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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,

$$a=9\cdot706,\ b=13\cdot520,\ c=8\cdot760\ \text{Å};\ \beta=91^\circ 51'.$$

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 ($a=5\cdot4306$ 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:

$$a=\ 9\cdot706\ \text{Å} \qquad \sigma(a)=0\cdot005\ \text{Å}$$
$$b=13\cdot520 \qquad \sigma(b)=0\cdot005$$
$$c=\ 8\cdot760 \qquad \sigma(c)=0\cdot005$$
$$\beta=91^\circ 51' \qquad \sigma(\beta)=4'$$

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 data for the nine layers $0 \leq l \leq 8$. These crystals can be described as exhibiting a roughly quadrilateral prismatic habit, the length of the prism varying from 0·16 to 0·30 mm, while in cross section the edges varied from 0·05 to 0·08 mm. Equi-inclination Weissenberg photographs were taken with the crystals rotating around the *c* axis. The layers 0–3 were recorded with the first crystal, layer 4 with the second, and layers 5 and 6 with the third, while for each of the layers 7 and 8 a new crystal (nos. 4 and 5) was used. Immediately the crystals 2, 3, 4 and 5 had been adjusted a part ($w=90°$) of layer one ($l=1$) was recorded. For the recording of subsequent layers each crystal was then rotated through the same angle relative to the reciprocal lattice as crystal 1. Inspection showed that in the repeated photographs of the layer $l=1$ the intensities of the diffraction spots altered very little and such variations as occurred were uniform for each film. This provided the sole purpose of this repeated recording of the first layer. An intensity scale was prepared for each crystal. The films 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.

The intensities of each layer were estimated visually, using the scale prepared from the corresponding crystal. The intensities of reflexions of the first layer for crystals 2 to 5 were estimated with the corresponding scale and also with the scale from crystal 1. These values were used for correlating the different intensity scales and also for scaling the intensities from different crystals.

The scaled intensities, $I(h, k, l)$ obtained from crystals 2–5 were then compared with those obtained from crystal 1 by a Wilson plot. It was found that there were no appreciable differences between the temperature factors of the different crystals.

1962 independent intensities were estimated*. The data were corrected for the Lorentz and polarization effects.

Observed extinctions were $h+l$ odd for $h0l$ and k odd for $0k0$ reflexions, from which it was assumed that the structure belongs to the space group $P2_1/n$.

On the basis of a unit cell containing four formula units $SbCl_5 . HCON(CH_3)_2$ the calculated density is 2·15 $g.cm^{-3}$. A density determination by the flotation method using an aqueous solution of thallium(I) formate gave a value of approximately 2·16 $g.cm^{-3}$.

Determination of the atomic positions

All atoms in the formula unit $SbCl_5 . HCON(CH_3)_2$ were assumed to occupy general positions, 4(*e*), in the space group $P2_1/n$. Approximate parameters for the antimony and five chlorine atomic positions were derived from a three-dimensional Patterson function by locating the corresponding vectors. 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, pp. 202, 211). Programs devised by Liminga & Olovsson (1964) for the Swedish electronic computer FACIT EDB were employed for the calculation of structure factors and Fourier functions. Approximate parameters for the oxygen, nitrogen and carbon atoms were derived from an F_o synthesis. The atomic positions of the antimony and chlorine atoms were then used to calculate a Fourier synthesis in which values of $F_o - F_h$ were used as Fourier coefficients. F_o refers to observed structure factors, for which signs were determined from the positions of all the atoms in the structure, and F_h refers to structure factors calculated for the antimony and chlorine atoms. From this 'difference' synthesis it was possible to derive more accurate parameters for the oxygen, nitrogen and carbon atoms.

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 nine 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 $a=20·0$ and $c=0·01$. 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 $\sin\theta$. The values of a and c

Table 1. *Final weight analysis*

$\sin\theta$ interval	$\overline{\omega\Delta^2}$	Number of reflexions
0·00–0·25	0·96	361
0·25–0·32	1·05	344
0·32–0·36	0·99	308
0·36–0·40	0·97	243
0·40–0·43	1·03	179
0·43–0·46	0·97	121
0·46–0·48	0·91	85
0·48–0·50	1·20	37
0·50–0·52	1·34	9
0·52–0·54	1·73	5

$\lvert F_o\rvert$ interval	$\overline{\omega\Delta^2}$	Number of reflexions
0–10	0·78	22
10–20	1·03	424
20–30	1·11	469
30–40	1·04	280
40–50	0·91	148
50–60	0·87	99
60–70	1·03	84
70–80	0·76	51
80–90	0·74	39
90–225	0·71	76

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

were adjusted between the refinement cycles so that this mean value was as constant as possible in all the 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 0·084 at this point and the shifts for all the parameters were less than one-tenth of their estimated standard deviations.

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 previous block-diagonal matrix approximation with those derivied from a full-matrix calculation. No significant deviations were found. During the subsequent 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 one-tenth of 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 0·050 and 0·067 respectively.

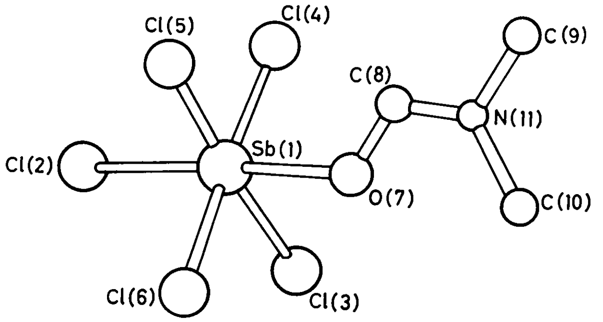

Fig. 1. The molecular structure of $SbCl_5\,.\,HCON(CH_3)_2$.

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.

The carbonyl oxygen of the *N*,*N*-dimethylformamide acts as the donor atom. Evidence from spectroscopic studies of several amide adducts (Gompper & Altreuther, 1959; Cook, 1960; Gerrard, Lappert, Pyszora & Wallis, 1960; Archambault & Rivest, 1960; Bystrov,

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	$\sigma(z)$
Sb(1)	0·3462	0·0005	0·1764	0·0006	0·1471	0·0006
Cl(2)	0·1448	0·0028	0·2494	0·0037	0·0486	0·0036
Cl(3)	0·2476	0·0028	0·0191	0·0029	0·1584	0·0033
Cl(4)	0·4290	0·0033	0·1440	0·0033	−0·0961	0·0032
Cl(5)	0·4684	0·0026	0·3267	0·0027	0·1497	0·0030
Cl(6)	0·2852	0·0030	0·2050	0·0031	0·3986	0·0031
O(7)	0·5175	0·0057	0·1093	0·0066	0·2423	0·0070
C(8)	0·6417	0·0086	0·1201	0·0092	0·1938	0·0100
C(9)	0·8877	0·0102	0·0904	0·0139	0·2086	0·0146
C(10)	0·7234	0·0116	0·0053	0·0108	0·3924	0·0118
N(11)	0·7435	0·0074	0·0759	0·0082	0·2621	0·0083

Table 3. *Final iansotropic 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}	$\sigma(\beta_{23})$
Sb(1)	7·14	0·05	4·87	0·03	9·95	0·10	−0·18	0·04	0·57	0·04	0·27	0·04
Cl(2)	8·78	0·27	9·84	0·23	22·00	0·56	0·00	0·21	−1·81	0·28	5·60	0·30
Cl(3)	11·98	0·32	6·14	0·17	19·57	0·52	−2·04	0·19	1·52	0·30	−0·22	0·23
Cl(4)	15·36	0·39	8·58	0·21	13·39	0·46	−1·40	0·23	2·24	0·31	−1·51	0·24
Cl(5)	10·80	0·27	5·35	0·14	16·52	0·46	−0·73	0·17	0·30	0·25	0·55	0·20
Cl(6)	13·64	0·35	7·50	0·19	14·66	0·48	1·01	0·20	3·84	0·31	−0·42	0·21
O(7)	6·94	0·62	5·43	0·40	15·09	1·10	0·49	0·41	0·64	0·61	1·52	0·52
C(8)	8·18	0·93	4·26	0·52	13·98	1·59	−0·18	0·53	1·51	0·88	−0·15	0·64
C(9)	6·97	0·99	9·20	0·94	26·55	2·62	0·36	0·81	4·13	1·28	−0·28	1·27
C(10)	13·07	1·35	5·88	0·67	14·39	1·80	0·66	0·73	−1·40	1·13	0·45	0·79
N(11)	8·02	0·77	5·08	0·45	13·14	1·29	0·32	0·47	−0·11	0·72	−0·32	0·58

Table 4. *Observed and calculated structure factors*

$|F_o|$ for reflexions marked with an asterisk are threshold values

h	k	l	$\|F_o\|$	$\|F_c\|$
-12	0	0	19.5	17.9
-10	0	0	72.1	72.8
-8	0	0	38.3	38.1
-6	0	0	72.9	73.3
-4	0	0	46.9	42.4
-2	0	0	123.6	115.5
-13	1	0	16.9	17.6
-12	1	0	15.9	16.2
•-11	1	0	15.0	7.4
•-10	1	0	14.0	9.7
-9	1	0	20.7	19.6
-8	1	0	47.0	44.7
-7	1	0	26.3	24.4
-6	1	0	16.2	17.2
-5	1	0	18.5	17.7
-4	1	0	36.9	39.0
-3	1	0	85.0	82.9
-2	1	0	173.9	165.0
•-13	2	0	17.0	5.6
•-12	2	0	16.0	2.0
-11	2	0	38.3	41.7
-10	2	0	29.9	30.4
• -9	2	0	13.2	6.4
• -8	2	0	12.2	10.1
-7	2	0	16.0	17.3
-6	2	0	103.0	100.2
-5	2	0	92.1	89.2
-4	2	0	115.1	115.4
-3	2	0	7.4	11.3
-2	2	0	24.6	20.4
-1	2	0	132.0	131.3
-13	3	0	26.9	30.5
•-12	3	0	16.1	0.2
•-11	3	0	15.2	11.9
•-10	3	0	14.2	5.7
-9	3	0	41.0	40.7
• -8	3	0	12.4	0.8
-7	3	0	58.5	55.4
-6	3	0	35.1	33.3
• -5	3	0	9.7	2.0
-4	3	0	34.4	32.9
-3	3	0	181.0	180.2
• -2	3	0	15.5	12.4
-1	3	0	111.4	111.2
•-12	4	0	16.2	2.4
-11	4	0	34.2	35.1
•-10	4	0	14.4	1.9
-9	4	0	21.3	21.5
-8	4	0	15.4	14.9
-7	4	0	18.5	18.9
-6	4	0	26.5	25.4
-5	4	0	114.9	111.6
-4	4	0	40.9	35.6
-3	4	0	15.6	13.8
-2	4	0	121.0	112.9
-1	4	0	172.2	177.9
0	4	0	34.0	32.2
-12	5	0	23.2	23.7
•-11	5	0	15.5	8.8
•-10	5	0	14.6	2.7
-9	5	0	16.8	18.6
-8	5	0	55.2	55.8
-7	5	0	28.1	25.7
-6	5	0	15.8	18.0
-5	5	0	10.4	10.0
-4	5	0	26.3	25.7
-3	5	0	149.1	147.9
-2	5	0	145.4	149.5
-1	5	0	18.4	18.9
•-12	6	0	16.6	14.0
•-11	6	0	15.7	8.6
-10	6	0	37.8	38.5
-9	6	0	17.1	19.7
• -8	6	0	13.1	3.2
• -7	6	0	12.3	3.4
-6	6	0	39.1	40.9
-5	6	0	33.2	32.0
-4	6	0	24.7	22.3
-3	6	0	39.6	39.0
-2	6	0	27.6	26.8
-1	6	0	92.9	89.7
0	6	0	157.3	158.5
-12	7	0	20.7	21.5
•-11	7	0	16.0	0.1
•-10	7	0	15.1	1.7
• -9	7	0	14.3	7.5
-8	7	0	78.0	79.6
• -7	7	0	12.7	7.8
-6	7	0	29.3	26.0
-5	7	0	23.9	25.2
-4	7	0	53.1	57.4
• -3	7	0	10.1	3.7
-2	7	0	147.1	146.5
-1	7	0	27.2	27.4
-11	8	0	20.0	21.6
-10	8	0	18.9	19.4
-9	8	0	14.7	19.0
• -8	8	0	13.8	3.1
• -7	8	0	13.1	7.6
-6	8	0	47.2	50.3
-5	8	0	30.0	30.4
-4	8	0	30.6	31.0
-3	8	0	13.1	14.8
-2	8	0	21.8	21.7
-1	8	0	60.7	61.6
0	8	0	66.0	62.6
•-10	9	0	15.8	6.9
-9	9	0	23.8	27.2
-8	9	0	26.7	27.6
-7	9	0	39.5	38.7
-6	9	0	15.8	14.9
-5	9	0	21.2	20.0
-4	9	0	50.5	51.7
-3	9	0	77.4	77.9
-2	9	0	59.4	61.3
-1	9	0	13.1	12.5
•-10	10	0	16.2	3.7
• -9	10	0	15.4	13.3
• -8	10	0	14.7	6.5
-7	10	0	22.2	22.8
• -6	10	0	13.4	1.1
-5	10	0	86.4	90.0
-4	10	0	23.0	23.9
-3	10	0	23.8	27.0
-2	10	0	24.6	26.3
-1	10	0	34.2	35.4
0	10	0	17.9	16.4
•-10	11	0	16.6	0.4
-9	11	0	15.9	15.9
-8	11	0	18.6	18.1
-7	11	0	29.0	31.5
• -6	11	0	13.9	3.7
• -5	11	0	13.4	10.5
• -4	11	0	12.9	7.6
-3	11	0	62.7	67.0
-2	11	0	22.9	22.3
-1	11	0	12.1	13.1
-10	12	0	20.9	20.6
• -9	12	0	16.4	13.2
• -8	12	0	15.7	8.4
• -7	12	0	15.0	0.9
-6	12	0	27.1	26.0
-5	12	0	26.1	26.5
-4	12	0	23.4	25.5
-3	12	0	18.6	19.2
• -2	12	0	12.9	6.0
-1	12	0	39.3	40.4
0	12	0	55.3	55.8
-8	13	0	30.3	30.7
• -7	13	0	15.6	13.0
-6	13	0	15.0	14.5
• -5	13	0	14.6	3.3
-4	13	0	17.3	16.1
-3	13	0	13.8	12.1
-2	13	0	35.9	36.7
• -1	13	0	13.4	8.5
-6	14	0	34.9	35.9
• -5	14	0	15.2	7.6
-4	14	0	25.6	25.7
• -3	14	0	14.5	1.7
• -2	14	0	14.2	0.4
• -1	14	0	14.1	8.9
0	14	0	43.3	44.5
• -5	15	0	15.8	4.1
-4	15	0	15.4	13.4
-3	15	0	18.5	17.1
-2	15	0	18.3	16.4
• -1	15	0	14.8	2.1
-5	16	0	30.7	29.0
• -4	16	0	16.1	9.4
• -3	16	0	15.8	4.4
• -2	16	0	15.6	4.0
• -1	16	0	15.5	10.9
0	16	0	15.4	14.8
-3	17	0	23.3	24.9
• -2	17	0	16.3	2.6
• -1	17	0	16.1	8.1
•-13	0	1	16.0	11.7
-11	0	1	30.0	31.8
-9	0	1	87.4	88.3
• -7	0	1	10.6	2.9
-5	0	1	65.3	62.2
-3	0	1	44.5	36.2
3	0	1	23.3	18.5
5	0	1	91.8	92.0
7	0	1	78.2	76.4
• 9	0	1	12.4	5.4
11	0	1	28.5	30.4
• 13	0	1	16.0	9.9
•-14	1	1	16.9	0.0
-13	1	1	16.0	16.6
-12	1	1	21.3	18.1
-11	1	1	44.9	44.4
•-10	1	1	13.3	9.3
-9	1	1	12.4	13.4
-8	1	1	11.5	10.0
-7	1	1	96.9	91.8
-6	1	1	48.0	46.3
-5	1	1	15.2	14.7
-4	1	1	12.3	15.4
-3	1	1	21.3	18.3
-2	1	1	47.7	48.0
2	1	1	21.5	15.2
3	1	1	173.6	179.3
4	1	1	88.6	87.7
5	1	1	130.3	130.1
6	1	1	33.1	33.0
7	1	1	25.0	23.3
8	1	1	23.1	22.8
9	1	1	67.6	66.8
10	1	1	28.3	28.2
11	1	1	14.2	14.5
• 12	1	1	15.2	1.4
13	1	1	16.1	17.1
• 14	1	1	16.9	5.6
•-14	2	1	16.9	14.9
•-13	2	1	16.0	8.0
•-12	2	1	15.1	0.9
•-11	2	1	14.2	10.5
-10	2	1	46.2	46.8
-9	2	1	39.4	39.9
-8	2	1	56.1	57.4
-7	2	1	22.7	22.9
-6	2	1	23.0	22.8
-5	2	1	61.8	65.6
-4	2	1	71.8	70.2
-3	2	1	27.6	26.6
-2	2	1	22.8	21.4
-1	2	1	68.9	71.7
1	2	1	139.6	127.5
2	2	1	191.8	190.9
3	2	1	50.5	44.9
4	2	1	41.0	37.6
5	2	1	69.6	64.3
6	2	1	97.1	92.9
7	2	1	51.6	50.3
• 8	2	1	11.6	0.1
• 9	2	1	12.5	6.6
• 10	2	1	13.4	11.7
• 11	2	1	14.3	7.6
12	2	1	30.4	28.1
• 13	2	1	16.1	2.5
• 14	2	1	17.0	0.6
•-14	3	1	17.0	2.4
•-13	3	1	16.1	1.4
-12	3	1	37.3	38.0
•-11	3	1	14.4	7.0
-10	3	1	13.5	15.4
-9	3	1	17.8	17.2
-8	3	1	39.8	40.1
• -7	3	1	10.9	2.4
-6	3	1	96.2	94.3
-5	3	1	65.6	63.4
-4	3	1	15.5	16.2
-3	3	1	11.7	10.0
-2	3	1	82.6	88.4
-1	3	1	24.0	20.2
0	3	1	75.5	71.2
1	3	1	8.4	6.8
2	3	1	81.9	87.1
3	3	1	69.9	64.7
4	3	1	220.6	221.1
5	3	1	59.0	54.4
• 6	3	1	10.1	1.4
7	3	1	21.8	20.5
8	3	1	30.1	27.8
9	3	1	21.9	22.7
10	3	1	37.1	35.8
• 11	3	1	14.4	7.1
• 12	3	1	15.3	11.2
• 13	3	1	16.2	2.4
14	3	1	20.9	20.8
-14	4	1	24.2	21.6
•-13	4	1	16.3	10.5
•-12	4	1	15.4	5.0
•-11	4	1	14.5	9.9
-10	4	1	43.1	43.7
• -9	4	1	12.8	7.9
-8	4	1	31.5	31.2
-7	4	1	11.1	10.5
-6	4	1	29.0	27.6
-5	4	1	41.2	41.4
-4	4	1	127.6	130.1
-3	4	1	67.9	64.9
-2	4	1	7.2	4.1
-1	4	1	139.8	138.2
0	4	1	35.7	38.5
1	4	1	40.4	37.1
2	4	1	142.1	139.9
3	4	1	46.3	44.6
4	4	1	61.6	60.9
5	4	1	34.3	33.7
6	4	1	118.1	115.5
7	4	1	36.1	36.0
8	4	1	41.5	42.2
9	4	1	12.8	14.7
• 10	4	1	13.7	10.2
• 11	4	1	14.6	14.2
12	4	1	26.7	27.3
• 13	4	1	16.3	6.7
• 14	4	1	17.2	3.4
-12	5	1	31.1	31.4
-11	5	1	23.2	21.3
-10	5	1	13.8	18.1
-9	5	1	20.5	19.7
-8	5	1	25.8	24.2
-7	5	1	81.1	80.0
-6	5	1	47.3	47.9
-5	5	1	17.0	12.6
-4	5	1	12.9	15.0
-3	5	1	20.6	19.9
-2	5	1	97.8	106.3
-1	5	1	88.3	93.0
0	5	1	13.7	13.2
1	5	1	48.2	41.6
2	5	1	55.8	56.8
3	5	1	105.4	102.1
4	5	1	110.9	110.1
5	5	1	23.1	22.4
• 6	5	1	10.6	10.2
7	5	1	27.9	28.4
8	5	1	41.4	43.7
9	5	1	22.6	20.4
10	5	1	29.5	29.0
• 11	5	1	14.7	5.5
• 12	5	1	15.6	4.3
•-12	6	1	15.7	4.0
•-11	6	1	14.9	8.1
-10	6	1	14.1	19.0
-9	6	1	72.5	71.8
-8	6	1	21.5	19.8
-7	6	1	26.1	25.6
-6	6	1	37.8	35.9
-5	6	1	33.9	32.8
-4	6	1	17.9	18.5
-3	6	1	68.3	69.9
-2	6	1	62.1	60.1
-1	6	1	18.3	17.8
0	6	1	57.6	60.6
1	6	1	192.2	202.0
2	6	1	58.7	59.2
3	6	1	62.1	62.0
4	6	1	15.2	13.5
5	6	1	32.5	36.0
6	6	1	20.5	20.3
7	6	1	66.8	68.3
8	6	1	21.6	23.1
9	6	1	13.3	14.0
• 10	6	1	14.1	8.5
11	6	1	29.9	31.5
• 12	6	1	15.8	9.5
•-12	7	1	16.0	3.3
-11	7	1	28.4	26.2
•-10	7	1	14.3	0.7
• -9	7	1	13.5	9.9
• -8	7	1	12.8	8.6
-7	7	1	64.7	63.1
• -6	7	1	11.3	0.3
-5	7	1	16.8	14.2
-4	7	1	12.3	14.2
-3	7	1	63.3	64.0
• -2	7	1	9.1	6.4
-1	7	1	109.1	115.6
0	7	1	51.5	49.5
1	7	1	15.4	15.3
2	7	1	34.9	36.5
3	7	1	84.8	89.4
• 4	7	1	10.1	4.1
5	7	1	32.1	30.9
6	7	1	24.1	23.6
7	7	1	27.0	25.3
• 8	7	1	12.8	3.9
9	7	1	46.1	48.5
• 10	7	1	14.4	5.0
• 11	7	1	15.2	2.0
• 12	7	1	16.0	0.6
•-12	8	1	16.3	0.3
•-11	8	1	15.4	3.1
-10	8	1	23.2	24.0
-9	8	1	38.0	38.3
-8	8	1	16.1	15.3
• -7	8	1	12.4	7.1
-6	8	1	11.7	12.1
-5	8	1	47.9	50.0
-4	8	1	50.8	50.9
-3	8	1	82.8	85.2
• -2	8	1	9.7	0.5
-1	8	1	16.5	17.8
• 0	8	1	9.5	7.4
1	8	1	95.9	95.7
2	8	1	87.5	84.0
3	8	1	12.4	12.0
• 4	8	1	10.6	7.3
5	8	1	37.9	37.1
6	8	1	25.0	25.9
7	8	1	77.8	79.4
• 8	8	1	13.2	0.5
• 9	8	1	13.9	0.6
• 10	8	1	14.7	12.5
11	8	1	15.5	18.2
• 12	8	1	16.3	16.0
-12	9	1	16.5	18.0
•-11	9	1	15.8	9.3
•-10	9	1	15.0	3.2
• -9	9	1	14.2	6.4
-8	9	1	34.5	33.3
-7	9	1	28.7	26.5
-6	9	1	53.2	54.1
-5	9	1	11.6	12.2
• -4	9	1	11.1	5.5
-3	9	1	21.4	22.6
-2	9	1	72.3	76.1
-1	9	1	20.4	21.3
0	9	1	37.8	41.2
1	9	1	55.3	53.7
2	9	1	16.4	17.2
3	9	1	39.4	40.2
4	9	1	69.2	72.1
5	9	1	40.4	39.4
• 6	9	1	12.2	7.4
• 7	9	1	12.9	3.2
8	9	1	27.1	29.1
9	9	1	14.3	14.7
10	9	1	15.0	17.1
• 11	9	1	15.8	3.1
• 12	9	1	16.6	5.9
•-12	10	1	16.9	1.3
•-11	10	1	16.1	3.3
-10	10	1	26.6	22.9
• -9	10	1	14.6	0.9
-8	10	1	17.1	16.6
-7	10	1	21.0	21.3
-6	10	1	12.7	12.3
• -5	10	1	12.1	8.3
-4	10	1	95.6	96.7
• -3	10	1	11.3	0.4
-2	10	1	11.0	15.2
-1	10	1	17.1	15.9
0	10	1	31.4	31.7
• 1	10	1	10.8	8.4
2	10	1	63.3	64.7
3	10	1	19.6	16.9
4	10	1	20.3	16.8
• 5	10	1	12.2	2.6
6	10	1	53.3	54.8
7	10	1	16.3	16.6
8	10	1	17.1	18.4
• 9	10	1	14.7	8.0
• 10	10	1	15.4	13.2
• 11	10	1	16.2	5.8
12	10	1	20.7	19.6
•-10	11	1	15.7	4.5
• -9	11	1	15.0	2.4
-8	11	1	14.4	14.4
-7	11	1	19.5	18.4
-6	11	1	44.8	46.5
-5	11	1	20.0	16.8
• -4	11	1	12.2	2.7
• -3	11	1	11.9	6.6
-2	11	1	68.7	71.0
-1	11	1	28.1	29.1
0	11	1	19.8	20.2
1	11	1	19.8	20.6
2	11	1	21.8	23.3
3	11	1	25.3	22.9
4	11	1	54.9	56.5
5	11	1	20.1	16.7
• 6	11	1	13.2	1.3
• 7	11	1	13.8	2.3
8	11	1	22.8	22.8
• 9	11	1	15.1	13.2
10	11	1	19.4	18.6
-10	12	1	16.2	16.2
-9	12	1	26.8	22.3
-8	12	1	18.2	18.0
• -7	12	1	14.3	11.4
• -6	12	1	13.7	0.8
-5	12	1	35.0	36.7
-4	12	1	32.7	34.0
-3	12	1	36.4	37.7
• -2	12	1	12.2	4.9
• -1	12	1	12.1	6.8
0	12	1	45.9	48.3
1	12	1	41.0	40.2
2	12	1	33.6	32.2
• 3	12	1	12.5	6.5
• 4	12	1	12.9	5.0
5	12	1	16.2	15.0
6	12	1	21.7	23.7
7	12	1	24.8	23.7
• 8	12	1	14.9	6.5
• 9	12	1	15.5	11.2
• 10	12	1	16.2	9.6
• -9	13	1	16.0	0.3
• -8	13	1	15.3	1.4
-7	13	1	31.3	30.1
• -6	13	1	14.3	7.7
-5	13	1	13.8	12.4
• -4	13	1	13.4	0.0
-3	13	1	20.7	19.3
-2	13	1	12.9	11.9
-1	13	1	69.7	69.2
• 0	13	1	12.7	2.7
• 1	13	1	12.7	7.9
• 2	13	1	12.9	3.9
3	13	1	18.6	16.7
• 4	13	1	13.4	9.9
5	13	1	24.0	24.0
• 6	13	1	14.3	6.5
• 7	13	1	14.8	12.7
• 8	13	1	15.4	2.5
9	13	1	27.7	29.3
-9	14	1	20.1	19.0
• -8	14	1	15.8	4.2
• -7	14	1	15.3	2.6
• -6	14	1	14.8	5.5
-5	14	1	24.9	27.1
• -4	14	1	14.0	5.4
-3	14	1	25.7	27.1
• -2	14	1	13.5	4.5
-1	14	1	16.4	16.5
• 0	14	1	13.3	5.1
1	14	1	43.4	43.6
2	14	1	16.5	16.3
• 3	14	1	13.7	7.3
• 4	14	1	14.0	7.4
• 5	14	1	14.4	8.9
• 6	14	1	14.8	0.7
7	14	1	21.7	21.8
• 8	14	1	15.9	5.2
• 9	14	1	16.5	5.3
-7	15	1	25.1	23.8
-6	15	1	18.8	18.3
-5	15	1	15.0	14.3
• -4	15	1	14.6	3.2
• -3	15	1	14.3	8.6
-2	15	1	26.5	26.8
-1	15	1	29.7	31.5
• 0	15	1	14.0	12.9
• 1	15	1	14.0	8.5
• 2	15	1	14.2	0.4
3	15	1	20.3	20.2
4	15	1	17.9	16.9
5	15	1	15.0	18.9
• 6	15	1	15.4	5.7
• 7	15	1	15.9	5.1
• -6	16	1	16.0	10.0
• -5	16	1	15.6	11.2
-4	16	1	35.7	35.4
• -3	16	1	15.0	10.3
• -2	16	1	14.8	10.4
• -1	16	1	14.7	[illegible]
• 0	16	1	14.6	9.5
• 1	16	1	14.7	8.4
• 2	16	1	14.8	11.5
• 3	16	1	15.0	0.4
• 4	16	1	15.3	7.5
• 5	16	1	15.6	5.7
6	16	1	22.6	22.6
-6	17	1	16.5	17.6
• -5	17	1	16.2	0.4
• -4	17	1	15.8	0.4
• -3	17	1	15.6	4.7
-2	17	1	24.4	22.2
• -1	17	1	15.3	0.4
• 0	17	1	15.3	10.1
• 1	17	1	15.3	5.9
• 2	17	1	15.4	4.7
• 3	17	1	15.6	0.7
4	17	1	25.1	22.0
• 5	17	1	16.2	0.8
• 6	17	1	16.5	1.6
• -2	18	1	16.1	1.2
• -1	18	1	16.0	1.0
0	18	1	15.9	14.1
• 1	18	1	16.0	8.3
2	18	1	16.1	17.2
-1	19	1	20.3	17.0
• 0	19	1	16.6	7.1
• 1	19	1	16.6	2.7
•-12	0	2	17.8	6.0
-10	0	2	15.7	17.3
-8	0	2	110.4	110.6
-6	0	2	31.2	27.9
-4	0	2	30.2	33.2
-2	0	2	86.3	80.8
2	0	2	98.1	88.4
4	0	2	91.6	85.0
6	0	2	52.3	49.4
8	0	2	66.4	65.1
• 10	0	2	15.8	5.2
12	0	2	22.0	20.3
•-13	1	2	18.9	9.0
-12	1	2	25.2	23.2
-11	1	2	26.5	26.0
-10	1	2	53.2	54.1
-9	1	2	23.1	20.1
• -8	1	2	13.6	5.8
-7	1	2	17.7	14.0
-6	1	2	146.6	146.4
-5	1	2	21.9	25.8
-4	1	2	73.7	72.2
-3	1	2	85.3	76.7
-2	1	2	60.9	61.5
2	1	2	60.2	53.9
3	1	2	61.5	53.8
4	1	2	138.7	127.8
5	1	2	57.5	52.4
6	1	2	81.2	75.1
7	1	2	26.9	26.5
8	1	2	61.4	56.7
9	1	2	27.6	27.8
10	1	2	54.9	52.8
11	1	2	16.9	20.3
• 12	1	2	18.0	2.9
-13	2	2	19.0	23.1
•-12	2	2	17.9	7.2
•-11	2	2	16.8	4.5
•-10	2	2	15.8	7.4
-9	2	2	34.5	35.0
-8	2	2	43.2	42.7
-7	2	2	80.9	78.3
• -6	2	2	11.6	8.1
-5	2	2	45.8	44.7
-4	2	2	21.0	22.6
-3	2	2	109.2	115.4
-2	2	2	70.5	76.1
-1	2	2	10.3	12.2
1	2	2	34.9	27.7
• 2	2	2	7.2	5.4
3	2	2	157.6	144.8
• 4	2	2	9.6	2.8
5	2	2	43.4	39.9
6	2	2	39.8	38.1
7	2	2	87.2	83.5
8	2	2	67.7	65.9
9	2	2	33.2	34.0
• 10	2	2	15.9	11.1
11	2	2	17.0	17.9
• 12	2	2	18.0	8.0
• 13	2	2	19.1	17.9
•-12	3	2	18.0	12.8
-11	3	2	37.9	37.2
-10	3	2	19.5	18.9
• -9	3	2	14.9	12.9
-8	3	2	21.9	25.0
-7	3	2	69.7	68.7
-6	3	2	31.2	31.7
-5	3	2	168.9	165.9
-4	3	2	32.4	34.0
• -3	3	2	8.7	2.2
-2	3	2	9.5	10.9
-1	3	2	11.0	15.1
0	3	2	19.4	20.3
• 1	3	2	7.0	5.0
2	3	2	82.3	74.8
3	3	2	86.6	80.2
4	3	2	56.5	49.4
5	3	2	176.1	167.6
6	3	2	18.9	16.9
• 7	3	2	13.0	4.7
8	3	2	19.8	19.9
9	3	2	31.9	31.2
• 10	3	2	16.1	10.0
11	3	2	29.6	28.9
• 12	3	2	18.1	3.3
•-12	4	2	18.1	7.9
•-11	4	2	17.1	0.9
•-10	4	2	16.1	0.3
-9	4	2	48.8	50.8
-8	4	2	39.8	38.4
-7	4	2	75.7	76.2
-6	4	2	22.7	19.0
-5	4	2	23.7	21.9
-4	4	2	68.5	69.0
-3	4	2	144.2	139.9
-2	4	2	35.6	39.8
-1	4	2	7.9	7.1
0	4	2	67.3	67.5
1	4	2	48.3	50.1
2	4	2	35.0	32.3
3	4	2	135.9	126.3
4	4	2	20.7	18.3
5	4	2	41.5	41.1
6	4	2	49.0	48.4
7	4	2	77.7	75.1
• 8	4	2	14.2	13.2
9	4	2	26.4	26.1
• 10	4	2	16.2	13.2
11	4	2	17.3	17.8
• 12	4	2	18.3	4.8
•-12	5	2	18.4	4.7
-11	5	2	34.7	33.6
-10	5	2	16.3	20.6
-9	5	2	15.3	17.2
• -8	5	2	14.4	0.2
-7	5	2	13.4	15.0
-6	5	2	61.1	60.5
-5	5	2	87.8	90.0
-4	5	2	26.3	24.4
-3	5	2	23.3	21.5
• -2	5	2	9.3	0.7
-1	5	2	74.4	80.3
0	5	2	56.9	56.7
1	5	2	94.5	89.1
2	5	2	24.8	24.8
3	5	2	48.7	44.7
4	5	2	47.3	43.5
5	5	2	53.7	48.1
6	5	2	77.2	74.3
• 7	5	2	13.5	7.4
• 8	5	2	14.5	4.1
9	5	2	36.3	37.6
10	5	2	23.3	21.6
11	5	2	30.3	29.9
• 12	5	2	18.5	4.8
•-12	6	2	18.6	16.9
•-11	6	2	17.6	6.2
•-10	6	2	16.6	16.4
-9	6	2	35.0	33.4
-8	6	2	70.5	74.3
-7	6	2	23.9	21.7
• -6	6	2	12.9	5.1
-5	6	2	22.6	21.1
-4	6	2	94.1	94.4
-3	6	2	33.5	35.2
-2	6	2	94.5	95.1
• -1	6	2	9.7	8.1
0	6	2	35.8	36.0
1	6	2	38.8	41.0
2	6	2	125.7	123.1
• 3	6	2	10.7	4.9
4	6	2	34.2	31.9
5	6	2	27.2	25.7
6	6	2	53.7	52.8
7	6	2	29.5	26.1
8	6	2	63.8	64.3
9	6	2	15.8	15.6
10	6	2	16.8	20.1
• 11	6	2	17.7	2.4
12	6	2	18.8	21.1
•-11	7	2	17.9	0.1
-10	7	2	35.9	37.7
• -9	7	2	16.0	11.0
-8	7	2	15.1	12.6
• -7	7	2	14.2	5.9
-6	7	2	50.0	49.8
• -5	7	2	12.6	1.0
-4	7	2	29.1	28.3
-3	7	2	60.7	58.9
-2	7	2	34.1	34.4
-1	7	2	36.3	37.9
0	7	2	119.6	116.7
1	7	2	42.1	44.1
• 2	7	2	10.9	3.1
3	7	2	40.1	39.7
4	7	2	28.1	29.5
• 5	7	2	12.7	6.8
6	7	2	54.0	57.3
• 7	7	2	14.3	12.9
8	7	2	26.3	23.8
• 9	7	2	16.1	4.8
10	7	2	36.2	36.4
• 11	7	2	18.0	0.5
•-11	8	2	18.2	0.7
-10	8	2	17.3	19.2
-9	8	2	16.4	18.0
-8	8	2	57.0	59.1
-7	8	2	31.1	29.7
• -6	8	2	13.9	14.2
-5	8	2	16.1	17.6
-4	8	2	45.1	46.0
-3	8	2	47.1	50.5
-2	8	2	79.5	83.7
-1	8	2	30.9	29.6
0	8	2	35.4	34.8
1	8	2	32.0	32.4
2	8	2	97.0	98.2
3	8	2	75.1	71.9
• 4	8	2	12.6	2.6
• 5	8	2	13.2	2.0
6	8	2	40.8	41.9
7	8	2	14.8	20.5
8	8	2	50.7	54.3
• 9	8	2	16.5	0.3
• 10	8	2	17.4	6.8
• 11	8	2	18.4	6.5
-11	9	2	18.6	19.8
•-10	9	2	17.7	7.2
• -9	9	2	16.8	8.0
• -8	9	2	16.0	13.4
-7	9	2	15.2	18.6
-6	9	2	32.2	31.0
-5	9	2	74.0	77.0
-4	9	2	37.2	42.3
-3	9	2	15.5	16.9
-2	9	2	21.3	21.3
-1	9	2	43.4	47.4
0	9	2	28.1	27.9
1	9	2	60.3	58.0
2	9	2	35.9	36.7
3	9	2	32.4	34.8
4	9	2	28.1	29.8
5	9	2	67.8	70.0
6	9	2	27.2	27.2
• 7	9	2	15.3	12.3
• 8	9	2	16.1	6.1
9	9	2	16.9	18.4
• 10	9	2	17.8	11.8
• 11	9	2	18.8	17.4
•-11	10	2	19.0	1.5
•-10	10	2	18.1	7.4
-9	10	2	21.2	23.6
• -8	10	2	16.5	10.3
-7	10	2	15.7	15.5
• -6	10	2	15.0	2.5
-5	10	2	30.5	32.6
• -4	10	2	13.8	2.4
-3	10	2	88.1	89.9
-2	10	2	24.3	21.3
-1	10	2	15.7	16.6
0	10	2	23.8	21.9
1	10	2	32.7	34.8
• 2	10	2	13.0	11.1
3	10	2	53.6	57.0
• 4	10	2	13.9	12.0
5	10	2	20.4	21.9
6	10	2	14.1	12.5

Table 4 (*cont.*)

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
7	10	2	38.7	37.9
• 8	10	2	16.6	1.7
• 9	10	2	17.4	17.1
• 10	10	2	18.3	1.2
• 11	10	2	19.1	9.8
-11	11	2	23.8	22.2
•-10	11	2	18.6	9.8
• -9	11	2	17.8	6.7
• -8	11	2	17.0	12.2
• -7	11	2	16.3	14.6
-6	11	2	27.0	26.0
-5	11	2	41.1	42.5
• -4	11	2	14.5	8.8
• -3	11	2	14.1	4.4
-2	11	2	21.7	20.2
-1	11	2	59.1	63.8
0	11	2	25.3	27.7
1	11	2	45.0	48.5
2	11	2	13.8	14.7
3	11	2	22.3	20.4
4	11	2	17.8	21.3
5	11	2	45.2	46.3
6	11	2	22.2	21.7
• 7	11	2	16.4	4.2
• 8	11	2	17.1	7.5
• 9	11	2	17.9	17.6
• 10	11	2	18.7	2.7
• 11	11	2	19.6	19.3
-9	12	2	18.3	18.7
-8	12	2	17.5	18.5
-7	12	2	16.9	18.4
• -6	12	2	16.2	2.5
• -5	12	2	15.6	0.7
-4	12	2	15.2	18.8
-3	12	2	27.6	28.9
-2	12	2	36.9	39.8
• -1	12	2	14.3	4.9
• 0	12	2	14.3	12.8
1	12	2	32.0	34.8
2	12	2	43.6	48.3
3	12	2	31.4	34.7
4	12	2	24.1	24.4
• 5	12	2	15.7	8.3
• 6	12	2	16.3	3.1
• 7	12	2	17.0	13.6
8	12	2	17.7	18.7
• 9	12	2	18.4	11.8
• -8	13	2	18.1	2.8
• -7	13	2	17.5	10.2
-6	13	2	23.8	26.3
• -5	13	2	16.3	10.3
• -4	13	2	15.9	7.2
• -3	13	2	15.5	10.2
-2	13	2	37.3	35.7
• -1	13	2	15.1	12.6
0	13	2	68.8	75.5
• 1	13	2	15.1	1.9
• 2	13	2	15.3	4.4
• 3	13	2	15.5	11.3
4	13	2	22.5	20.8
• 5	13	2	16.4	9.0
6	13	2	16.9	18.2
• 7	13	2	17.5	0.1
• 8	13	2	18.2	13.5
-8	14	2	18.7	21.4
• -7	14	2	18.1	3.7
• -6	14	2	17.5	3.5
• -5	14	2	17.0	2.1
-4	14	2	16.6	15.5
• -3	14	2	16.2	5.7
-2	14	2	40.7	40.5
• -1	14	2	15.8	5.0
• 0	14	2	15.8	14.8
• 1	14	2	15.8	4.8
2	14	2	32.0	32.8
• 3	14	2	16.3	12.3
• 4	14	2	16.6	9.1
• 5	14	2	17.1	2.0
• 6	14	2	17.6	12.8
• 7	14	2	18.2	2.2
8	14	2	18.8	22.2
-6	15	2	18.2	22.2
• -5	15	2	17.7	15.0
• -4	15	2	17.3	14.3
• -3	15	2	17.0	4.9
• -2	15	2	16.7	8.7
-1	15	2	20.3	21.3
0	15	2	33.1	32.4
1	15	2	16.6	15.0
• 2	15	2	16.8	6.9
• 3	15	2	17.0	4.2
4	15	2	24.5	23.2
• 5	15	2	17.8	16.3
6	15	2	22.4	18.0
-3	16	2	30.7	27.3
• -2	16	2	17.5	9.2
• -1	16	2	17.3	6.4
• 0	16	2	17.3	2.6
1	16	2	17.4	15.8
• 2	16	2	17.5	10.6
3	16	2	28.1	26.6
-1	17	2	22.2	22.7
• 0	17	2	18.1	0.9
• 1	17	2	18.1	12.7
-13	0	3	25.1	24.0
-11	0	3	24.9	23.7
-9	0	3	13.8	16.5
-7	0	3	97.7	104.9
-5	0	3	33.5	36.8
-3	0	3	124.8	133.4
3	0	3	83.9	79.2
5	0	3	65.0	61.0
7	0	3	71.9	71.7
9	0	3	83.8	87.5
• 11	0	3	16.0	10.3
13	0	3	22.0	21.1
•-14	1	3	18.8	8.0
•-13	1	3	17.8	1.8
•-12	1	3	16.8	8.4
-11	1	3	22.3	23.2
-10	1	3	25.6	21.4
-9	1	3	32.3	33.8
-8	1	3	31.3	34.1
-7	1	3	37.3	40.5
• -6	1	3	10.8	8.0
-5	1	3	80.6	85.1
-4	1	3	69.6	69.8
-3	1	3	89.3	84.6
-2	1	3	52.0	54.2
2	1	3	61.7	61.6
• 3	1	3	7.7	2.5
• 4	1	3	8.9	2.1
5	1	3	17.3	17.6
6	1	3	24.6	22.7
7	1	3	44.9	43.9
• 8	1	3	13.0	0.0
9	1	3	28.0	27.6
10	1	3	23.7	25.8
11	1	3	25.3	25.0
• 12	1	3	17.0	14.0
• 13	1	3	18.0	6.6
• 14	1	3	19.0	0.0
•-14	2	3	18.8	5.8
•-13	2	3	17.8	8.6
-12	2	3	20.6	21.1
-11	2	3	15.8	17.0
•-10	2	3	14.8	8.4
-9	2	3	13.9	15.3
-8	2	3	35.3	36.9
-7	2	3	66.3	68.6
-6	2	3	79.5	81.6
-5	2	3	33.6	30.0
-4	2	3	36.0	35.6
-3	2	3	80.5	80.7
-2	2	3	156.1	160.6
-1	2	3	157.6	158.9
0	2	3	29.3	31.7
1	2	3	13.5	14.0
2	2	3	18.2	19.2
3	2	3	67.9	68.2
4	2	3	88.3	87.0
5	2	3	49.6	45.5
6	2	3	19.3	18.2
7	2	3	34.3	33.5
8	2	3	34.7	35.5
9	2	3	37.3	38.9
10	2	3	23.8	23.8
• 11	2	3	16.1	7.5
• 12	2	3	17.1	16.0
13	2	3	18.1	18.7
• 14	2	3	19.0	13.2
-14	3	3	18.9	19.9
•-13	3	3	17.9	1.1
•-12	3	3	17.0	6.0
•-11	3	3	16.0	0.6
-10	3	3	28.0	26.1
• -9	3	3	14.0	1.9
• -8	3	3	13.0	12.8
-7	3	3	29.6	29.4
-6	3	3	70.4	70.9
-5	3	3	48.7	47.9
-4	3	3	195.6	200.6
-3	3	3	8.2	9.2
• -2	3	3	7.3	1.6
-1	3	3	32.1	34.3
0	3	3	62.3	69.8
1	3	3	14.2	10.8
2	3	3	69.2	70.4
3	3	3	45.0	40.8
4	3	3	56.8	52.3
• 5	3	3	10.4	5.3
6	3	3	87.8	85.7
• 7	3	3	12.3	6.1
8	3	3	21.0	18.7
• 9	3	3	14.2	3.5
10	3	3	30.4	33.7
• 11	3	3	16.2	2.6
12	3	3	21.0	23.2
• 13	3	3	18.1	2.5
• 14	3	3	19.1	6.7
-12	4	3	29.6	29.3
•-11	4	3	16.1	0.6
•-10	4	3	15.2	7.6
• -9	4	3	14.2	0.1
-8	4	3	38.7	39.4
• -7	4	3	12.3	11.0
-6	4	3	74.9	75.3
• -5	4	3	10.5	5.7
-4	4	3	66.6	66.7
-3	4	3	29.1	28.8
-2	4	3	149.5	155.5
-1	4	3	16.7	15.4
0	4	3	67.5	68.4
1	4	3	49.9	47.3
2	4	3	40.8	38.9
• 3	4	3	8.9	3.2
4	4	3	85.3	83.2
5	4	3	13.1	13.8
6	4	3	27.2	27.3
• 7	4	3	12.5	0.9
8	4	3	50.4	53.7
9	4	3	14.4	13.2
10	4	3	24.3	25.8
• 11	4	3	16.3	7.7
12	4	3	17.3	18.4
•-12	5	3	12.2	9.8
•-11	5	3	16.3	6.7
-10	5	3	32.6	35.7
-9	5	3	32.3	32.7
• -8	5	3	13.5	9.6
• -7	5	3	12.6	3.0
-6	5	3	25.0	24.2
-5	5	3	69.9	70.8
-4	5	3	75.0	73.1
-3	5	3	90.6	94.9
-2	5	3	21.4	20.6
-1	5	3	62.4	59.8
0	5	3	60.6	60.1
1	5	3	65.9	67.7
2	5	3	94.1	95.8
3	5	3	9.5	9.6
4	5	3	14.5	11.3
5	5	3	50.9	49.8
6	5	3	36.8	36.7
7	5	3	69.1	68.9
• 8	5	3	13.7	4.6
9	5	3	17.9	15.5
10	5	3	19.1	22.9
11	5	3	23.4	23.5
12	5	3	24.8	22.7
•-11	6	3	16.6	16.2
•-10	6	3	15.6	5.2
-9	6	3	23.3	22.2
-8	6	3	29.4	29.5
-7	6	3	58.1	59.5
-6	6	3	24.3	25.1
-5	6	3	13.9	11.2
-4	6	3	29.2	29.4
-3	6	3	65.9	62.3
-2	6	3	44.4	42.5
-1	6	3	73.1	74.1
0	6	3	68.8	69.3
1	6	3	81.4	78.1
2	6	3	26.2	25.9
3	6	3	52.6	50.4
4	6	3	18.7	18.5
5	6	3	30.5	34.2
6	6	3	24.7	22.8
7	6	3	24.6	24.1
8	6	3	22.2	20.3
9	6	3	31.7	32.4
• 10	6	3	15.8	7.4
• 11	6	3	16.8	3.4
•-11	7	3	16.9	16.5
•-10	7	3	16.0	8.7
-9	7	3	54.4	54.9
-8	7	3	22.5	21.3
• -7	7	3	13.4	0.0
-6	7	3	28.2	28.0
-5	7	3	72.7	75.6
• -4	7	3	11.2	1.3
-3	7	3	60.2	62.1
-2	7	3	46.7	46.4
-1	7	3	58.6	62.7
0	7	3	36.1	33.7
1	7	3	145.9	158.0
• 2	7	3	10.3	6.2
• 3	7	3	10.7	6.4
• 4	7	3	11.3	3.1
5	7	3	39.0	40.4
6	7	3	15.6	14.5
7	7	3	53.4	55.4
• 8	7	3	14.4	3.8
9	7	3	32.4	30.8
• 10	7	3	16.1	6.7
11	7	3	31.9	32.4
•-10	8	3	16.3	0.7
-9	8	3	21.8	23.3
• -8	8	3	14.6	2.2
-7	8	3	41.5	39.5
-6	8	3	34.6	34.4
-5	8	3	17.6	18.3
-4	8	3	18.7	18.8
-3	8	3	44.4	44.0
-2	8	3	40.8	42.0
-1	8	3	78.6	77.6
• 0	8	3	10.6	6.3
• 1	8	3	10.7	9.4
2	8	3	24.5	24.9
3	8	3	31.2	32.2
4	8	3	35.8	37.8
• 5	8	3	12.6	7.6
• 6	8	3	13.2	1.6
7	8	3	28.0	26.4
8	8	3	25.6	27.0
9	8	3	22.1	22.3
• 10	8	3	16.5	15.3
-10	9	3	23.6	22.5
-9	9	3	15.8	17.2
• -8	9	3	15.1	8.5
-7	9	3	24.8	21.5
-6	9	3	21.5	21.9
-5	9	3	46.7	47.1
-4	9	3	65.1	69.6
-3	9	3	50.0	49.7
-2	9	3	24.6	21.7
-1	9	3	11.4	13.2
0	9	3	40.8	42.3
1	9	3	52.3	52.9
2	9	3	39.5	41.4
• 3	9	3	12.0	1.3
4	9	3	37.6	35.5
5	9	3	42.5	44.1
6	9	3	49.6	49.2
7	9	3	28.9	26.4
• 8	9	3	15.2	7.8
• 9	9	3	16.0	7.0
• 10	9	3	16.9	12.3
•-10	10	3	17.1	2.1
• -9	10	3	16.3	6.1
-8	10	3	26.9	25.5
• -7	10	3	14.8	3.8
-6	10	3	48.0	48.4
-5	10	3	13.5	18.1
-4	10	3	22.6	21.6
• -3	10	3	12.6	1.7
-2	10	3	51.4	52.4
• -1	10	3	12.1	5.9
0	10	3	20.9	18.4
1	10	3	14.8	14.8
2	10	3	53.8	57.2
• 3	10	3	12.7	1.7
4	10	3	67.0	70.7
• 5	10	3	13.7	10.5
• 6	10	3	14.3	7.8
• 7	10	3	15.0	1.8
8	10	3	22.2	22.2
• 9	10	3	16.5	3.2
• 10	10	3	17.3	15.5
-10	11	3	27.7	23.3
• -9	11	3	16.8	9.0
-8	11	3	16.0	13.5
• -7	11	3	15.3	1.9
-6	11	3	27.5	24.7
-5	11	3	20.0	14.6
-4	11	3	43.2	43.9
• -3	11	3	13.3	10.4
• -2	11	3	13.0	11.7
• -1	11	3	12.8	7.3
0	11	3	43.3	44.2
• 1	11	3	12.8	11.4
2	11	3	44.2	46.7
3	11	3	26.7	24.7
4	11	3	32.3	33.5
5	11	3	17.5	13.5
6	11	3	31.5	33.0
7	11	3	24.5	23.4
• 8	11	3	16.2	2.9
• 9	11	3	16.9	0.1
• 10	11	3	17.7	13.3
• -9	12	3	17.2	2.8
-8	12	3	16.6	15.9
-7	12	3	22.5	21.4
• -6	12	3	15.3	11.3
• -5	12	3	14.8	2.7
• -4	12	3	14.3	13.2
• -3	12	3	13.9	14.7
-2	12	3	30.6	34.5
-1	12	3	39.4	39.7
0	12	3	19.0	19.9
1	12	3	23.5	22.0
2	12	3	13.7	11.2
3	12	3	35.7	37.3
4	12	3	28.8	28.0
5	12	3	18.2	21.7
6	12	3	15.4	14.2
• 7	12	3	16.0	13.9
• 8	12	3	16.7	12.5
9	12	3	24.6	19.6
-9	13	3	25.1	25.5
• -8	13	3	17.1	1.3
• -7	13	3	16.5	4.3
• -6	13	3	15.9	11.9
• -5	13	3	15.4	12.7
• -4	13	3	15.0	9.8
• -3	13	3	14.6	8.0
• -2	13	3	14.4	2.5
-1	13	3	30.2	30.7
0	13	3	17.4	14.1
1	13	3	49.4	52.7
2	13	3	14.4	14.6
• 3	13	3	14.7	3.0
• 4	13	3	15.1	8.7
5	13	3	15.5	18.5
• 6	13	3	16.0	6.8
7	13	3	16.6	16.8
• 8	13	3	17.2	0.4
• 9	13	3	17.9	9.7
• -9	14	3	18.3	6.8
• -8	14	3	17.6	1.3
-7	14	3	27.0	29.5
• -6	14	3	16.5	10.2
• -5	14	3	16.0	2.5
• -4	14	3	15.6	3.7
-3	14	3	15.3	14.0
• -2	14	3	15.1	7.2
-1	14	3	38.1	38.9
• 0	14	3	14.9	0.7
1	14	3	15.0	15.1
• 2	14	3	15.1	9.6
3	14	3	42.1	38.9
• 4	14	3	15.7	9.4
5	14	3	16.1	15.6
• 6	14	3	16.6	3.6
• 7	14	3	17.2	14.8
• 8	14	3	17.8	2.8
9	14	3	18.4	18.1
-5	15	3	16.7	16.9
• -4	15	3	16.3	11.7
• -3	15	3	16.0	12.6
• -2	15	3	15.8	6.7
• -1	15	3	15.7	6.9
0	15	3	15.6	13.8
1	15	3	15.7	15.2
2	15	3	15.8	18.6
• 3	15	3	16.1	6.3
• 4	15	3	16.4	8.7
5	15	3	16.8	18.6
• -4	16	3	17.0	7.2
• -3	16	3	16.7	9.1
-2	16	3	20.2	18.5
• -1	16	3	16.4	11.5
• 0	16	3	16.4	3.8
• 1	16	3	16.4	4.3
• 2	16	3	16.5	14.5
• 3	16	3	16.8	15.0
4	16	3	24.1	23.7
-4	17	3	17.7	18.2
• -3	17	3	17.4	7.0
• -2	17	3	17.2	1.9
• -1	17	3	17.1	3.6
• 0	17	3	17.1	13.7
• 1	17	3	17.1	1.4
• 2	17	3	17.2	17.1
• 3	17	3	17.5	2.9
• 4	17	3	17.7	13.7
• -1	18	3	17.8	7.3
• 0	18	3	17.8	2.7
• 1	18	3	17.8	6.0
-12	0	4	23.6	25.4
-10	0	4	38.3	37.6
-8	0	4	42.6	40.7
-6	0	4	46.9	47.9
• -4	0	4	7.6	6.6
-2	0	4	173.4	170.2
2	0	4	61.0	64.1
4	0	4	67.4	61.3
6	0	4	23.1	24.0
8	0	4	35.9	34.5
10	0	4	34.2	34.4
• 12	0	4	15.2	5.0
•-13	1	4	15.8	8.0
•-12	1	4	14.9	14.8
•-11	1	4	14.1	11.7
•-10	1	4	13.2	13.7
-9	1	4	23.0	22.4
-8	1	4	46.3	45.9
-7	1	4	14.9	15.3
-6	1	4	22.5	20.8
-5	1	4	8.7	10.1
-4	1	4	61.3	57.0
-3	1	4	50.6	48.7
-2	1	4	119.6	129.5
1	1	4	65.3	70.7
2	1	4	127.7	135.2
3	1	4	79.9	78.4
4	1	4	35.3	33.8
5	1	4	11.0	9.1
6	1	4	26.1	23.1
• 7	1	4	10.8	7.7
8	1	4	57.1	55.6
• 9	1	4	12.5	7.2
• 10	1	4	13.4	11.7
• 11	1	4	14.3	17.3
12	1	4	18.6	22.1
• 13	1	4	16.1	9.5
•-13	2	4	15.9	13.8
-12	2	4	15.0	16.1
-11	2	4	31.6	30.6
-10	2	4	13.2	16.8
• -9	2	4	12.4	0.3
-8	2	4	32.5	30.8
-7	2	4	28.1	27.8
-6	2	4	49.6	46.6
-5	2	4	47.5	46.3
• -4	2	4	7.9	5.5
-3	2	4	47.4	46.7
-2	2	4	73.9	76.1
-1	2	4	138.5	150.4
0	2	4	75.6	84.0
1	2	4	62.1	67.2
2	2	4	68.6	74.0
3	2	4	71.3	69.2
4	2	4	64.6	62.5
5	2	4	46.4	45.0
6	2	4	31.6	29.3
7	2	4	10.9	9.3
8	2	4	23.5	22.5
9	2	4	35.7	34.4
• 10	2	4	13.5	10.0
11	2	4	17.6	18.5
• 12	2	4	15.3	7.4
• 13	2	4	16.1	10.1
-13	3	4	25.2	26.0
•-12	3	4	15.1	3.8
•-11	3	4	14.2	6.3
•-10	3	4	13.4	6.7
-9	3	4	33.1	29.4
• -8	3	4	11.6	6.0
-7	3	4	13.2	15.3
• -6	3	4	9.9	2.9
-5	3	4	54.0	50.7
-4	3	4	14.2	11.9
-3	3	4	139.5	142.9
-2	3	4	17.2	16.3
• -1	3	4	5.8	3.8
0	3	4	30.9	29.2
1	3	4	101.0	98.7
2	3	4	35.0	34.5
3	3	4	87.7	91.0
4	3	4	52.1	47.9
5	3	4	55.9	55.6
• 6	3	4	10.2	7.2
7	3	4	49.3	50.8
8	3	4	14.6	14.9
9	3	4	27.0	26.7
• 10	3	4	13.6	5.4
11	3	4	22.9	23.0
• 12	3	4	15.4	6.5
• 13	3	4	16.2	16.3
•-13	4	4	16.1	7.4
•-12	4	4	15.2	0.9
-11	4	4	30.5	31.5
•-10	4	4	[illegible]	6.9
• -9	4	4	12.7	3.4
• -8	4	4	11.8	9.8
-7	4	4	36.5	38.1
-6	4	4	10.2	10.1
-5	4	4	76.2	75.8
-4	4	4	75.5	70.2
-3	4	4	58.5	58.7
-2	4	4	28.6	25.4
-1	4	4	103.5	106.4
0	4	4	11.3	10.7
1	4	4	46.0	46.0
2	4	4	27.9	27.2
3	4	4	83.9	83.2
4	4	4	30.5	28.7
5	4	4	77.4	78.7
6	4	4	35.3	32.5
• 7	4	4	11.2	2.3
8	4	4	12.1	13.2
9	4	4	20.4	19.9
10	4	4	13.8	15.9
11	4	4	14.6	18.0
• 12	4	4	15.5	3.6
• 13	4	4	16.3	14.3
-13	5	4	16.2	16.5
•-12	5	4	15.4	7.2
•-11	5	4	14.6	3.1
-10	5	4	21.7	23.9
-9	5	4	28.8	26.9
-8	5	4	37.2	33.2
-7	5	4	27.6	28.5
-6	5	4	23.5	25.3
-5	5	4	60.1	57.4
-4	5	4	49.4	49.4
-3	5	4	69.5	68.2
-2	5	4	86.6	80.7
-1	5	4	24.7	24.5
0	5	4	74.3	78.3
1	5	4	103.8	101.0
2	5	4	60.1	58.1
3	5	4	88.0	85.0
4	5	4	38.0	34.8
5	5	4	9.9	11.9
6	5	4	39.4	35.1
7	5	4	28.2	27.9
8	5	4	24.6	27.8
• 9	5	4	13.1	0.6
10	5	4	13.9	16.5
11	5	4	14.8	19.3
• 12	5	4	15.6	11.2
• 13	5	4	16.5	13.9
-12	6	4	15.6	18.6
•-11	6	4	14.8	8.9
-10	6	4	29.6	29.7
• -9	6	4	13.1	3.8
• -8	6	4	12.4	10.7
• -7	6	4	11.6	3.3
-6	6	4	32.6	33.4
• -5	6	4	10.2	5.5
-4	6	4	19.0	18.6
-3	6	4	61.2	57.0
-2	6	4	65.8	61.4
-1	6	4	40.0	36.7
0	6	4	147.7	148.3
1	6	4	48.4	44.8
2	6	4	12.1	10.8
• 3	6	4	9.1	7.0
4	6	4	33.6	31.5
5	6	4	26.4	25.4
6	6	4	40.7	39.5
• 7	6	4	11.8	7.8
8	6	4	33.3	33.3
• 9	6	4	13.4	7.2
10	6	4	34.8	35.8
• 11	6	4	15.0	8.3
• 12	6	4	15.8	5.9
•-12	7	4	15.8	6.4
•-11	7	4	15.0	5.5
-10	7	4	30.2	28.2
• -9	7	4	13.4	6.8
-8	7	4	46.6	46.5
• -7	7	4	11.9	6.6
• -6	7	4	11.2	12.7
-5	7	4	21.2	17.8
-4	7	4	53.9	52.2
-3	7	4	9.5	8.4
-2	7	4	48.6	45.0
• -1	7	4	8.8	5.4
0	7	4	82.0	80.3
1	7	4	8.9	7.5
2	7	4	95.7	93.6
3	7	4	9.6	11.8
4	7	4	10.2	11.6
• 5	7	4	10.8	3.2
6	7	4	43.6	41.6
• 7	7	4	12.1	6.6
8	7	4	28.8	27.2
• 9	7	4	13.7	2.9
10	7	4	14.5	17.2
• 11	7	4	15.3	3.0
12	7	4	16.1	17.0
• -9	8	4	13.8	0.5
-8	8	4	13.0	14.4
-7	8	4	12.3	13.1
-6	8	4	52.9	54.0
-5	8	4	44.3	45.8
-4	8	4	10.5	11.8
• -3	8	4	10.1	6.0
-2	8	4	33.0	31.5
-1	8	4	38.7	38.8
0	8	4	65.6	66.8
1	8	4	17.9	17.9
2	8	4	24.1	22.3
3	8	4	36.8	33.6
4	8	4	56.1	54.6
5	8	4	19.5	21.2
6	8	4	48.2	47.1
7	8	4	12.5	9.7
8	8	4	16.2	18.2
9	8	4	14.0	16.0
-9	9	4	26.5	25.6
-8	9	4	13.4	14.9
-7	9	4	29.9	27.6
-6	9	4	29.8	28.5
-5	9	4	30.6	29.5
-4	9	4	50.8	50.9
-3	9	4	52.3	52.2
-2	9	4	14.6	16.9
• -1	9	4	10.2	1.3
0	9	4	20.2	21.3
1	9	4	40.9	41.7
2	9	4	29.5	27.8
3	9	4	30.5	28.5
• 4	9	4	11.2	3.9
5	9	4	37.1	36.7
6	9	4	28.9	25.8
7	9	4	36.6	33.4
• 8	9	4	13.6	9.9
• 9	9	4	14.3	10.5
• -9	10	4	14.5	2.2
• -8	10	4	13.9	7.6
-7	10	4	26.4	25.[illegible]
• -6	10	4	12.6	1.9
-5	10	4	53.4	54.6
-4	10	4	14.2	13.5
-3	10	4	23.9	23.0
-2	10	4	15.5	18.0
-1	10	4	41.9	41.1
• 0	10	4	10.8	7.7
1	10	4	32.6	32.0
2	10	4	32.2	30.5
3	10	4	39.4	40.8
• 4	10	4	11.8	4.9
5	10	4	54.1	53.8
• 6	10	4	12.8	6.7
• 7	10	4	13.4	8.7
• 8	10	4	14.0	2.4
9	10	4	20.8	20.5
-9	11	4	21.1	20.4
• -8	11	4	14.3	5.7
-7	11	4	16.8	17.8
• -6	11	4	13.1	1.5
-5	11	4	23.6	28.8
• -4	11	4	12.2	9.9
-3	11	4	41.1	41.3
-2	11	4	36.7	36.1
• -1	11	4	11.4	10.9
• 0	11	4	11.4	9.0
1	11	4	28.1	28.6
• 2	11	4	11.7	3.1
3	11	4	45.5	47.6
• 4	11	4	12.3	4.3
5	11	4	20.2	21.6
6	11	4	13.3	12.8
7	11	4	21.9	21.8
8	11	4	14.5	16.2
• 9	11	4	15.1	3.3
• -8	12	4	14.8	13.3
-7	12	4	14.2	16.0
-6	12	4	30.5	31.8
-5	12	4	16.1	18.7
• -4	12	4	12.8	9.1
-3	12	4	19.7	22.9
-2	12	4	24.4	20.5
-1	12	4	34.2	30.8
0	12	4	31.9	29.8
1	12	4	19.1	20.9
2	12	4	27.5	26.6
3	12	4	15.4	15.8
4	12	4	20.4	24.1
5	12	4	26.6	25.5
• 6	12	4	13.8	10.4
• 7	12	4	14.3	6.5
8	12	4	14.9	16.3
-8	13	4	32.3	30.1
• -7	13	4	14.7	0.1
• -6	13	4	14.2	1.9
• -5	13	4	13.7	4.8
-4	13	4	16.4	15.3
• -3	13	4	13.1	6.0
-2	13	4	22.3	23.2
• -1	13	4	12.7	7.1
0	13	4	23.7	21.1
• 1	13	4	12.7	1.4
2	13	4	31.6	33.8
• 3	13	4	13.1	10.1
• 4	13	4	13.5	10.8
• 5	13	4	13.9	2.2
6	13	4	17.5	18.7
• 7	13	4	14.8	5.2
8	13	4	18.9	19.0
-6	14	4	23.3	25.9
• -5	14	4	14.3	4.4
• -4	14	4	13.9	6.0
• -3	14	4	13.7	1.6
-2	14	4	21.3	22.5
• -1	14	4	13.4	1.1
0	14	4	23.1	24.7
• 1	14	4	13.4	7.3
2	14	4	13.5	9.0
• 3	14	4	13.7	1.1
4	14	4	22.2	23.3
• 5	14	4	14.4	1.7
• 6	14	4	14.9	9.6
• -5	15	4	14.9	6.5
-4	15	4	17.8	18.3
-3	15	4	14.3	16.2
-2	15	4	17.3	17.5
• -1	15	4	14.0	2.1
• 0	15	4	14.0	7.1
• 1	15	4	14.0	7.5
2	15	4	17.3	15.7
3	15	4	14.4	16.1
• 4	15	4	14.6	1.2
• 5	15	4	15.0	13.9
•-13	0	5	14.6	7.0
-11	0	5	31.2	32.2
-9	0	5	57.7	58.5
-7	0	5	23.3	24.4
• -5	0	5	8.0	4.6
• -3	0	5	6.0	5.4
3	0	5	20.3	19.0
5	0	5	52.6	50.1
7	0	5	34.7	31.9
9	0	5	24.1	25.9
11	0	5	20.0	19.6
• 13	0	5	14.9	8.7
-13	1	5	20.7	19.7
•-12	1	5	13.8	12.9
-11	1	5	22.6	23.9
•-10	1	5	12.2	3.1
-9	1	5	33.7	33.8
-8	1	5	34.3	33.6
-7	1	5	65.5	63.7
-6	1	5	14.1	15.7
• -5	1	5	8.0	1.0
-4	1	5	21.1	19.8
-3	1	5	48.2	50.1
-2	1	5	18.7	19.1
2	1	5	55.9	60.9
3	1	5	120.3	130.5
4	1	5	34.0	35.9
5	1	5	13.9	14.8
6	1	5	21.1	18.6
7	1	5	58.2	57.1
8	1	5	13.3	12.8
9	1	5	36.1	36.2
• 10	1	5	12.5	6.6
• 11	1	5	13.3	11.9
• 12	1	5	14.1	6.3
13	1	5	14.9	16.3
•-12	2	5	13.9	8.3
•-11	2	5	13.1	11.1
-10	2	5	38.8	37.8
-9	2	5	16.2	17.3
-8	2	5	16.0	13.5
-7	2	5	24.1	25.3
-6	2	5	39.9	37.4
-5	2	5	33.0	33.1
-4	2	5	54.8	54.2
-3	2	5	26.0	26.5
-2	2	5	29.2	29.1
-1	2	5	9.5	11.0

Table 4 (*cont.*)

h	k	l	|F_o|	|F_c|
0	2	5	50.3	58.2
1	2	5	20.7	20.8
2	2	5	69.2	77.0
3	2	5	32.6	35.1
4	2	5	82.3	85.4
5	2	5	44.5	45.6
6	2	5	44.2	44.0
7	2	5	37.3	37.5
• 8	2	5	11.0	7.1
• 9	2	5	11.8	0.4
10	2	5	21.8	21.3
• 11	2	5	13.4	6.9
• 12	2	5	14.2	14.6
-12	3	5	25.2	28.0
•-11	3	5	13.2	9.7
•-10	3	5	12.4	6.4
• -9	3	5	11.6	1.7
-8	3	5	48.3	47.6
-7	3	5	20.0	20.1
-6	3	5	31.2	31.3
• -5	3	5	8.4	7.7
-4	3	5	63.0	60.5
-3	3	5	34.5	31.1
-2	3	5	68.1	70.0
-1	3	5	10.5	8.9
0	3	5	16.0	15.7
1	3	5	48.6	52.7
2	3	5	91.2	98.4
3	3	5	17.0	18.2
4	3	5	69.5	69.1
5	3	5	9.7	11.2
6	3	5	48.2	46.5
7	3	5	23.0	23.0
8	3	5	34.6	33.9
• 9	3	5	11.9	6.9
10	3	5	12.7	15.0
• 11	3	5	13.5	5.0
12	3	5	14.3	15.9
•-11	4	5	13.3	3.8
-10	4	5	39.1	36.5
-9	4	5	11.7	11.6
-8	4	5	17.3	16.6
-7	4	5	43.3	39.9
-6	4	5	37.8	37.9
-5	4	5	34.8	32.1
-4	4	5	61.0	55.9
-3	4	5	44.9	39.1
-2	4	5	35.6	33.2
-1	4	5	7.6	6.6
0	4	5	73.3	77.5
1	4	5	43.1	43.9
2	4	5	56.4	57.4
3	4	5	28.6	28.6
4	4	5	74.7	77.7
5	4	5	31.4	32.6
6	4	5	65.2	63.2
• 7	4	5	10.5	5.4
• 8	4	5	11.2	1.9
9	4	5	18.1	15.2
10	4	5	24.0	23.2
• 11	4	5	13.6	5.0
•-11	5	5	13.5	13.4
•-10	5	5	12.7	9.8
-9	5	5	18.9	19.7
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-7	5	5	24.0	24.3
-6	5	5	49.2	46.6
-5	5	5	20.2	18.3
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-2	5	5	28.1	29.4
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2	5	5	76.1	76.8
3	5	5	45.1	44.3
4	5	5	67.1	65.9
• 5	5	5	9.3	8.0
6	5	5	22.4	21.5
7	5	5	17.0	17.8
8	5	5	29.3	26.2
9	5	5	17.3	16.6
10	5	5	13.0	10.8
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-7	6	5	27.4	25.2
• -6	6	5	10.1	0.9
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• -4	6	5	8.8	8.8
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-2	6	5	40.3	36.3
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• 2	6	5	8.0	5.7
3	6	5	24.0	25.8
• 4	6	5	9.0	6.6
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6	6	5	26.8	26.2
7	6	5	28.6	29.2
• 8	6	5	11.7	0.1
9	6	5	29.9	27.3
• 10	6	5	13.2	9.6
11	6	5	18.5	20.2
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• -8	7	5	11.8	10.2
-7	7	5	49.3	45.8
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-5	7	5	12.1	11.6
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-3	7	5	37.5	34.2
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-1	7	5	50.1	49.9
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2	7	5	9.6	10.6
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• 8	7	5	12.0	2.9
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• 10	7	5	13.5	1.0
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4	8	5	15.7	16.8
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8	8	5	17.4	15.4
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• 9	10	5	13.7	4.9
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2	11	5	30.2	30.2
• 3	11	5	11.1	10.6
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• 6	11	5	12.4	9.5
7	11	5	12.9	14.7
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• 3	14	5	12.8	3.9
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• 2	15	5	13.1	6.5
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• -2	16	5	13.7	6.1
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•-12	0	6	13.6	3.5
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• 4	0	6	7.3	0.5
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2	1	6	37.7	42.8
3	1	6	31.9	33.4
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• 13	1	6	14.7	4.6
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• 5	13	6	12.7	1.9
-4	14	6	16.9	17.8
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-2	14	6	12.3	13.8
• -1	14	6	12.2	8.2
0	14	6	27.3	27.0
• 1	14	6	12.2	12.0
2	14	6	28.4	26.2
3	14	6	12.6	11.2
• 4	14	6	12.9	9.3
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• 0	15	6	12.8	11.0
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• 3	15	6	13.1	9.5
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-7	0	7	41.9	43.0
-5	0	7	14.1	12.5
-3	0	7	80.6	86.6
3	0	7	43.4	47.2
5	0	7	14.0	14.1
7	0	7	45.7	44.0
• 9	0	7	18.3	9.8
• 11	0	7	20.7	17.5
•-11	1	7	20.2	13.3
•-10	1	7	18.9	12.8
• -9	1	7	17.7	11.6
• -8	1	7	16.4	5.3
-7	1	7	29.2	32.1
-6	1	7	13.8	13.2
-5	1	7	59.7	60.3
-4	1	7	18.2	18.8
-3	1	7	16.0	18.0
-2	1	7	39.0	43.8
1	1	7	38.1	44.5
2	1	7	20.6	22.9
• 3	1	7	10.3	8.1
• 4	1	7	11.8	9.7
5	1	7	31.1	29.4
6	1	7	14.5	14.4
7	1	7	23.9	21.3
• 8	1	7	17.1	6.7
9	1	7	30.2	27.1
• 10	1	7	19.6	12.9
• 11	1	7	20.8	14.1
•-11	2	7	20.3	3.1
•-10	2	7	19.0	13.7
-9	2	7	20.2	19.1
-8	2	7	25.8	25.4
-7	2	7	18.3	17.1
-6	2	7	25.9	26.0
-5	2	7	33.6	34.9
-4	2	7	65.0	72.3
-3	2	7	62.6	70.5
-2	2	7	44.5	48.7
-1	2	7	46.5	44.9
0	2	7	9.5	10.5
1	2	7	26.1	27.0
2	2	7	36.9	38.5
• 3	2	7	10.6	10.7
4	2	7	22.3	20.6
5	2	7	13.4	13.2
6	2	7	26.0	25.0
7	2	7	35.1	33.8
8	2	7	31.8	27.8
• 9	2	7	18.4	9.4
• 10	2	7	19.7	1.0
• 11	2	7	20.9	10.1
•-11	3	7	20.4	1.4
•-10	3	7	19.2	13.6
• -9	3	7	18.0	0.6
• -8	3	7	16.8	7.0
• -7	3	7	15.5	12.4
-6	3	7	56.7	59.4
• -5	3	7	13.0	1.7
-4	3	7	61.5	68.5
-3	3	7	13.2	14.0
-2	3	7	41.1	45.9
• -1	3	7	8.5	0.3
0	3	7	37.9	44.0
1	3	7	12.5	12.6
2	3	7	20.6	21.0
3	3	7	12.7	11.3
4	3	7	43.3	46.3
• 5	3	7	13.7	3.5
6	3	7	38.7	36.2
• 7	3	7	16.2	4.6
• 8	3	7	17.4	8.9
• 9	3	7	18.6	2.3
10	3	7	27.0	24.5
• 11	3	7	21.0	5.5
•-10	4	7	19.4	14.1
• -9	4	7	18.2	2.4
-8	4	7	24.9	26.6
• -7	4	7	15.9	2.9
-6	4	7	17.5	18.3
• -5	4	7	13.5	7.4
-4	4	7	58.2	65.7
-3	4	7	21.7	21.7
-2	4	7	55.9	61.5
• -1	4	7	9.7	6.9
• 0	4	7	9.5	7.2
• 1	4	7	10.0	0.6
2	4	7	41.8	45.4
• 3	4	7	11.8	0.8
4	4	7	31.7	29.1
5	4	7	16.0	14.7
6	4	7	27.7	28.9
• 7	4	7	16.4	12.4
8	4	7	22.1	21.4
• 9	4	7	18.8	9.4
• 10	4	7	20.0	1.6
•-10	5	7	19.7	13.1
• -9	5	7	18.5	14.7
• -8	5	7	17.4	2.6
-7	5	7	20.4	19.1
-6	5	7	39.6	39.6
-5	5	7	38.3	40.9
-4	5	7	30.7	30.0
• -3	5	7	12.1	0.9
-2	5	7	28.7	30.2
-1	5	7	56.3	57.6
0	5	7	57.2	56.2
1	5	7	14.4	13.2
2	5	7	26.1	24.8
3	5	7	27.2	26.5
4	5	7	38.3	35.0
5	5	7	33.6	32.4
• 6	5	7	15.7	14.2
7	5	7	16.8	12.8
• 8	5	7	18.0	9.1
9	5	7	24.0	21.4
10	5	7	21.7	19.1
•-10	6	7	20.0	8.9
-9	6	7	21.4	20.3
• -8	6	7	17.8	12.9
-7	6	7	26.8	29.4
• -6	6	7	15.7	5.3
• -5	6	7	14.7	10.5
-4	6	7	13.7	13.1
-3	6	7	44.2	43.6
-2	6	7	22.7	22.4
-1	6	7	25.4	26.3
• 0	6	7	11.8	8.1
1	6	7	47.7	45.4
2	6	7	14.2	14.0
3	6	7	33.4	30.4
• 4	6	7	14.2	5.6
5	6	7	19.0	15.3
• 6	6	7	16.2	11.1
7	6	7	26.9	28.8
• 8	6	7	18.4	2.1
• 9	6	7	19.5	17.6
• 10	6	7	20.6	2.1
-9	7	7	19.3	16.6
• -8	7	7	18.2	11.9
-7	7	7	28.4	31.0
• -6	7	7	16.2	7.5
-5	7	7	32.2	33.5
• -4	7	7	14.5	0.3
• -3	7	7	13.8	6.1
-2	7	7	17.3	17.0
-1	7	7	67.1	68.2
• 0	7	7	12.8	4.0
1	7	7	40.2	38.0
• 2	7	7	13.5	5.1
3	7	7	17.7	17.8
• 4	7	7	14.9	0.4
5	7	7	33.7	31.9
• 6	7	7	16.7	7.3
• 7	7	7	17.7	5.4
• 8	7	7	18.8	1.3
9	7	7	26.0	24.4
-9	8	7	19.8	18.1
• -8	8	7	18.8	13.1
-7	8	7	17.8	17.9
-6	8	7	23.8	23.8
-5	8	7	19.1	19.1
-4	8	7	15.2	13.1
-3	8	7	33.6	35.1
• -2	8	7	14.1	13.6
-1	8	7	40.5	38.2
0	8	7	22.7	19.0
1	8	7	29.8	26.7
2	8	7	29.2	27.3
3	8	7	27.6	24.6
4	8	7	24.3	23.8
• 5	8	7	16.4	1.3
• 6	8	7	17.3	10.8
7	8	7	22.9	20.9
• 8	8	7	19.3	11.9
• 9	8	7	20.3	12.0
• -8	9	7	19.3	2.2
-7	9	7	25.1	23.7
-6	9	7	26.5	27.7
-5	9	7	21.0	20.2
-4	9	7	21.0	21.5
• -3	9	7	15.5	9.2
-2	9	7	23.4	26.2
-1	9	7	17.7	17.7
0	9	7	28.4	27.3
1	9	7	21.8	19.6
• 2	9	7	15.2	4.8
3	9	7	22.2	20.8
4	9	7	35.5	32.9
5	9	7	19.4	18.7
• 6	9	7	18.0	14.6
• 7	9	7	18.9	1.4
• 8	9	7	19.8	4.0
• -8	10	7	19.9	16.2
• -7	10	7	19.0	3.2
• -6	10	7	18.2	8.7
• -5	10	7	17.5	2.8
-4	10	7	31.1	31.3
• -3	10	7	16.3	1.0
-2	10	7	34.6	34.0
• -1	10	7	15.7	8.3
• 0	10	7	15.7	1.1
• 1	10	7	15.8	5.1
2	10	7	36.0	33.6
• 3	10	7	16.5	6.9
4	10	7	19.4	18.8
• 5	10	7	17.8	1.1
6	10	7	25.4	21.8
• 7	10	7	19.5	2.6
8	10	7	21.8	18.8
• -7	11	7	19.7	1.6
-6	11	7	22.6	19.7
• -5	11	7	18.2	4.8
• -4	11	7	17.6	11.6
• -3	11	7	17.2	11.0
-2	11	7	22.0	21.8
• -1	11	7	16.6	7.0
0	11	7	29.4	27.2
• 1	11	7	16.7	2.4
• 2	11	7	17.0	8.9
• 3	11	7	17.4	4.4
4	11	7	28.7	28.9
• 5	11	7	18.6	12.1
• 6	11	7	19.3	10.6
• 7	11	7	20.1	11.0
• -5	12	7	19.0	3.7
• -4	12	7	18.4	14.1
• -3	12	7	18.0	15.5
• -2	12	7	17.7	13.0
• -1	12	7	17.5	6.6
• 0	12	7	17.5	0.2
1	12	7	29.7	31.9
2	12	7	26.1	26.6
3	12	7	21.8	19.9
• 4	12	7	18.7	10.5
• 5	12	7	19.3	0.0
• -3	13	7	18.9	3.3
• -2	13	7	18.6	1.9
-1	13	7	25.1	22.9
• 0	13	7	18.4	4.3
1	13	7	20.9	21.4
• 2	13	7	18.7	1.9
• 3	13	7	19.1	8.9
• -1	14	7	19.3	12.0
• 0	14	7	19.3	2.7
1	14	7	22.0	19.6
•-12	0	8	18.9	17.3
•-10	0	8	16.8	4.3
-8	0	8	27.7	28.0
-6	0	8	13.0	12.5
-4	0	8	22.3	19.3
-2	0	8	63.2	71.4
2	0	8	46.4	51.3
4	0	8	17.4	17.3
• 6	0	8	12.9	8.1
8	0	8	26.3	27.0
• 10	0	8	17.4	10.1
• 12	0	8	19.5	3.9
•-11	1	8	17.9	9.0
-10	1	8	22.2	21.4
• -9	1	8	15.7	9.0
-8	1	8	15.5	13.3
• -7	1	8	13.5	3.7
-6	1	8	19.0	18.8
-5	1	8	18.8	16.6
-4	1	8	42.5	41.0
-3	1	8	16.0	14.2
-2	1	8	15.2	15.0
1	1	8	36.5	38.4
2	1	8	40.7	45.5
• 3	1	8	9.2	4.3
• 4	1	8	10.6	8.2
• 5	1	8	11.8	10.0
6	1	8	34.0	34.6
• 7	1	8	14.1	5.8
• 8	1	8	15.2	12.6

Table 4 (*cont.*)

	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
•	9	1	8	16.3	4.6
	10	1	8	18.5	18.0
•	11	1	8	18.5	8.8
•	-11	2	8	17.9	12.1
•	-10	2	8	16.9	4.8
•	-9	2	8	15.8	9.4
	-8	2	8	18.0	13.0
	-7	2	8	15.2	16.0
•	-6	2	8	12.5	4.7
	-5	2	8	27.1	25.1
	-4	2	8	15.5	14.4
	-3	2	8	37.4	39.6
	-2	2	8	36.4	38.8
	-1	2	8	41.8	46.6
	0	2	8	11.5	13.7
•	1	2	8	6.9	6.4
	2	2	8	26.1	29.5
	3	2	8	44.0	48.0
	4	2	8	20.5	21.2
	5	2	8	21.6	19.6
•	6	2	8	13.1	7.8
•	7	2	8	14.2	9.2
•	8	2	8	15.3	9.2
	9	2	8	18.4	16.3
•	10	2	8	17.5	3.2
•	11	2	8	18.5	3.2
•	-11	3	8	18.1	14.5
•	-10	3	8	17.0	1.3
	-9	3	8	17.9	14.7
•	-8	3	8	14.9	4.0
•	-7	3	8	13.8	2.9
	-6	3	8	18.0	15.6
	-5	3	8	46.8	46.4
	-4	3	8	12.9	13.0
	-3	3	8	41.2	38.8
•	-2	3	8	8.3	2.5
	-1	3	8	32.6	35.6
	0	3	8	13.5	15.0
	1	3	8	54.0	59.4
	2	3	8	15.4	15.0
•	3	3	8	10.0	5.4
•	4	3	8	11.1	5.6
	5	3	8	37.5	38.6
	6	3	8	14.9	13.7
	7	3	8	26.0	21.8
•	8	3	8	15.5	2.3
•	9	3	8	16.6	0.9
•	10	3	8	17.6	4.7
•	11	3	8	18.7	15.1
•	-11	4	8	18.2	14.3
•	-10	4	8	17.2	1.6
•	-9	4	8	16.2	6.7
•	-8	4	8	15.1	9.3
	-7	4	8	22.3	21.4
•	-6	4	8	13.0	10.0
•	-5	4	8	12.0	8.7
•	-4	4	8	11.0	7.4
	-3	4	8	50.2	52.0
	-2	4	8	20.6	21.4
	-1	4	8	49.2	50.4
	0	4	8	10.9	12.3
•	1	4	8	8.9	1.9
	2	4	8	21.6	24.8
	3	4	8	43.0	47.8
•	4	4	8	11.6	4.5
	5	4	8	20.9	19.6
•	6	4	8	13.7	4.2
	7	4	8	14.7	14.0
•	8	4	8	15.7	12.3
	9	4	8	21.4	19.6
•	10	4	8	17.8	4.5
•	11	4	8	18.8	3.8
•	-11	5	8	18.5	9.9
•	-10	5	8	17.5	13.3
•	-9	5	8	16.4	15.9
•	-8	5	8	15.4	4.2
•	-7	5	8	14.5	1.6
	-6	5	8	15.1	13.2
	-5	5	8	26.9	27.1
	-4	5	8	26.6	27.2
	-3	5	8	10.7	11.2
	-2	5	8	21.9	22.2
	-1	5	8	33.2	35.4
	0	5	8	35.1	36.0
	1	5	8	42.0	45.2
•	2	5	8	10.4	4.3
	3	5	8	27.5	26.0
	4	5	8	13.5	12.9
	5	5	8	23.5	24.5
	6	5	8	17.9	17.8
•	7	5	8	15.0	8.1
•	8	5	8	16.0	9.2
•	9	5	8	17.0	4.6
•	10	5	8	18.0	7.1
•	11	5	8	19.0	13.1
•	-11	6	8	18.7	3.4
•	-10	6	8	17.7	6.7
•	-9	6	8	16.8	0.6
	-8	6	8	27.9	24.1
•	-7	6	8	14.8	10.6
	-6	6	8	26.5	25.0
•	-5	6	8	13.0	7.1
•	-4	6	8	12.2	3.1
	-3	6	8	24.1	21.5
	-2	6	8	52.3	52.5
	-1	6	8	10.6	9.4
	0	6	8	26.6	26.8
•	1	6	8	10.7	4.7
	2	6	8	42.6	40.9
	3	6	8	18.3	18.2
	4	6	8	34.2	32.5
•	5	6	8	13.5	11.4
•	6	6	8	14.5	4.4
•	7	6	8	15.4	3.8
	8	6	8	25.2	24.3
•	9	6	8	17.3	4.6
•	10	6	8	18.3	10.1
•	11	6	8	19.3	0.2
•	-11	7	8	19.0	6.1
	-10	7	8	20.2	17.6
•	-9	7	8	17.1	4.4
	-8	7	8	16.2	15.5
•	-7	7	8	15.3	6.8
	-6	7	8	24.0	22.0
•	-5	7	8	13.6	5.3
	-4	7	8	20.4	20.7
•	-3	7	8	12.2	8.3
•	-2	7	8	11.8	2.1
•	-1	7	8	11.5	1.2
	0	7	8	53.1	53.1
•	1	7	8	11.6	3.8
	2	7	8	26.6	26.2
•	3	7	8	12.6	3.2
•	4	7	8	13.3	7.9
•	5	7	8	14.1	2.4
	6	7	8	20.5	20.3
•	7	7	8	15.8	0.1
•	8	7	8	16.7	4.9
•	9	7	8	17.7	0.9
•	10	7	8	18.6	11.9
•	11	7	8	19.5	3.3
•	-10	8	8	18.4	8.5
•	-9	8	8	17.5	6.8
	-8	8	8	16.7	16.2
	-7	8	8	17.7	16.3
	-6	8	8	19.1	16.7
	-5	8	8	14.2	13.3
•	-4	8	8	13.6	11.4
	-3	8	8	13.0	12.5
	-2	8	8	37.2	38.3
	-1	8	8	16.3	17.5
	0	8	8	23.4	22.8
•	1	8	8	12.5	6.1
	2	8	8	21.2	22.4
	3	8	8	16.2	19.5
	4	8	8	31.2	32.1
•	5	8	8	14.7	1.0
•	6	8	8	15.5	2.0
•	7	8	8	16.3	9.3
	8	8	8	21.9	20.3
•	9	8	8	18.1	9.4
•	10	8	8	19.0	8.2
•	-10	9	8	18.8	5.6
•	-9	9	8	18.0	12.3
•	-8	9	8	17.1	3.2
•	-7	9	8	16.3	4.2
	-6	9	8	20.6	17.5
	-5	9	8	23.5	22.9
•	-4	9	8	14.3	11.3
	-3	9	8	26.2	24.5
•	-2	9	8	13.4	5.5
•	-1	9	8	13.2	7.9
	0	9	8	16.1	11.5
	1	9	8	23.0	22.0
•	2	9	8	13.6	10.5
•	3	9	8	14.0	10.3
•	4	9	8	14.6	4.8
	5	9	8	26.4	25.3
•	6	9	8	16.0	11.7
•	7	9	8	16.8	13.3
•	8	9	8	17.6	2.0
•	9	9	8	18.5	2.1
•	10	9	8	19.3	3.1
•	-9	10	8	18.4	6.8
•	-8	10	8	17.7	0.2
	-7	10	8	26.7	23.6
•	-6	10	8	16.2	1.1
•	-5	10	8	15.5	10.7
•	-4	10	8	15.0	12.4
	-3	10	8	28.1	28.2
•	-2	10	8	14.2	4.7
	-1	10	8	23.7	18.6
•	0	10	8	14.0	5.1
•	1	10	8	14.1	3.0
•	2	10	8	14.4	1.1
	3	10	8	33.0	33.9
•	4	10	8	15.3	7.5
•	5	10	8	15.9	9.4
•	6	10	8	16.6	1.0
•	7	10	8	17.3	12.8
•	8	10	8	18.1	3.9
•	9	10	8	18.9	10.5
•	-8	11	8	18.2	5.2
•	-7	11	8	17.5	3.1
•	-6	11	8	16.8	6.3
	-5	11	8	21.4	22.3
•	-4	11	8	15.7	11.9
	-3	11	8	15.3	12.8
	-2	11	8	18.3	13.8
•	-1	11	8	14.8	9.2
•	0	11	8	14.8	9.0
	1	11	8	21.7	21.7
•	2	11	8	15.1	0.9
	3	11	8	15.5	12.0
•	4	11	8	16.0	8.6
	5	11	8	18.5	19.0
•	6	11	8	17.2	9.9
•	7	11	8	17.9	11.0
•	8	11	8	18.6	4.2
•	-6	12	8	17.4	9.9
•	-5	12	8	16.9	3.9
•	-4	12	8	16.4	0.8
	-3	12	8	21.9	18.1
	-2	12	8	15.7	14.4
•	-1	12	8	15.6	8.7
•	0	12	8	15.6	9.2
•	1	12	8	15.7	0.1
•	2	12	8	15.9	9.6
	3	12	8	18.1	16.7
•	4	12	8	16.7	8.6
•	5	12	8	17.2	6.5
•	6	12	8	17.8	0.2
•	-6	13	8	18.1	8.8
•	-5	13	8	17.6	4.2
	-4	13	8	19.1	14.3
•	-3	13	8	16.8	2.2
•	-2	13	8	16.5	3.5
•	-1	13	8	16.4	5.2
	0	13	8	20.0	20.6
•	1	13	8	16.4	6.1
	2	13	8	18.6	15.3
•	3	13	8	17.0	3.3
•	4	13	8	17.4	4.9
•	5	13	8	17.9	1.7
	6	13	8	19.5	14.7

Table 5. *Bond distances and bond angles in* $SbCl_5$. $HCON(CH_3)_2$ *with their standard deviations*

	Distance	σ
Sb(1)-Cl(2)	2·330 Å	0·003 Å
Sb(1)-Cl(3)	2·336	0·003
Sb(1)-Cl(4)	2·343	0·003
Sb(1)-Cl(5)	2·353	0·003
Sb(1)-Cl(6)	2·332	0·003
Sb(1)-O(1)	2·048	0·006
O(7)—C(8)	1·300	0·010
C(8)—N(11)	1·287	0·012
N(11)-C(9)	1·504	0·012
N(11)-C(10)	1·505	0·014

	Angle	σ
Cl(2)-Sb(1)-Cl(3)	93·49°	0·12°
Cl(2)-Sb(1)-Cl(4)	92·90	0·14
Cl(2)-Sb(1)-Cl(5)	93·15	0·11
Cl(2)-Sb(1)-Cl(6)	92·54	0·13
Cl(2)-Sb(1)-O(7)	177·11	0·19
Cl(3)-Sb(1)-Cl(4)	91·18	0·12
Cl(3)-Sb(1)-Cl(5)	173·33	0·10
Cl(3)-Sb(1)-Cl(6)	89·68	0·12
Cl(3)-Sb(1)-O(7)	84·69	0·20
Cl(4)-Sb(1)-Cl(5)	89·02	0·11
Cl(4)-Sb(1)-Cl(6)	174·43	0·11
Cl(4)-Sb(1)-O(7)	89·39	0·22
Cl(5)-Sb(1)-Cl(6)	89·49	0·11
Cl(5)-Sb(1)-O(7)	88·65	0·20
Cl(6)-Sb(1)-O(7)	85·21	0·21
Sb(1)-O(7)—C(8)	124·49	0·60
O(7) -C(8)—N(11)	120·15	0·89
C(8) -N(11)-C(9)	120·20	0·92
C(8) -N(11)-C(10)	122·08	0·82
C(9) -N(11)-C(10)	117·67	0·89

Table 6. *Intramolecular, non-covalent distances less than* 4·0 Å *in* $SbCl_5$. $HCON(CH_3)_2$

Sb(1)-C(8)	2·98 Å
Cl(2)-Cl(3)	3·40
Cl(2)-Cl(4)	3·39
Cl(2)-Cl(5)	3·40
Cl(2)-Cl(6)	3·37
Cl(3)-Cl(4)	3·34
Cl(3)-Cl(6)	3·29
Cl(3)-O(7)	2·96 Å
Cl(4)-Cl(5)	3·29
Cl(4)-O(7)	3·10
Cl(4)-C(8)	3·24
Cl(5)-Cl(6)	3·30
Cl(5)-O(7)	3·08
Cl(5)-C(8)	3·28
Cl(6)-O(7)	2·97
O(7) -C(9)	3·62
O(7) -C(10)	2·74
O(7) -N(11)	2·24
C(8) -C(9)	2·42
C(8) -C(10)	2·44
C(9) -C(10)	2·57

Table 7. *Intermolecular distances less than* 4·0 Å *in* $SbCl_5$. $HCON(CH_3)_2$

Cl(2)*A*-Cl(5)*G*	3·98 Å	Cl(3)*A*-N(11)*C*	3·90 Å
Cl(2)*A*-Cl(6)*G*	3·74	Cl(4)*A*-O(7)*C*	3·70
Cl(2)*A*-O(7)*G*	3·49	Cl(4)*A*-C(8)*C*	3·73
Cl(2)*A*-C(8)*G*	3·57	Cl(4)*A*-C(9)*G*	3·99
Cl(2)*A*-C(9)*B*	3·61	Cl(4)*A*-C(10)*C*	3·57
Cl(2)*A*-C(10)*G*	3·68	Cl(4)*A*-N(11)*C*	3·69
Cl(2)*A*-N(11)*G*	3·60	Cl(5)*A*-Cl(6)*F*	3·86
Cl(3)*A*-Cl(4)*C*	3·89	Cl(5)*A*-C(10)*I*	3·87
Cl(3)*A*-Cl(5)*H*	3·77	Cl(5)*A*-C(10)*G*	3·94
Cl(3)*A*-C(8)*C*	3·80	Cl(6)*A*-C(8)*E*	3·80
Cl(3)*A*-C(9)*B*	3·66	Cl(6)*A*-C(9)*E*	3·98
Cl(3)*A*-C(9)*C*	3·74	Cl(6)*A*-C(10)*D*	3·38
Cl(3)*A*-C(10)*D*	3·95		

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

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

Sumarokova & Filimonov, 1961) and crystal structure determinations of adducts between $CdCl_2$ and a number of amides (Cavalca, Nardelli & Coghi, 1957; Nardelli, Cavalca & Fava, 1957; Nardelli, Coghi & Azzoni, 1958; Cavalca, Nardelli & Fava, 1960) demonstrate that addition to the carbonyl oxygen is of frequent occurrence. The acceptor atom in the adduct molecule $SbCl_5 . HCON(CH_3)_2$ exhibits a change of coordination from trigonal bipyramidal in free $SbCl_5$ to distorted octahedral in the adduct. The average Sb–Cl bond length is 2·34 Å. Corresponding values for the adducts $SbCl_5 . (CH_3)_3PO$ and $SbCl_5 . POCl_3$ (Brändén & Lindqvist, 1963) are 2·34 Å and 2·33 Å respectively.

Lindqvist and co-workers (Brändén, Hansson, Hermodsson & Lindqvist, 1962; Lindqvist, 1963) have shown that the observed deviations from ideal octahedral coordination of the acceptor atom in the last two adducts can be interpreted as arising from two steric factors, the van der Waals radii of the ligand atoms and their distances from the antimony atom. The Sb–O bond length in the $SbCl_5 . HCON(CH_3)_2$ molecule is 2·05 Å, the average of the Cl–Sb–O bond angles is 87·0° and the averages of the Cl–Sb–Cl bond angles and the Cl*–Sb–Cl bond angles are 89·8° and 93·0°, respectively. (Cl* is the chlorine atom opposite the oxygen atom.) These values are compared in Table 8 with those of the other two $SbCl_5$ adducts. The steric influence of the Sb–O distance on the magnitude of the bond angles is clearly demonstrated in this table. An increasing Sb–O distance is accompanied by a decrease in the bond angle Cl–Sb–O and an increase in the bond angle Cl*–Sb–Cl. From the Sb–O distances obtained in these adducts it may be concluded that, with $SbCl_5$ as acceptor, the amide is a stronger donor than $POCl_3$ but weaker than $(CH_3)_3PO$. Similar results were obtained in the thermochemical study by Zackrisson (Lindqvist & Zackrisson, 1960; Zackrisson, 1961).

Table 8. *Bond angles (average values) around the acceptor atom in* $SbCl_5 . D$ *adducts*

D	$(CH_3)_3PO$	$HCON(CH_3)_2$	$POCl_3$
Sb–O	1·94 Å	2·05 Å	2·18 Å
Cl—Sb–O	88·3°	87·0°	85·3°
Cl—Sb–Cl	90·0	89·8	89·6
Cl*–Sb–Cl	91·8	93·0	94·7

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 Sb–O–C bond angle of 124·5° in the $SbCl_5 . HCON(CH_3)_2$ molecule is considerably less than the Sb–O–P angles of 144·9° and 145·0° in the adduct molecules $SbCl_5 . (CH_3)_3PO$ and $SbCl_5 . POCl_3$, respectively.

A recent electron diffraction study of $HCON(CH_3)_2$ in the vapor phase by Vilkov, Akishin & Presnyakova (1962) indicates that the amide molecule possesses a nearly planar framework. In that investigation the angle OCN was assumed to be 123° and the C–H bond lengths 1·09 Å. The following structural parameters were determined: angle CNC′ = angle CNC″ = 117·5° ± 2°, r(C–N) = 1·34 ± 0·04 Å, r(C′–N) = r(C″–N) = 1·45 ± 0·02 Å and r(C=O) = 1·20 Å. (C′ is the methyl carbon atom *trans* to the oxygen atom and C″ is the other methyl carbon atom.) These values can be compared with microwave studies of formamide (Kurland & Wilson, 1957; Costain & Dowling, 1960) which yield 1·193 ± 0·020 Å (r_0) and 1·243 ± 0·070 Å (r_0) for the C=O bond length and 1·376 ± 0·010 Å (r_0) and 1·343 ± 0·007 Å (r_0) for the C–N bond length. These studies indicate that r(C=O) = 1·20 Å is a fairly accurate value. Lide (1962) has suggested that the length of a C–N bond with carbon hybridized in the sp^2 state is probably 1·36 ± 0·02 Å.

The coordination of nitrogen in the present adduct is almost planar, according to a least-squares fit of the atoms C(8), C(9), C(10) and N(11) to a plane using a

Table 9. *Deviations from the plane* $0·0941x+0·7619y+0·6409z-2·9107=0$ *found by a least-squares fit of the atoms* C(8), C(9), C(10) *and* N(11)

C(8)	−0·005 Å
C(9)	−0·004
C(10)	−0·004
N(11)	+0·013
O(7)	+0·040
Sb(1)	+0·044

Deviations from the plane $0·1150x+0·7894y+0·6030z-3·0155=0$ defined by the atoms O(7), C(8) and N(11)

C(9)	+0·034 Å
C(10)	−0·092
Sb(1)	+0·026

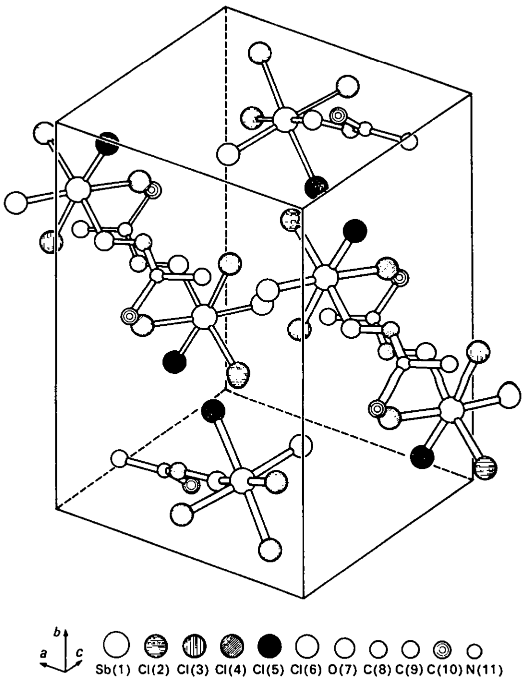
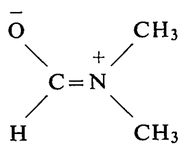


Fig. 2. The crystal structure of $SbCl_5 . HCON(CH_3)_2$.

method devised by Blow (1960). A dihedral angle of 2° 56′ has been found between this plane and that defined by the atoms O(7), C(8) and N(11). Vertical deviations of atoms from the coplanar positions are listed in Table 9.

The length of the carbon–oxygen bond of the adduct, 1·300 ± 0·030 Å seems to be significantly greater than that of the carbonyl bond of the free donor. A major consequence of donor–acceptor interaction is an electron density withdrawal from the oxygen atom leading to an increase in the heteropolarity of the carbonyl bond, a reduction of the bond order and consequently an increase in the bond length (Lindqvist, 1963).

The increase in the electronegativity of the carbonyl carbon atom which attends the formation of the adduct increases the σ-bond order of the C–N bond in the OCN group. It can be expected that the electron density withdrawal from the amide molecule increases the delocalization of the lone pair of electrons of the nitrogen atom. (The contribution of the ionic structure



increases). Thus the π-bond order of the C–N bond in the OCN group also increases. It is to be expected that these changes in the σ- and π-bond orders could lead to a decrease in the length of the bond. Owing, however, to the low accuracy of the determination of the C–N bond length in the free donor molecule the observed difference in length is not significant, but a comparison of the value 1·287 ± 0·036 Å for the adduct with the value 1·36 ± 0·02 Å proposed by Lide (1962) for free amides strongly supports these arguments. Spectroscopic evidence for a strengthening of the C–N bond in adducts of *N*,*N*-dimethylformamide with titanium(IV) halides as compared with the free donor have been reported (Archambault & Rivest, 1960).

The heteropolarity of the bonds from nitrogen to the methyl carbon atoms ought to increase owing to the withdrawal of electron density from the nitrogen atom. A bond length increase from 1·45 ± 0·02 Å in the free *N*,*N*-dimethylformamide to 1·504 ± 0·036 Å and 1·505 ± 0·042 Å respectively has been observed in the present adduct.

A similar change in the dimensions of the donor molecule accompanying adduct formation has been found in the adduct ($TiCl_4 . CH_3COOC_2H_5)_2$ (Brun, 1965). In this instance the acetyl–oxygen bond length decreases and the ethyl–oxygen bond length increases.

An X-ray crystal structure determination of the adduct $NaI . 3HCON(CH_3)_2$ has been reported (Gobillon, Piret & Van Meerssche, 1962). The carbon, nitrogen and oxygen atoms in the amide molecule were found to be coplanar. The structural parameters were: angle OCN = 123·6 ± 2°, angle CNC′ = 119·5 ± 2°, angle CNC″ = 119·6 ± 2°, r(C=O) = 1·23 ± 0·04 Å, r(C–N) = 1·34 ± 0·04 Å, r(C′–N) = 1·52 ± 0·04 Å and r(C″–N) = 1·45 ± 0·04 Å. Although the accuracy of this determination is not very high the dimensions obtained are nevertheless consistent with the picture given by the preceding discussion of the effects produced by a donor–acceptor interaction which is substantially weaker than that found in the present adduct.

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A Reinvestigation of the Crystal Structure of $LiIO_3$*

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The crystal structure of $LiIO_3$ has been reinvestigated with the use of single-crystal Mo $K\alpha$ diffractometer intensity data. Morphological measurements and diffraction photographs establish $P6_3$ to be the correct space group. The values for the lattice constants, $a_0 = 5{\cdot}1815$ and $c_0 = 5{\cdot}1709$, were determined by a least-squares fit of back-reflection powder lines. The structure consists of lithium ions, surrounded by six oxygen atoms in a distorted octahedral arrangement, and discrete trigonal iodate groups with a 1·817 Å iodine–oxygen bond distance and 98·65° O–I–O bond angle.

Introduction

As a result of discussions concerning naturally occurring iodates (Kaplan, 1966), we reviewed the literature on the configuration of iodate groups in crystalline solids. It was noted that the structure of $LiIO_3$ reported by Zachariasen & Barta (1931) (hereafter ZB) placed the iodine in an octahedral coordination with six equidistant oxygens, rather than in trigonal, pyramidal configuration as in other iodates. That the structure might merit reinvestigation was pointed out by Wyckoff (1960). This anomalous behavior of iodine in several alkali metal iodates has also been noted by Ibers (1956). On examination of the original paper of ZB, it became apparent that the structure was interpreted largely from powder diffraction data, and that the crystals available were extremely small. It is then not too surprising that an incorrect space group was chosen and erroneous positions were deduced for the lighter atoms. Since occasionally discrete molecules rearrange in the solid state when crystallized from gaseous or liquid state, (*e.g.* gaseous Al_2Cl_6 and infinite molecular sheets in crystalline $AlCl_3$), the structure of $LiIO_3$ merits reinvestigation.

Our structure results are reported here.

Experimental

Crystals of lithium iodate were prepared in the following manner: (1) stoichiometric quantities of reagent grade iodic acid and lithium carbonate were dissolved in water; (2) the solution was then warmed to remove any remaining carbon dioxide; (3) the solution was allowed to evaporate at room temperature until crystals began to form.

The crystals obtained are brilliant pseudo-prisms up to 0·5 mm long and 0·2 mm in diameter. Careful examination reveals that the apparent prisms are actually portions of extremely steep hexagonal pyramids. Morphological measurements made with a reflecting goniometer yielded results which permit the indexing of all but the very steep faces. The polar angle of these steep faces is so great that indexing becomes ambiguous. The approximate index of these faces, orienting them so that they taper toward the negative end of **c**, is $\{20\cdot0\cdot\overline{20}\cdot\bar{1}\}$. These are terminated by the forms $\{10\bar{1}1\}$, $\{10\bar{1}\bar{1}\}$, and very small faces of $\{12\bar{3}\bar{2}\}$. Mor-

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