anisotropic refinement). Since the results from all of the refinements were quite close, the fact that the standard errors for the isotropic group *A* refinement were the smallest was the deciding factor in listing the group *A* parameters in Table 1 and calculating from them the bond lengths and angles given in Table 2. The observed and calculated structure factors presented in Table 3 were obtained from the complete, anisotropic, refinement.

Discussion

The essential structural features of the original proposal of McCarroll, Katz & Ward (1957) were found to be correct. The structure consists of a distorted double-hexagonal closest packing (*abcb*) of oxygen atoms in which the oxygen layers are held together by alternate layers of zinc and molybdenum ions. Half of the zinc ions are in approximately tetrahedral coordination with oxygen; the other half are in approximately octahedral coordination. The molybdenum ions are in approximately octahedral coordination with oxygen with the octahedra sharing edges. The molybdenum ions lie in rows with alternately long and short spacings. The rows are arranged with threefold symmetry giving a pattern of molybdenum triangles. Fig. 1 shows this pattern of molybdenum ions and the edge sharing oxygen octahedra about one of the bonded groups (Mo–Mo distance = 2·52 Å). Fig. 2 shows the bonding scheme in the structure in more detail. Oxygen atoms in Fig. 2 are numbered as in Tables 1 and 2.

A final remark on the observed data: the 220 reflection, the one with the largest calculated structure factor, had an observed *F* too small by a factor of almost two in the original work; the new observed value agrees well with the calculated value.

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The Crystal Structure of Sodium Naphthionate Tetrahydrate

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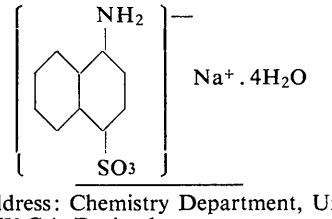
Three-dimensional X-ray diffraction data and electronic computing have been used to determine the positional and thermal atomic parameters in crystalline sodium naphthionate tetrahydrate. 2293 structure amplitudes were used, resulting in $R = 10{\cdot}1\,\%$. The sodium ion is coordinated approximately octahedrally to six oxygen atoms, with a mean Na–O length of 2·424 Å. In the anion the distances are S–O 1·454, S–C 1·765, and C–N 1·411 Å, while in the aromatic ring, four C–C have mean distance 1·366 Å and the other seven C–C 1·420 Å, similar to the values found in naphthalene.

Introduction

Sodium naphthionate



is of importance as an intermediate in dyestuffs manufacture, and as the crystal structures of relatively few metal-organic compounds were known in 1945 when this work was commenced, it was chosen as the first substance in this class to be investigated. The unit-cell dimensions and space groups of a number of related compounds have already been published (Corbridge, Brown & Wallwork, 1966), and a paper describing the structure of this substance was presented at the Glasgow Conference of the X-Ray Analysis Group (*Brit. J. Appl. Phys.* 1961). Other structure determinations of metal salts of organic sulphonic acids include zinc and

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magnesium benzenesulphonates (Broomhead & Nicol, 1948), and zinc toluene-*p*-sulphonate hexahydrate (Hargreaves, 1957).

Experimental

Good monoclinic prisms of sodium naphthionate tetrahydrate were readily grown by recrystallizing commercial material from water, and from a number of batches suitable samples for X-ray analysis were chosen. The unit-cell dimensions were determined in the first instance from rotation photographs, and subsequently improved by measuring high-order reflexions on Weissenberg photographs:

$a=11{\cdot}613$, $b=12{\cdot}053$, $c=10{\cdot}045$ Å; $\beta=98°48'$.

The calculated specific gravity, assuming four molecules of $Na[C_{10}H_6 . NH_2 . SO_3] . 4H_2O$ per unit cell, is 1·516, while that observed by flotation in a mixture of organic liquids was 1·513. The space group derived from absent reflexions is unambigously $P2_1/c$.

Intensity data were obtained from Weissenberg photographs about **a** (zero layer), **b** (zero and ten layers) and **c** (zero layer). Multiple film packs were used with three different time exposures in order to cover as complete a range of intensities as possible, and these were estimated by visual comparison with a calibrated film strip. Although the linear absorption coefficient for Cu $K\alpha$ radiation is moderately high (26 cm^{-1}), no correction was applied owing to the difficult shape of the crystal; it was realized that this would limit the ultimate accuracy of the results, but the best was made of the situation by using crystals with a maximum cross-section of 0·3 mm. Geometrical and polarization corrections were applied in the usual way, and the scale factor adjustment to the structure amplitudes was made during the refinement on the computer.

Determination of the trial structure

A Patterson projection on (010) was first computed; although b is the longest of the principal axes, it was chosen for simplicity of calculation, and for the sake of fewer ambiguities. The highest peak was assumed to be a S–S vector, which gave for the coordinates of the sulphur atom $x=0{\cdot}17$ and $z=0{\cdot}29$. A Harker section of the three-dimensional vector map at $y=\frac{1}{2}$ confirmed these x and z values for sulphur, so a set of $F(h0l)$ was calculated for the sulphur atom only; this resulted in moderate agreement with many of the experimental values of $F(h0l)$. Taking as criterion $F(\text{calc}) \geq \frac{1}{3} F(\text{obs})$, an electron density projection was calculated for these terms only. Later it was observed that 94 out of the 121 phases of the $F(h0l)$ had been correctly determined by the sulphur atom contribution alone.

There was sufficient detail in this first electron density projection to enable the oxygen atoms of the SO_3 group, the naphthalene ring and the sodium ion to be located approximately. Several sets of structure factor calculations and electron density projections followed until the majority of the atoms were resolved. The four water oxygen atoms presented difficulties as no peaks were found which could definitely be assigned to them; they were located by difference syntheses. All the four water oxygen atoms overlap other atoms in the **b** projection, the final version of which is shown in Fig. 1.

The determination of the y coordinates was more difficult because the (100) and (001) Patterson maps did not yield much useful information. The most probable value for the sulphur coordinate from these maps was $y=0$, and the naphthalene rings were probably inclined at 45° to (010). On the basis of this hypothesis a molecular model was made, and likely space-filling arrangements were tested by structure factor calculations. Attempts at refining these coordinates were not successful until the y coordinates of the sodium ion and water oxygen atoms had been determined. These were found by a succession of three-dimensional Patterson syntheses along lines parallel to **b** at such values of x and z as would give S–Na and S–O vectors. On account of the symmetry of the Patterson function there was an inherent ambiguity as to whether the deduced coordinate was $(y+y')$ or $(y-y')$ with respect to the sulphur atom. Pairs of Patterson lines using symmetry-related sulphur atoms as reference points eliminated stray peaks and gave S(1)–Na, S(2)–Na, S(1)–O(n) and S(2)–O(n) in turn. The ambiguities were finally resolved by further trial-and-error structure factor calculations, after which refinement was continued on the computer.

Refinement of the structure

The approximate atomic coordinates derived above were refined by least-squares on a Pegasus computer with programs written by Cruickshank & Pilling (1961). Eight cycles were carried out, the first three with a limited number of terms, and five with all the 2293 observed $F\{hkl\}$. The R value fell from 41% to 10·1% during the process. Individual isotropic temperature factors as well as the atomic positional coordinates were refined, but no hydrogen atoms were included. Half of the hydrogen atoms in the molecule formed part of the water molecules; it was not feasible to guess their positions with any certainty, and the experimental data were not good enough to enable them to be located by difference syntheses.

The conclusion of the refinement was judged to have been reached when the shifts indicated for both the positional and thermal parameters were less than the standard deviations for the corresponding atom, and the predicted fall in R' for a further cycle was negligibly small. The final values of the parameters are listed in Table 1, and electron density projections on (100) and (001) are shown in Figs. 2 and 3 respectively. Table 2 shows the agreement between the observed and calculated structure amplitudes, and Table 3 gives the values of the bond-lengths and inter-bond angles.

Table 1. *Final atomic parameters*

	x/a	*y/b*	*z/c*	*B*
C(1)	0·5606	0·0320	0·2996	2·52 Å
C(2)	0·4951	−0·0385	0·2110	3·02
C(3)	0·3735	−0·0444	0·2073	2·93
C(4)	0·3182	0·0213	0·2885	2·42
C(5)	0·3816	0·1015	0·3759	2·39
C(6)	0·3298	0·1740	0·4612	2·67
C(7)	0·3953	0·2472	0·5442	3·17
C(8)	0·5171	0·2533	0·5460	3·00
C(9)	0·5695	0·1841	0·4662	2·80
C(10)	0·5044	0·1062	0·3797	2·43
N	0·6831	0·0324	0·3076	3·11
O(1)	0·1559	−0·0286	0·4287	3·16
O(2)	0·1077	0·1006	0·2470	3·28
O(3)	0·1356	−0·0929	0·1975	3·09
O(4)	0·1220	0·4406	0·4459	3·67
O(5)	0·0092	0·6854	0·0176	3·66
O(6)	0·1816	0·6923	0·3388	3·96
O(7)	0·1570	0·3295	0·2185	3·77
Na	0·0467	0·6267	0·4648	3·06
S	0·1682	−0·0019	0·2897	2·30

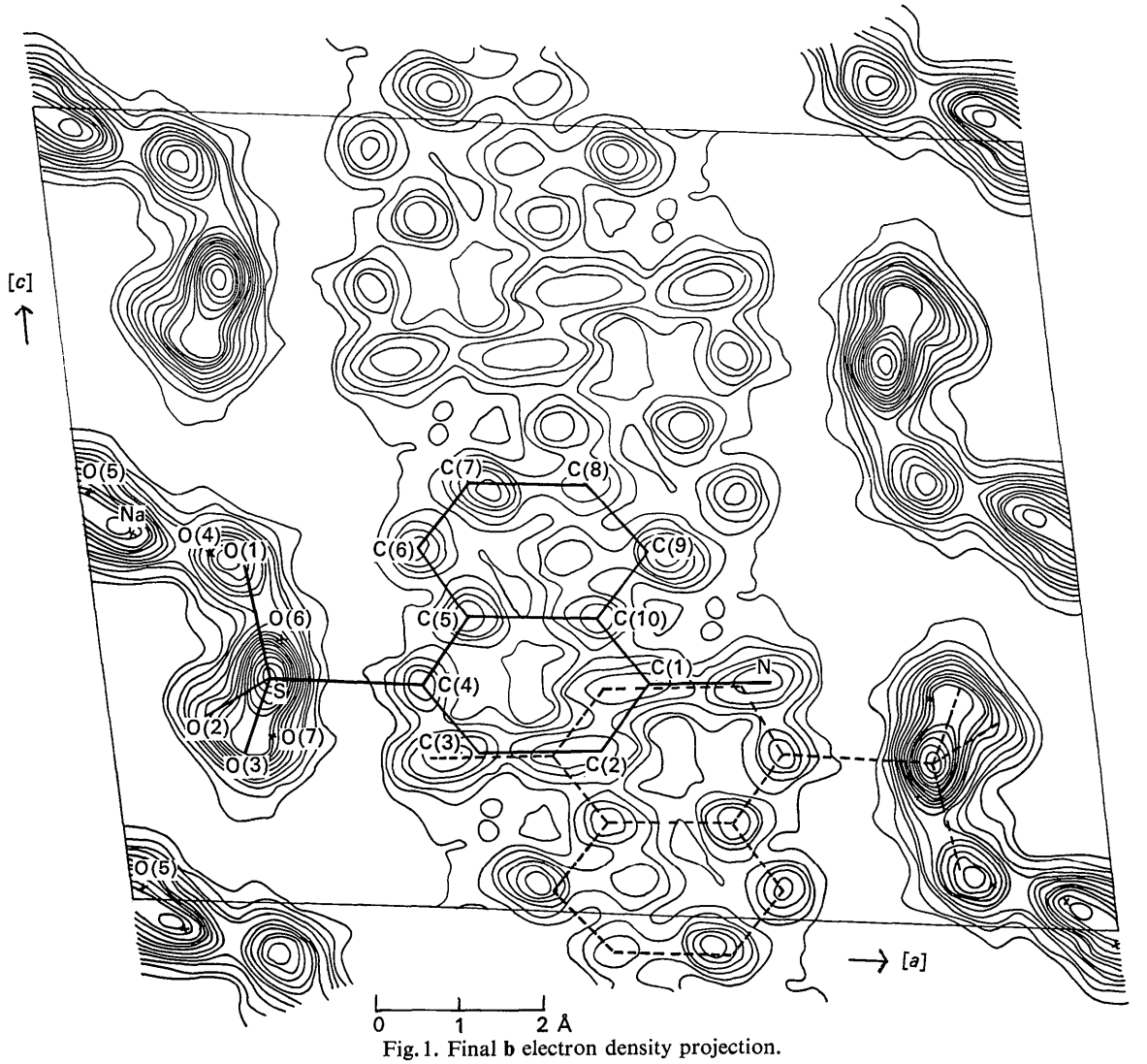

Fig. 1. Final **b** electron density projection.

Table 2. *Observed and calculated structure amplitudes*

H	K	L	F(OBS)	F(CAL)
0	0	2	49.2	-51.9
0	0	4	113.4	+110.4
0	0	8	30.6	-35.3
0	0	10	10.1	+9.6
0	0	12	39.3	-35.0
1	0	-12	16.0	+16.9
1	0	-10	8.7	-10.3
1	0	-6	12.2	-11.6
1	0	-4	14.8	+13.4
1	0	-2	41.2	-43.3
1	0	0	22.7	+21.8
1	0	2	58.3	+59.0
1	0	4	89.0	+82.4
1	0	6	7.2	+5.1
1	0	10	3.1	+2.5
1	0	12	2.7	+2.2
2	0	-12	2.2	-2.9
2	0	-10	7.9	-8.2
2	0	-8	12.9	+11.3
2	0	-6	43.9	-47.2
2	0	-4	2.2	+3.9
2	0	-2	32.4	+35.4
2	0	0	45.3	+49.2
2	0	2	149.2	+157.5
2	0	4	43.3	+44.2
2	0	6	52.3	+52.4
2	0	8	13.4	+15.5
2	0	10	10.9	-10.6
2	0	12	3.3	-4.7
3	0	-12	7.9	+8.4
3	0	-10	7.9	-7.4
3	0	-8	6.8	+5.4
3	0	-6	45.3	+45.5
3	0	-4	45.3	-45.2
3	0	-2	102.7	+104.0
3	0	0	104.7	-105.7
3	0	2	87.9	+85.7
3	0	4	45.3	+47.4
3	0	6	7.9	+9.7
3	0	8	22.7	+25.6
3	0	10	10.4	-9.3
3	0	12	4.5	+4.0
4	0	-10	13.6	-14.4
4	0	-4	55.5	-60.6
4	0	-2	82.8	+79.3
4	0	0	100.7	-95.6
4	0	2	44.5	+50.1
4	0	4	20.7	+22.2
4	0	6	32.7	+35.4
4	0	8	32.1	+32.3
4	0	10	4.5	+7.4
5	0	-12	5.1	-6.7
5	0	-10	5.1	+7.2
5	0	-8	11.3	-11.8
5	0	-6	22.2	+25.0
5	0	-2	52.8	+55.1
5	0	6	9.1	+12.4
5	0	8	11.3	+11.9
6	0	-12	16.6	-22.2
6	0	-10	10.4	+11.9
6	0	-8	18.9	-22.1
6	0	-4	48.7	+48.3
6	0	-2	63.8	-63.3
6	0	0	116.2	+107.7
6	0	2	18.9	-17.5
6	0	4	8.1	-9.0
6	0	8	10.9	-10.7
6	0	10	19.6	+19.9
7	0	-12	3.9	+3.7
7	0	-8	16.0	-15.9
7	0	-6	40.5	-44.0
7	0	-4	28.1	+26.8
7	0	-2	41.4	-38.9
7	0	0	41.4	+35.4
7	0	2	10.9	+13.3
7	0	4	15.3	+17.4
7	0	6	32.1	+35.1
7	0	8	14.7	-12.5
7	0	10	13.6	+13.6
8	0	-10	3.2	-6.0
8	0	-8	24.9	+27.7
8	0	-6	17.6	-18.5
8	0	-2	3.6	-2.6
8	0	2	22.7	+22.6
8	0	4	20.3	-18.7
8	0	6	3.9	-6.1
9	0	-10	2.8	-5.1
9	0	-8	7.5	-7.8
9	0	-4	25.4	-27.2
9	0	-2	10.9	+10.9
9	0	0	34.2	-35.6
9	0	2	16.0	+12.1
9	0	4	27.8	+29.0
9	0	6	4.5	+3.6
9	0	8	11.3	+11.4
10	0	-10	2.4	-2.3
10	0	-8	7.9	+7.8
10	0	-6	10.1	+9.4
10	0	-4	32.1	-30.0
10	0	-2	16.0	+16.0
10	0	0	10.1	-6.6
10	0	2	16.0	-15.9
10	0	4	20.1	+9.0
10	0	6	10.4	-7.4
10	0	8	13.8	+12.8
11	0	-10	4.5	+5.6
11	0	-8	1.7	-2.2
11	0	-6	13.0	+13.1
11	0	-4	8.7	-9.9
11	0	-2	10.1	-11.7
11	0	0	11.3	-13.5
11	0	2	16.8	-18.4
11	0	4	7.9	+4.4
11	0	6	9.6	-8.2
12	0	-6	4.5	+3.4
12	0	-4	20.7	+20.0
12	0	-2	13.6	-13.3
12	0	0	16.8	+17.2
12	0	2	13.0	-12.6
12	0	6	3.9	-4.0
13	0	-8	7.9	+6.6
13	0	-6	15.7	-17.3
13	0	-4	18.8	+16.9
13	0	-2	19.0	-18.3
13	0	4	14.0	-13.1
14	0	-6	7.9	+6.3
14	0	-4	3.9	+3.4
14	0	-2	5.1	+4.3
14	0	0	11.1	-10.0
14	0	2	10.1	+7.0
15	0	-2	16.5	+18.6
0	1	1	44.7	-41.9
0	1	2	2.8	+2.7
0	1	3	50.7	+53.6
0	1	4	5.1	-4.2
0	1	5	17.4	-16.1
0	1	6	12.6	-9.9
0	1	7	29.1	+23.6
0	1	8	4.8	-7.7
0	1	9	27.7	-24.4
0	1	10	5.1	+5.1
0	1	11	3.5	+2.3
0	1	12	7.5	+6.9
1	1	-12	7.2	+4.5
1	1	-11	10.9	+8.9
1	1	-10	15.9	+12.4
1	1	-9	27.7	-24.8
1	1	-8	10.6	-8.2
1	1	-7	6.4	+4.0
1	1	-6	25.3	+21.9
1	1	-5	10.9	+11.3
1	1	-4	42.4	-37.9
1	1	-3	36.1	-34.6
1	1	-2	29.0	+26.4
1	1	-1	131.1	+133.7
1	1	0	9.1	-7.9
1	1	1	27.6	-24.4
1	1	2	43.6	-36.9
1	1	3	46.2	+44.0
1	1	4	2.2	-3.6
1	1	5	28.5	-26.7
1	1	6	26.1	+21.0
1	1	7	29.1	+25.9
1	1	8	6.8	-6.0
1	1	10	4.5	-4.9
1	1	11	15.3	-13.6
2	1	-12	6.0	-4.3
2	1	-11	3.2	-2.2
2	1	-10	3.9	-4.5
2	1	-9	20.1	-16.7
2	1	-7	39.7	-37.3
2	1	-6	35.8	+37.1
2	1	-5	41.9	+42.3
2	1	-4	9.6	+5.1
2	1	-3	70.3	-69.5
2	1	-2	28.9	+29.2
2	1	-1	78.5	+75.6
2	1	0	23.8	+26.6
2	1	1	36.3	-32.1
2	1	2	60.0	+55.8
2	1	3	44.7	+41.4
2	1	4	57.3	-48.6
2	1	5	29.1	+26.8
2	1	6	2.2	+3.6
2	1	7	29.1	-27.0
2	1	8	16.0	-11.5
2	1	9	27.7	+24.1
2	1	11	11.6	-9.6
3	1	-11	9.9	-10.1
3	1	-9	8.7	+9.7
3	1	-8	9.6	-10.6
3	1	-7	44.2	-43.7
3	1	-5	25.9	-22.8
3	1	-4	27.3	+25.3
3	1	-3	35.8	-32.5
3	1	-2	3.2	+2.3
3	1	-1	27.9	+28.5
3	1	0	6.4	+6.0
3	1	1	22.5	-17.7
3	1	2	58.7	+51.1
3	1	3	37.6	+30.4
3	1	4	7.5	+3.1
3	1	5	13.8	+15.5
3	1	6	24.1	+19.3
3	1	8	5.6	-2.5
3	1	9	16.0	+14.2
3	1	10	6.4	+4.1
3	1	12	6.4	-5.4
4	1	-11	14.0	-13.0
4	1	-9	17.4	+16.9
4	1	-8	10.6	+7.7
4	1	-7	29.1	-25.1
4	1	-5	13.4	-12.2
4	1	-4	24.6	+20.6
4	1	-3	19.6	-18.2
4	1	-2	10.1	+11.5
4	1	-1	23.0	-20.4
4	1	0	19.5	-17.8
4	1	1	18.3	+20.1
4	1	3	5.1	+2.7
4	1	4	6.8	+4.5
4	1	5	17.1	+16.5
4	1	6	9.3	-8.4
4	1	9	3.9	-3.1
4	1	10	3.2	+5.0
4	1	11	2.2	+2.8
5	1	-12	10.1	-10.9
5	1	-11	13.4	-13.8
5	1	-10	11.8	-11.4
5	1	-9	5.1	+3.3
5	1	-5	39.9	-41.9
5	1	-4	20.7	+20.2
5	1	-3	2.2	+1.6
5	1	-2	64.7	+59.8
5	1	-1	89.8	-85.7
5	1	0	55.1	+53.8
5	1	1	57.3	+46.4
5	1	2	19.4	+16.7
5	1	3	14.5	-13.0
5	1	4	41.2	+37.2
5	1	5	12.3	+13.6
5	1	6	7.5	-4.8
5	1	7	27.6	+25.2
5	1	9	13.0	-13.0
5	1	10	5.6	-3.6
5	1	11	20.9	+17.9
6	1	-11	8.7	+10.3
6	1	-10	9.3	-8.6
6	1	-9	20.1	-21.0
6	1	-7	21.5	+24.4
6	1	-5	35.7	-34.5
6	1	-4	7.9	+3.5
6	1	-3	18.4	+16.8
6	1	-2	3.9	+5.1
6	1	-1	32.1	-32.1
6	1	0	16.4	+14.7
6	1	1	41.2	-32.8
6	1	2	2.2	-1.6
6	1	3	9.1	+8.3
6	1	4	24.2	+23.0
6	1	5	9.6	-6.8
6	1	7	22.5	+23.3
6	1	8	6.0	+4.1
6	1	9	8.1	-5.1
7	1	-12	5.6	-4.8
7	1	-11	3.9	+6.3
7	1	-10	9.9	-9.8
7	1	-9	21.5	-21.4
7	1	-8	16.0	-14.2
7	1	-7	22.5	+23.2
7	1	-6	9.6	-12.8
7	1	-5	18.4	-19.0
7	1	-4	9.3	-9.7
7	1	-3	6.4	+2.8
7	1	-2	17.8	+15.4
7	1	-1	21.9	-18.8
7	1	0	50.4	+43.4
7	1	1	16.5	-13.3
7	1	2	23.3	+19.7
7	1	3	7.9	+7.7
7	1	4	15.3	+14.4
7	1	5	35.7	-32.6
7	1	6	16.0	+15.5
7	1	7	17.4	+16.9
7	1	8	11.3	+10.5
7	1	9	5.6	+5.0
7	1	10	8.7	-6.1
8	1	-11	2.2	+4.3
8	1	-10	6.4	-4.3
8	1	-9	9.3	-9.0
8	1	-7	39.1	-40.5
8	1	-6	8.7	+9.9
8	1	-5	37.4	+37.9
8	1	-4	13.0	+16.3
8	1	-3	35.8	-33.5
8	1	-2	7.5	-6.1
8	1	-1	27.9	+22.5
8	1	0	14.0	+10.0
8	1	1	13.0	-9.1
8	1	2	25.3	+22.9
8	1	3	26.3	-22.2
8	1	5	45.1	+37.7
8	1	7	35.8	-28.8
8	1	9	24.8	+17.7
9	1	-11	4.5	-3.2
9	1	-10	5.6	-3.9
9	1	-8	18.0	-17.4
9	1	-7	7.9	-7.9
9	1	-6	31.9	-30.7
9	1	-5	22.5	-19.0
9	1	-4	6.0	-6.2
9	1	-3	20.4	-18.3
9	1	-2	8.5	-5.2
9	1	-1	15.3	+11.5
9	1	0	6.8	+7.7
9	1	1	7.5	-7.1
9	1	2	24.6	+21.1
9	1	3	9.9	-9.4
9	1	4	21.7	+18.9
9	1	6	21.7	+20.0
9	1	7	13.6	-9.2
9	1	8	7.5	+8.1
9	1	9	12.6	+11.4
10	1	-9	10.9	+11.2
10	1	-8	7.5	+5.1
10	1	-7	30.4	-22.9
10	1	-5	3.9	-2.7
10	1	-3	7.2	-5.4
10	1	-2	3.9	-2.7
10	1	-1	27.7	-24.8
10	1	1	22.5	+17.2
10	1	2	3.2	+4.2
10	1	3	12.4	-11.0
10	1	5	13.0	+11.2
10	1	7	7.2	-5.6
11	1	-9	3.9	+3.7
11	1	-8	5.6	-5.2
11	1	-7	2.2	+2.4
11	1	-6	4.5	-3.4
11	1	-5	21.5	-17.8
11	1	-4	11.3	-9.1
11	1	-3	10.1	-7.8
11	1	-2	3.9	+2.3
11	1	-1	16.0	-10.4
11	1	1	3.2	-3.4
11	1	2	4.8	-4.1
11	1	4	9.9	+10.0
11	1	5	4.5	-3.8
11	1	6	5.1	+5.1
11	1	7	11.6	+8.3
12	1	-8	7.2	-6.5
12	1	-7	17.4	+14.1
12	1	-5	22.1	-18.1
12	1	-4	10.4	-9.3
12	1	-2	3.9	+2.5
12	1	-1	24.1	-20.7
12	1	1	18.6	-13.7
12	1	2	4.5	+2.8
12	1	3	11.6	+7.8
12	1	4	7.5	+7.0
12	1	5	17.6	-14.0
12	1	6	5.6	+5.9
13	1	-7	18.7	+12.7
13	1	-6	4.5	+3.1
13	1	-5	3.9	+3.6
13	1	-4	5.6	-4.8
13	1	-3	3.9	-3.8
13	1	-1	3.2	+2.1
13	1	0	7.2	-4.4
13	1	1	21.9	-20.6
13	1	3	10.1	+9.7
13	1	4	7.9	-6.0
14	1	-6	3.9	-3.2
14	1	-5	15.0	+16.1
14	1	-3	9.1	-8.7
14	1	-2	3.2	-3.2
14	1	-1	9.6	+7.9
14	1	0	4.5	-3.7
14	1	1	10.4	-9.3
14	1	2	6.8	+5.0
0	2	0	111.4	+110.3
0	2	1	31.5	-30.1
0	2	2	142.6	-147.7
0	2	3	51.3	-48.7
0	2	4	15.0	+13.7
0	2	5	17.4	-11.6
0	2	6	25.6	-23.8
0	2	7	11.1	-9.8
0	2	8	26.2	-24.5
0	2	9	35.4	-33.8
0	2	10	34.0	+31.3
0	2	11	7.5	-6.2
0	2	12	15.3	-13.9
1	2	-12	4.3	+3.6
1	2	-11	8.7	-8.6
1	2	-10	27.7	-24.4
1	2	-9	20.1	+17.6
1	2	-8	10.6	+10.6
1	2	-7	9.9	+9.6
1	2	-6	55.5	-52.3
1	2	-5	49.5	+48.0
1	2	-4	21.4	-12.7
1	2	-3	62.9	-55.9
1	2	-2	49.9	+45.4
1	2	0	12.9	+14.3
1	2	1	48.1	+46.4
1	2	2	86.7	+83.6
1	2	3	16.8	-13.6
1	2	4	31.5	+28.4
1	2	6	12.9	+8.8
1	2	7	11.1	-9.1
1	2	8	35.5	-32.6
1	2	9	5.1	-7.4
1	2	12	12.9	-9.5
2	2	-12	10.1	+8.5
2	2	-11	12.4	+11.6
2	2	-10	7.9	-7.1
2	2	-9	14.1	+12.5
2	2	-8	40.0	+37.3
2	2	-6	51.3	-45.1
2	2	-5	71.7	+66.0
2	2	-4	14.9	-12.5
2	2	-3	5.1	+4.4
2	2	-2	70.8	-72.1
2	2	-1	13.8	+15.7
2	2	0	53.1	-53.0
2	2	1	18.6	-21.8
2	2	2	11.1	+8.9
2	2	3	50.2	-47.6
2	2	4	46.9	-41.9
2	2	5	12.0	+7.9
2	2	6	45.9	+41.8
2	2	7	7.9	-8.4
2	2	8	18.7	-17.4
2	2	9	12.4	-12.9
2	2	11	3.9	-4.0
2	2	12	3.2	+3.6
3	2	-12	9.3	+10.0
3	2	-11	6.8	+7.7
3	2	-10	9.6	-9.7
3	2	-9	5.1	+2.7
3	2	-8	8.1	-6.8
3	2	-7	28.9	+28.0
3	2	-6	16.2	+16.0
3	2	-5	52.5	+49.7
3	2	-4	72.4	-66.3
3	2	-2	36.3	-33.8
3	2	-1	41.5	+44.1
3	2	0	57.8	-54.8
3	2	1	25.0	-25.9
3	2	2	12.9	-5.5
3	2	3	24.9	-18.4
3	2	4	16.0	+7.2
3	2	5	30.4	-28.1
3	2	6	12.0	+13.5
3	2	7	23.9	-22.3
3	2	8	25.0	+20.1
3	2	9	5.1	+3.9
3	2	10	9.1	-8.9
3	2	11	8.1	-9.1
3	2	12	7.5	+6.5
4	2	-12	2.2	+3.2
4	2	-9	12.4	-12.4
4	2	-7	20.4	+19.0
4	2	-6	35.5	+36.6
4	2	-5	13.2	+12.6
4	2	-4	12.2	-12.4
4	2	-3	70.6	+71.0
4	2	-2	10.1	+12.9
4	2	-1	55.5	+54.0
4	2	0	68.1	-63.6
4	2	1	16.2	+15.0
4	2	2	24.4	-22.0
4	2	3	27.0	+25.9
4	2	4	17.1	-17.0
4	2	5	8.5	-9.8
4	2	6	25.0	-21.2
4	2	7	19.5	-18.1
4	2	8	22.5	+18.8
4	2	10	12.0	-10.3
4	2	11	10.6	-11.1
5	2	-12	9.6	-9.9
5	2	-10	10.6	+10.6
5	2	-9	7.9	-10.7
5	2	-8	30.2	-26.6
5	2	-7	21.4	+21.2
5	2	-6	19.6	+19.2
5	2	-5	22.4	-24.7
5	2	-4	10.9	-13.2
5	2	-3	60.4	+65.2
5	2	-2	27.8	+21.4
5	2	0	45.6	-39.7
5	2	1	11.3	+10.6
5	2	2	35.8	-29.0
5	2	3	17.1	+15.9
5	2	5	9.1	-7.8
5	2	6	33.6	-31.1
5	2	7	10.1	-10.5
5	2	8	22.5	+19.6
5	2	9	7.9	-7.7
5	2	11	2.2	-1.5
6	2	-12	17.3	-16.6
6	2	-11	6.8	-6.8
6	2	-10	14.5	+14.8
6	2	-8	20.1	-18.3
6	2	-7	7.2	+7.4
6	2	-6	14.5	-13.3
6	2	-5	21.5	-21.5
6	2	-4	16.2	+17.7
6	2	-3	36.2	+37.9
6	2	-2	35.1	-33.4
6	2	-1	27.8	+24.5
6	2	0	40.4	+37.7
6	2	1	53.9	+51.1
6	2	2	39.3	-32.0
6	2	3	8.5	-7.3
6	2	4	3.2	+5.3
6	2	5	10.6	+10.8
6	2	6	5.1	-6.6
6	2	8	10.6	-10.8
6	2	9	6.0	-6.4
6	2	10	17.0	+13.9
7	2	-11	7.2	-7.7
7	2	-10	7.5	-7.8
7	2	-9	11.3	-9.9
7	2	-8	12.4	+13.8
7	2	-6	25.5	-20.9
7	2	-5	5.6	+8.1
7	2	-4	21.5	+24.2
7	2	-3	6.0	+6.6
7	2	0	18.2	+16.5
7	2	1	42.4	+35.7
7	2	2	6.8	-7.8
7	2	3	27.8	+25.6
7	2	4	30.3	-24.0
7	2	5	10.1	+8.1
7	2	6	10.1	+7.3
7	2	7	5.1	-3.9
7	2	8	34.4	-32.8
7	2	9	5.6	-5.1
7	2	10	10.6	+7.5
8	2	-11	5.6	-5.8
8	2	-10	18.4	-18.9
8	2	-9	7.2	+9.1
8	2	-8	15.9	+16.3
8	2	-7	31.9	-31.3
8	2	-6	31.7	-33.8
8	2	-5	7.5	-6.4
8	2	-4	13.4	-13.5
8	2	-3	7.9	-9.1
8	2	-2	12.4	-13.5
8	2	-1	7.5	-7.5
8	2	0	9.9	-7.3
8	2	1	20.4	+20.6
8	2	2	33.8	+32.5
8	2	3	6.8	-6.8
8	2	4	14.1	-12.1
8	2	5	17.4	+16.8
8	2	6	24.8	+22.2
8	2	7	20.7	+19.3
8	2	9	3.2	-2.7
9	2	-11	1.6	-2.3
9	2	-10	3.6	-4.6
9	2	-9	3.3	-1.9
9	2	-8	4.8	-3.5
9	2	-7	7.9	-7.0
9	2	-6	10.1	+10.5
9	2	-5	24.6	+24.9
9	2	-4	10.1	-10.1
9	2	-3	26.1	-30.0
9	2	-1	15.3	+13.6
9	2	0	16.5	-14.5
9	2	1	3.9	-3.5
9	2	2	11.1	+8.8
9	2	3	17.4	+16.4
9	2	4	3.2	-4.7
9	2	6	6.4	-4.0
9	2	7	6.0	-4.6
10	2	-10	2.2	+1.7
10	2	-9	3.2	-3.2
10	2	-8	6.8	-6.3
10	2	-7	13.4	-14.2
10	2	-6	8.7	+8.3
10	2	-5	10.1	-8.3
10	2	-4	20.1	-19.9
10	2	-3	7.2	-5.1
10	2	-1	10.1	+7.7
10	2	0	12.2	-12.6
10	2	1	20.1	-18.8
10	2	2	11.3	-10.6
10	2	3	11.3	+10.8
10	2	4	13.6	+11.5
10	2	5	4.5	+4.4
10	2	6	9.1	-7.7
10	2	7	9.6	+7.2
10	2	8	15.3	+14.0
11	2	-9	3.2	-4.0
11	2	-8	12.2	-12.6
11	2	-7	4.5	-2.1
11	2	-6	9.1	+9.3
11	2	-5	9.6	-8.3
11	2	-4	7.9	-4.7
11	2	-3	12.4	-13.7
11	2	-2	7.2	+7.1
11	2	1	3.2	-3.7
11	2	2	11.8	-8.8
11	2	3	5.1	+3.8
11	2	4	15.3	+13.0
11	2	6	15.3	-13.0
11	2	7	5.1	+2.5
12	2	-9	4.5	-4.4
12	2	-8	7.5	-7.4
12	2	-7	6.4	+6.0
12	2	-6	6.0	-4.9
12	2	-5	10.9	-10.3
12	2	-3	2.8	-1.9
12	2	-2	16.6	-14.0
12	2	-1	7.5	-6.4
12	2	0	9.3	+7.5
12	2	1	7.9	-7.2
12	2	2	19.8	-16.7
12	2	3	3.2	-3.6
12	2	4	6.4	+5.1
12	2	5	5.1	-3.9
13	2	-7	2.2	-2.1
13	2	-6	11.7	-12.0
13	2	-5	7.5	-7.8
13	2	-4	13.8	+14.6
13	2	-2	11.6	-9.5
13	2	-1	8.1	-7.5
13	2	0	7.9	+7.2
13	2	4	15.3	-12.1
14	2	-5	9.6	-8.1

Table 2 (*cont.*)

H	K	L	F(OBS)	F(CAL)
14	2	-4	6.8	-3.7
14	2	-1	10.1	-10.7
14	2	0	6.8	-5.2
14	2	1	3.9	+2.8
14	2	2	12.6	+11.7
0	3	2	82.7	+84.1
0	3	3	64.1	+67.4
0	3	4	43.6	-44.5
0	3	5	25.0	-26.3
0	3	6	14.3	+15.6
0	3	7	28.5	+29.3
0	3	8	9.9	-11.9
0	3	9	3.2	-1.3
0	3	10	4.5	+3.1
0	3	11	3.2	-2.5
1	3	-11	16.4	+18.9
1	3	-10	18.9	+22.8
1	3	-9	11.1	-11.0
1	3	-8	12.2	-13.2
1	3	-7	14.3	+15.1
1	3	-6	20.1	+25.3
1	3	-5	10.1	+11.5
1	3	-4	23.9	+26.2
1	3	-3	23.3	-24.6
1	3	-2	42.1	+45.7
1	3	-1	36.2	+34.9
1	3	0	13.0	+13.9
1	3	1	108.3	-114.4
1	3	2	50.0	-51.6
1	3	3	27.8	+34.3
1	3	4	10.0	-7.4
1	3	5	14.7	-15.6
1	3	6	7.2	-9.2
1	3	7	6.8	+5.5
1	3	8	15.7	-18.2
1	3	9	9.9	+11.4
1	3	10	4.5	-5.2
1	3	12	3.2	-4.9
2	3	-11	9.6	+10.5
2	3	-10	5.1	+6.7
2	3	-8	12.2	+11.4
2	3	-6	14.3	+17.4
2	3	-5	30.0	+32.2
2	3	-4	24.4	-26.7
2	3	-3	34.9	-38.4
2	3	-2	2.1	+2.9
2	3	-1	101.4	+104.2
2	3	0	21.0	-20.8
2	3	1	37.0	-38.7
2	3	2	21.3	+24.6
2	3	3	22.7	-24.7
2	3	4	15.1	-15.2
2	3	5	13.2	+14.2
2	3	7	21.0	-21.7
2	3	8	7.2	-7.7
2	3	9	22.4	+19.9
2	3	10	8.2	+7.4
2	3	11	7.9	-8.1
2	3	12	3.9	-5.2
3	3	-11	3.2	+3.4
3	3	-10	10.6	+11.7
3	3	-9	9.9	+10.4
3	3	-7	6.4	+7.2
3	3	-6	32.1	+32.1
3	3	-5	30.9	+31.1
3	3	-4	16.4	+13.6
3	3	-3	18.6	+16.8
3	3	-2	32.1	+29.9
3	3	-1	29.7	+26.5
3	3	0	4.8	+8.1
3	3	1	36.3	+40.7
3	3	2	20.1	-21.7
3	3	3	23.2	-21.9
3	3	7	21.2	-19.3
3	3	8	19.9	-22.1
3	3	9	3.2	-3.6
3	3	11	2.2	-3.7
3	3	12	3.2	-5.7
4	3	-9	18.7	+18.0
4	3	-8	5.6	+4.9
4	3	-7	9.3	-11.5
4	3	-6	33.3	+33.9
4	3	-5	3.9	+4.4
4	3	-4	8.7	-6.8
4	3	-3	4.5	+4.2
4	3	-2	42.4	+46.8
4	3	-1	45.1	-49.2
4	3	0	7.2	+4.0
4	3	1	59.6	+64.4
4	3	2	4.5	+5.2
4	3	3	22.5	-23.7
4	3	5	14.8	+14.7
4	3	6	3.2	-3.3
4	3	10	6.0	-5.7
4	3	11	6.4	+5.9
5	3	-10	3.2	-5.1
5	3	-9	24.4	+28.3
5	3	-8	3.9	+6.5
5	3	-7	18.9	+22.8
5	3	-6	15.5	+15.5
5	3	-5	10.1	+11.6
5	3	-4	6.0	+4.1
5	3	-3	71.7	+67.7
5	3	-2	25.9	+28.5
5	3	-1	51.3	-52.1
5	3	0	3.2	+3.8
5	3	1	42.1	+46.7
5	3	3	24.3	-26.3
5	3	4	4.5	-4.4
5	3	6	11.6	-11.5
5	3	7	3.2	-2.0
5	3	8	7.9	+9.0
5	3	9	19.6	-20.9
5	3	10	3.2	-5.0
5	3	11	7.5	+7.6
6	3	-12	3.9	-2.9
6	3	-11	3.2	+3.6
6	3	-10	17.6	-17.8
6	3	-7	35.1	+38.2
6	3	-6	13.4	-15.9
6	3	-4	45.3	+47.3
6	3	-3	29.7	+32.9
6	3	-2	11.6	+14.5
6	3	-1	12.9	+13.7
6	3	0	22.1	+18.8
6	3	1	24.2	-22.1
6	3	2	37.6	+38.0
6	3	3	30.4	+28.1
6	3	4	9.1	+10.4
6	3	5	21.0	-18.6
6	3	6	5.1	-6.0
6	3	7	7.2	+4.6
6	3	8	3.9	-3.8
6	3	9	3.9	-3.4
6	3	10	5.6	-6.3
7	3	-12	2.3	-1.6
7	3	-11	3.3	+6.9
7	3	-10	2.3	+2.9
7	3	-9	7.5	-9.2
7	3	-7	22.2	+23.4
7	3	-6	18.3	-20.1
7	3	-5	13.4	+14.7
7	3	-4	9.9	+12.5
7	3	-3	21.6	+22.7
7	3	-2	4.5	+6.9
7	3	-1	45.3	+49.4
7	3	0	22.7	+21.6
7	3	1	36.1	-35.6
7	3	2	4.5	-5.6
7	3	3	35.1	+37.0
7	3	4	4.5	-2.1
7	3	5	17.3	-16.6
7	3	7	11.6	+11.7
7	3	8	6.0	+6.1
7	3	9	3.5	-4.1
7	3	10	7.5	-5.3
8	3	-11	4.5	+5.9
8	3	-10	12.6	-15.1
8	3	-9	9.1	+9.7
8	3	-8	9.6	-9.4
8	3	-6	15.7	-18.0
8	3	-5	54.6	+56.3
8	3	-3	28.5	-31.5
8	3	-2	12.9	-15.3
8	3	-1	57.2	+60.7
8	3	0	24.9	+25.0
8	3	1	10.1	-9.8
8	3	2	29.8	+25.3
8	3	3	17.3	-19.2
8	3	4	24.9	+24.1
8	3	7	19.6	-21.9
8	3	8	2.2	-2.3
8	3	9	13.4	+10.8
9	3	-11	2.2	-4.0
9	3	-10	8.1	+11.0
9	3	-9	7.2	-5.9
9	3	-6	9.9	-8.1
9	3	-5	15.7	+18.4
9	3	-3	17.2	+18.9
9	3	-2	7.2	-6.1
9	3	-1	29.9	+29.5
9	3	0	8.1	+8.4
9	3	1	22.2	+21.9
9	3	2	14.1	-15.3
9	3	3	12.2	+13.3
9	3	4	3.2	+4.2
9	3	5	6.4	+4.3
9	3	6	7.5	+8.0
9	3	7	7.9	-5.6
10	3	-10	3.2	-3.5
10	3	-9	14.5	+15.0
10	3	-8	5.6	-6.9
10	3	-7	11.1	-12.1
10	3	-4	20.1	-21.3
10	3	-3	17.2	+19.9
10	3	-2	14.1	-15.4
10	3	-1	12.2	-13.8
10	3	1	38.7	+41.9
10	3	2	8.7	+10.8
10	3	3	14.1	-10.7
10	3	4	5.1	+4.8
10	3	5	8.7	+8.0
10	3	6	8.7	+8.2
11	3	-8	5.1	-6.0
11	3	-7	5.1	+5.6
11	3	-6	8.7	+8.6
11	3	-5	7.2	-9.9
11	3	-4	6.8	-6.7
11	3	-3	16.6	+17.7
11	3	-1	12.2	-13.4
11	3	0	11.1	-11.8
11	3	1	17.8	+16.9
11	3	2	6.8	-5.0
11	3	4	2.7	+2.6
11	3	5	6.0	+4.6
12	3	-7	15.9	+16.9
12	3	-5	10.4	-11.0
12	3	-4	4.5	-5.7
12	3	-3	20.6	+20.9
12	3	0	10.1	-10.7
12	3	1	6.4	+6.4
12	3	3	13.4	+12.0
12	3	4	2.2	-2.6
12	3	5	3.9	-1.9
13	3	-7	9.1	+6.8
13	3	-6	3.2	-4.1
13	3	-5	3.2	-3.0
13	3	-4	3.9	-4.6
13	3	-3	6.8	-7.9
13	3	-2	5.1	+4.3
13	3	-1	9.6	+12.5
13	3	0	5.6	-6.2
13	3	1	14.5	-15.5
13	3	2	4.5	+4.1
13	3	3	13.4	+13.2
13	3	4	7.9	-4.7
14	3	-5	19.2	+18.3
14	3	-4	3.9	+4.7
14	3	-3	11.1	-12.4
14	3	-1	14.7	+14.8
14	3	1	3.2	-2.7
0	4	0	35.1	+38.9
0	4	1	8.7	+10.2
0	4	2	36.6	-40.8
0	4	3	53.7	+54.8
0	4	4	14.0	+15.0
0	4	5	23.1	+24.2
0	4	6	3.2	-2.9
0	4	7	32.5	+35.0
0	4	8	30.8	-33.5
0	4	10	11.1	+17.4
0	4	12	6.4	-9.7
1	4	-12	6.4	+6.7
1	4	-10	3.2	+4.8
1	4	-9	12.0	+14.6
1	4	-8	37.6	+38.7
1	4	-6	29.2	-30.6
1	4	-5	8.1	+9.4
1	4	-4	15.7	-18.2
1	4	-3	26.8	-31.1
1	4	-2	18.9	-22.8
1	4	-1	43.3	-48.6
1	4	0	57.4	-60.8
1	4	1	23.8	-27.1
1	4	2	6.4	+10.3
1	4	3	30.6	+37.4
1	4	4	80.1	-80.5
1	4	5	13.2	-14.5
1	4	6	16.6	+19.4
1	4	7	13.0	+14.6
1	4	8	13.8	-15.1
1	4	10	9.1	+11.9
1	4	12	3.2	-3.0
2	4	-12	6.0	+7.6
2	4	-10	9.3	-10.6
2	4	-8	19.5	+23.4
2	4	-6	29.4	-32.8
2	4	-5	11.6	-13.1
2	4	-4	29.3	+32.8
2	4	-3	17.6	+18.1
2	4	-2	52.7	-52.2
2	4	-1	40.7	-41.3
2	4	0	45.3	-50.4
2	4	1	33.9	-35.2
2	4	2	51.7	+59.5
2	4	3	6.0	-6.0
2	4	4	38.7	-43.1
2	4	5	15.6	+19.6
2	4	6	27.8	+28.9
2	4	7	9.3	+14.9
2	4	8	19.5	-24.2
2	4	11	9.9	+11.6
2	4	12	3.2	+4.2
3	4	-12	9.3	+11.6
3	4	-11	4.5	-4.8
3.	4	-10	7.2	+7.5
3	4	-9	8.5	-10.1
3	4	-8	16.8	+21.2
3	4	-7	13.0	+16.7
3	4	-6	13.2	+16.7
3	5	-5	3.9	-5.3
3	4	-4	5.1	-4.5
3	4	-3	3.2	+2.8
3	4	-2	13.4	-13.6
3	4	-1	27.2	+31.8
3	4	0	38.7	-41.6
3	4	1	16.5	-17.6
3	4	2	36.6	-44.4
3	4	3	13.0	-17.3
3	4	4	23.2	-27.2
3	4	5	18.6	+19.9
3	4	6	6.4	-8.3
3	4	8	3.2	+5.0
3	4	9	10.6	+12.5
3	4	10	6.4	-8.2
4	4	-12	2.2	+5.7
4	4	-9	3.9	-4.8
4	4	-8	5.1	+5.8
4	4	-7	3.2	+6.4
4	4	-6	30.9	+35.6
4	4	-5	3.2	+4.3
4	4	-4	3.9	+3.6
4	4	-2	6.8	+10.1
4	4	0	7.2	-8.9
4	4	2	51.7	-53.1
4	4	3	44.7	-44.9
4	4	6	29.2	-32.7
4	4	7	12.0	-12.6
4	4	8	8.5	+8.7
4	4	9	9.1	+10.4
4	4	10	8.7	-10.7
5	4	-12	2.2	-2.5
5	4	-11	3.9	-4.8
5	4	-10	7.2	+9.9
5	4	-9	7.5	-12.8
5	4	-8	7.5	-12.8
5	4	-7	3.9	-4.2
5	4	-6	32.4	+36.7
5	4	-5	6.0	+5.0
5	4	-4	5.6	-6.2
5	4	-3	20.4	+28.4
5	4	-2	9.6	+13.4
5	4	-1	7.9	+15.9
5	4	0	16.5	+21.5
5	4	1	44.2	+45.2
5	4	2	40.2	-44.0
5	4	3	9.6	+9.3
5	4	4	18.7	+23.0
5	4	6	43.5	-43.1
5	4	8	13.2	+13.4
5	4	9	2.2	-3.7
5	4	10	2.2	-5.0
6	4	-12	6.2	-7.3
6	4	-10	14.5	+17.7
6	4	-8	3.2	-3.9
6	4	-7	13.8	-15.9
6	4	-6	11.3	+11.3
6	4	-5	4.5	-4.9
6	4	-4	41.8	+43.5
6	4	-3	5.6	-4.2
6	4	-1	3.2	+4.7
6	4	0	41.6	+44.7
6	4	1	24.2	+25.4
6	4	2	43.8	-49.2
6	4	3	7.5	+9.0
6	4	4	3.2	+3.3
6	4	6	19.5	-19.5
6	4	8	14.3	-16.0
7	4	-10	3.2	-4.8
7	4	-9	4.5	-6.3
7	4	-8	17.0	+20.8
7	4	-6	9.6	-13.3
7	4	-5	11.3	-14.6
7	4	-4	9.9	+12.6
7	4	-2	7.2	-10.3
7	4	-1	2.7	-3.8
7	4	0	18.7	+20.8
7	4	1	13.2	-15.9
7	4	2	17.6	+20.2
7	4	3	41.0	+41.7
7	4	4	19.5	-17.9
7	4	6	5.1	+6.8
7	4	7	3.2	+4.0
7	4	8	11.8	-14.0
8	4	-11	5.6	-6.6
8	4	-10	10.4	-13.2
8	4	-9	10.6	+13.4
8	4	-8	16.4	+19.2
8	4	-6	6.8	-9.4
8	4	-5	5.6	-7.2
8	4	-4	32.6	+32.3
8	4	-3	20.7	+23.1
8	4	-2	32.3	+34.5
8	4	-1	7.9	-8.1
8	4	0	18.3	-21.6
8	4	1	14.5	+15.8
8	4	2	41.2	+42.4
8	4	3	3.9	-4.9
8	4	4	19.2	-18.7
8	4	5	6.9	+7.3
8	4	6	8.1	+9.7
8	4	7	9.3	+10.8
8	4	8	16.5	-16.7
8	4	9	10.6	-11.9
9	4	-10	2.2	+2.6
9	4	-9	7.9	-9.4
9	4	-8	7.5	+8.9
9	4	-6	3.9	+7.4
9	4	-4	15.3	-18.2
9	4	-3	30.9	-31.6
9	4	-2	13.8	+15.0
9	4	-1	8.5	+10.4
9	4	0	13.8	-13.9
9	4	1	6.8	-9.0
9	4	2	19.5	+19.9
9	4	3	4.9	+4.5
9	4	4	10.9	-13.0
9	4	5	9.3	+11.8
9	4	6	7.5	+7.7
9	4	8	7.5	+7.6
10	4	-10	2.2	-2.3
10	4	-8	8.1	-11.4
10	4	-6	18.9	+24.0
10	4	-3	4.9	+5.5
10	4	-2	19.5	+23.6
10	4	2	4.9	+6.5
10	4	3	4.7	-4.8
10	4	4	9.1	+11.8
10	4	6	6.4	-7.3
10	4	7	4.2	+4.8
11	4	-9	3.9	+4.9
11	4	-8	7.5	-11.5
11	4	-7	4.5	-4.5
11	4	-6	12.2	+11.9
11	4	-5	11.1	+12.7
11	4	-4	3.9	-4.9
11	4	-3	3.9	-4.9
11	4	-2	6.8	+8.7
11	4	0	13.2	+13.1
11	4	1	3.2	+5.4
11	4	2	10.1	-9.2
11	4	3	7.5	-7.2
11	4	4	11.6	+10.5
11	4	6	5.3	-4.5
12	4	-8	9.6	-10.9
12	4	-4	8.5	+8.7
12	4	-2	8.7	-8.0
12	4	-1	4.3	+5.6
12	4	0	19.4	+22.9
12	4	2	9.6	-9.2
12	4	3	10.4	+11.5
12	4	4	8.7	+10.6
13	4	-7	3.2	+4.5
13	4	-6	10.9	-13.6
13	4	-4	12.2	+13.6
13	4	-2	6.4	-8.8
13	4	0	12.9	+13.5
13	4	1	7.9	-7.2
13	4	2	6.3	+7.2
14	4	-5	3.2	-5.1
14	4	-3	5.6	+7.1
14	4	-2	3.9	+5.3
14	4	0	5.9	-6.4
14	4	1	6.3	+6.9
0	5	1	66.1	-65.5
0	5	2	23.1	+23.5
0	5	3	17.3	-16.2
0	5	4	55.5	-55.3
0	5	5	74.6	-73.9
0	5	6	29.9	+26.8
0	5	7	48.2	+48.2
0	5	8	15.1	-15.7
0	5	9	8.5	-9.3
0	5	10	3.2	+3.5
0	5	11	7.2	+6.2
1	5	-11	13.0	+14.4
1	5	-9	26.2	-24.2
1	5	-8	33.6	-29.8
1	5	-7	15.3	+15.0
1	5	-6	18.6	-13.7
1	5	-5	10.4	+9.7
1	5	-4	45.3	-44.3
1	5	-3	11.1	+10.0
1	5	-2	44.7	-44.3
1	5	-1	64.1	-61.0
1	5	0	19.9	+24.4
1	5	1	39.3	-36.3
1	5	2	20.6	-20.4
1	5	3	2.2	-2.4
1	5	4	52.9	+49.9
1	5	5	43.0	-37.6
1	5	6	9.3	+8.4
1	5	7	3.2	+4.5
1	5	8	10.1	+17.3
1	5	9	4.5	-4.1
1	5	10	12.0	+12.5
1	5	11	2.2	-3.0
2	5	-12	4.5	+3.0
2	5	-11	7.5	+8.5
2	5	-9	10.6	+7.7
2	5	-8	6.8	+6.9
2	5	-7	16.6	-15.0
2	5	-6	18.6	-16.1
2	5	-5	8.1	+8.3
2	5	-4	10.1	-8.3
2	5	-3	7.9	-9.1
2	5	-2	8.5	-6.5
2	5	-1	22.7	-21.4
2	5	0	18.0	-17.2
2	5	1	6.4	-9.6
2	5	2	9.6	-9.3
2	5	3	61.5	-68.9
2	5	5	7.9	-8.4
2	5	6	5.1	-5.2
2	5	7	29.8	-27.7
2	5	8	4.5	+3.2
2	5	9	17.8	+18.5
2	5	11	14.7	-13.3
3	5	-11	6.0	-5.4
3	5	-10	15.3	+13.2
3	5	-9	13.6	+12.3
3	5	-7	28.3	-27.4
3	5	-5	8.5	+9.1
3	5	-4	16.8	-17.4
3	5	-3	10.6	-9.8
3	5	-2	55.1	-52.4
3	5	-1	44.2	-46.6
3	5	0	19.1	-15.6
3	5	1	12.0	+9.6
3	5	2	41.8	-36.1
3	5	3	53.1	-49.4
3	5	5	22.9	+16.8
3	5	7	42.4	-38.4
3	5	9	14.0	+13.2
3	5	10	6.8	+6.6
4	5	-12	3.2	+3.1
4	5	-11	5.1	-5.0
4	5	-10	2.2	-2.5
4	5	-9	19.4	+20.7
4	5	-7	11.6	-10.1
4	5	-6	12.6	+12.5
4	5	-5	15.3	+14.4
4	5	-4	25.4	-21.8
4	5	-3	4.5	-4.3
4	5	-2	11.8	+7.3
4	5	-1	3.9	+3.1
4	5	0	26.3	-26.6
4	5	1	12.2	+10.0
4	5	2	5.1	-5.0
4	5	3	50.7	-49.9
4	5	4	6.0	-4.5
4	5	5	15.3	+13.3
4	5	7	39.9	-37.0
4	5	8	4.5	+5.1
4	5	9	7.5	-7.5
4	5	10	3.2	-3.4
5	5	-11	4.5	-4.4
5	5	-7	6.0	+3.2
5	5	-6	12.6	+12.7
5	5	-5	25.1	-22.8
5	5	-4	11.1	-13.4
5	5	-3	11.3	-11.3
5	5	-1	10.6	-12.3
5	5	0	33.6	-33.5
5	5	1	5.1	-3.8
5	5	2	16.6	-16.4
5	5	3	19.4	-18.9
5	5	4	14.5	-12.2
5	5	5	4.5	+5.7
5	5	6	9.6	-9.7
5	5	7	8.1	+7.5
5	5	9	16.0	-16.3
6	5	-11	5.6	+5.4
6	5	-9	14.1	-14.3
6	5	-8	10.9	+12.0
6	5	-7	36.9	+37.1
6	5	-6	11.6	-9.2
6	5	-5	12.6	-13.3
6	5	-4	16.8	+17.2
6	5	-3	8.7	-9.2
6	5	-2	8.5	-9.4
6	5	0	26.5	-22.8
6	5	1	27.8	-24.5
6	5	2	9.3	-9.6
6	5	3	31.1	+25.8
6	5	4	28.1	-28.6
6	5	5	42.5	-40.7
6	5	7	16.0	+15.1
6	5	9	10.4	-9.4
7	5	-11	12.0	+13.8
7	5	-9	11.8	-11.1
7	5	-8	9.1	-8.8
7	5	-7	9.6	+10.1
7	5	-6	3.9	-4.0
7	5	-5	3.9	+4.5
7	5	-4	6.4	+6.7
7	5	-3	7.5	+8.0
7	5	-2	2.2	+3.6
7	5	-1	4.5	+4.2
7	5	0	18.7	+14.5
7	5	1	60.0	-54.0
7	5	2	4.5	+3.1
7	5	3	29.7	+27.7
7	5	5	33.8	-32.9
7	5	6	6.4	-5.8
7	5	7	14.0	+11.9
7	5	8	8.7	-7.5
7	5	9	8.1	-8.1
8	5	-11	6.8	-6.6
8	5	-10	5.1	+5.9
8	5	-9	6.4	+6.5
8	5	-8	5.6	+6.2
8	5	-7	13.6	-13.1
8	5	-6	6.8	-5.3
8	5	-5	21.3	+21.1
8	5	-4	9.3	-8.3
8	5	-3	21.0	-19.3
8	5	-2	14.1	-12.6
8	5	-1	24.4	+27.4
8	5	0	8.7	-8.5
8	5	2	21.3	-19.6
8	5	4	7.5	-5.7
8	5	6	6.8	-6.4
8	5	7	8.7	-8.5
8	5	9	15.3	+12.6
9	5	-10	8.5	+7.0
9	5	-9	6.4	+7.6
9	5	-7	14.0	-14.7
9	5	-5	10.6	+12.8
9	5	-3	8.1	+8.0
9	5	-2	10.6	-10.3
9	5	-1	9.6	-9.0
9	5	0	6.8	+6.3
9	5	1	8.1	-4.6
9	5	3	13.6	-9.3
9	5	4	4.5	+3.3
9	5	5	8.7	+8.1
9	5	6	2.2	-4.0

Table 2 (*cont.*)

H	K	L	F(OBS)	F(CAL)
9	5	7	17.3	-15.0
9	5	8	3.9	-3.7
10	5	-9	12.4	+12.5
10	5	-8	7.5	+7.9
10	5	-7	10.1	-11.2
10	5	-6	10.9	+10.8
10	5	-3	7.5	+7.2
10	5	0	11.8	-10.8
10	5	1	30.4	+28.7
10	5	2	5.1	-5.4
10	5	3	25.3	-22.8
10	5	4	8.5	-8.9
10	5	5	10.9	+11.1
11	5	-9	10.6	-7.3
11	5	-6	11.3	+9.0
11	5	-5	6.0	-4.4
11	5	-4	5.6	-4.1
11	5	-3	9.3	+7.7
11	5	-1	11.3	-8.6
11	5	0	10.4	-8.2
11	5	1	19.9	+18.1
11	5	2	4.5	-3.7
11	5	3	5.1	-2.7
11	5	5	4.5	+4.6
11	5	6	2.2	-2.3
12	5	-8	8.7	+6.8
12	5	-7	7.2	+8.8
12	5	-6	8.5	+7.7
12	5	-5	16.8	-16.6
12	5	-4	12.6	+10.5
12	5	-3	4.1	+4.2
12	5	-2	4.1	+4.3
12	5	-1	9.3	-7.9
12	5	2	9.1	-7.6
12	5	3	8.1	+6.7
12	5	4	7.5	-7.6
13	5	-5	3.9	-3.1
13	5	-4	9.9	+9.0
13	5	-2	9.9	+9.2
13	5	-1	12.0	+11.6
13	5	0	3.2	+2.6
13	5	1	12.4	-12.1
13	5	2	4.5	+4.3
13	5	3	13.8	+13.2
14	5	-3	13.8	-12.1
14	5	-1	6.0	+5.7
14	5	0	6.8	+6.4
0	6	0	43.5	+40.2
0	6	1	12.6	+12.1
0	6	2	23.8	-25.7
0	6	3	23.6	+26.6
0	6	4	28.8	+29.1
0	6	5	33.1	+31.3
0	6	6	11.8	+11.1
0	6	7	12.9	-10.6
0	6	8	13.2	-12.0
0	6	9	7.9	+8.1
0	6	10	17.8	+15.5
1	6	-8	11.7	+12.8
1	6	-7	10.9	-9.4
1	6	-6	26.3	-25.1
1	6	-5	28.6	-30.3
1	6	-4	17.7	+17.1
1	6	-3	26.4	-25.7
1	6	-2	11.1	-9.3
1	6	-1	27.8	-29.0
1	6	0	29.6	+28.9
1	6	1	20.3	-19.1
1	6	2	37.4	+34.6
1	6	4	26.2	-24.1
1	6	5	34.0	+35.9
1	6	6	32.8	+28.6
1	6	7	22.2	+21.6
1	6	8	9.3	-8.0
1	6	9	8.7	+6.9
1	6	10	8.7	+7.5
1	6	11	4.5	-3.4
2	6	-10	2.2	-4.0
2	6	-8	22.9	+20.9
2	6	-7	12.7	+10.9
2	6	-5	3.9	-3.2
2	6	-4	35.7	+33.8
2	6	-3	23.8	-25.0
2	6	-1	49.2	-52.7
2	6	0	39.9	-41.3
2	6	1	2.1	+0.6
2	6	2	52.1	+46.6
2	6	3	23.8	-23.2
2	6	4	33.3	-33.3
2	6	5	3.2	-2.3
2	6	6	17.6	+15.0
2	6	7	20.7	+20.1
2	6	8	8.0	-6.9
2	6	9	7.5	+5.8
2	6	11	8.3	+6.9
3	6	-11	5.1	+5.1
3	6	-10	6.4	-6.5
3	6	-9	2.8	-2.6
3	6	-8	8.1	+7.1
3	6	-7	7.9	-6.9
3	6	-6	7.4	+5.5
3	6	-5	7.5	+7.2
3	6	-4	6.8	+6.3
3	6	-3	26.6	-15.4

H	K	L	F(OBS)	F(CAL)
3	6	-2	45.9	+49.8
3	6	-1	17.1	-20.1
3	6	0	3.2	-6.2
3	6	1	53.1	-50.8
3	6	2	33.1	+32.9
3	6	3	13.6	-11.4
3	6	4	3.9	-3.3
3	6	5	18.7	-16.7
3	6	6	6.3	+4.7
3	6	7	6.5	+6.7
3	6	9	10.6	+9.8
3	6	10	13.8	-12.1
3	6	11	6.6	+3.3
4	6	-11	5.1	-4.4
4	6	-10	6.8	-6.1
4	6	-9	6.8	+6.6
4	6	-8	6.5	-6.4
4	6	-7	14.5	-14.9
4	6	-6	10.6	+8.8
4	6	-5	8.1	+7.1
4	6	-4	16.5	-17.2
4	6	-2	19.5	+20.6
4	6	-1	9.6	-5.3
4	6	0	9.1	+6.2
4	6	1	19.5	-18.8
4	6	2	3.3	-3.7
4	6	3	10.4	-9.0
4	6	4	25.6	+22.9
4	6	5	15.3	-14.8
4	6	7	8.1	-7.2
4	6	8	17.4	+15.0
4	6	9	5.6	+5.2
5	6	-10	7.5	+7.6
5	6	-9	7.5	+7.0
5	6	-8	6.4	-6.7
5	6	-7	6.4	-5.6
5	6	-6	28.2	+29.0
5	6	-5	17.1	-16.6
5	6	-4	2.5	+3.0
5	6	-3	4.7	-4.9
5	6	-2	7.9	+9.1
5	6	-1	7.5	-7.5
5	6	0	37.5	+38.0
5	6	1	17.4	-16.8
5	6	2	31.5	-31.0
5	6	3	14.0	-12.1
5	6	4	23.6	+25.4
5	6	5	20.2	-20.0
5	6	6	29.6	-27.8
5	6	8	6.0	+5.3
5	6	9	7.2	-6.5
6	6	-11	3.2	+2.7
6	6	-10	8.7	+8.6
6	6	-8	14.3	-13.3
6	6	-6	14.5	-14.0
6	6	-4	16.8	+15.9
6	6	-3	21.9	-23.8
6	6	-2	24.9	-28.4
6	6	-1	2.2	-2.5
6	6	0	48.1	+50.3
6	6	1	5.6	-5.6
6	6	2	26.1	-23.6
6	6	3	10.6	-11.7
6	6	4	28.5	+30.1
6	6	5	6.4	+6.3
6	6	6	4.5	+6.0
6	6	7	13.8	-13.7
6	6	9	6.8	-6.1
7	6	-11	12.2	+10.3
7	6	-10	2.2	-2.5
7	6	-8	12.4	+12.5
7	6	-7	13.0	+12.4
7	6	-6	10.4	-10.1
7	6	-5	9.1	-9.9
7	6	-4	19.9	+19.9
7	6	-3	17.4	-17.7
7	6	-2	15.9	-16.2
7	6	-1	8.5	+8.5
7	6	0	26.8	+26.1
7	6	1	23.6	-24.9
7	6	2	14.0	+12.7
7	6	4	6.4	-5.1
7	6	5	10.4	-8.8
7	6	6	6.4	+5.5
7	6	8	7.5	-6.8
8	6	-9	9.1	+6.5
8	6	-8	13.2	+15.4
8	6	-7	5.1	+4.8
8	6	-6	13.0	-13.1
8	6	-2	7.9	+4.5
8	6	-1	44.7	-46.2
8	6	0	45.0	-47.5
8	6	1	13.4	+10.6
8	6	2	29.2	+22.7
8	6	3	16.2	-14.6
8	6	4	18.4	-13.5
8	6	5	6.4	-5.2
8	6	6	16.6	+13.2
9	6	-10	4.5	-3.7
9	6	-8	9.3	+6.7
9	6	-7	7.2	+7.5
9	6	-6	10.1	+10.6
9	6	-5	13.4	+10.9
9	6	-4	8.1	-7.4
9	6	-2	35.8	+34.1
9	6	-1	10.4	+8.9
9	6	0	9.3	-8.8

H	K	L	F(OBS)	F(CAL)
9	6	1	25.5	-25.6
9	6	2	25.5	+25.0
9	6	3	9.3	-9.0
9	6	4	12.4	-11.3
9	6	6	3.7	+3.2
9	6	7	7.2	-7.6
10	6	-9	5.1	+4.1
10	6	-8	3.2	-5.2
10	6	-7	10.6	+11.4
10	6	-6	18.6	+17.8
10	6	-5	5.6	-3.9
10	6	-4	12.9	-13.5
10	6	-3	13.0	+11.9
10	6	-2	10.0	+8.3
10	6	-1	13.0	-12.1
10	6	0	20.6	-18.5
10	6	1	4.5	-4.9
10	6	3	6.4	-4.9
10	6	4	3.2	+3.1
10	6	5	13.8	-12.3
11	6	-8	5.6	-7.6
11	6	-7	4.5	-2.8
11	6	-6	10.4	+9.9
11	6	-5	9.1	+7.6
11	6	-3	8.5	+7.9
11	6	-2	4.5	+3.9
11	6	0	12.2	+11.7
11	6	1	4.2	+2.7
11	6	2	11.3	-11.0
11	6	3	11.6	-11.0
11	6	4	5.1	+3.5
11	6	5	3.2	+1.3
12	6	-7	10.4	+8.6
12	6	-6	7.2	+3.8
12	6	-5	2.1	+2.4
12	6	-4	18.3	+14.8
12	6	-2	8.5	-9.1
12	6	-1	3.9	+2.8
12	6	0	25.9	+24.2
12	6	2	13.8	-10.6
12	6	3	3.9	-4.0
12	6	4	10.4	+6.2
13	6	-5	5.6	+5.5
13	6	-4	10.1	+9.0
13	6	-3	2.2	-1.8
13	6	-2	14.1	-14.1
13	6	-1	10.1	+8.2
13	6	0	9.1	+7.1
0	7	1	10.7	-9.6
0	7	2	3.9	+3.4
0	7	3	49.2	+46.6
0	7	4	23.2	+19.3
0	7	5	29.7	-29.5
0	7	6	52.3	+50.3
0	7	7	34.5	+32.6
0	7	8	15.5	+14.3
0	7	9	11.9	-10.8
0	7	10	8.1	+8.8
0	7	11	4.5	+2.9
1	7	-11	6.0	+5.7
1	7	-10	3.9	-4.7
1	7	-9	10.4	-11.1
1	7	-8	11.1	-9.5
1	7	-7	15.3	+16.1
1	7	-6	36.9	+32.6
1	7	-5	5.6	+4.8
1	7	-4	36.1	-34.7
1	7	-3	18.0	+17.4
1	7	-2	4.5	+9.6
1	7	-1	25.8	+25.0
1	7	0	19.1	+21.3
1	7	1	20.7	-20.1
1	7	2	22.5	-22.5
1	7	3	30.6	+26.3
1	7	4	13.8	+13.2
1	7	5	11.1	-9.5
1	7	6	33.0	-31.5
1	7	7	5.6	+5.4
1	7	8	10.9	+9.6
1	7	9	6.4	+3.2
1	7	10	5.1	+3.1
1	7	11	6.4	-4.1
2	7	-10	10.4	-11.2
2	7	-9	6.4	-5.8
2	7	-7	8.7	-8.4
2	7	-6	41.4	-38.7
2	7	-5	22.7	+19.6
2	7	-4	16.4	-15.5
2	7	-3	7.2	-6.8
2	7	-2	14.1	-11.9
2	7	-1	44.2	+44.9
2	7	0	26.2	-27.8
2	7	1	5.0	+5.7
2	7	2	20.1	+19.0
2	7	4	5.1	+4.9
2	7	5	22.1	+19.9
2	7	6	17.3	+14.8
2	7	7	10.0	-9.1
2	7	8	15.3	+14.5
2	7	9	14.0	+13.3
2	7	10	4.5	-4.3
2	7	11	8.5	-7.5
3	7	-11	10.9	-9.0
3	7	-10	3.9	-3.2
3	7	-9	4.5	+4.7

H	K	L	F(OBS)	F(CAL)
3	7	-8	6.4	+5.2
3	7	-7	22.4	-21.5
3	7	-6	30.0	-29.0
3	7	-5	27.8	+24.4
3	7	-4	19.6	+16.5
3	7	-3	5.6	-5.0
3	7	-2	45.3	-46.2
3	7	-1	20.4	+18.8
3	7	0	20.1	+18.0
3	7	1	44.7	+43.6
3	7	2	23.8	+23.7
3	7	3	21.9	-19.4
3	7	5	26.1	+25.2
3	7	6	14.1	+13.2
3	7	7	15.5	-14.7
3	7	9	7.5	+6.6
3	7	10	4.5	+3.3
4	7	-11	8.1	-9.1
4	7	-9	3.9	+4.4
4	7	-8	10.9	+9.9
4	7	-7	24.6	-25.8
4	7	-6	13.6	-14.2
4	7	-5	11.6	+7.8
4	7	-3	2.5	-2.7
4	7	-2	32.6	-36.0
4	7	-1	2.4	-2.5
4	7	0	30.8	-30.5
4	7	1	46.2	+44.4
4	7	2	10.9	-11.7
4	7	3	10.9	-7.8
4	7	4	7.2	-7.6
4	7	5	27.3	+26.4
4	7	6	4.5	+4.7
4	7	7	6.4	-4.6
4	7	8	6.0	+4.8
4	7	10	3.9	+3.9
5	7	-11	6.4	-6.6
5	7	-9	3.9	-2.8
5	7	-8	6.8	-6.4
5	7	-7	6.8	-5.7
5	7	-6	7.9	+9.0
5	7	-5	23.2	-21.9
5	7	-3	14.7	+13.6
5	7	-2	4.5	-1.3
5	7	-1	13.2	-11.9
5	7	0	5.1	-4.0
5	7	1	30.1	+26.7
5	7	2	21.0	-21.2
5	7	3	11.6	+14.5
5	7	4	16.0	+19.5
5	7	5	9.1	+7.4
5	7	7	12.0	+12.1
5	7	8	3.9	+1.9
5	7	9	9.1	-6.7
5	7	10	5.1	+5.3
6	7	-11	3.9	+4.0
6	7	-9	13.4	-13.5
6	7	-7	12.6	+14.2
6	7	-5	34.0	-36.1
6	7	-4	7.2	-7.8
6	7	-3	5.6	+4.6
6	7	-2	7.9	+8.8
6	7	-1	12.4	-12.3
6	7	0	8.7	+8.7
6	7	1	15.3	-14.6
6	7	2	13.0	-12.9
6	7	3	36.2	+32.1
6	7	4	8.7	-8.8
6	7	5	12.6	-10.7
6	7	6	4.6	+6.1
6	7	7	19.9	+21.1
6	7	9	5.1	-3.7
7	7	-10	3.2	+3.9
7	7	-9	10.1	-11.9
7	7	-8	14.0	-14.7
7	7	-7	8.7	+7.9
7	7	-6	22.5	+23.6
7	7	-5	14.3	-11.9
7	7	-4	17.8	-17.2
7	7	-3	15.1	-14.7
7	7	-2	6.4	-4.9
7	7	-1	15.5	+14.6
7	7	0	17.8	-15.6
7	7	1	33.3	-31.5
7	7	2	6.4	-7.0
7	7	3	28.3	+25.7
7	7	4	6.8	-6.7
7	7	5	7.5	-5.6
7	7	6	6.0	-4.5
7	7	7	10.4	+10.2
8	7	-8	4.5	-4.6
8	7	-7	4.5	-5.8
8	7	-5	7.9	+7.7
8	7	-4	9.1	-9.2
8	7	-3	28.3	-26.8
8	7	-2	31.6	+30.1
8	7	-1	9.9	+8.2
8	7	0	6.4	+5.7
8	7	1	20.1	-15.6
8	7	2	10.1	+8.6
8	7	4	4.5	-2.6
8	7	5	4.5	+5.1
8	7	8	3.9	-2.1
9	7	-9	10.4	+9.7
9	7	-8	7.5	+7.5
9	7	-7	13.2	-14.1
9	7	-6	3.9	-3.8

H	K	L	F(OBS)	F(CAL)
9	7	-5	15.1	+12.6
9	7	-3	10.9	-11.0
9	7	-2	15.5	-15.4
9	7	-1	10.9	-10.6
9	7	0	14.1	-11.7
9	7	1	4.5	+5.3
9	7	2	14.0	+13.3
9	7	3	19.1	-17.4
9	7	4	7.2	-5.6
9	7	5	11.8	+10.5
9	7	6	3.2	-3.5
9	7	7	7.2	-6.0
10	7	-8	7.9	+7.7
10	7	-7	8.1	-7.6
10	7	-6	8.5	-10.4
10	7	-5	5.6	+3.5
10	7	-4	7.2	+6.8
10	7	-3	3.2	+3.1
10	7	-1	13.8	-14.6
10	7	0	7.5	-6.9
10	7	1	10.4	+10.2
10	7	2	3.2	+3.3
10	7	3	17.4	-16.1
10	7	5	3.2	+3.4
10	7	6	9.3	+8.1
11	7	-8	12.0	+11.3
11	7	-7	2.2	+2.9
11	7	-6	11.0	+8.3
11	7	-5	7.2	-7.5
11	7	-4	5.6	+6.0
11	7	-3	12.4	+10.3
11	7	-1	15.9	-14.3
11	7	0	3.2	+3.0
11	7	1	8.5	+6.7
11	7	2	10.1	-9.0
11	7	3	5.7	-5.3
11	7	5	2.2	-2.7
12	7	-5	11.3	-10.6
12	7	-4	9.6	+8.7
12	7	-3	7.5	+6.9
12	7	-2	2.2	-2.4
12	7	-1	4.5	-3.1
12	7	0	12.6	+11.0
12	7	1	6.8	-6.4
12	7	2	5.6	-4.5
12	7	3	5.6	+4.9
13	7	-4	7.2	+5.5
13	7	-3	5.6	-4.8
13	7	-1	11.3	+9.9
13	-7	1	14.7	-13.2
0	8	0	19.5	+18.1
0	8	1	10.6	+13.7
0	8	2	13.2	-12.2
0	8	3	5.6	+7.3
0	8	4	9.6	+8.7
0	8	5	6.0	+6.1
0	8	6	9.3	-10.0
0	8	7	21.3	-20.2
0	8	8	3.9	-2.5
0	8	9	7.5	+7.1
0	8	10	6.0	+5.2
0	8	11	5.1	-4.5
1	8	-10	6.4	-6.1
1	8	-9	7.9	+5.6
1	8	-8	15.7	+15.2
1	8	-7	2.5	-1.9
1	8	-6	18.4	-21.1
1	8	-5	9.1	-10.6
1	8	-4	39.9	+39.6
1	8	-3	18.0	+17.7
1	8	-2	21.9	-19.7
1	8	-1	15.5	-17.4
1	8	0	6.4	+5.2
1	8	1	5.6	-7.4
1	8	2	7.2	-5.6
1	8	3	2.2	+1.7
1	8	4	8.5	-7.1
1	8	5	17.3	+15.4
1	8	6	18.6	+18.6
1	8	7	4.5	+3.5
1	8	8	22.7	-23.4
1	8	9	3.2	+2.1
1	8	10	16.8	+13.6
2	8	-11	6.4	-4.2
2	8	-10	17.0	-19.8
2	8	-9	3.2	+2.2
2	8	-8	6.4	+8.8
2	8	-7	12.0	+11.7
2	8	-6	18.4	-21.2
2	8	-4	3.2	-3.2
2	8	-2	15.7	+15.6
2	8	-1	18.7	-18.3
2	8	0	6.8	+6.3
2	8	1	5.1	+2.6
2	8	2	23.4	+21.6
2	8	3	5.6	-5.7
2	8	4	16.0	-15.7
2	8	5	6.0	-5.0
2	8	6	18.9	+20.3
2	8	7	8.5	+6.9
2	8	8	7.2	-7.6
2	8	9	5.6	+3.4
2	8	10	3.9	-3.3
3	8	-10	14.5	-15.7

H	K	L	F(OBS)	F(CAL)
3	8	-8	6.0	-5.7
3	8	-7	4.3	+2.9
3	8	-6	4.1	-3.7
3	8	-5	13.4	+14.2
3	8	-4	15.3	-14.7
3	8	-3	5.6	+5.2
3	8	-2	5.1	+4.3
3	8	-1	14.1	+16.2
3	8	0	12.6	-12.6
3	8	1	28.4	-31.8
3	8	2	19.8	+18.4
3	8	3	3.2	+3.0
3	8	4	8.5	-9.3
3	8	5	11.6	-13.8
3	8	6	8.5	+8.4
3	8	8	8.7	+6.9
3	8	10	6.4	-4.4
4	8	-11	6.4	-7.0
4	8	-9	3.2	+3.1
4	8	-8	18.4	-20.5
4	8	-7	13.4	-14.4
4	8	-6	12.0	+12.3
4	8	-5	11.3	+11.6
4	8	-4	20.6	-19.8
4	8	-2	14.5	+15.7
4	8	-1	17.0	+18.5
4	8	1	6.4	+7.3
4	8	2	10.9	+10.5
4	8	4	6.9	+7.0
4	8	5	3.2	-3.3
4	8	6	13.4	-14.5
4	8	8	9.3	+10.3
4	8	10	10.1	-10.4
5	8	-10	2.2	+4.2
5	8	-8	39.9	-36.6
5	8	-7	6.0	-6.2
5	8	-6	6.4	-6.7
5	8	-4	33.0	-34.0
5	8	-3	3.9	-2.7
5	8	-2	7.2	-6.1
5	8	1	11.3	+11.6
5	8	2	5.6	-2.2
5	8	4	37.6	+35.4
5	8	5	11.3	-12.4
5	8	6	5.6	-5.4
5	8	7	6.8	+7.5
5	8	8	15.0	+16.6
5	8	9	7.2	-7.4
6	8	-10	3.9	+5.2
6	8	-8	7.5	-7.5
6	8	-7	6.4	-6.8
6	8	-6	13.4	-12.3
6	8	-5	8.5	+10.0
6	8	-4	7.2	-6.1
6	8	-3	9.1	-10.4
6	8	-2	21.5	-21.7
6	8	0	8.7	+7.6
6	8	1	6.8	+7.9
6	8	2	11.6	-11.0
6	8	3	2.2	+2.5
6	8	4	8.5	+9.5
6	8	5	8.5	+9.7
6	8	7	7.2	-8.8
6	8	8	6.4	-3.3
6	8	9	5.1	-4.7
7	8	-10	3.9	-2.5
7	8	-7	5.1	+5.4
7	8	-6	32.4	-32.3
7	8	-5	9.6	-9.5
7	8	-4	4.5	-4.3
7	8	-3	3.9	-4.6
7	8	-2	34.7	-35.4
7	8	-1	16.6	+16.1
7	8	0	9.3	-10.8
7	8	1	10.4	-11.3
7	8	2	9.3	-10.1
7	8	3	8.5	+8.6
7	8	6	20.3	+21.8
7	8	8	7.2	-8.4
8	8	-8	9.1	+12.0
8	8	-7	3.2	+4.3
8	8	-6	13.8	-15.1
8	8	-4	9.6	-7.7
8	8	-3	4.5	+4.3
8	8	-2	5.6	-3.7
8	8	-1	27.0	-27.1
8	8	0	10.4	-10.6
8	8	1	9.6	+10.9
8	8	2	15.7	+15.4
8	8	4	17.8	-18.1
8	8	5	3.9	+3.4
8	8	6	11.8	+13.3
8	8	7	2.2	+1.9
9	8	-9	5.1	-5.7
9	8	-8	2.2	+1.4
9	8	-7	5.1	+5.2
9	8	-6	5.1	-4.1
9	8	-5	3.2	+2.2
9	8	-4	14.1	-14.4
9	8	-2	18.7	-17.5
9	8	-1	16.8	+15.9
9	8	0	32.5	-31.3
9	8	1	18.6	-19.3
9	8	2	7.2	-7.2
9	8	3	3.2	-2.6
9	8	4	7.2	-9.1
9	8	5	2.2	+2.8

Table 2 (*cont.*)

H	K	L	F(OBS)	F(CAL)
10	8	-8	6.8	-7.8
10	8	-7	6.8	+5.5
10	8	-6	6.4	+8.2
10	8	-5	5.6	-5.7
10	8	-4	22.9	-22.0
10	8	-3	8.7	+8.1
10	8	-2	5.6	+5.7
10	8	-1	5.6	-4.3
10	8	0	7.9	-5.6
10	8	1	8.5	+7.4
10	8	2	5.1	-6.4
10	8	5	5.6	-6.8
11	8	-7	9.1	-9.1
11	8	-6	4.5	+6.0
11	8	-4	4.5	-4.2
11	8	-3	4.5	+3.0
11	8	-2	6.0	-4.8
11	8	-1	6.8	-5.9
11	8	0	5.6	-3.3
11	8	1	7.9	+6.5
11	8	2	15.3	-14.1
11	8	3	8.7	-8.0
11	8	4	5.1	+6.1
12	8	-5	3.9	-3.3
12	8	-4	2.2	-1.9
12	8	-3	3.2	+1.6
12	8	-2	11.1	-12.3
12	8	0	4.5	+4.4
12	8	1	3.2	+2.8
12	8	2	13.0	-13.8
0	9	2	12.3	-10.9
0	9	3	32.8	+31.0
0	9	4	45.2	-46.2
0	9	5	2.2	-1.2
0	9	6	10.4	-9.7
0	9	7	14.9	+13.9
0	9	8	18.4	-16.4
0	9	9	13.2	-13.6
0	9	10	6.0	-5.3
1	9	-9	2.2	-2.4
1	9	-8	9.8	-9.9
1	9	-7	6.0	+5.5
1	9	-6	11.1	+9.5
1	9	-5	2.2	+3.6
1	9	-4	9.1	-7.8
1	9	-3	28.0	-23.9
1	9	-2	10.9	+11.0
1	9	-1	45.0	+45.4
1	9	0	10.9	+10.1
1	9	1	34.0	-27.2
1	9	2	6.0	-5.2
1	9	3	21.1	+19.3
1	9	4	14.9	+14.5
1	9	5	11.6	-8.6
1	9	6	25.6	-23.8
1	9	7	8.7	+9.0
1	9	8	7.5	+6.4
1	9	9	12.6	+11.8
2	9	-9	9.6	-7.1
2	9	-8	17.1	+14.3
2	9	-6	5.6	-5.4
2	9	-5	39.9	+32.4
2	9	-4	25.6	+22.4
2	9	-3	21.2	-18.6
2	9	-2	32.1	+32.2
2	9	-1	42.1	+44.0
2	9	0	5.6	+4.9
2	9	1	31.5	-26.8
2	9	2	8.7	+8.5
2	9	3	31.8	+30.2
2	9	5	3.2	-2.9
2	9	6	19.6	-20.0
2	9	7	8.7	-9.0
2	9	8	9.1	-10.3
2	9	9	8.5	+8.1
2	9	10	9.9	-10.4
3	9	-10	6.4	+4.7
3	9	-9	6.4	+6.8
3	9	-8	12.0	+12.0
3	9	-7	11.3	-13.3
3	9	-6	7.9	-8.7
3	9	-5	15.1	+15.1
3	9	-4	8.5	+6.6
3	9	-2	10.4	-10.4
3	9	-1	27.4	+28.0
3	9	0	13.8	+13.7
3	9	1	14.0	+12.2
3	9	4	3.2	-1.8
3	9	5	11.1	+10.3
3	9	6	3.2	+2.5
3	9	7	5.6	-4.0
3	9	8	8.1	-8.8
4	9	-10	5.6	-4.8
4	9	-8	6.4	+5.6
4	9	-7	17.6	-15.5
4	9	-6	8.7	+8.0
4	9	-5	6.8	-6.6
4	9	-4	5.6	+4.3
4	9	-3	10.6	+10.4
4	9	-2	6.4	+5.2
4	9	-1	10.4	-11.2
4	9	0	10.4	+10.5
4	9	1	31.5	+32.1
4	9	2	14.8	+16.2
4	9	3	3.2	-2.1
4	9	5	17.7	+16.7
4	9	6	7.9	+9.1
4	9	7	6.4	+5.1
5	9	-10	6.0	+5.3
5	9	-8	5.6	-5.3
5	9	-7	3.2	+4.8
5	9	-6	14.8	+15.4
5	9	-5	17.6	-17.0
5	9	-4	6.4	+4.2
5	9	-3	25.4	+22.2
5	9	-1	26.7	-24.7
5	9	0	6.8	+4.0
5	9	1	29.7	+28.7
5	9	2	5.6	-5.9
5	9	4	3.2	+2.6
5	9	7	7.9	+7.1
6	9	-9	8.5	-10.2
6	9	-5	25.2	-25.2
6	9	-4	10.4	+11.1
6	9	-3	21.3	+20.6
6	9	-1	14.7	-13.5
6	9	1	8.6	+8.1
6	9	3	12.6	+12.5
6	9	4	7.9	-8.1
6	9	6	3.2	+3.0
6	9	7	19.1	+15.6
6	9	8	2.2	+2.8
7	9	-9	6.8	-8.7
7	9	-8	10.0	-11.2
7	9	-7	5.1	+4.7
7	9	-6	5.1	+5.2
7	9	-5	5.6	-4.5
7	9	-4	6.8	+5.8
7	9	-3	30.6	-27.8
7	9	-2	12.6	+14.7
7	9	-1	13.5	+13.7
7	9	0	9.6	+9.1
7	9	1	9.6	-9.0
7	9	2	8.7	+8.4
7	9	3	12.6	+12.8
7	9	4	6.8	+5.7
7	9	6	4.5	-3.9
7	9	7	2.2	+1.8
8	9	-9	3.2	-2.5
8	9	-5	8.5	+9.5
8	9	-4	13.6	-13.2
8	9	-3	14.8	-14.5
8	9	-2	11.3	+11.7
8	9	-1	3.9	+3.7
8	9	0	3.9	-2.6
8	9	1	27.5	-25.5
8	9	2	9.6	-8.3
8	9	3	3.9	+3.1
8	9	4	3.2	+4.8
8	9	5	7.5	+5.2
8	9	6	2.2	-3.4
9	9	-7	8.1	-8.4
9	9	-6	7.2	-7.3
9	9	-5	8.5	+9.1
9	9	-4	3.9	-1.9
9	9	-3	12.0	-12.5
9	9	-1	6.0	+5.0
9	9	0	6.8	+8.5
9	9	1	9.3	+9.5
9	9	2	12.6	+12.5
9	9	3	14.0	-14.3
9	9	4	3.2	+3.4
9	9	5	11.1	+10.0
10	9	-5	4.5	+2.6
10	9	-4	2.2	-2.2
10	9	-3	5.1	+3.7
10	9	-1	12.4	-12.8
10	9	0	6.8	-5.1
10	9	2	2.2	+2.6
10	9	3	5.1	-4.6
10	9	4	4.5	-3.8
11	9	-5	9.9	-10.1
11	9	-4	7.5	-5.6
11	9	-3	13.0	+12.1
11	9	-2	3.2	-4.8
11	9	-1	12.6	-12.2
11	9	1	6.0	+4.9
11	9	2	3.9	+3.8
11	9	3	8.7	-6.2
12	9	-3	8.7	+8.9
12	9	-2	8.7	-8.3
12	9	1	2.2	-1.5
0	10	0	26.7	+25.2
0	10	1	11.2	-13.3
0	10	2	26.3	-27.1
0	10	3	9.6	+10.0
0	10	6	3.2	+2.4
0	10	8	8.1	+10.1
1	10	-9	6.8	+8.1
1	10	-7	12.4	+12.4
1	10	-6	9.1	-9.4
1	10	-5	8.7	+8.7
1	10	-4	42.4	+43.2
1	10	-3	16.5	+14.5
1	10	-2	34.0	-35.1
1	10	-1	3.2	-4.6
1	10	0	29.1	+24.9
1	10	1	4.5	-4.7
1	10	2	6.8	-5.7
1	10	3	4.5	+5.2
1	10	5	16.4	-16.0
1	10	6	11.6	+12.5
1	10	7	3.2	-2.6
1	10	8	17.6	-18.4
1	10	9	5.1	-5.3
2	10	-8	12.4	+14.5
2	10	-7	10.1	+9.5
2	10	-6	3.9	-3.6
2	10	-5	2.2	+2.2
2	10	-4	3.2	+3.5
2	10	-3	23.6	+24.4
2	10	-2	19.5	+18.2
2	10	0	11.3	-12.4
2	10	1	2.2	+3.0
2	10	2	8.5	+7.2
2	10	4	19.5	-18.0
2	10	5	6.4	-4.4
2	10	6	2.2	+2.8
2	10	7	2.2	+3.1
2	10	8	4.5	+4.6
2	10	9	6.8	-7.3
3	10	-9	8.7	-8.6
3	10	-8	5.6	+6.6
3	10	-7	5.6	+5.5
3	10	-4	2.2	-2.5
3	10	-3	13.6	+14.2
3	10	-2	30.3	+29.8
3	10	-1	17.6	+20.1
3	10	0	20.6	-23.0
3	10	1	8.5	+8.0
3	10	2	29.1	+27.9
3	10	3	11.3	+12.4
3	10	4	6.4	-6.9
3	10	6	7.9	-6.0
4	10	-9	5.1	+5.8
4	10	-8	6.4	-7.6
4	10	-7	6.8	-6.3
4	10	-6	10.4	+12.7
4	10	-5	9.1	+9.5
4	10	-4	17.4	-20.9
4	10	-3	6.0	+5.5
4	10	-2	29.1	+30.8
4	10	-1	5.6	+6.0
4	10	0	12.2	-10.8
4	10	1	12.6	+12.4
4	10	2	8.5	+9.8
4	10	3	11.3	-14.1
4	10	4	9.1	+8.3
4	10	5	5.6	+4.6
4	10	6	8.5	-8.4
4	10	7	8.7	-7.4
4	10	8	6.8	+7.1
5	10	-9	3.2	-2.8
5	10	-8	8.5	-10.8
5	10	-7	6.0	-6.6
5	10	-6	14.5	+16.4
5	10	-5	5.1	+5.0
5	10	-4	10.4	-9.0
5	10	-3	7.2	+8.2
5	10	-2	11.3	+12.1
5	10	-1	9.9	+11.5
5	10	0	10.9	+11.9
5	10	1	27.7	+27.7
5	10	2	7.2	-9.3
5	10	3	8.1	+10.3
5	10	4	8.7	+10.8
5	10	5	5.6	+6.3
5	10	6	4.5	-4.5
6	10	-8	3.9	-3.9
6	10	-7	7.2	-5.9
6	10	-5	2.2	+2.7
6	10	-3	3.9	-6.0
6	10	-2	23.1	-23.8
6	10	-1	10.4	+10.3
6	10	0	16.4	+17.0
6	10	1	9.1	+8.7
6	10	3	6.4	+7.1
6	10	4	2.2	+2.9
6	10	5	6.8	+9.2
6	10	6	8.5	+7.0
7	10	-8	2.2	+4.0
7	10	-7	3.2	+3.8
7	10	-6	7.5	-9.6
7	10	-5	4.5	-3.8
7	10	-4	32.5	+32.5
7	10	-3	6.4	-5.8
7	10	-2	10.9	-12.3
7	10	-1	6.4	+5.1
7	10	0	10.4	+10.3
7	10	1	7.5	-7.5
7	10	3	14.1	+18.4
7	10	4	5.1	-4.8
7	10	5	3.2	-3.1
7	10	6	12.6	+12.1
8	10	-8	15.1	+14.2
8	10	-7	2.2	+3.3
8	10	-6	6.8	-8.4
8	10	-4	3.2	-3.3
8	10	-3	13.4	+16.5
8	10	-2	5.6	-5.0
8	10	-1	2.2	-1.8
8	10	0	6.4	-6.9
8	10	1	9.9	+10.0
8	10	2	9.6	+9.8
8	10	4	10.9	-12.2
8	10	6	7.5	+7.0
9	10	-4	7.2	+6.5
9	10	-3	7.5	-6.6
9	10	-2	14.8	+15.2
9	10	-1	8.1	+8.6
9	10	0	7.5	-8.0
9	10	1	5.6	-3.6
9	10	2	4.5	+3.8
9	10	3	7.9	+8.6
9	10	4	6.8	+5.7
9	10	5	5.6	+4.7
10	10	-6	7.5	+9.0
10	10	-5	2.2	-2.7
10	10	-4	11.6	-14.4
10	10	-3	5.1	+5.1
10	10	-2	9.9	+12.8
10	10	1	4.5	+4.5
10	10	2	7.3	-7.7
11	10	0	6.0	+8.3
11	10	1	7.3	+9.6
0	11	1	26.6	-25.7
0	11	2	10.5	+6.0
0	11	3	11.6	-5.2
0	11	4	16.2	-14.0
0	11	5	18.4	-17.8
0	11	6	3.6	+1.8
0	11	7	10.5	+10.9
0	11	8	7.5	-6.4
0	11	9	8.6	-10.8
1	11	0	18.1	+17.4
2	11	0	12.9	+12.1
3	11	0	10.8	+9.4
4	11	0	10.6	-8.3
5	11	0	4.0	-3.5
6	11	0	3.4	+1.1
7	11	0	11.5	+9.9
8	11	0	9.4	+11.8
10	11	0	1.8	+1.6
0	12	0	13.4	+9.9
0	12	1	18.3	-15.3
0	12	2	13.8	-9.9
0	12	3	6.9	-3.5
0	12	4	9.8	+8.3
0	12	5	4.5	-2.5
1	12	0	5.9	+4.6
2	12	0	12.9	-14.6
3	12	0	17.9	-20.2
4	12	0	13.3	-14.1
5	12	0	7.5	+7.3
6	12	0	11.7	+12.9
7	12	0	8.7	+10.3
9	12	0	4.2	-5.6
0	13	1	5.1	+2.3
0	13	2	9.7	+5.6
0	13	3	11.6	+9.3
0	13	4	5.4	-3.8
0	13	5	11.3	-12.7
0	13	7	7.6	+9.2
1	13	0	7.5	-4.4
2	13	0	8.7	+9.0
3	13	0	4.0	-3.1
4	13	0	11.8	-13.6
6	13	0	10.2	-12.2
0	14	0	16.9	-19.8
0	14	2	7.6	-6.8
0	14	3	4.7	+4.0
1	14	0	16.2	+19.0
2	14	0	10.4	-12.9
3	14	0	6.4	-7.4
5	14	0	5.2	+7.4
0	15	1	8.3	+9.2
0	15	3	4.0	+4.7
2	15	0	4.5	+4.8

Description of the structure

Sodium naphthionate is the trivial name for sodium 1-aminonaphthalene-4-sulphonate, and the crystals investigated are the tetrahydrate, which is the common form reported in the literature (Groth, 1919). A metastable orthorhombic modification has also been reported, which may be a monohydrate, but this form has not been encountered in the course of this work. The crystals of the tetrahydrate effloresce slowly on keeping, resulting in pseudomorphs.

There are no particular abnormalities in the dimensions of the molecule; the ionic region resembles an inorganic salt, and the organic region of the molecule behaves as a covalent naphthalene derivative. The dimensions of the anion are shown in Fig. 4 alongside the corresponding values for naphthalene (Cruickshank, 1957). The shortening of the four symmetrical outer C–C bonds and the lengthening of the four symmetrical inner C–C bonds are common to both molecules, indicating similar electronic orbits in both cases, the substituent bonds having no resultant effect on the resonance.

The C–N length of 1·412 Å is within the range 1·35–1·47 Å quoted for similar bonds in other structures. It is probable that this length is quite sensitive to the environment and hydrogen bonding of the nitrogen atom.

The C–S length of 1·766 Å agrees with other published values, *e.g.* 1·752 Å in *β*-isoprene sulphone (Jeffrey, 1951). The S–O bonds in the sulphonate group have a mean length of 1·454 Å, in good agreement with 1·456 Å in potassium ethyl sulphate (Truter, 1958) and 1·447 Å in potassium aminedisulphonate (Jeffrey & Jones, 1956). This distance appears to correspond to a formal S=O double bond as it occurs in a wide variety of sulphur–oxygen compounds (Cruickshank, 1961) under different conditions of valency in the sulphur atom.

The oxygen atoms coordinated to the sodium ion form a slightly distorted octahedron. Pairs of these

octahedra share an edge so that there are five coordinated oxygens per sodium ion; three of these oxygen atoms belong to water molecules and two are from different sulphonate groups, the mean Na–O distance being 2·424 Å. The angles subtended at the sodium ion by the edges of the octahedron, which would be 90° in a regular figure, vary from 76·4° to 111·1° over the twelve angles of this distorted version.

In addition to the van der Waals forces between the naphthalene rings and the ionic coordination around the sodium, there are a number of hydrogen bonds in the structure. As there are four water molecules and one amino group per structural unit, ten hydrogen atoms are available to form hydrogen bonds. The hydrogen atoms have not been located during this structure determination, so the hydrogen bonds can only be inferred from the closeness of approach of the relevant atoms. Table 4 lists these distances; whether these are all true hydrogen bonds is difficult to assess; some of the distances are rather longer than usual, but this may perhaps be expected in the neighbourhood of the much stronger sodium ionic field.

The thermal parameters of the atoms have been determined isotropically only; the relatively low accuracy of the intensity data would have made any attempt at calculating anisotropic temperature factors not very meaningful. The values of B for each atom are given in Table 1. The sulphur atom, as expected, has

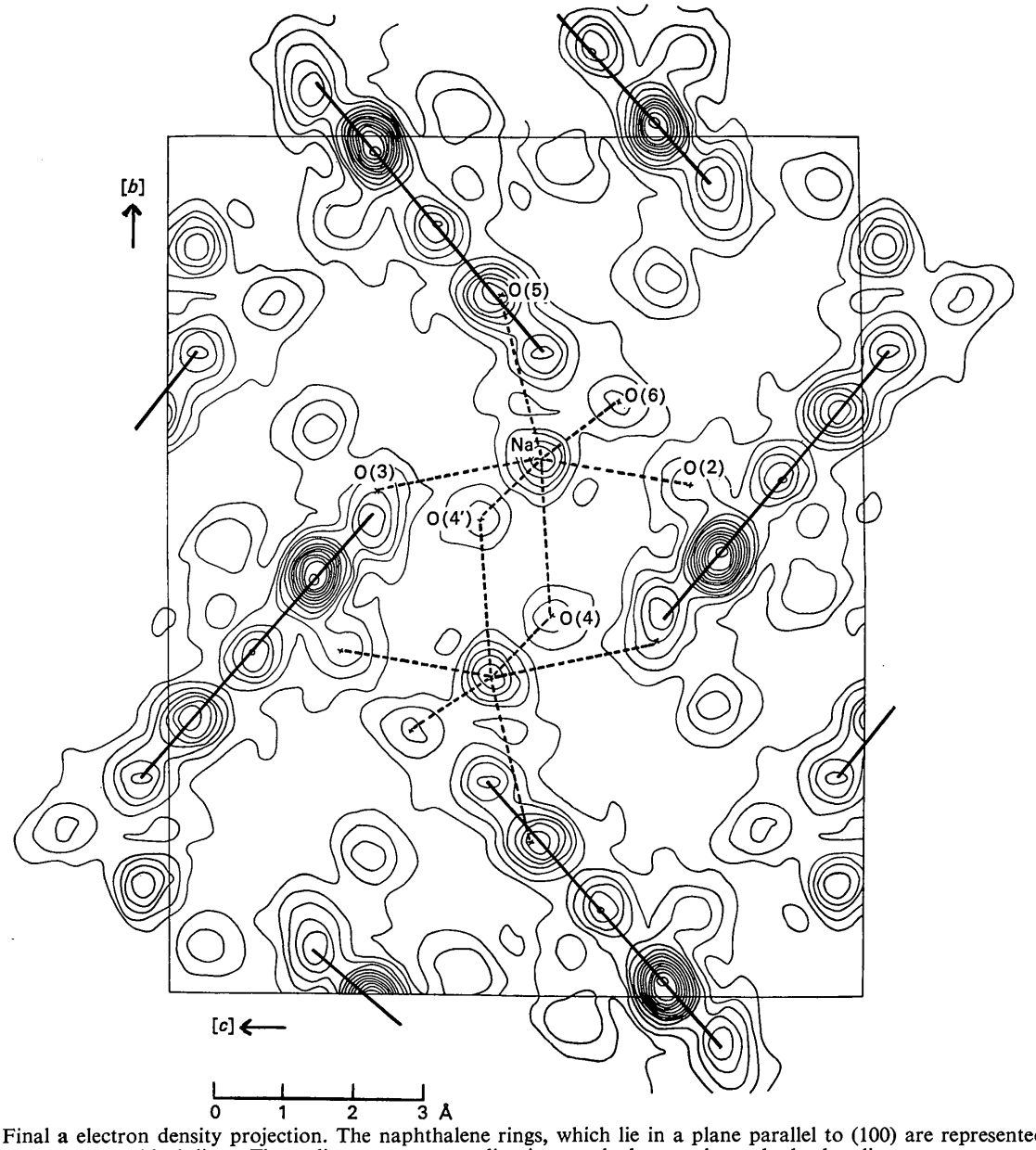

Fig. 2. Final a electron density projection. The naphthalene rings, which lie in a plane parallel to (100) are represented by full black lines. The sodium–oxygen coordination octahedra are shown by broken lines.

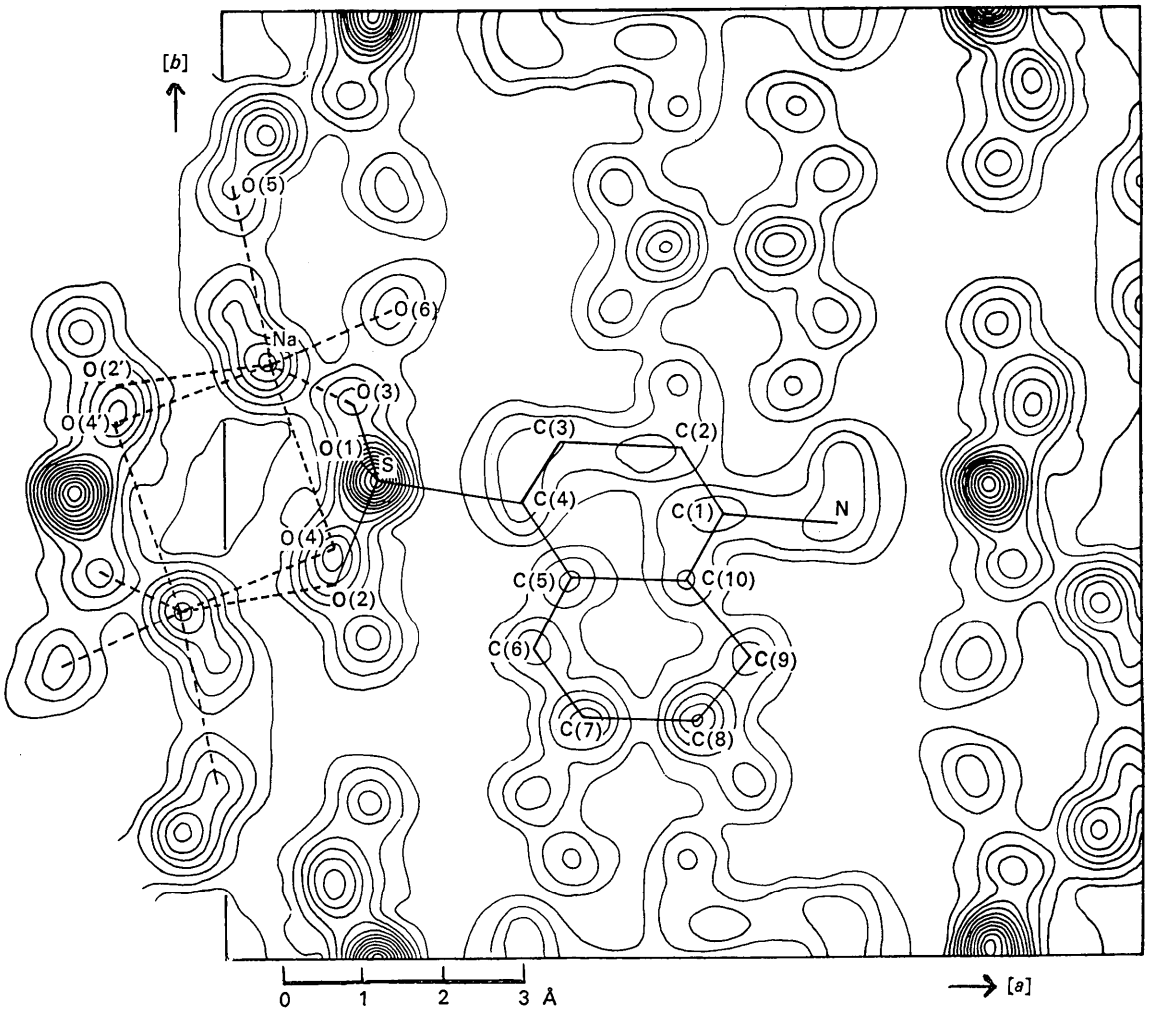

Fig. 3. Final c electron density projection. The sodium–oxygen coordination octahedra are shown by broken lines.

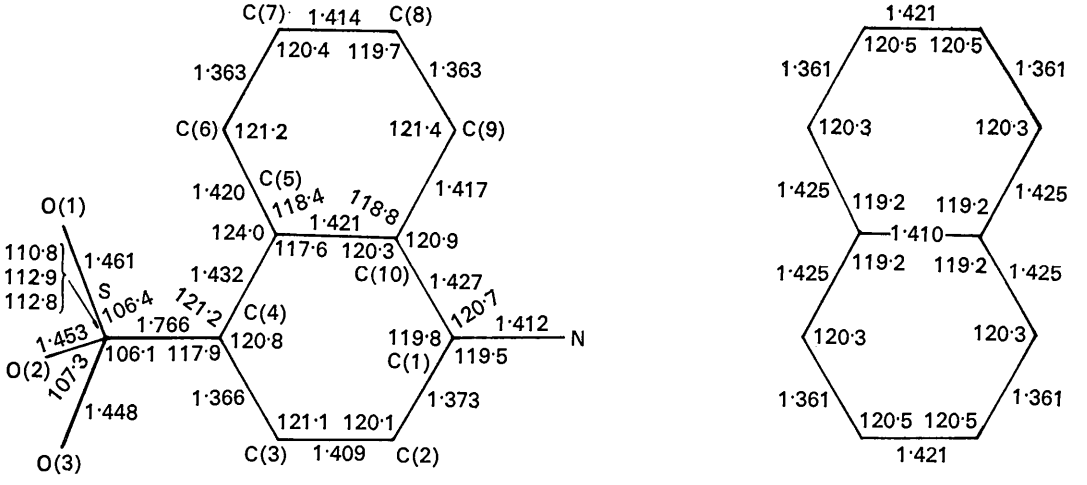

Fig. 4. Covalent bond-lengths and inter-bond angles in sodium naphthionate compared with those in naphthalene.

Table 3. *Bond lengths and inter-bond angles*

C(1)—C(2)	1·373 Å	C(1)—C(2)—C(3)	120·1°
C(2)—C(3)	1·409	C(2)—C(3)—C(4)	121·1
C(3)—C(4)	1·366	C(3)—C(4)—C(5)	120·8
C(4)—C(5)	1·432	C(3)—C(4)—S	117·8
C(5)—C(6)	1·420	C(5)—C(4)—S	121·2
C(6)—C(7)	1·363	C(4)—C(5)—C(6)	124·0
C(7)—C(8)	1·414	C(4)—C(5)—C(10)	117·6
C(8)—C(9)	1·363	C(6)—C(5)—C(10)	118·4
C(9)—C(10)	1·417	C(5)—C(6)—C(7)	121·2
C(10)-C(1)	1·427	C(6)—C(7)—C(8)	120·4
C(10)-C(5)	1·421	C(7)—C(8)—C(9)	119·7
C(1)—N	1·412	C(8)—C(9)—C(10)	121·4
C(4)—S	1·766	C(9)—C(10)-C(5)	118·8
S ——O(1)	1·461	C(9)—C(10)-C(1)	120·9
S ——O(2)	1·453	C(5)—C(10)-C(1)	120·3
S ——O(3)	1·448	C(10)-C(1)—C(2)	119·8
Na——O(2)	2·583	C(10)-C(1)—N	120·7
Na——O(3)	2·440	C(2)—C(1)—N	119·5
Na——O(4)	2·416	C(4)—S ——O(1)	106·4
Na——O(4′)	2·426	C(4)—S ——O(2)	107·3
Na——O(5)	2·381	C(4)—S ——O(3)	106·1
Na——O(6)	2·300	O(1) -S ——O(2)	110·8
		O(1) -S ——O(3)	113·0
		O(2) -S ——O(3)	112·8

Mean standard deviation for bond-lengths, 0·007 Å.
Mean standard deviation for inter-bond angles, 0·5°.

Table 4. *Hydrogen bond lengths*

O(4)-O(7)	2·731 Å
O(4)-O(2)	3·094
O(5)-O(1)	2·782
O(5)-O(2)	3·076
O(6)-O(3)	2·961
O(6)-N	3·010
O(7)-O(5)	2·825
O(7)-O(2)	2·841
N——O(1)	3·000
N——O(7)	3·106

the lowest factor in the whole molecule, while the three sulphonate oxygen atoms have higher vibration amplitudes. The naphthalene ring is subject to oscillatory motion about an axis situated somewhere between the C(4)–C(1) and C(5)–C(10) lines. The vibration amplitudes of the four water oxygen atoms, independent apart from hydrogen bondings, are higher still. The average value of B for the whole molecular unit is 3·02 Å^2.

The equation of the mean plane through the ten carbon atoms of the naphthalene ring, determined by least-squares, is

$$0{\cdot}0126X - 0{\cdot}6849Y + 0{\cdot}7285Z = 1{\cdot}9352$$

where X, Y, and Z are orthogonal axes. The mean displacement of the carbon atoms out of this plane is 0·014 Å, the sulphur atom is 0·194 Å out of the plane, and the nitrogen atom 0·116 Å, both on the same side of the naphthalene ring. The normal to the naphthalene ring makes an angle of 46·8° with the b axis.

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