	-7	14.6	13.6
	5	3	-6	34.6	32.5
	5	3	-5	31.6	29.5
	5	3	-4	14.7	13.0
	5	3	-3	64.0	63.9
	5	3	-2	97.9	108.8
	5	3	-1	100.7	109.5
	5	3	0	47.4	43.8
	5	3	1	7.2	6.4
	5	3	2	14.8	13.2
	5	3	3	22.2	21.2
	5	3	4	24.9	23.4
	5	3	5	29.1	27.9
	5	3	6	18.3	17.9
•	5	3	7	3.9	1.4
	5	3	8	6.0	6.4
	6	3	-11	11.0	11.0
	6	3	-10	11.9	12.4
	6	3	-9	11.1	10.2
	6	3	-8	21.6	21.4
	6	3	-7	9.0	8.2
	6	3	-6	25.0	26.1
	6	3	-5	9.7	8.5
	6	3	-4	17.6	17.6
	6	3	-3	59.2	60.5
	6	3	-2	35.8	32.7
	6	3	-1	22.9	20.1
••	6	3	0	2.5	3.0
	6	3	1	23.1	23.2
	6	3	2	18.5	15.5
	6	3	3	30.5	29.4
	6	3	4	9.8	8.8
•	6	3	5	3.5	1.2
	6	3	6	15.2	15.0
•	6	3	7	4.1	2.5
	7	3	-12	6.7	6.8
	7	3	-11	6.3	6.9
	7	3	-10	13.3	13.2
	7	3	-9	5.6	7.1
	7	3	-8	5.2	5.8
	7	3	-7	11.4	11.8
	7	3	-6	15.1	15.0
	7	3	-5	3.0	4.6
	7	3	-4	35.4	35.8
	7	3	-3	15.3	14.5
	7	3	-2	5.9	6.3
	7	3	-1	18.8	17.2
	7	3	0	9.8	9.1
	7	3	1	8.0	7.7
	7	3	2	13.5	13.8
	7	3	3	47.2	48.6
	7	3	4	37.9	37.4
	7	3	5	26.1	26.0
	7	3	6	3.9	4.2
	7	3	7	5.9	5.9
	8	3	-11	6.4	7.0
•	8	3	-10	4.3	1.8
•	8	3	-9	4.0	2.3
	8	3	-8	15.5	16.8
•	8	3	-7	3.5	2.3
	8	3	-6	23.5	22.9
	8	3	-5	16.0	15.5
	8	3	-4	23.9	22.9
	8	3	-3	40.8	41.0
•	8	3	-2	2.8	1.1
	8	3	-1	8.5	8.5
•	8	3	0	2.9	1.6
	8	3	1	13.3	12.9
	8	3	2	4.5	4.9
	8	3	3	12.7	12.2
	8	3	4	17.0	16.5
	8	3	5	10.2	10.2
	8	3	6	4.1	5.0
•	9	3	-10	4.3	0.1
	9	3	-9	10.7	9.6
	9	3	-8	14.8	14.1
	9	3	-7	3.6	3.7
•	9	3	-6	3.4	4.2
	9	3	-5	12.2	10.9
	9	3	-4	9.9	9.0
	9	3	-3	28.4	26.6
	9	3	-2	4.3	3.9
	9	3	-1	9.2	9.9
	9	3	0	14.0	14.3
	9	3	1	13.8	12.3
	9	3	2	27.8	27.5
	9	3	3	19.6	18.8
•	9	3	4	3.8	0.5
	9	3	5	4.0	6.2
	9	3	6	9.5	8.8
	9	3	7	6.4	6.9
	10	3	-10	7.6	8.0
	10	3	-9	4.1	4.8
	10	3	-8	7.8	8.8
	10	3	-7	9.1	8.9
	10	3	-6	15.9	16.1
•	10	3	-5	3.4	4.4
•	10	3	-4	3.3	1.8
·	10	3	-3	15.9	15.7
·	10	3	-2	25.0	23.5
•	10	3	-1	3.3	3.0
•	10	3	0	3.3	1.5
	10	3	1	23.1	22.5
	10	3	2	10.8	10.6
	10	3	3	3.8	4.4
•	10	3	4	4.0	1.0
•	10	3	5	4.2	0.0
	11	3	-11	8.1	8.0
	11	3	-10	8.9	9.5
	11	3	-9	14.6	14.9
	11	3	-8	14.5	14.5
	11	3	-7	3.8	4.6
	11	3	-6	11.1	11.6
	11	3	-5	3.6	4.2
	11	3	-4	17.0	16.0
	11	3	-3	10.8	10.9
	11	3	-2	14.9	15.2
	11	3	-1	3.5	4.9
	11	3	0	20.0	19.8
	11	3	1	8.9	7.9
•	11	3	2	3.8	1.4
	11	3	3	11.9	12.4
	11	3	4	11.0	10.9
	11	3	5	6.2	6.5
	11	3	6	6.5	6.0
	11	3	7	4.8	6.1
	12	3	-11	6.7	6.9
•	12	3	-10	4.5	2.7
•	12	3	-9	4.3	0.8
•	12	3	-8	4.1	1.2
	12	3	-7	5.6	6.7
•	12	3	-6	3.8	3.7
	12	3	-5	9.9	9.5
•	12	3	-4	3.6	1.7
	12	3	-3	14.0	13.5
	12	3	-2	20.1	21.2
	12	3	-1	14.6	13.6
	12	3	0	6.5	6.6
	12	3	1	7.7	6.6
	12	3	2	8.9	8.5
	12	3	3	13.1	13.6
	12	3	4	6.1	6.6
	13	3	-11	4.8	5.9
	13	3	-10	8.0	7.6
	13	3	-9	14.0	14.0
	13	3	-8	10.4	10.6
•	13	3	-7	4.1	2.6
	13	3	-6	8.0	8.9
	13	3	-5	30.4	30.9
	13	3	-4	34.9	34.8
	13	3	-3	18.2	18.5
	13	3	-2	6.6	6.2
•	13	3	-1	3.9	2.8
•	13	3	0	3.9	0.2
•	13	3	1	4.0	0.0
•	13	3	2	4.2	2.5
	13	3	3	4.3	5.0
	14	3	-7	6.0	6.0
•	14	3	-6	4.1	2.0
	14	3	-5	5.7	5.4
	14	3	-4	5.7	6.0
	14	3	-3	4.0	5.2
	14	3	-2	12.0	12.1
	14	3	-1	4.1	4.2
•	14	3	0	4.1	1.5
	14	3	1	4.2	5.8
	14	3	2	8.8	9.3
	14	3	3	6.4	8.1
	15	3	-9	6.6	6.8
•	15	3	-8	4.5	0.7
	15	3	-7	7.6	8.0
	15	3	-6	12.2	12.1
	15	3	-5	12.0	12.7
	15	3	-4	11.1	12.1
	15	3	-3	8.4	9.1
	15	3	-2	5.9	6.0
•	15	3	-1	4.3	0.1
	15	3	0	9.7	11.3
	15	3	1	12.6	13.7
	15	3	2	12.1	11.6
	15	3	3	6.7	6.9
	16	3	-7	6.5	7.5
	16	3	-6	6.3	6.2
	16	3	-5	8.8	8.6
	16	3	-4	4.4	6.1
	17	3	-1	8.1	8.4
	17	3	0	12.6	12.3
	17	3	1	4.9	5.6
•	0	4	-12	5.0	4.2
•	0	4	-11	4.7	2.2
	0	4	-10	4.4	4.7
	0	4	-9	9.1	8.9
	0	4	-8	3.8	4.6
•	0	4	-7	3.5	0.3
	0	4	-6	5.5	5.4
	0	4	-5	27.4	27.0
	0	4	-4	31.8	32.5
	0	4	-3	18.1	15.7
	0	4	-2	12.4	10.2
	0	4	-1	21.4	23.4
	1	4	-12	8.5	8.0
	1	4	-11	6.5	6.7
	1	4	-10	4.3	5.8
•	1	4	-9	4.0	2.6
	1	4	-8	14.8	14.0
	1	4	-7	22.8	23.2
	1	4	-6	25.6	26.4
	1	4	-5	33.0	32.5
	1	4	-4	27.2	27.4
	1	4	-3	36.4	36.2
	1	4	-2	5.9	7.3
	1	4	-1	15.2	12.4
	1	4	0	3.8	3.1
	1	4	1	25.0	25.4
	1	4	2	57.4	63.0
	1	4	3	81.5	89.1
	1	4	4	28.0	28.3
	1	4	5	13.4	15.0
	1	4	6	14.1	13.7
	1	4	7	24.2	24.5
•	1	4	8	3.8	2.7
•	1	4	9	4.1	0.8
	1	4	10	6.3	6.7
•	2	4	-11	4.6	3.4
•	2	4	-10	4.3	4.5
	2	4	-9	5.6	5.3
	2	4	-8	13.2	14.2
	2	4	-7	8.2	7.2
	2	4	-6	4.3	4.5
	2	4	-5	31.5	30.5
	2	4	-4	27.0	27.4
	2	4	-3	23.9	23.5
	2	4	-2	48.7	49.5
	2	4	-1	7.4	7.4
	2	4	0	18.3	17.2
	2	4	1	5.1	5.0
	2	4	2	34.9	35.5
	2	4	3	49.9	49.6
	2	4	4	13.8	13.9
	2	4	5	5.2	6.2
	2	4	6	13.3	13.5
•	2	4	7	3.6	1.9
•	2	4	8	3.9	3.9
•	2	4	9	4.2	4.3
	3	4	-12	10.8	8.9
•	3	4	-11	4.5	1.9
	3	4	-10	13.4	14.4
	3	4	-9	6.8	6.8
	3	4	-8	17.9	17.8
	3	4	-7	19.0	19.3
	3	4	-6	16.5	17.2
	3	4	-5	8.3	7.8
	3	4	-4	4.9	3.5
	3	4	-3	33.2	31.5
	3	4	-2	27.9	28.0
	3	4	-1	5.4	5.3
	3	4	0	45.7	46.7
	3	4	1	78.6	85.6
	3	4	2	66.4	71.1
	3	4	3	6.7	6.4
	3	4	4	25.0	24.8
	3	4	5	11.7	11.4
	3	4	6	15.0	15.0
	3	4	7	20.4	20.0
	3	4	8	9.0	8.1
	3	4	9	7.5	8.9
	4	4	-11	7.8	8.1
•	4	4	-10	4.2	1.2
•	4	4	-9	3.9	0.1
	4	4	-8	11.5	11.5
	4	4	-7	8.9	9.2
	4	4	-6	19.9	17.7
•	4	4	-5	2.8	1.1
	4	4	-4	21.6	21.4
•	4	4	-3	2.3	0.1
	4	4	-2	22.9	23.2
	4	4	-1	7.6	6.6
••	4	4	0	2.0	4.4
	4	4	1	7.6	6.3
	4	4	2	34.2	34.1
	4	4	3	46.1	44.7
	4	4	4	25.0	23.6
	4	4	5	10.3	9.8
	4	4	6	5.0	5.9
	4	4	7	9.4	10.5
	4	4	8	7.2	7.0
	5	4	-11	10.1	10.1
	5	4	-10	15.2	15.3
	5	4	-9	3.9	4.4
	5	4	-8	26.1	26.6
	5	4	-7	27.0	27.0
•	5	4	-6	2.3	0.2
	5	4	-5	13.4	13.3
	5	4	-4	43.4	42.5
	5	4	-3	62.9	66.0
	5	4	-2	12.4	12.6
	5	4	-1	34.7	35.6
	5	4	0	21.9	20.3
	5	4	1	14.4	12.4
	5	4	2	4.6	4.6
	5	4	3	20.4	18.9
	5	4	4	8.9	7.9
	5	4	5	11.8	12.2
	5	4	6	20.8	20.8
	5	4	7	20.6	20.6
	5	4	8	6.0	6.1
	6	4	-11	4.5	4.2
	6	4	-10	6.0	5.1
•	6	4	-9	4.0	1.3
	6	4	-8	3.7	4.0
	6	4	-7	20.2	18.9
	6	4	-6	18.8	17.9
	6	4	-5	23.0	23.4
	6	4	-4	46.0	44.6
	6	4	-3	20.9	21.0
	6	4	-2	7.0	6.5
	6	4	-1	6.5	6.4
	6	4	0	31.1	31.2
	6	4	1	32.5	32.1
	6	4	2	4.0	4.5
	6	4	3	7.5	8.9
	6	4	4	3.3	3.9
•	6	4	5	3.6	1.4
•	6	4	6	3.8	1.4
	6	4	7	5.8	6.8
•	6	4	8	4.4	4.4
	7	4	-11	9.0	9.3
	7	4	-10	12.0	12.2
	7	4	-9	8.0	8.6
	7	4	-8	18.3	18.1
	7	4	-7	6.0	6.0
	7	4	-6	40.8	42.1
	7	4	-5	28.7	28.3
	7	4	-4	32.2	31.6
	7	4	-3	31.2	31.9
	7	4	-2	11.0	10.8
••	7	4	-1	8.0	2.6
	7	4	0	17.5	16.4
	7	4	1	20.1	19.2
	7	4	2	15.5	13.4
	7	4	3	9.7	8.5
	7	4	4	4.9	5.0
	7	4	5	16.6	16.0
	7	4	6	15.9	15.9
•	7	4	7	4.2	1.7
	7	4	8	6.4	6.7
	8	4	-10	9.6	8.5
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	8	4	-8	7.6	7.5
•	8	4	-7	3.6	1.4
	8	4	-6	3.3	3.5
	8	4	-5	10.5	11.1
	8	4	-4	24.9	23.7
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	8	4	-2	9.9	9.3
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	8	4	0	25.4	24.8
	8	4	1	41.8	42.4
	8	4	2	27.1	25.8
	8	4	3	10.3	9.6
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	8	4	5	9.5	8.0
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	9	4	-11	10.3	10.0
	9	4	-10	4.3	5.5
•	9	4	-9	4.1	3.7
	9	4	-8	3.9	4.8
	9	4	-7	22.8	22.7
	9	4	-6	32.7	34.7
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	9	4	-4	17.4	17.1
	9	4	-3	18.3	18.3
	9	4	-2	9.7	9.8
	9	4	-1	13.1	11.9
	9	4	0	33.1	33.6
	9	4	1	44.6	44.3
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	9	4	3	6.3	7.0
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•	9	4	5	4.1	2.4
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•	10	4	-11	4.6	2.6
•	10	4	-10	4.4	2.8
	10	4	-9	5.9	5.2
	10	4	-8	7.9	8.5
	10	4	-7	16.8	16.3
	10	4	-6	26.9	27.3
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	10	4	-4	8.2	7.9
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•	10	4	-2	3.3	2.3
	10	4	-1	10.4	9.7
•	10	4	0	3.4	2.3
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•	10	4	3	3.8	3.1
•	10	4	4	4.0	4.0
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	11	4	-11	8.2	7.8
•	11	4	-10	4.5	1.3
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	11	4	-7	10.3	9.6
	11	4	-6	12.3	12.1
	11	4	-5	5.1	5.1
	11	4	-4	15.3	15.5
	11	4	-3	12.5	11.0
	11	4	-2	45.5	45.7
	11	4	-1	32.0	31.6
	11	4	0	25.2	24.0
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	11	4	2	5.4	6.0
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•	11	4	4	4.2	1.7
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	12	4	-7	8.0	6.9
	12	4	-6	19.3	19.2
	12	4	-5	11.9	11.9
	12	4	-4	5.2	5.6
	12	4	-3	5.2	6.2
	12	4	-2	12.6	12.6
	12	4	-1	18.8	18.8
	12	4	0	12.5	12.0
	12	4	1	15.5	13.8
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	13	4	-10	4.7	5.6
	13	4	-9	4.5	6.0
	13	4	-8	4.3	3.6
	13	4	-7	14.9	13.5
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•	13	4	-5	3.9	0.9
	13	4	-4	3.9	3.7
	13	4	-3	18.0	16.9
	13	4	-2	17.2	17.7
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	13	4	4	10.2	9.8
	13	4	5	10.7	10.3
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	14	4	-2	8.1	8.1
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	15	4	-7	9.9	10.0
	15	4	-6	4.3	5.6
•	15	4	-5	4.3	0.5
•	15	4	-4	4.2	3.5
•	15	4	-3	4.2	2.3
•	15	4	-2	4.2	1.2
•	15	4	-1	4.3	0.3
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	15	4	2	10.3	10.8
	15	4	3	8.3	8.7
	16	4	-8	8.2	7.5
•	16	4	-7	4.6	4.5
•	16	4	-6	4.5	1.0
•	16	4	-5	4.4	0.7
•	16	4	-4	4.4	3.2
•	16	4	-3	4.4	4.8
•	16	4	-2	4.4	4.0
	16	4	-1	7.8	7.3
	16	4	0	6.5	5.0
	17	4	-2	9.3	8.1
	19	4	-3	7.1	7.2
•	0	5	-10	4.1	3.5
•	0	5	-9	3.8	2.8
•	0	5	-8	3.5	0.2
	0	5	-7	8.0	7.6
•	0	5	-6	3.0	0.9
	0	5	-5	15.6	13.5
	0	5	-4	17.1	17.2
	0	5	-3	37.0	37.1
	0	5	-2	67.1	72.5
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	1	5	-9	5.3	6.2
	1	5	-8	10.5	9.8
	1	5	-7	10.1	11.0
	1	5	-6	37.3	38.8
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	1	5	-4	6.9	7.9
	1	5	-3	10.3	10.0
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	1	5	-1	40.5	44.9
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•	1	5	7	3.3	0.4
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	2	5	-11	4.3	4.8
	2	5	-10	5.7	6.0
	2	5	-9	9.9	9.0
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	2	5	-4	12.4	12.0
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•	2	5	6	3.1	1.1
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	2	5	8	9.0	9.5
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	3	5	-5	2.6	1.5
	3	5	-4	25.5	25.4
	3	5	-3	42.9	44.2
	3	5	-2	29.8	31.4
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	4	5	-7	16.7	16.6
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	4	5	7	12.0	12.2
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	5	5	4	12.7	11.8
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	2	6	-4	12.5	12.0
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	2	6	-1	25.5	25.6
	2	6	0	8.1	7.5
	2	6	1	1.5	1.9
•	2	6	2	1.8	0.3
	2	6	3	14.0	14.4

Table 4 (*cont.*)

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	2	6	4	2.4	2.2
	2	6	5	12.7	12.5
	2	6	6	22.0	21.6
	2	6	7	3.2	3.7
*	2	6	8	3.5	2.4
*	3	6	-11	4.0	1.3
	3	6	-10	7.6	8.0
	3	6	-9	3.5	3.7
	3	6	-8	5.6	6.4
	3	6	-7	5.2	4.8
	3	6	-6	10.2	10.2
	3	6	-5	6.1	5.3
	3	6	-4	7.9	7.7
	3	6	-3	39.8	39.7
	3	6	-2	49.8	48.6
	3	6	-1	49.1	50.1
	3	6	0	20.5	20.5
	3	6	1	12.8	13.8
	3	6	2	18.6	17.5
	3	6	3	6.8	6.5
	3	6	4	2.5	2.5
	3	6	5	9.3	9.2
	3	6	6	9.2	8.8
*	3	6	7	3.3	0.2
*	3	6	8	3.6	1.3
	4	6	-11	9.8	9.6
*	4	6	-10	3.8	2.3
*	4	6	-9	3.5	2.4
*	4	6	-8	3.2	0.6
	4	6	-7	23.2	23.8
	4	6	-6	13.5	12.3
	4	6	-5	10.3	9.3
*	4	6	-4	2.3	0.7
	4	6	-3	4.1	3.9
	4	6	-2	18.6	17.2
	4	6	-1	8.5	7.3
	4	6	0	14.2	14.5
	4	6	1	4.8	5.2
	4	6	2	9.0	8.7
	4	6	3	16.5	15.4
	4	6	4	6.6	7.0
	4	6	5	14.3	14.1
	4	6	6	7.1	7.3
	4	6	7	9.7	9.3
	4	6	8	5.2	5.7
*	5	6	-10	3.7	1.5
	5	6	-9	8.6	8.3
	5	6	-8	6.5	6.3
*	5	6	-7	3.0	2.3
	5	6	-6	15.2	14.6
	5	6	-5	12.5	11.6
	5	6	-4	23.5	23.8
	5	6	-3	14.5	13.7
	5	6	-2	19.8	18.9
	5	6	-1	31.1	29.8
	5	6	0	16.5	15.5
	5	6	1	13.8	12.9
	5	6	2	4.7	4.8
	5	6	3	13.9	13.7
	5	6	4	12.3	12.3
	5	6	5	11.4	11.9
*	5	6	6	3.3	2.8
	5	6	7	3.5	2.9
	6	6	-12	6.0	5.9
	6	6	-11	5.7	6.5
	6	6	-10	3.8	4.1
	6	6	-9	3.5	4.0
	6	6	-8	10.4	9.7
	6	6	-7	25.6	25.6
	6	6	-6	11.0	9.5
	6	6	-5	5.9	5.3
	6	6	-4	9.8	9.0
	6	6	-3	6.5	5.5
	6	6	-2	25.9	25.1
	6	6	-1	9.8	8.5
	6	6	0	8.4	7.1
*	6	6	1	2.4	0.2
	6	6	2	24.4	24.4
	6	6	3	10.3	9.4
	6	6	4	4.2	4.3
*	6	6	5	3.2	1.9
	6	6	6	5.9	5.3
	6	6	7	8.9	8.7
	7	6	-10	6.6	6.2
	7	6	-9	3.5	3.4
	7	6	-8	3.3	3.9
	7	6	-7	8.8	8.2
	7	6	-6	20.3	21.1
	7	6	-5	9.0	8.8
	7	6	-4	5.1	5.0
	7	6	-3	23.2	22.1
	7	6	-2	44.6	43.6
	7	6	-1	34.0	33.4
	7	6	0	23.5	22.8
	7	6	1	17.4	16.7
	7	6	2	11.9	11.1
*	7	6	3	2.9	1.0
	7	6	4	11.2	10.8
	7	6	5	15.6	15.7
	7	6	6	11.2	11.4
	7	6	7	5.3	5.2
	8	6	-10	3.8	4.8
*	8	6	-9	3.6	0.0
	8	6	-8	6.8	7.3
	8	6	-7	22.5	23.1
	8	6	-6	9.5	9.9
	8	6	-5	2.8	3.4
	8	6	-4	2.7	3.1
	8	6	-3	30.8	31.3
	8	6	-2	32.8	33.4
	8	6	-1	9.9	8.9
	8	6	0	5.9	6.2
	8	6	1	10.3	10.4
	8	6	2	17.1	16.4
*	8	6	3	3.1	1.2
	8	6	4	5.6	6.2
*	8	6	5	3.5	1.0
*	8	6	6	3.7	0.4
	9	6	-12	4.3	3.3
	9	6	-11	10.0	9.6
	9	6	-10	12.2	12.8
	9	6	-9	8.2	9.0
	9	6	-8	6.9	6.5
	9	6	-7	5.6	5.3
	9	6	-6	12.4	12.7
	9	6	-5	5.9	5.6
	9	6	-4	4.9	4.4
	9	6	-3	5.5	5.8
	9	6	-2	9.9	9.4
	9	6	-1	16.1	15.4
	9	6	0	23.3	22.8
	9	6	1	13.1	13.7
	9	6	2	7.5	8.1
	9	6	3	22.4	22.8
	9	6	4	19.9	20.4
	9	6	5	12.0	12.7
	9	6	6	6.6	6.8
*	10	6	-10	3.9	1.5
	10	6	-9	3.7	3.5
	10	6	-8	3.5	4.7
	10	6	-7	16.1	15.9
*	10	6	-6	3.2	0.3
	10	6	-5	8.7	8.2
	10	6	-4	12.3	12.3
	10	6	-3	24.1	24.1
	10	6	-2	7.1	7.1
	10	6	-1	4.1	2.8
	10	6	0	5.2	5.3
	10	6	1	6.2	5.1
	10	6	2	11.7	12.3
	10	6	3	7.6	8.0
	10	6	4	3.6	5.1
	11	6	-11	8.4	7.1
	11	6	-10	5.6	6.7
*	11	6	-9	3.8	3.4
*	11	6	-8	3.6	3.7
*	11	6	-7	3.5	1.9
	11	6	-6	14.8	14.7
	11	6	-5	20.8	20.4
	11	6	-4	28.9	28.7
	11	6	-3	16.6	16.5
	11	6	-2	5.3	4.6
	11	6	-1	8.8	7.3
*	11	6	0	3.2	1.6
*	11	6	1	3.3	1.1
	11	6	2	5.9	6.1
	11	6	3	5.0	3.5
	11	6	4	3.7	3.0
	12	6	-10	4.0	3.0
*	12	6	-9	3.9	1.3
*	12	6	-8	3.7	2.5
*	12	6	-7	3.6	3.3
	12	6	-6	3.4	4.2
*	12	6	-5	3.3	2.3
*	12	6	-4	3.3	0.3
	12	6	-3	7.3	7.1
*	12	6	-2	3.3	1.6
*	12	6	-1	3.3	1.8
*	12	6	0	3.4	1.0
	12	6	1	9.2	9.5
	12	6	2	12.4	13.4
	12	6	3	5.3	5.9
*	13	6	-10	4.1	0.0
*	13	6	-9	4.0	1.4
*	13	6	-8	3.8	2.5
	13	6	-7	9.8	9.9
	13	6	-6	12.9	12.7
	13	6	-5	4.9	5.9
	13	6	-4	6.0	6.5
*	13	6	-3	3.4	2.6
*	13	6	-2	3.4	2.0
*	13	6	-1	3.5	0.2
	13	6	0	3.5	4.7
	13	6	1	8.9	8.5
	13	6	2	6.5	6.2
	13	6	3	3.9	4.3
*	14	6	-5	3.6	3.5
*	14	6	-4	3.6	2.4
	14	6	-3	5.1	6.3
*	14	6	-2	3.6	0.4
	14	6	-1	5.2	5.3
	14	6	0	3.7	4.8
	14	6	1	5.4	5.4
	15	6	-9	4.2	4.7
*	15	6	-8	4.0	2.8
	15	6	-7	4.0	2.8
*	15	6	-6	3.9	2.8
	15	6	-5	9.3	8.8
	15	6	-4	6.5	7.3
	15	6	-3	5.3	6.1
	15	6	-2	5.3	6.4
	15	6	-1	5.4	5.9
	15	6	0	8.7	8.4
	16	6	-4	5.6	5.9
	16	6	-3	3.9	4.7
*	16	6	-2	3.9	1.4
*	16	6	-1	4.0	2.9
*	16	6	0	4.1	0.4
	17	6	-5	4.1	4.7
	17	6	-4	5.8	5.7
	17	6	-3	8.2	8.5
	17	6	-2	5.8	6.7
*	17	6	-1	4.2	0.6
*	17	6	0	4.2	3.5
	17	6	1	4.3	5.5
*	0	7	-10	3.8	3.9
	0	7	-9	5.0	5.0
	0	7	-8	8.1	8.0
	0	7	-7	17.5	17.7
	0	7	-6	14.7	14.9
	0	7	-5	9.4	9.8
	0	7	-4	26.4	23.1
**	0	7	-3	1.9	1.8
	0	7	-2	34.6	32.2
	0	7	-1	11.2	10.8
	1	7	-10	5.3	4.0
	1	7	-9	7.0	8.0
*	1	7	-8	3.3	0.8
	1	7	-7	3.0	3.7
	1	7	-6	9.5	10.0
	1	7	-5	25.1	23.4
	1	7	-4	15.0	13.6
*	1	7	-3	1.9	1.0
	1	7	-2	12.8	11.7
	1	7	-1	5.4	5.7
	1	7	0	24.0	27.4
	1	7	1	26.2	25.6
	1	7	2	15.8	15.4
*	1	7	3	2.0	0.1
	1	7	4	22.6	20.9
	1	7	5	18.6	19.6
*	1	7	6	2.8	2.5
*	1	7	7	3.1	1.0
*	1	7	8	3.4	0.8
	1	7	9	5.1	5.6
	2	7	-10	5.3	6.1
	2	7	-9	4.9	4.0
	2	7	-8	7.9	7.6
	2	7	-7	19.7	19.2
*	2	7	-6	2.7	3.8
	2	7	-5	17.2	17.2
	2	7	-4	23.4	22.1
	2	7	-3	40.4	38.4
	2	7	-2	36.3	36.4
**	2	7	-1	3.6	4.6
	2	7	0	3.3	3.6
	2	7	1	1.5	2.0
	2	7	2	12.2	11.5
	2	7	3	9.0	8.5
	2	7	4	13.6	12.5
*	2	7	5	2.7	1.4
	2	7	6	11.0	11.6
	2	7	7	13.5	14.5
	2	7	8	3.4	3.7
*	2	7	9	3.7	1.1
*	2	7	10	4.0	4.2
	2	7	11	7.3	7.1
*	3	7	-9	3.5	0.5
	3	7	-8	7.9	7.5
	3	7	-7	3.0	2.8
	3	7	-6	4.7	4.7
	3	7	-5	12.7	12.7
	3	7	-4	9.2	8.9
	3	7	-3	13.8	13.0
	3	7	-2	10.5	9.6
	3	7	-1	17.2	17.2
	3	7	0	24.2	23.0
	3	7	1	11.7	11.0
	3	7	2	10.3	10.0
**	3	7	3	3.2	2.7
	3	7	4	5.0	4.4
	3	7	5	3.9	4.4
*	3	7	6	3.0	0.2
	3	7	7	3.3	4.4
*	3	7	8	3.5	2.1
	3	7	9	3.8	3.7
	4	7	-10	5.2	5.5
*	4	7	-9	3.4	2.5
	4	7	-8	4.5	4.3
	4	7	-7	3.0	2.4
	4	7	-6	22.0	21.6
	4	7	-5	36.3	36.3
	4	7	-4	27.6	27.8
	4	7	-3	32.9	32.5
	4	7	-2	14.1	13.4
	4	7	-1	3.9	3.5
**	4	7	0	1.8	1.9
	4	7	1	20.9	20.8
	4	7	2	46.7	46.4
	4	7	3	23.5	23.0
	4	7	4	7.9	6.9
*	4	7	5	2.9	0.5
	4	7	6	10.8	11.3
	4	7	7	7.6	7.1
*	4	7	8	3.6	3.7
*	5	7	-9	3.4	2.5
	5	7	-8	4.5	5.6
	5	7	-7	5.9	5.7
	5	7	-6	2.7	3.3
*	5	7	-5	2.5	2.1
	5	7	-4	11.8	11.4
	5	7	-3	5.2	5.4
	5	7	-2	5.7	5.1
	5	7	-1	10.2	9.9
	5	7	0	7.5	6.9
	5	7	1	10.8	9.8
*	5	7	2	2.3	2.0
	5	7	3	6.7	7.1
	5	7	4	2.8	2.2
	5	7	5	6.7	5.7
	5	7	6	3.2	3.4
*	5	7	7	3.5	1.6
*	5	7	8	3.7	2.1
	5	7	9	4.0	3.2
	6	7	-10	6.4	5.5
*	6	7	-9	3.5	0.5
*	6	7	-8	3.2	1.3
*	6	7	-7	3.0	1.3
	6	7	-6	8.4	8.6
	6	7	-5	5.2	5.1
	6	7	-4	6.4	7.1
	6	7	-3	20.4	20.4
	6	7	-2	3.8	4.0
	6	7	-1	17.7	16.7
	6	7	0	27.0	25.8
	6	7	1	44.7	42.7
	6	7	2	43.5	43.5
	6	7	3	9.8	9.2
	6	7	4	2.9	3.0
	6	7	5	3.1	3.8
	6	7	6	8.2	9.0
	6	7	7	3.6	3.9
	7	7	-9	3.5	4.7
	7	7	-8	8.0	8.7
	7	7	-7	3.1	2.8
	7	7	-6	4.1	4.1
	7	7	-5	9.7	9.5
	7	7	-4	23.4	23.9
	7	7	-3	9.7	9.8
*	7	7	-2	2.3	2.3
*	7	7	-1	2.3	0.6
	7	7	0	6.4	5.7
	7	7	1	6.7	6.9
	7	7	2	9.7	9.2
	7	7	3	11.8	12.0
	7	7	4	9.2	9.3
*	7	7	5	3.3	0.6
	7	7	6	4.9	4.4
	8	7	-11	4.0	5.4
	8	7	-10	5.3	4.6
	8	7	-9	3.5	4.2
	8	7	-8	8.8	9.5
	8	7	-7	9.9	9.9
	8	7	-6	6.6	6.5
	8	7	-5	4.0	5.0
	8	7	-4	7.0	7.0
	8	7	-3	7.7	7.7
	8	7	-2	10.7	10.5
	8	7	-1	22.8	22.2
	8	7	0	8.2	7.6
	8	7	1	6.1	6.5
	8	7	2	2.9	2.6
	8	7	3	5.2	6.5
	8	7	4	4.5	4.3
	8	7	5	6.8	6.9
	8	7	6	12.0	12.9
	8	7	7	5.4	6.4
*	9	7	-11	4.0	1.4
*	9	7	-10	3.8	1.0
	9	7	-9	8.8	8.8
	9	7	-8	8.3	9.4
	9	7	-7	3.2	4.0
	9	7	-6	4.3	5.2
*	9	7	-5	2.9	0.6
	9	7	-4	6.3	7.1
	9	7	-3	6.1	5.9
	9	7	-2	11.5	11.6
	9	7	-1	11.2	11.5
*	9	7	0	2.8	3.2
	9	7	1	11.9	12.5
	9	7	2	10.0	10.4
	9	7	3	8.4	8.6
*	9	7	4	3.4	1.5
	9	7	5	3.6	3.6
	9	7	6	3.8	2.7
	10	7	-11	4.0	6.4
	10	7	-10	3.9	5.0
	10	7	-9	5.2	6.1
*	10	7	-8	3.5	4.2
	10	7	-7	3.3	4.4
	10	7	-6	4.5	5.4
*	10	7	-5	3.0	1.6
*	10	7	-4	2.9	1.3
*	10	7	-3	2.9	2.1
*	10	7	-2	2.9	1.0
	10	7	-1	5.0	5.1
	10	7	0	14.5	14.6
	10	7	1	6.9	7.4
	10	7	2	3.2	4.1
	10	7	3	5.8	6.4
	10	7	4	5.0	5.2
	10	7	5	8.3	8.7
	10	7	6	5.5	6.7
	11	7	-8	3.6	4.0
	11	7	-7	4.8	5.1
	11	7	-6	7.3	8.1
	11	7	-5	3.2	2.8
	11	7	-4	6.9	6.7
	11	7	-3	5.3	6.6
	11	7	-2	9.6	10.1
	11	7	-1	7.5	7.9
*	11	7	0	3.1	2.2
*	11	7	1	3.2	1.3
*	11	7	2	3.4	0.6
*	11	7	3	3.5	2.2
	12	7	-8	10.3	9.9
	12	7	-7	15.3	16.2
	12	7	-6	10.2	10.5
	12	7	-5	3.3	2.8
*	12	7	-4	3.2	1.7
	12	7	-3	5.6	5.3
*	12	7	-2	3.2	1.1
*	12	7	-1	3.2	0.7
*	12	7	0	3.3	2.9
*	12	7	1	3.4	3.1
*	12	7	2	3.5	2.7
	12	7	3	3.7	5.0
*	13	7	-7	3.6	0.8
*	13	7	-6	3.5	0.9
	13	7	-5	3.4	4.0
	13	7	-4	3.4	4.7
*	13	7	-3	3.4	2.2
*	13	7	-2	3.4	0.4
	13	7	-1	3.4	2.9
*	13	7	0	3.5	2.6
	13	7	1	3.6	3.7
*	13	7	2	3.7	2.0
	13	7	3	3.8	4.6
	14	7	-10	4.2	3.3
	14	7	-9	4.0	4.7
	14	7	-8	7.7	8.0
	14	7	-7	9.9	10.4
	14	7	-6	8.2	7.9
*	14	7	-5	3.6	2.6
*	14	7	-4	3.5	1.8
	14	7	-3	9.3	8.9
	14	7	-2	13.7	14.1
	14	7	-1	11.9	12.9
	14	7	0	8.2	7.9
*	14	7	1	3.7	1.9
	15	7	-8	4.0	3.3
	15	7	-7	5.5	5.9
	15	7	-6	3.8	3.2
*	15	7	-5	3.7	1.7
*	15	7	-4	3.7	1.3
*	15	7	-3	3.7	2.7
*	15	7	-2	3.7	0.2
*	15	7	-1	3.8	2.8
	15	7	0	3.8	4.1
*	15	7	1	3.9	2.0
	16	7	-5	3.9	2.7
	16	7	-4	9.5	8.2
	16	7	-3	10.9	11.5
	16	7	-2	6.7	8.0
	16	7	-1	3.9	4.1
*	16	7	0	4.0	1.6
*	16	7	1	4.1	0.2
	17	7	-1	5.8	4.8
*	0	8	-10	3.9	4.1
*	0	8	-9	3.6	0.0
	0	8	-8	3.3	3.2
	0	8	-7	4.4	3.8
*	0	8	-6	2.8	0.8
*	0	8	-5	2.5	0.8
	0	8	-4	7.1	7.3
	0	8	-3	6.1	5.7
*	0	8	-2	1.6	0.5
	0	8	-1	4.1	4.7
	1	8	-10	5.4	5.4
*	1	8	-9	3.6	0.9
	1	8	-8	3.3	2.2
	1	8	-7	8.6	8.1
	1	8	-6	3.9	3.0
	1	8	-5	2.5	3.5
	1	8	-4	13.6	12.7
*	1	8	-3	1.9	1.7
	1	8	-2	7.5	7.4
	1	8	-1	1.9	2.1
	1	8	0	8.2	8.8
	1	8	1	19.4	20.0
	1	8	2	9.5	8.6
	1	8	3	21.2	19.0
	1	8	4	21.1	20.2
	1	8	5	3.7	3.2
*	1	8	6	2.9	3.3
	1	8	7	7.1	6.0
	1	8	8	3.4	2.4
*	1	8	9	3.7	1.2
*	1	8	10	3.9	0.2
	2	8	-10	3.8	3.5
*	2	8	-9	3.5	1.0
	2	8	-8	4.6	4.5
	2	8	-7	10.4	10.4
	2	8	-6	11.3	11.6
	2	8	-5	12.8	12.3
	2	8	-4	4.4	4.2
	2	8	-3	23.2	22.0
	2	8	-2	35.0	33.0
	2	8	-1	21.3	22.6
*	2	8	0	1.3	1.3
	2	8	1	17.8	17.2
	2	8	2	13.8	12.7
	2	8	3	3.0	3.3
	2	8	4	8.4	8.0
	2	8	5	8.1	7.1
	2	8	6	5.1	5.1
*	2	8	7	3.2	0.5
	2	8	8	3.5	4.1
	2	8	9	5.3	5.6
	2	8	10	5.6	3.9
*	3	8	-10	3.8	2.1
	3	8	-9	3.5	3.9
*	3	8	-8	3.2	0.4
*	3	8	-7	3.0	1.9
	3	8	-6	6.7	6.6
	3	8	-5	8.2	7.7
	3	8	-4	8.6	8.0
	3	8	-3	22.7	20.9
	3	8	-2	16.9	15.7
	3	8	-1	1.5	1.1
	3	8	0	15.6	15.4
	3	8	1	16.6	16.1
	3	8	2	2.9	3.4
	3	8	3	2.3	2.1
*	3	8	4	2.5	1.2
	3	8	5	6.3	5.6
*	3	8	6	3.1	0.6
*	3	8	7	3.3	3.4
	3	8	8	9.5	9.5
	3	8	9	3.8	4.4
*	3	8	10	4.1	1.5
	4	8	-11	5.6	6.4
	4	8	-10	5.3	5.9
*	4	8	-9	3.5	0.7
	4	8	-8	10.8	11.0
	4	8	-7	21.6	22.6
	4	8	-6	18.5	19.0
	4	8	-5	4.3	5.2
**	4	8	-4	10.1	8.8
	4	8	-3	25.1	24.5
	4	8	-2	23.7	23.1
	4	8	-1	21.1	20.4
	4	8	0	12.9	13.2
*	4	8	1	2.0	1.2
	4	8	2	6.6	6.6
	4	8	3	16.1	15.4
	4	8	4	24.5	23.5
	4	8	5	14.0	13.7
*	4	8	6	3.2	0.4
	4	8	7	4.8	5.8
	4	8	8	6.3	7.3
	4	8	9	3.9	3.4
	5	8	-10	3.7	4.1
	5	8	-9	6.0	6.7
*	5	8	-8	3.3	1.6
	5	8	-7	3.0	2.7
	5	8	-6	9.2	9.6
*	5	8	-5	2.6	0.1
	5	8	-4	4.1	4.3
	5	8	-3	8.9	8.3
	5	8	-2	6.7	6.5
	5	8	-1	6.9	6.5
	5	8	0	2.0	1.2
	5	8	1	15.1	14.4
	5	8	2	19.1	17.9
	5	8	3	3.7	3.6
	5	8	4	6.9	6.7
	5	8	5	9.6	10.0
*	5	8	6	3.3	1.9
	5	8	7	3.5	3.8
*	5	8	8	3.8	3.6
	6	8	-11	7.9	6.2
*	6	8	-10	3.7	3.5
*	6	8	-9	3.5	1.8
	6	8	-8	8.7	9.2
	6	8	-7	15.9	15.2
	6	8	-6	11.0	11.6
	6	8	-5	8.3	7.9
	6	8	-4	4.2	4.3
	6	8	-3	5.6	5.3
	6	8	-2	21.1	20.2
	6	8	-1	32.6	30.3
	6	8	0	23.5	22.8
	6	8	1	4.1	4.7
	6	8	2	16.9	17.2
	6	8	3	17.6	17.5
	6	8	4	11.5	11.5
	6	8	5	3.2	2.8
*	6	8	6	3.4	0.7
*	6	8	7	3.6	1.8
	6	8	8	3.9	4.1
	7	8	-12	4.2	2.8
*	7	8	-11	4.0	0.4
	7	8	-10	3.8	3.7
	7	8	-9	5.0	5.2
*	7	8	-8	3.3	2.9
	7	8	-7	5.4	5.0
	7	8	-6	4.1	5.3
	7	8	-5	14.9	15.1
	7	8	-4	15.8	14.8
	7	8	-3	4.9	4.3
	7	8	-2	11.2	11.0
	7	8	-1	9.2	9.8
*	7	8	0	2.4	1.1
	7	8	1	8.1	8.3
	7	8	2	5.4	5.2
	7	8	3	2.9	2.6
	7	8	4	3.1	3.6
*	7	8	5	3.3	1.7
	7	8	6	3.5	4.4
*	7	8	7	3.8	3.3
*	8	8	-9	3.6	0.4
	8	8	-8	3.4	2.4
	8	8	-7	9.5	9.6
	8	8	-6	12.3	12.4
	8	8	-5	9.0	8.8
*	8	8	-4	2.7	0.1
	8	8	-3	12.2	11.4
	8	8	-2	14.7	14.6
	8	8	-1	10.3	9.7
*	8	8	0	2.6	0.3
	8	8	1	8.2	8.3
	8	8	2	5.0	5.2
*	8	8	3	3.1	1.5
*	8	8	4	3.3	2.2
*	8	8	5	3.5	1.7
*	8	8	6	3.7	1.8
*	9	8	-10	3.8	0.1
*	9	8	-9	3.6	0.1
	9	8	-8	6.9	6.6
	9	8	-7	4.6	4.9
	9	8	-6	5.4	5.5
	9	8	-5	11.4	12.0
	9	8	-4	6.3	6.9
	9	8	-3	2.8	1.9
	9	8	-2	4.7	4.7
	9	8	-1	6.8	7.1
	9	8	0	13.8	13.6
	9	8	1	6.5	6.8
	9	8	2	4.3	5.1
	9	8	3	6.5	6.2
	9	8	4	3.4	3.0
	9	8	5	5.1	4.8
	9	8	6	5.4	4.6
	10	8	-9	3.7	3.2
	10	8	-8	5.0	4.4
	10	8	-7	8.2	7.1
*	10	8	-6	3.2	1.3
	10	8	-5	9.2	9.0
	10	8	-4	10.3	10.6
	10	8	-3	6.5	6.7
	10	8	-2	2.9	2.9
	10	8	-1	2.9	3.9
*	10	8	0	3.0	0.7
*	10	8	1	3.1	0.7
	10	8	2	3.2	2.9
	10	8	3	3.4	4.5
*	10	8	4	3.6	2.4
*	10	8	5	3.7	2.0
	11	8	-11	4.1	3.2
*	11	8	-10	4.0	0.0
*	11	8	-9	3.6	0.7
*	11	8	-8	3.6	1.5
	11	8	-7	4.9	5.4
	11	8	-6	4.7	4.8
*	11	8	-5	3.2	0.0
	11	8	-4	5.4	5.4
	11	8	-3	6.2	6.9
	11	8	-2	7.5	7.5
	11	8	-1	9.8	10.0
	11	8	0	7.8	6.8
	11	8	1	3.3	2.3
	11	8	2	4.8	4.5
	11	8	3	3.6	4.1
*	11	8	4	3.7	0.7
	12	8	-10	7.0	6.0
	12	8	-9	5.5	6.3
*	12	8	-8	3.7	2.6
*	12	8	-7	3.6	0.2
	12	8	-6	6.9	6.5
	12	8	-5	8.9	9.4
	12	8	-4	7.3	8.3
	12	8	-3	6.5	6.8
	12	8	-2	3.2	2.7
*	12	8	-1	3.3	0.7
	12	8	0	4.7	4.4
	12	8	1	9.8	9.7
	12	8	2	8.8	9.1
	12	8	3	3.7	3.6
*	13	8	-9	3.9	1.5
*	13	8	-8	3.8	1.6
	13	8	-7	5.2	5.5
	13	8	-6	5.0	4.5
	13	8	-5	6.0	5.6
	13	8	-4	6.9	6.7
*	13	8	-3	3.4	1.2
*	13	8	-2	3.4	1.8
*	13	8	-1	3.5	1.2
*	13	8	0	3.5	1.6
	13	8	1	3.6	3.5
*	13	8	2	3.7	2.9
*	13	8	3	3.9	3.5
	13	8	4	4.0	4.8
	14	8	-10	5.9	4.8
	14	8	-9	4.0	4.2
*	14	8	-8	3.9	2.2
*	14	8	-7	3.8	1.3
*	14	8	-6	3.7	2.1
	14	8	-5	6.3	5.3
	14	8	-4	9.5	9.9
	14	8	-3	10.1	10.6
	14	8	-2	3.6	2.8
	14	8	-1	5.1	6.1
	14	8	0	9.8	9.0
	14	8	1	8.5	7.7
	14	8	2	3.9	3.7
*	15	8	-12	4.5	0.7
*	15	8	-11	4.4	0.3
*	15	8	-10	4.3	0.7
*	15	8	-9	4.1	1.3
*	15	8	-8	4.0	0.9
*	15	8	-7	3.9	0.2
*	15	8	-6	3.8	2.1
*	15	8	-5	3.8	1.1
*	15	8	-4	3.7	1.3
*	15	8	-3	3.7	3.8
	15	8	-2	5.2	4.5
*	15	8	-1	3.8	2.6
*	15	8	0	3.9	2.8
*	15	8	1	4.0	4.1
*	15	8	2	4.1	3.1
*	16	8	0	4.0	2.4
	17	8	-6	4.1	3.8
*	0	9	-9	2.6	2.2
	0	9	-8	2.4	2.2
	0	9	-7	5.0	5.3
	0	9	-6	4.6	3.9
	0	9	-5	5.2	4.2
	0	9	-4	10.9	10.7
	0	9	-3	12.4	10.9
	0	9	-2	18.7	17.4
	0	9	-1	19.2	21.8
*	1	9	-9	2.6	1.2
*	1	9	-8	2.4	0.8
	1	9	-7	2.2	1.8
	1	9	-6	6.3	6.0
*	1	9	-5	1.8	1.3
**	1	9	-4	2.3	2.3
	1	9	-3	4.3	3.8
	1	9	-2	5.9	5.6
	1	9	-1	7.8	8.7
	1	9	0	3.9	4.8
	1	9	1	10.1	10.3
	1	9	2	7.2	6.3
*	1	9	3	1.5	0.3
*	1	9	4	1.7	0.9
	1	9	5	6.0	5.1
	1	9	6	8.1	7.9
*	1	9	7	2.3	2.3
*	1	9	8	2.5	1.2
*	1	9	9	2.6	0.3
*	2	9	-9	2.5	2.8
	2	9	-8	4.1	3.6
	2	9	-7	2.2	1.6
	2	9	-6	5.6	5.6
	2	9	-5	7.1	7.3
	2	9	-4	19.8	18.8
	2	9	-3	7.5	7.1
	2	9	-2	3.6	3.7
	2	9	-1	12.7	14.6
	2	9	0	27.2	31.8
	2	9	1	28.0	28.8
	2	9	2	15.6	14.5
	2	9	3	11.0	9.9
	2	9	4	8.2	7.9
	2	9	5	2.0	2.0
	2	9	6	6.4	5.8
	2	9	7	7.7	7.9
	2	9	8	7.9	8.9
	2	9	9	2.7	2.9
*	3	9	-9	2.5	1.8
	3	9	-8	4.7	4.1
*	3	9	-7	2.2	0.1
	3	9	-6	4.4	4.0
*	3	9	-5	1.8	0.7
**	3	9	-4	4.8	3.7
	3	9	-3	7.3	6.3
*	3	9	-2	1.2	1.4
*	3	9	-1	1.1	0.2
	3	9	0	3.4	3.1
	3	9	1	6.5	6.1
*	3	9	2	1.5	0.7
	3	9	3	4.9	4.8
*	3	9	4	1.8	0.9
*	3	9	5	2.0	1.5
	3	9	6	2.2	2.7
*	3	9	7	2.4	0.2
*	3	9	8	2.6	0.2
	4	9	-10	3.8	3.5
	4	9	-9	11.8	11.9
	4	9	-8	9.9	11.0
	4	9	-7	8.1	8.7
	4	9	-6	6.6	6.5
	4	9	-5	11.4	10.9
	4	9	-4	15.5	14.2
	4	9	-3	1.5	1.9
**	4	9	-2	1.3	1.6
*	4	9	-1	1.3	1.4
	4	9	0	10.7	10.6
	4	9	1	17.1	15.2

Table 4 (*cont.*)

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	4	9	2	17.0	16.0
	4	9	3	10.4	9.8
	4	9	4	7.2	7.1
	4	9	5	19.2	18.8
	4	9	6	15.8	15.9
	4	9	7	8.9	9.9
	4	9	8	5.9	6.4
•	5	9	-11	2.8	1.7
•	5	9	-10	2.7	0.9
•	5	9	-9	2.5	0.8
	5	9	-8	3.3	3.4
•	5	9	-7	2.2	1.2
	5	9	-6	3.5	3.2
•	5	9	-5	1.8	0.4
	5	9	-4	3.4	3.1
•	5	9	-3	1.6	1.0
•	5	9	-2	1.5	0.7
	5	9	-1	5.2	5.2
	5	9	0	4.9	4.9
	5	9	1	1.6	1.3
	5	9	2	3.4	3.5
	5	9	3	3.2	2.8
	5	9	4	2.9	2.6
	5	9	5	3.1	2.8
•	5	9	6	2.4	0.1
•	5	9	7	2.5	1.2
•	5	9	8	2.7	0.1
	6	9	-10	6.6	7.0
	6	9	-9	10.7	10.5
	6	9	-8	3.3	3.2
	6	9	-7	2.2	2.5
	6	9	-6	4.6	4.9
	6	9	-5	8.1	7.9
	6	9	-4	15.8	15.4
	6	9	-3	19.6	17.9
	6	9	-2	25.2	24.2
	6	9	-1	12.3	12.1
	6	9	0	4.9	5.3
	6	9	1	10.9	9.9
	6	9	2	8.0	7.6
•	6	9	3	2.0	0.1
	6	9	4	9.0	9.9
	6	9	5	9.4	10.4
	6	9	6	4.9	4.8
•	6	9	7	2.6	2.5
	6	9	8	2.8	2.6
	7	9	-9	2.5	1.8
	7	9	-8	2.4	1.8
	7	9	-7	3.2	3.4
•	7	9	-6	2.1	0.5
	7	9	-5	2.8	2.5
•	7	9	-4	1.9	0.6
	7	9	-3	4.0	4.4
	7	9	-2	3.4	3.4
	7	9	-1	3.9	3.5
	7	9	0	6.1	6.4
•	7	9	1	1.9	2.0
•	7	9	2	2.0	1.3
•	7	9	3	2.1	0.3
•	7	9	4	2.2	1.9
•	7	9	5	2.4	0.2
•	7	9	6	2.5	1.2
•	8	9	-9	2.6	0.7
	8	9	-8	5.9	4.9
	8	9	-7	3.2	2.6
	8	9	-6	2.2	1.9
	8	9	-5	13.4	13.6
	8	9	-4	15.5	16.0
	8	9	-3	12.6	12.1
	8	9	-2	7.2	7.6
	8	9	-1	3.2	3.6
	8	9	0	6.0	6.1
•	8	9	1	2.0	0.4
	8	9	2	4.7	4.2
	8	9	3	8.0	7.6
	8	9	4	4.7	4.4
•	8	9	5	2.5	0.5
	9	9	-8	3.5	3.5
	9	9	-7	4.7	4.2
•	9	9	-6	2.2	0.0
	9	9	-5	3.7	3.7
	9	9	-4	5.4	4.9
	9	9	-3	6.0	6.4
	9	9	-2	6.6	6.1
•	9	9	-1	2.0	1.5
•	9	9	0	2.0	1.0
•	9	9	1	2.1	0.5
	9	9	2	3.8	4.1
	9	9	3	4.0	3.2
•	9	9	4	2.4	0.1
•	10	9	-9	2.6	1.2
	10	9	-8	7.6	7.4
	10	9	-7	7.6	7.7
	10	9	-6	5.6	6.2
	10	9	-5	3.8	4.6
	10	9	-4	6.1	6.2
	10	9	-3	11.4	11.8
	10	9	-2	8.4	8.5
	10	9	-1	8.5	9.0
	10	9	0	6.9	6.4
	10	9	1	4.5	4.3
	10	9	2	7.0	7.9
	10	9	3	5.5	5.5
•	10	9	4	2.6	1.1
	11	9	-8	2.6	2.4
	11	9	-7	3.5	3.0
•	11	9	-6	2.4	1.2
•	11	9	-5	2.3	0.9
	11	9	-4	3.2	3.1
	11	9	-3	7.0	7.1
	11	9	-2	7.4	7.3
	11	9	-1	2.2	2.1
•	11	9	0	2.3	0.4
	11	9	1	4.1	3.2
	11	9	2	4.2	4.3
•	11	9	3	2.6	1.4
•	11	9	4	2.7	0.1
	12	9	-10	4.1	3.2
•	12	9	-9	2.8	0.1
	12	9	-8	6.5	5.8
	12	9	-7	5.1	5.0
•	12	9	-6	2.5	0.9
	12	9	-5	2.4	3.5
	12	9	-4	9.5	9.7
	12	9	-3	8.1	8.6
	12	9	-2	6.2	6.8
	12	9	-1	11.1	11.0
	12	9	0	7.2	7.3
•	12	9	1	2.5	0.1
	12	9	2	3.6	4.0
	12	9	3	6.5	6.7
	12	9	4	6.2	6.3
	12	9	5	2.9	3.0
•	13	9	-6	2.6	1.4
•	13	9	-5	2.5	0.7
•	13	9	-4	2.5	0.3
•	13	9	-3	2.5	2.8
•	13	9	-2	2.5	1.7
•	13	9	-1	2.5	0.9
•	13	9	0	2.5	1.6

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
•	13	9	1	2.6	1.7
•	13	9	2	2.7	0.8
•	13	9	3	2.8	0.2
	14	9	-6	5.3	4.9
	14	9	-5	5.2	4.5
•	14	9	-4	2.6	0.6
•	14	9	-3	2.6	2.3
	14	9	-2	3.6	3.8
	14	9	-1	3.7	4.6
•	14	9	0	2.6	1.4
	14	9	1	6.1	6.2
	14	9	2	5.6	6.0
	14	9	3	5.0	4.8
	16	9	-8	4.2	3.1
	16	9	-7	5.0	4.9
	16	9	-6	6.4	6.6
	16	9	-5	4.0	4.2
	0	10	-9	2.0	1.9
	0	10	-8	3.7	3.5
	0	10	-7	3.4	3.8
•	0	10	-6	1.6	0.5
	0	10	-5	5.1	4.5
	0	10	-4	6.5	6.7
	0	10	-3	1.5	1.3
	0	10	-2	3.8	3.8
••	0	10	-1	0.6	2.1
•	1	10	-10	2.1	2.0
•	1	10	-9	2.0	0.7
	1	10	-8	2.6	2.5
	1	10	-7	1.7	1.7
•	1	10	-6	1.5	1.1
	1	10	-5	2.4	1.6
	1	10	-4	10.4	8.9
	1	10	-3	9.8	9.2
	1	10	-2	7.8	8.0
	1	10	-1	7.6	8.6
••	1	10	0	0.5	1.8
	1	10	1	11.4	13.2
	1	10	2	17.5	18.0
	1	10	3	22.6	21.8
	1	10	4	16.8	16.0
	1	10	5	3.8	3.7
	1	10	6	2.3	1.9
	1	10	7	3.0	3.1
	1	10	8	3.8	3.6
•	1	10	9	2.0	1.2
	2	10	-10	2.9	2.5
•	2	10	-9	1.9	0.1
	2	10	-8	5.1	5.0
	2	10	-7	5.3	5.7
	2	10	-6	7.1	7.3
	2	10	-5	13.6	13.0
	2	10	-4	8.0	7.3
	2	10	-3	7.5	7.3
	2	10	-2	10.7	10.2
	2	10	-1	8.6	9.4
••	2	10	0	4.2	5.1
	2	10	1	5.6	6.4
•	2	10	2	1.0	0.8
	2	10	3	5.9	5.2
	2	10	4	3.3	3.1
	2	10	5	4.7	4.2
•	2	10	6	1.6	0.4
	2	10	7	1.8	1.3
	2	10	8	1.9	2.0
	2	10	9	3.5	3.7
•	3	10	-11	2.2	1.2
•	3	10	-10	2.0	0.3
	3	10	-9	1.9	1.6
	3	10	-8	2.5	2.7
	3	10	-7	3.7	3.7
	3	10	-6	9.5	9.0
	3	10	-5	11.0	10.2
	3	10	-4	4.9	4.7
	3	10	-3	1.9	2.0
	3	10	-2	2.5	2.1
	3	10	-1	3.6	3.4
	3	10	0	4.3	4.7
	3	10	1	9.2	8.7
	3	10	2	8.2	7.9
	3	10	3	8.5	8.0
	3	10	4	2.0	2.1
	3	10	5	4.9	4.9
	3	10	6	4.8	5.0
	3	10	7	3.6	3.7
	3	10	8	4.4	4.0
	3	10	9	2.1	1.9
•	3	10	10	2.2	0.9
	4	10	-10	2.0	3.5
•	4	10	-9	1.9	0.2
	4	10	-8	5.9	6.5
	4	10	-7	9.4	9.5
	4	10	-6	7.6	8.1
	4	10	-5	5.7	5.7
••	4	10	-4	3.8	4.0
	4	10	-3	11.0	10.2
	4	10	-2	7.9	7.4
	4	10	-1	10.3	10.6
	4	10	0	12.3	11.4
	4	10	1	1.9	1.8
	4	10	2	2.1	2.6
	4	10	3	1.3	1.7
	4	10	4	10.2	10.1
	4	10	5	4.6	4.4
	4	10	6	1.7	1.7
	4	10	7	1.9	1.7
	4	10	8	2.0	2.6
•	4	10	9	2.1	1.3
	5	10	-10	2.0	2.0
	5	10	-9	3.3	3.6
	5	10	-8	4.0	3.8
	5	10	-7	2.9	3.1
	5	10	-6	5.1	5.0
	5	10	-5	3.5	3.1
•	5	10	-4	1.3	0.5
•	5	10	-3	1.2	0.7
	5	10	-2	1.6	2.0
	5	10	-1	2.5	1.8
•	5	10	0	1.1	0.4
	5	10	1	5.1	4.7
	5	10	2	10.7	9.5
	5	10	3	7.3	7.1
	5	10	4	5.2	5.1
	5	10	5	5.8	5.1
	5	10	6	3.1	3.0
	5	10	7	2.7	3.1
	5	10	8	2.1	2.0
•	5	10	9	2.2	0.7
	6	10	-10	2.0	2.2
•	6	10	-9	1.9	1.1
	6	10	-8	4.4	4.5
	6	10	-7	2.9	3.2
•	6	10	-6	1.6	1.4
•	6	10	-5	1.5	0.4
	6	10	-4	3.0	3.1
	6	10	-3	5.4	4.7
	6	10	-2	6.5	6.7
	6	10	-1	16.1	16.0
	6	10	0	9.7	9.6
	6	10	1	6.2	5.8

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	6	10	2	8.6	7.9
	6	10	3	6.8	6.8
	6	10	4	5.7	6.1
•	6	10	5	1.7	0.6
•	6	10	6	1.9	0.7
•	6	10	7	2.0	0.7
•	6	10	8	2.1	1.4
	7	10	-12	2.3	1.7
	7	10	-11	3.1	2.3
	7	10	-10	2.9	2.9
	7	10	-9	2.7	2.6
•	7	10	-8	1.8	1.0
	7	10	-7	5.1	5.0
	7	10	-6	9.2	8.6
	7	10	-5	10.6	11.0
	7	10	-4	6.8	7.0
•	7	10	-3	1.4	1.2
•	7	10	-2	1.3	0.9
•	7	10	-1	1.3	1.0
•	7	10	0	1.3	0.2
	7	10	1	2.0	2.2
	7	10	2	2.6	2.6
	7	10	3	1.6	0.9
	7	10	4	2.4	2.4
	7	10	5	2.6	3.0
•	7	10	6	1.9	0.8
•	7	10	7	2.0	0.1
•	7	10	8	2.2	1.9
	7	10	9	3.2	2.9
••	8	10	-10	2.1	0.3
•	8	10	-9	2.0	1.3
	8	10	-8	1.9	1.6
	8	10	-7	1.7	1.2
	8	10	-6	2.9	3.4
	8	10	-5	1.6	1.1
	8	10	-4	6.0	5.9
	8	10	-3	6.9	6.8
	8	10	-2	3.5	4.0
	8	10	-1	2.8	2.6
	8	10	0	5.5	5.0
	8	10	1	9.2	9.0
	8	10	2	4.2	4.3
	8	10	3	3.8	3.5
	8	10	4	3.1	3.7
	8	10	5	1.9	1.6
•	8	10	6	2.0	0.9
•	8	10	7	2.1	1.0
	8	10	8	3.1	2.8
•	9	10	-10	2.1	2.1
•	9	10	-9	2.0	0.0
	9	10	-8	4.2	4.0
	9	10	-7	6.2	6.8
	9	10	-6	9.6	9.3
	9	10	-5	9.1	9.7
	9	10	-4	5.4	5.8
•	9	10	-3	1.5	1.1
	9	10	-2	3.0	2.6
	9	10	-1	7.6	7.6
	9	10	0	11.6	11.7
	9	10	1	9.8	9.7
	9	10	2	5.9	6.1
	9	10	3	2.5	2.0
	9	10	4	2.6	2.0
•	9	10	5	2.0	1.4
•	9	10	6	2.1	0.3
•	9	10	7	2.2	1.0
•	10	10	-10	2.1	1.1
	10	10	-9	4.0	4.1
	10	10	-8	4.7	4.5
	10	10	-7	4.1	4.1
•	10	10	-6	1.8	2.4
	10	10	-5	3.8	4.1
	10	10	-4	7.7	7.6
	10	10	-3	2.3	2.1
	10	10	-2	1.6	1.9
	10	10	-1	1.6	1.8
	10	10	0	2.3	2.4
	10	10	1	3.4	3.4
	10	10	2	3.1	3.3
	10	10	3	4.2	4.3
	10	10	4	2.0	1.7
	10	10	5	2.0	2.2
	10	10	6	3.0	2.8
	10	10	7	2.2	2.2
	11	10	-10	2.1	2.1
•	11	10	-9	2.1	1.4
•	11	10	-8	2.0	1.0
•	11	10	-7	1.9	0.9
	11	10	-6	3.2	2.1
	11	10	-5	2.5	2.9
•	11	10	-4	1.7	1.1
	11	10	-3	2.4	2.0
	11	10	-2	5.4	5.7
	11	10	-1	9.7	9.6
	11	10	0	9.4	9.7
	11	10	1	5.4	5.4
	11	10	2	1.9	1.6
•	11	10	3	2.0	1.1
•	11	10	4	2.0	2.0
	11	10	5	2.1	1.6
•	11	10	6	2.2	1.5
•	12	10	-12	2.3	0.2
•	12	10	-11	2.3	0.6
	12	10	-10	3.1	3.1
	12	10	-9	5.6	5.4
	12	10	-8	3.5	3.4
	12	10	-7	2.0	2.1
•	12	10	-6	1.9	0.7
	12	10	-5	3.2	3.3
	12	10	-4	4.4	4.8
	12	10	-3	4.0	4.2
	12	10	-2	4.0	3.8
	12	10	-1	1.8	2.5
•	12	10	0	1.8	1.5
	12	10	1	3.8	4.2
	12	10	2	4.4	3.4
•	12	10	3	2.0	1.0
•	12	10	4	2.1	1.9
	12	10	5	2.2	3.1
	13	10	-9	2.1	2.1
	13	10	-8	2.1	2.7
	13	10	-7	2.0	2.1
•	13	10	-6	2.0	0.4
•	13	10	-5	1.9	0.3
•	13	10	-4	1.9	0.7
•	13	10	-3	1.9	1.5
•	13	10	-2	1.9	0.8
•	13	10	-1	1.9	0.5
•	13	10	0	1.9	1.7
	13	10	1	2.0	1.8
•	13	10	2	2.0	1.2
	13	10	3	3.0	1.9
	13	10	4	2.2	2.5
•	14	10	-6	2.0	0.4
	14	10	-5	3.4	2.7
	14	10	-4	5.9	5.7
	14	10	-3	6.5	6.3
	14	10	-2	2.8	3.1
•	14	10	-1	2.0	0.8
	14	10	0	3.5	2.7

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	14	10	1	2.1	1.6
•	14	10	2	2.1	0.6
•	15	10	-4	2.0	0.6
•	15	10	-3	2.0	1.7
•	15	10	-2	2.0	2.5
	15	10	-1	2.9	2.7
	15	10	0	2.1	2.5
	16	10	-4	2.1	1.7
•	16	10	-3	2.1	0.7
•	16	10	-2	2.1	0.5
•	16	10	-1	2.2	1.7
•	16	10	0	2.2	1.4
•	16	10	1	2.2	1.2
	16	10	2	2.3	1.4
	19	10	-3	3.3	3.0
	0	11	-9	3.2	3.2
	0	11	-8	4.0	4.0
	0	11	-7	5.3	4.0
	0	11	-6	3.3	4.4
	0	11	-5	3.0	1.0
	0	11	-4	1.3	1.3
	0	11	-3	2.3	1.8
	0	11	-2	5.6	6.7
	0	11	-1	5.0	6.8
	1	11	-10	3.0	3.7
	1	11	-9	3.7	3.8
•	1	11	-8	1.7	0.8
	1	11	-7	4.5	4.0
	1	11	-6	6.6	6.6
	1	11	-5	11.1	11.1
	1	11	-4	7.5	7.4
	1	11	-3	3.4	3.6
	1	11	-2	3.9	4.1
	1	11	-1	1.4	2.0
	1	11	0	8.9	9.6
	1	11	1	6.8	7.5
	1	11	2	5.1	4.5
•	1	11	3	1.1	0.7
	1	11	4	8.1	7.3
	1	11	5	9.1	9.1
	1	11	6	3.7	3.4
•	1	11	7	1.6	0.5
	1	11	8	2.5	2.3
	1	11	9	4.2	4.4
	1	11	10	2.8	2.8
	2	11	-9	1.8	2.1
	2	11	-8	2.4	3.6
	2	11	-7	5.0	4.4
	2	11	-6	3.9	3.7
•	2	11	-5	1.3	1.4
	2	11	-4	7.9	7.8
	2	11	-3	11.2	10.7
	2	11	-2	11.0	11.5
	2	11	-1	8.2	9.0
	2	11	0	4.3	4.7
	2	11	1	2.0	2.1
•	2	11	2	1.0	0.5
•	2	11	3	1.1	0.6
	2	11	4	2.2	2.0
	2	11	5	1.4	1.4
•	2	11	6	1.5	1.8
	2	11	7	2.4	2.9
	2	11	8	1.8	2.2
•	2	11	9	1.9	0.0
•	3	11	-9	1.8	0.3
	3	11	-8	3.4	3.4
	3	11	-7	2.2	2.2
	3	11	-6	3.8	3.9
	3	11	-5	7.2	7.1
	3	11	-4	4.5	4.3
	3	11	-3	4.0	3.0
	3	11	-2	2.4	1.9
	3	11	-1	7.8	8.2
	3	11	0	11.5	12.7
	3	11	1	7.5	7.3
	3	11	2	3.3	3.1
•	3	11	3	1.2	0.4
	3	11	4	3.0	2.9
	3	11	5	1.5	0.7
•	3	11	6	1.6	0.5
•	3	11	7	1.7	0.5
•	3	11	8	1.8	0.6
•	4	11	-9	1.8	0.2
•	4	11	-8	1.7	0.2
•	4	11	-7	1.6	0.5
	4	11	-6	1.4	1.9
	4	11	-5	5.9	6.3
	4	11	-4	7.5	7.1
	4	11	-3	4.3	4.0
	4	11	-2	4.1	4.2
	4	11	-1	5.3	5.4
	4	11	0	3.6	3.7
	4	11	1	3.1	2.9
	4	11	2	9.2	8.5
	4	11	3	7.2	7.1
	4	11	4	3.4	3.4
	4	11	5	1.5	0.8
•	4	11	6	1.6	0.2
•	4	11	7	1.8	0.8
•	5	11	-9	1.8	1.1
	5	11	-8	2.4	2.6
•	5	11	-7	1.6	0.5
	5	11	-6	2.5	2.7
	5	11	-5	3.0	2.1
	5	11	-4	6.3	6.1
	5	11	-3	8.9	9.1
	5	11	-2	7.3	7.3
	5	11	-1	6.6	6.9
•	5	11	0	1.1	1.5
	5	11	1	2.6	2.8
•	5	11	2	1.2	0.3
•	5	11	3	1.3	0.2
	5	11	4	2.1	1.7
•	5	11	5	1.6	1.0
•	5	11	6	1.7	1.0
•	5	11	7	1.8	1.3
•	6	11	-9	1.8	0.6
	6	11	-8	3.0	2.8
	6	11	-7	3.2	2.9
•	6	11	-6	1.5	0.0
	6	11	-5	1.4	0.9
	6	11	-4	1.3	1.3
	6	11	-3	2.1	2.1
	6	11	-2	3.3	3.0
	6	11	-1	5.8	5.5
	6	11	0	7.3	7.3
	6	11	1	8.4	8.1
	6	11	2	6.0	6.1
	6	11	3	2.0	2.0
•	6	11	4	1.5	0.1
	6	11	5	1.6	1.0
•	6	11	6	1.8	0.5
•	6	11	7	1.9	0.9
	7	11	-9	1.8	2.3
	7	11	-8	4.2	4.4
	7	11	-7	2.3	2.6
	7	11	-6	1.5	1.8
	7	11	-5	3.2	3.0
	7	11	-4	10.8	10.7
	7	11	-3	8.7	9.3

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	7	11	-2	4.5	4.8
	7	11	-1	1.3	1.2
	7	11	0	4.5	4.3
	7	11	1	6.0	6.2
	7	11	2	4.5	4.5
	7	11	3	6.1	6.2
	7	11	4	5.6	5.7
	7	11	5	2.4	1.9
•	7	11	6	1.8	0.8
•	8	11	-6	1.6	1.3
•	8	11	-5	1.5	0.9
•	8	11	-4	1.4	1.0
	8	11	-3	3.3	3.5
	8	11	-2	6.9	6.6
	8	11	-1	6.7	7.0
	8	11	0	3.4	3.4
•	8	11	1	1.4	0.5
	8	11	2	1.5	1.4
•	8	11	3	1.6	1.3
	8	11	4	1.7	2.3
	8	11	5	3.6	3.0
	8	11	6	2.8	2.8
	9	11	-9	4.2	3.5
	9	11	-8	5.3	5.1
	9	11	-7	3.4	3.0
	9	11	-6	3.6	3.9
•	9	11	-5	1.5	0.4
	9	11	-4	3.0	3.8
	9	11	-3	3.8	3.6
	9	11	-2	4.3	4.3
	9	11	-1	3.2	3.7
	9	11	0	3.6	2.0
	9	11	1	7.5	6.0
	9	11	2	7.5	7.5
	9	11	3	6.3	6.3
	9	11	4	2.5	2.2
	9	11	5	1.0	2.0
	9	11	6	1.9	2.5
	10	11	-11	2.0	2.2
	10	11	-10	2.8	2.4
•	10	11	-9	1.9	1.0
•	10	11	-8	1.8	0.4
	10	11	-7	3.0	2.9
	10	11	-6	4.1	3.5
	10	11	-5	3.6	1.3
	10	11	-4	1.5	1.8
•	10	11	-3	1.5	0.1
•	10	11	-2	1.5	0.3
•	10	11	-1	1.5	0.9
	10	11	0	1.6	1.2
•	10	11	1	1.6	1.1
•	10	11	2	1.7	0.8
	10	11	3	1.8	1.8
	10	11	4	3.2	3.2
	10	11	5	2.7	3.0
	10	11	6	2.0	1.5
•	11	11	-10	2.0	0.4
	11	11	-9	2.7	2.9
	11	11	-8	3.7	3.6
	11	11	-7	3.6	4.0
	11	11	-6	5.7	5.5
	11	11	-5	2.9	2.4
	11	11	-4	2.8	2.2
	11	11	-3	4.9	4.2
	11	11	-2	5.6	5.6
	11	11	-1	2.8	2.9
	11	11	0	2.9	2.3
	11	11	1	2.9	3.0
	11	11	2	2.5	1.5
•	11	11	3	1.8	0.7
	12	11	-8	2.7	2.6
	12	11	-7	4.1	4.3
	12	11	-6	3.6	3.6
	12	11	-5	3.0	3.4
	12	11	-4	3.0	3.4
	12	11	-3	2.4	3.1
•	12	11	-2	1.7	1.5
	12	11	-1	1.7	1.7
	12	11	0	3.0	2.6
•	12	11	1	1.8	1.1
•	12	11	2	1.8	0.0
	13	11	-8	1.9	1.5
•	13	11	-7	1.9	1.0
•	13	11	-6	1.8	0.4
	13	11	-5	2.5	2.1
	13	11	-4	3.6	3.1
	13	11	-3	1.8	2.1
	13	11	-2	2.5	2.4
•	13	11	-1	1.8	1.3
•	13	11	0	1.8	0.0
•	13	11	1	1.9	0.5
	14	11	-2	2.6	2.4
	14	11	-1	3.2	3.0
	16	11	-5	2.8	2.2
	16	11	-4	2.8	3.3
	17	11	0	3.0	2.7
•	0	12	-9	1.9	1.0
•	0	12	-8	1.7	1.2
	0	12	-7	2.3	2.1
	0	12	-6	3.0	2.4
•	0	12	-5	1.3	0.5
•	0	12	-4	1.2	0.1
•	0	12	-3	1.0	0.4
	0	12	-2	5.1	5.3
	0	12	-1	6.9	7.4
•	1	12	-10	2.0	0.7
	1	12	-9	3.7	3.1
	1	12	-8	4.9	5.1
	1	12	-7	4.2	4.6
	1	12	-6	3.3	3.5
•	1	12	-5	1.3	0.6
	1	12	-4	4.1	4.1
	1	12	-3	5.0	5.1
	1	12	-2	4.6	5.2
	1	12	-1	6.4	7.3
	1	12	0	3.7	4.1
••	1	12	1	0.7	1.1
	1	12	2	3.7	3.7
	1	12	3	6.1	6.0
	1	12	4	2.5	2.5
	1	12	5	4.6	4.4
	1	12	6	5.9	6.1
	1	12	7	4.4	4.2
	1	12	8	3.1	3.2
•	2	12	-9	1.8	0.2
•	2	12	-8	1.7	1.4
	2	12	-7	1.6	1.4
•	2	12	-6	1.5	1.0
•	2	12	-5	1.3	1.3
	2	12	-4	1.2	1.0
•	2	12	-3	1.0	0.3
	2	12	-2	3.4	3.8
	2	12	-1	2.0	2.3
•	2	12	0	.7	0.1
	2	12	1	2.5	2.4
	2	12	2	2.8	2.6
•	2	12	3	1.1	0.4
	2	12	4	1.3	1.6
	2	12	5	3.5	3.8
	2	12	6	4.7	4.6

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
	2	12	7	2.4	2.3
	2	12	8	1.8	1.3
	3	12	-9	2.6	2.5
•	3	12	-8	1.7	1.4
•	3	12	-7	1.6	0.6
•	3	12	-6	1.4	1.0
	3	12	-5	1.9	2.0
	3	12	-4	6.1	6.1
	3	12	-3	8.7	8.2
	3	12	-2	8.5	9.2
	3	12	-1	6.4	7.3
••	3	12	0	0.8	0.9
	3	12	1	6.1	6.0
	3	12	2	5.3	5.2
	3	12	3	4.4	4.4
•	3	12	4	1.3	1.2
	3	12	5	2.1	2.3
	3	12	6	1.6	1.6
•	3	12	7	1.7	1.2
•	4	12	-9	1.8	0.8
•	4	12	-8	1.7	1.1
•	4	12	-7	1.6	0.1
•	4	12	-6	1.5	0.7
	4	12	-5	1.9	2.2
	4	12	-4	1.7	1.6
	4	12	-3	3.8	3.5
	4	12	-2	2.4	3.6
	4	12	-1	4.8	5.6
	4	12	0	4.8	4.8
	4	12	1	1.5	1.7
	4	12	2	1.2	1.1
•	4	12	3	1.3	0.9
•	4	12	4	1.4	0.5
	4	12	5	1.5	0.8
•	4	12	6	1.7	0.8
•	4	12	7	1.8	0.4
•	5	12	-10	1.9	1.0
•	5	12	-9	1.8	1.3
•	5	12	-8	1.7	0.2
	5	12	-7	1.6	1.7
	5	12	-6	3.6	2.9
	5	12	-5	4.7	4.2
	5	12	-4	7.3	7.1
	5	12	-3	4.2	4.3
•	5	12	-2	1.1	0.2
	5	12	-1	4.3	4.7
	5	12	0	9.1	9.0
	5	12	1	7.1	7.1
	5	12	2	3.3	3.6
	5	12	3	4.1	3.9
	5	12	4	2.6	2.4
•	5	12	5	1.6	0.2
•	5	12	6	1.7	1.3
•	6	12	-9	1.8	1.5
	6	12	-8	1.7	1.7
	6	12	-7	3.2	2.7
•	6	12	-6	1.5	0.1
	6	12	-5	1.4	1.9
•	6	12	-4	1.3	1.0
	6	12	-3	2.1	2.0
	6	12	-2	1.2	1.7
	6	12	-1	2.6	2.9
	6	12	0	3.2	2.9
	6	12	1	3.1	3.0
	6	12	2	2.3	2.0
	6	12	3	1.5	1.5
	6	12	4	4.4	3.9
	6	12	5	1.7	2.2
•	6	12	6	1.8	1.0
	7	12	-10	1.9	2.3
	7	12	-9	2.6	3.1
	7	12	-8	2.5	1.9
•	7	12	-7	1.6	1.0
	7	12	-6	3.4	3.4
	7	12	-5	4.1	4.6
	7	12	-4	2.7	2.1
	7	12	-3	2.9	2.9
	7	12	-2	4.6	4.6
	7	12	-1	4.6	5.1
	7	12	0	6.8	6.5
	7	12	1	5.1	5.3
	7	12	2	3.8	3.4
•	7	12	3	1.5	1.7
	7	12	4	2.3	2.3
	7	12	5	4.6	4.3
	7	12	6	4.1	3.5
	7	12	7	1.9	2.2
	8	12	-10	2.8	2.1
	8	12	-9	2.6	2.0
	8	12	-8	1.8	2.2
	8	12	-7	2.4	2.9
•	8	12	-6	1.6	0.4
	8	12	-5	2.1	2.3
	8	12	-4	4.0	3.7
	8	12	-3	5.2	5.3
	8	12	-2	3.9	3.9
•	8	12	-1	1.4	0.9
•	8	12	0	1.4	0.3
•	8	12	1	1.5	0.0
•	8	12	2	1.5	0.1
•	8	12	3	1.6	1.2
	8	12	4	1.7	1.3
•	8	12	5	1.8	0.3
	9	12	-10	2.8	2.2
	9	12	-9	3.3	3.0
•	9	12	-8	1.8	1.2
•	9	12	-7	1.7	0.4
	9	12	-6	1.6	1.7
	9	12	-5	3.1	2.7
	9	12	-4	2.1	2.3
	9	12	-3	1.5	1.3
•	9	12	-2	1.4	0.7
	9	12	-1	1.5	1.8
	9	12	0	4.5	4.3
	9	12	1	3.1	2.8
•	9	12	2	1.6	0.5
	9	12	3	3.4	3.3
	9	12	4	4.3	4.7
	9	12	5	3.2	3.6
•	10	12	-7	1.7	1.5
•	10	12	-6	1.7	0.5
	10	12	-5	2.8	2.8
	10	12	-4	3.9	4.1
	10	12	-3	4.9	4.9
	10	12	-2	3.1	3.5
	10	12	-1	2.7	2.4
	10	12	0	2.2	1.9
•	10	12	1	1.6	0.6
	10	12	2	2.9	2.8
	10	12	3	1.8	2.3
•	10	12	4	1.8	1.3
•	11	12	-8	1.9	0.5
	11	12	-7	1.8	1.2
	11	12	-6	3.0	2.8
	11	12	-5	4.1	4.3
	11	12	-4	3.7	4.0
	11	12	-3	2.3	2.1
•	11	12	-2	1.6	0.0
	13	12	-6	2.6	2.9
	15	12	-4	2.7	2.5
	15	12	-3	2.7	2.8

Table 5. *Bond distances and bond angles with their standard deviations in* $(TiCl_4 . CH_3COOC_2H_5)_2$ *and* $(TiCl_4 . POCl_3)_2$

	$(TiCl_4 . CH_3COOC_2H_5)_2$		$(TiCl_4 . POCl_3)_2$	
	Distance	σ	Distance	σ
Ti(1) –Cl(2)	2·500 Å	0·002 Å	2·44 Å	0·01 Å
Ti(1) –Cl(2′)	2·497	0·002	2·54	0·01
Ti(1) –Cl(3)	2·224	0·002	2·24	0·01
Ti(1) –Cl(4)	2·220	0·002	2·23	0·01
Ti(1) –Cl(5)	2·232	0·002	2·20	0·01
Ti(1) –O(6)	2·029	0·003	2·10	0·02
C(9)—O(6)	1·234	0·005		
C(9)—O(7)	1·295	0·005		
C(9)—C(8)	1·484	0·006		
C(10)–O(7)	1·495	0·006		
C(10)–C(11)	1·481	0·009		
	Angle	σ	Angle	σ
Cl(2) –Ti(1) –Cl(2′)	79·08°	0·05°	78·5°	0·3°
Cl(2) –Ti(1) –Cl(3)	166·28	0·05	165·0	0·4
Cl(2) –Ti(1) –Cl(4)	89·85	0·06	92·8	0·4
Cl(2) –Ti(1) –Cl(5)	90·99	0·06	92·2	0·4
Cl(2) –Ti(1) –O(6)	80·42	0·10	83·0	0·6
Cl(2′)–Ti(1) –Cl(3)	89·85	0·06	89·1	0·4
Cl(2′)–Ti(1) –Cl(4)	167·55	0·05	167·5	0·4
Cl(2′)–Ti(1) –Cl(5)	89·34	0·06	91·7	0·4
Cl(2′)–Ti(1) –O(6)	83·60	0·09	82·2	0·6
Cl(3) –Ti(1) –Cl(4)	100·23	0·07	98·2	0·4
Cl(3) –Ti(1) –Cl(5)	97·01	0·07	96·2	0·4
Cl(3) –Ti(1) –O(6)	90·40	0·10	87·4	0·6
Cl(4) –Ti(1) –Cl(5)	96·57	0·06	97·4	0·4
Cl(4) –Ti(1) –O(6)	89·02	0·09	88·1	0·6
Cl(5) –Ti(1) –O(6)	169·77	0·10	173·0	0·6
Ti(1) –O(6)—C(9)	152·11	0·31		
O(6)—C(9)—C(8)	123·94	0·42		
O(6)—C(9)—O(7)	120·12	0·40		
C(8)—C(9)—O(7)	115·94	0·38		
C(9)—O(7) –C(10)	118·08	0·37		
O(7)—C(10)–C(11)	107·80	0·49		

Table 6. *Intramolecular non-covalent distances less than* 4·0 Å *in the* $(TiCl_4 . CH_3COOC_2H_5)_2$ *molecule*

	Distance		Distance
Ti(1)–Ti(1′)	3·85 Å	Cl(3)–C(8)	3·68 Å
Ti(1)–C(8)	3·87	Cl(3)–C(9)	3·64
Ti(1)–C(9)	3·17	Cl(4)–Cl(5)	3·32
Cl(2)–Cl(2′)	3·18	Cl(4)–O(6)	2·98
Cl(2)–Cl(3′)	3·34	Cl(5)–O(6′)	3·51
Cl(2)–Cl(4)	3·34	Cl(5)–O(7′)	3·71
Cl(2)–Cl(5)	3·38	Cl(5)–C(8′)	3·79
Cl(2)–Cl(5′)	3·33	Cl(5)–C(9′)	3·41
Cl(2)–O(6)	2·95	O(6) –O(7)	2·19
Cl(2)–O(6′)	3·04	O(6) –C(8)	2·40
Cl(2)–C(8′)	3·48	O(6) –C(10)	2·63
Cl(2)–C(9)	3·92	O(7) –C(8)	2·36
Cl(2)–C(9′)	3·55	O(7) –C(11)	2·40
Cl(3)–Cl(4)	3·41	C(8) –C(10)	3·75
Cl(3)–Cl(5)	3·34	C(9) –C(10)	2·40
Cl(3)–O(6)	3·02	C(9) –C(11)	3·58

Table 7. *Intermolecular distances less than* 4·0 Å *in* $(TiCl_4 . CH_3COOC_2H_5)_2$

	Distance		Distance
Cl(2)*A*–C(8)*G*	3·73 Å	Cl(4)*A*–O(7′)*B*	3·76 Å
Cl(3)*A*–Cl(4′)*B*	3·84	Cl(4)*A*–C(8)*G*	3·93
Cl(3)*A*–Cl(4)*E*	3·93	Cl(4)*A*–C(9′)*B*	3·61
Cl(3)*A*–C(10′)*B*	3·94	Cl(5)*A*–Cl(5′)*C*	3·99
Cl(3)*A*–C(11′)*B*	3·83	Cl(5)*A*–O(7)*C*	3·61
Cl(3)*A*–C(11)*F*	3·82	O(7)*A* –C(11′)*D*	3·51
Cl(4)*A*–Cl(4′)*B*	3·98	C(8)*A* –C(10)*E*	3·80
Cl(4)*A*–O(6′)*B*	3·63	C(8)*A* –C(11′)*D*	3·83

Table 7 (*cont.*)

The coordinates of the atoms of molecules *B*–*G* are related to those of molecule *A* by the following symmetry relations:

Molecule	Coordinates		
A	x	y	z
B	x	$1+y$	z
C	x	y	$1+z$
D	x	$1+y$	$-1+z$
E	$\frac{1}{2}+x$	$\frac{1}{2}-y$	z
F	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$1+z$
G	$-\frac{1}{2}+x$	$\frac{1}{2}-y$	z

ducts the acceptor molecule has changed its coordination from tetrahedral to octahedral. The frameworks formed by titanium, chlorine and donor oxygen atoms are very similar. The Ti–Cl and Ti–O bond lengths and the Cl–Ti–Cl and Cl–Ti–O bond angles of the two adducts are compared in Table 5.

The Ti–O distances in $(TiCl_4 . CH_3COOC_2H_5)_2$ and $(TiCl_4 . POCl_3)_2$, 2·03 Å and 2·10 Å respectively, are consistent with the relative orders of donor strength of $CH_3COOC_2H_5$ and $POCl_3$ with $SnCl_4$, $SbCl_5$ or $SbCl_3$ as acceptor molecules (Lindqvist & Zackrisson, 1960; Lindqvist, 1963). For both adducts the lengths of the octahedral non-bridging Ti–Cl bonds appear to be slightly longer than the tetrahedral Ti–Cl bond lengths of $2·18 \pm 0·04$ Å found in free $TiCl_4$ (Lister & Sutton,

1941). The differences in length between non-bridging and bridging Ti–Cl bonds are about the same in the two adducts. In $(TiCl_4 . CH_3COOC_2H_5)_2$ these latter bonds are both equal to 2·50 Å. In $(TiCl_4 . POCl_3)_2$ these bridging bonds are not quite symmetrical but exhibit an average length of 2·49 Å.

The bond angle subtended at a bridging oxygen atom often decreases with increasing electronegativity of the atoms bonded to the oxygen atom (Gillespie & Nyholm, 1957; Lindqvist, 1963). The difference in electronegativity between the phosphorus and the carbonyl carbon atoms in $(TiCl_4 . POCl_3)_2$ and $(TiCl_4 . CH_3COOC_2H_5)_2$ does not seem to cause any appreciable difference in the bond angle.

Discussion of the effect of adduct formation on the donor molecule would be assisted by information as to the dimensions and configuration of ethyl acetate. Although no direct experimental data appear to be available, there is good reason for believing that the molecule is nearly planar, in spite of some contradictory suggestions. The carbonyl C=O bond length is probably very near to 1·20 Å (Curl, 1959). The acetyl–oxygen and the ethyl–oxygen bond lengths can be assumed to be $1·34 \pm 0·02$ Å and $1·43 \pm 0·02$ Å, respectively (Curl, 1959; Kwei & Curl, 1960; Lide, 1962). Lide has also discussed carbon–carbon bond lengths and covalent radii for carbon atoms. He finds that one of the best measurements of the distance between two carbon atoms, both exhibiting sp^3 hybridization, is the value $1·526 \pm 0·002$ Å (r_s) found in propane (Lide, 1960). Accurate messurements of the distance between two carbon atoms with sp^3 and sp^2 hydribization are $1·501 \pm$

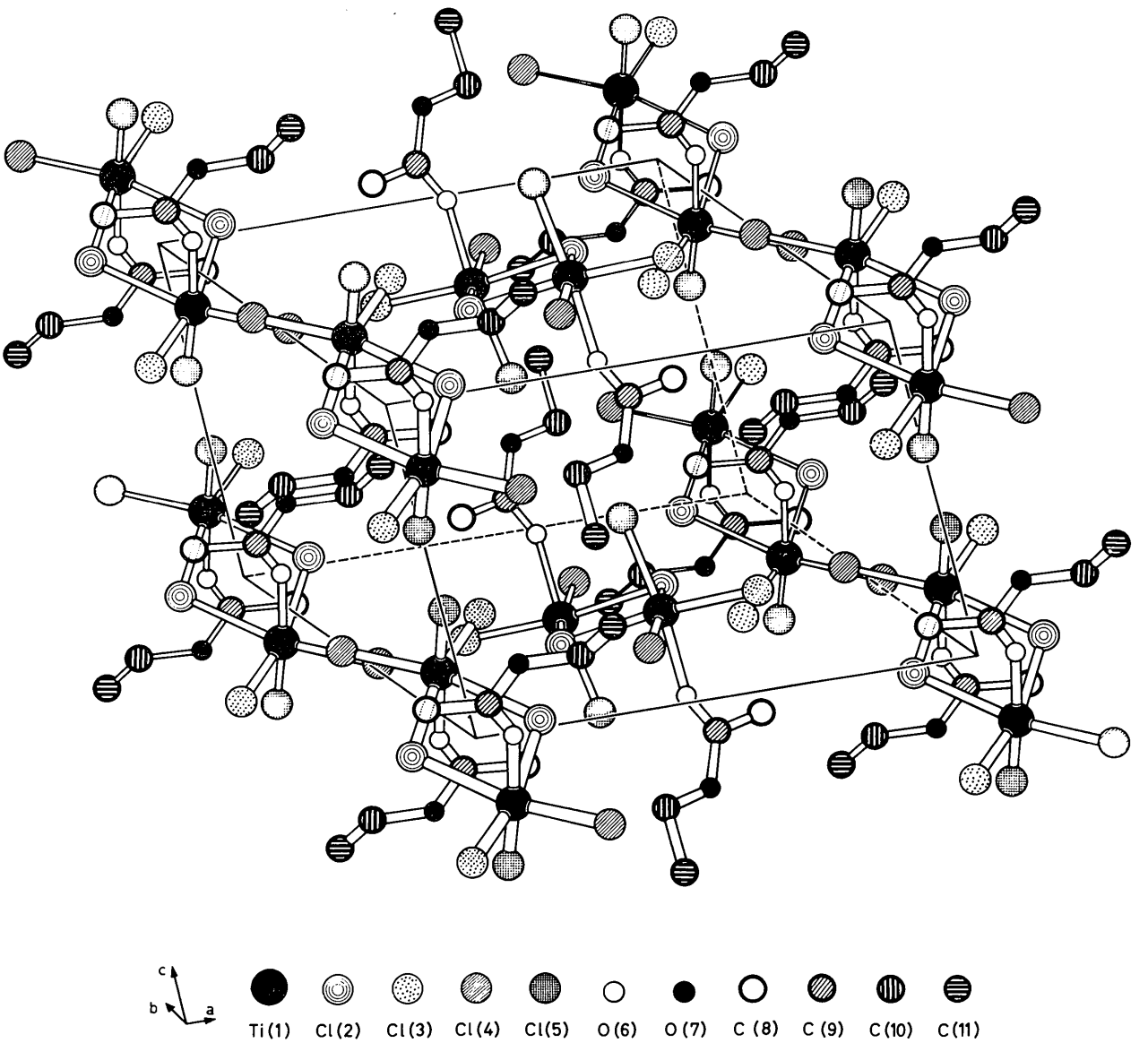


Fig. 2. The crystal structure of $(TiCl_4 . CH_3COOC_2H_5)_2$.

0·004 Å (r_s) found in propylene (Lide, 1962) and 1·500 ±0·005 Å (r_o) observed in acetaldehyde (Kilb, Lin & Wilson, 1957). The CH_2–CH_3 bond length in free ethyl acetate should deviate little from the value quoted for propane. The difference between the carbon–carbon distances in the acetyl groups of ethyl acetate and acetaldehyde is probably slight.

The coordination of carbonyl carbon in the present adduct is planar, according to a least-squares fit of the atoms O(6), O(7), C(8) and C(9) to a plane using a method devised by Blow (1960). A dihedral angle of 2°31′ has been found between this plane and that defined by the atoms O(7), C(9) and C(10). Vertical deviation of atoms from the coplanar positions are listed in Table 8. The ethyl–oxygen bond and the carbonyl bond are in cis position to the acetyl–oxygen bond.

Table 8. *Deviations from the plane* $0·2120x+0·9278y+0·3071z-1·8412=0$ *found by a least-squares fit of the atoms* O(6), O(7), C(8) *and* C(9)

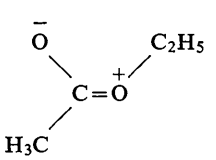
Atom	Distance
O(6)	0·000 Å
O(7)	0·000
C(8)	0·000
C(9)	0·000
C(10)	−0·056
C(11)	+0·517
Ti(1)	+0·050

Deviations from the plane $0·1715x+0·9305y+0·3237z-1·7575=0$ defined by the atoms O(7), C(9) and C(10).

Atom	Distance
O(6)	+0·048 Å
C(8)	−0·056
C(11)	+0·564
Ti(1)	+0·147

The changes attending adduct formation are an increase of the carbonyl C=O bond length to 1·23 Å, a shortening of the acetyl–oxygen bond to 1·30 Å and a lengthening of the ethyl–oxygen bond to 1·50 Å. The two carbon–carbon bonds have almost the same length, 1·48 Å.

The mathematical significance of the first change is not clearly established but the change is, nevertheless, supported by spectroscopic evidence. (Bystrov & Filimonov, 1960). All the first three changes can easily be explained as a result of the electron-density withdrawal from the donor molecule to the acceptor atom. Changes in heteropolarity as well as in delocalization take the same direction. The carbonyl C=O bond will thus be more heteropolar and the adjacent acetyl–oxygen bond less heteropolar owing to the electron density drift. At the same time delocalization according to the formula



will be favoured. The ethyl–oxygen bond will become more heteropolar, and thus weaker. The increase of the latter bond length is, however, surprisingly large, considering the fact that no delocalization effect is involved.

The shortness of the ethyl C–C bond is unexpected. It should theoretically be possible to suggest a hyperconjugation effect which would also account for the considerable lengthening of the adjacent ethyl–oxygen bond. It is, however, possible that the result is an artefact caused by an error in the parameter of the carbon atom bonded to the oxygen atom, although this is not indicated by the standard mathematical treatment of the experimental data.

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The Crystal Structure of $SbCl_5 . HCON(CH_3)_2$

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The crystal structure of $SbCl_5 . HCON(CH_3)_2$ has been determined from three-dimensional X-ray data. Crystals of this compound are monoclinic, space group $P2_1/n$, with 4 formula units in the unit cell. Cell dimensions are,

$$a=9{\cdot}706,\ b=13{\cdot}520,\ c=8{\cdot}760\ \text{Å};\ \beta=91°51'.$$

The atomic parameters were refined by the method of least squares. The structure is built up from discrete $SbCl_5 . HCON(CH_3)_2$ molecules. The antimony atom is octahedrally coordinated by five chlorine atoms and the carbonyl oxygen atom of *N,N*-dimethylformamide. Changes in the configurations and dimensions from that of the free acceptor and donor molecules are briefly discussed.

Introduction

It is well known that many amides are capable of forming addition compounds with metal halides and in this connection an adduct of acetamide with antimony(V) chloride was prepared as early as the turn of the century (Rosenheim & Stellmann, 1901).

The present structure determination of the adduct $SbCl_5 . HCON(CH_3)_2$ was undertaken as a part of an extensive investigation of adduct molecules of oxo-compounds undertaken at this Institute (Lindqvist, 1963). A thermochemical study of the reaction between antimony(V) chloride and various amides has been reported by Zackrisson (1961).

Experimental

The crystals were grown from a solution prepared by mixing equal volumes of 0·2*M* solutions of antimony(V) chloride and *N,N*-dimethylformamide in 1,2-dichlorethane. These solutions were kindly provided by Zackrisson, who has already described the preparation (Lindqvist & Zackrisson, 1960; Zackrisson, 1961). When heated the crystals decompose rapidly at 163 °C.

The unit-cell dimensions of the colourless monoclinic crystals were determined from powder photographs recorded in a camera of the Guinier type with Cr $K\alpha_1$ radiation (2·28962 Å) with silicon ($a=5{\cdot}4306$ Å) as an internal standard. The following values of the cell dimensions and angle and their standard deviations were calculated by the least-squares method from fourteen recorded powder reflexions:

$a=$ 9·706 Å	$\sigma(a)=0{\cdot}005$ Å
$b=13{\cdot}520$	$\sigma(b)=0{\cdot}005$
$c=$ 8·760	$\sigma(c)=0{\cdot}005$
$\beta=91°51'$	$\sigma(\beta)=4'$

The adduct is slowly decomposed on irradiation by X-rays. Five rod-shaped single crystals with the *c* axis parallel to the rod axis were used to provide intensity