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The Crystal Structure of Biringuccite, $Na_4[B_{10}O_{16}(OH)_2] \cdot 2H_2O$[1]

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Abstract

The crystal structure of biringuccite, $Na_4[B_{10}O_{16}(OH)_2] \cdot 2H_2O$, was determined on synthetic crystals from Weissenberg film data by direct methods; it was refined by least-squares, with anisotropic thermal parameters for non-hydrogen atoms to an R value of 0.073. The lattice constants, determined from high angle reflections, are: $a = 11.1955$, $b = 6.5607$, $c = 20.7566$ Å, $\beta = 93.891°$; space group $P2_1/c$, $Z = 4$. The basic structural element is the polyanion $[B_{10}O_{16}(OH)_2]^{4-}$ formed by four six-membered B-O rings and polymerized into sheets parallel to (001). These sheets are smooth on the side of closer approach, with projecting rings on the other side. Sodium-oxygen polyhedra, forming a three-dimensional framework, are found in both inter-sheet spaces. Connections between sheets are provided by these Na polyhedra and also by H-bonds on the side with projecting rings. A pseudosymmetry is dominant in the structure; the two halves of the polyanion as well as two Na atoms are quasi-equivalent. Two of the Na atoms and the hydrogen bonding arrangement do not follow the pseudosymmetry.

Introduction

This study of biringuccite, $2Na_2O \cdot 5B_2O_3 \cdot 3H_2O$, is a part of a program on the crystal-chemistry of hydrated sodium borates that includes structure determinations of phases obtained under hydrothermal conditions within the system Na_2O-B_2O_3-H_2O.

The only natural occurrence of biringuccite was described by Cipriani and Vannuccini (1961) and Cipriani (1961a), who reported its occurrence together with other borate minerals in the geothermal field of Larderello, Tuscany (Italy). The former name, hoeferite, was subsequently changed by Cipriani (1961b). From the data then available, Tennyson (1963) classified biringuccite as an inoborate with the crystal-chemical formula $Na_2[B_5O_7(OH)_3] \cdot \frac{1}{2}H_2O$.

Experimental

Colorless, well-formed crystals of synthetic biringuccite were obtained from a mixture of B_2O_3 and NaOH in a hydrothermal environment at 250°C, in sealed silica-glass vessels with runs of 48 hours. After the vessels were opened, the crystals were rinsed with cold water and dried with acetone.

The synthetic compound was identified as biringuccite by a comparison of powder diffraction patterns, as well as by optical and morphological characteristics. A density of 2.32 ± 0.01 g cm^{-3} was determined by flotation in a bromonaphthalene/bromoform solution. This agrees with the calculated value of 2.297 g cm^{-3} for four formula units per cell.

Lattice constants were determined at room temperature from Cu$K\alpha_1$ α_2, and β reflections obtained with a Straumanis type back-reflection Weissenberg camera (diameter 114.6 mm). The cell dimensions—$a = 11.1955(7)$, $b = 6.5607(4)$, $c = 20.7566(9)$ Å; $\beta = 93.891(6)°$; $V = 1521.06$ Å^3—were calculated by a least-squares treatment of 389 reflections from the $0kl$ and $h0l$ levels. The diffraction symmetry observed is $2/m$, and the systematic absences are $h0l$, $l = 2n + 1$ and $0k0$, $k = 2n + 1$. These results uniquely characterize the space group as $P2_1/c$.

A well-formed platy pseudohexagonal crystal, flattened on {001} and elongated along [010], with dimensions 0.664 × 0.150 × 0.056 mm was used for intensity measurement (Ni filtered CuK radiation) employing a Weissenberg camera and the multiple-film technique. Integrated intensities of reflections from $h0l$ to $h5l$ levels were measured by a microdensitometer. Of a total of 2760 observations, 648

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were below the detectable limit, and were given an intensity of half the minimum observable in each layer.

Corrections for Lorentz-polarization and α_1-α_2 splitting were applied by a standard data-reduction program. During the late stages of refinement a correction for the secondary extinction was applied, yielding a value of 2.1×10^{-6}. Because of the small size of the crystal and of the low absorption coefficient [$\mu = 27.16$ cm^{-1} (Cu$K\alpha$)], no allowance was made for absorption. Scattering factor curves for non-hydrogen atoms were those of Cromer and Waber (1965), and for hydrogens those of MacGillavry and Rieck (1962).

Structure Determination and Refinement

The structure was determined by means of the weighted tangent formula program (MULTAN) by Germain, Main, and Woolfson (1971), used in its fully automatic mode. The largest ($|E| \geq 1.60$) normalized structure amplitudes (computed on the basis of the overall temperature parameter and scale factors resulting from Wilson's method) were used for sign determinations. The phases of three reflections were assigned to fix the origin, and the phase of one structure invariant was known (from Σ_1 relationships). Besides these, three more symbols were chosen by the program and their signs were allowed to vary. Among the eight sign combinations thus obtained, the one with the best figures of merit was chosen. An F_o Fourier map, made with signs from this set, contained peaks corresponding to all sodium and oxygen atoms, the $R = \sum||F_o| - |F_c||/\sum|F_o|$ index being 0.45. In the next Fourier map all boron atoms were detected. No trace was found of another oxygen atom still missing according to the previously known formula. Further inspection of Fourier maps during the next stages of refinement confirmed its absence; as a consequence the correct formula of biringuccite is $Na_4B_{10}O_{16}(OH)_2 \cdot 2H_2O$.

The refinement of the structure was performed by the least-squares method (ORFLS program) with full matrix for the isotropic stages, and with the block-diagonal matrix following introduction of anisotropic thermal parameters. Positional and thermal parameters of hydrogen atoms were not refined. During all steps of refinement unit weight was given to observed reflections. The final R index for observed reflections is 0.073, and 0.094 for all reflections.

The final positional and thermal parameters are listed in Table 1. Table 2 lists the observed and calculated structure factors.

Hydrogen Atom Locations

In this structure there are six independent hydrogen atoms. Two hydrogens belong to the OH's attached to the B-O polyanion, and four hydrogens belong to the two water molecules in Na polyhedra. Towards the end of the refinement a difference Fourier synthesis was computed in an attempt to locate the hydrogen atoms directly. Together with several small spurious peaks, six maxima (0.35 to 0.45 e/Å^3) were found in positions suitable for hydrogen bonding. Attempts to refine hydrogen parameters were unsuccessful because of inconsistencies in shifts. The positional parameters given in Table 1 for hydrogen atoms are those derived from the ($F_o - F_c$) synthesis; thermal parameters were fixed at 4.0 Å^2 as the best average found in similar structures. Inspection of the final ($F_o - F_c$) map showed residual peaks of ± 0.3 e/Å^3, mostly surrounding the heavier atoms.

In Table 3 angles and distances involving the hydrogen-bonded atoms are given. Within 3.2 Å from the Ow(1) oxygen, only two distances corresponding to possible hydrogen bonds can be found (see Fig. 1). The hydrogens H(1) and H(2) as found in the Fourier map fit this assumption well.

Four oxygens (Fig. 1) at distances suitable for hydrogen bonding are found within a 3.2 Å radius around Ow(2); (a fifth distance from Ow(2) to its centrosymmetric mate Ow(2,2) of 3.195 Å is too long to be regarded as a symmetric hydrogen bond). Among the six angles formed around Ow(2) by the above four neighbors, two are at the very limits of the acceptor-donor-acceptor (ADA) angle range and two are well outside (Ferraris and Franchini-Angela, 1972) and are most unlikely to be ADA angles. The two remaining angles, O(7)-Ow(2)-O(10) and O(5)-Ow(2)-O(8), are both within the possible range. From a survey of the non-hydrogen environment of Ow(2) the tetrahedral arrangement involving O(7) and O(10) is seen to be more regular than that involving O(5) and O(8).

For the hydrogen atoms belonging to Ow(2), namely H(3) and H(4), it can be seen that besides the two configurations O(5)···H(3)-Ow(2)-H(4)···O(8) and O(7)···H(3)-Ow(2)-H(4)···O(10), a third one could exist by placing H(3) and H(4) in such positions as to make bifurcated bonds

TABLE 1. Atomic Parameters*

Atom	x/a	y/b	z/c	B eq.	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Na(1)	.0582(3)	.5021(5)	.2243(1)	1.82	27(2)	130(10)	11(1)	-1(4)	-2(1)	16(2)
Na(2)	.4394(2)	.1123(5)	.2650(1)	1.60	32(2)	100(9)	9(1)	-2(3)	1(1)	9(2)
Na(3)	.1531(3)	.5519(6)	.0447(2)	2.35	32(2)	181(11)	13(1)	11(4)	-3(1)	-13(2)
Na(4)	.4717(3)	.8478(5)	.0948(1)	1.76	37(2)	117(10)	8(1)	-10(4)	3(1)	-4(2)
O(1)	.3509(4)	.6534(8)	.1687(2)	1.02	13(3)	32(14)	11(1)	3(5)	0(1)	-1(3)
O(2)	.2911(4)	.9899(8)	.1748(2)	1.41	18(4)	13(15)	18(1)	1(5)	1(2)	-3(3)
O(3)	.2324(4)	.3425(8)	.1675(2)	1.12	21(3)	39(15)	9(1)	-5(5)	2(2)	2(3)
O(4)	.1444(4)	.7376(8)	.1465(2)	1.08	12(3)	62(15)	9(1)	4(5)	-2(1)	-4(3)
O(5)	.0842(4)	.0896(8)	.1657(2)	1.28	21(3)	42(15)	12(1)	-4(5)	2(2)	1(3)
O(6)	.9519(4)	.8115(7)	.1839(2)	0.79	15(3)	33(14)	6(1)	-4(5)	0(1)	-1(3)
O(7)	.9987(4)	.9050(9)	.0757(2)	1.44	22(4)	105(16)	8(1)	-10(6)	1(2)	6(3)
O(8)	.8168(4)	.7285(8)	.0905(2)	1.27	13(3)	104(16)	6(1)	-7(5)	0(1)	2(3)
OH(9)	.8532(4)	.8572(9)	-.0107(2)	1.53	26(4)	114(17)	8(1)	-2(6)	0(2)	2(3)
O(10)	.8494(4)	.4951(8)	.1792(2)	1.01	11(3)	44(15)	10(1)	-8(5)	1(1)	-2(3)
O(11)	.7349(4)	.8029(8)	.1911(2)	1.21	21(3)	49(15)	10(1)	7(5)	2(2)	0(3)
O(12)	.7901(4)	.1547(8)	.1908(2)	1.49	23(4)	23(15)	17(1)	-5(5)	0(2)	3(3)
O(13)	.5853(4)	.0516(8)	.1735(2)	1.11	14(3)	60(15)	9(1)	0(5)	-1(1)	1(3)
O(14)	.6471(4)	.4022(8)	.1519(2)	1.21	16(3)	69(15)	9(1)	-10(5)	-3(2)	6(3)
O(15)	.4505(4)	.3327(8)	.1795(2)	0.88	16(3)	49(14)	6(1)	4(5)	0(1)	1(3)
O(16)	.5159(4)	.2176(8)	.0761(2)	1.18	18(3)	84(15)	7(1)	10(5)	-2(1)	-2(3)
OH(17)	.4102(4)	.2959(9)	-.0210(2)	1.61	22(4)	142(17)	7(1)	11(6)	-1(2)	-3(3)
O(18)	.3435(4)	.4285(8)	.0778(2)	1.33	26(4)	87(16)	7(1)	10(6)	1(2)	0(3)
Ow(1)	.3087(5)	.8243(10)	.0150(3)	2.41	48(5)	127(19)	16(1)	15(7)	8(2)	8(4)
Ow(2)	-.0412(5)	.3782(10)	.0613(3)	2.66	64(5)	137(19)	15(1)	17(8)	11(2)	0(4)
B(1)	.2594(6)	.7871(14)	.1648(3)	0.95	20(5)	65(25)	4(2)	3(8)	4(2)	-1(4)
B(2)	.2029(6)	.1443(13)	.1691(3)	0.80	18(5)	39(24)	5(2)	16(8)	0(2)	-2(4)
B(3)	.0419(6)	.8854(13)	.1448(3)	0.72	12(5)	13(23)	8(2)	-2(8)	2(2)	-3(4)
B(4)	.8910(7)	.8321(13)	.0527(4)	0.95	25(5)	22(24)	7(2)	13(8)	1(2)	0(4)
B(5)	.8399(6)	.7129(13)	.1623(3)	0.77	9(5)	26(24)	8(2)	-1(7)	2(2)	1(4)
B(6)	.7034(6)	.0024(14)	.1852(3)	0.88	16(5)	65(25)	5(1)	-4(8)	3(2)	1(4)
B(7)	.7600(6)	.3537(14)	.1740(3)	0.88	16(5)	44(25)	7(2)	-2(8)	4(2)	-2(4)
B(8)	.5473(6)	.2560(13)	.1454(3)	0.71	12(5)	13(23)	8(2)	1(8)	2(2)	3(4)
B(9)	.4216(6)	.3173(14)	.0448(3)	0.99	17(5)	64(25)	6(2)	-18(8)	0(2)	1(4)
B(10)	.3467(6)	.4326(13)	.1491(4)	0.81	8(5)	30(24)	9(2)	-5(7)	2(2)	2(4)
H(1)	.360	.820	-.015	4.0						
H(2)	.280	.970	.010	4.0						
H(3)	-.029	.230	.067	4.0						
H(4)	-.055	.415	.103	4.0						
H(5)	.910	.930	-.035	4.0						
H(6)	.343	.310	-.037	4.0						

*The B equivalent factors, after Hamilton (1959), are in $Å^2$ units. Anisotropic thermal parameters ($\times 10^4$) are defined by: $\exp -(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)$. The standard deviations of the last digits are given in parentheses.

with O(5) and O(7), and with O(8) and O(10), respectively. The distances involving possible H(4) bonding, namely Ow(2)-O(10) = 2.912 and Ow(2)-O(8) = 2.882 Å, are shorter than the ones normally found in a bifurcated bond. For H(3), on the other hand, a bifurcated bond is more likely (Ferraris and Franchini-Angela, 1972), both distances being over 3.1 Å.

The positions found for H(3) and H(4) in the difference Fourier map lie very close to the directions from Ow(2) to O(7) and to O(10), thus confirming the above conclusions based on geometrical considerations. From the point of view of electrostatic valence balance, the choice for H(3) and H(4) bridging to O(7) and O(10) is not completely satisfactory; these oxygens seem overbonded, while the alternate pair O(5) and O(8) are underbonded.

No difficulty was encountered for positioning H(5) and H(6), close to OH(9) and OH(17) respectively (see Table 4).

TABLE 2. Observed and Calculated Structure Factors for Biringuccite

h	k	l	Fobs	Fcalc
0	0	2	59.9	-71.8
0	0	4	67.5	-83.5
0	0	6	137.4	190.2
0	0	8	152.4	-191.0
0	0	10	42.5	-43.1
0	0	12	151.9	166.4
0	0	14	47.2	-45.1
0	0	16	27.3	-24.5
0	0	18	21.8	18.3
0	0	20	39.8	-34.7
0	0	22	48.3	45.5
0	0	24	18.3	-12.2
1	0	-26	21.7	21.8
1	0	-24*	6.8	8.7
1	0	-22	23.8	-23.9
1	0	-20	46.1	42.8
1	0	-18	14.9	14.1
1	0	-16*	7.1	7.2
1	0	-14	79.2	83.9
1	0	-12	88.2	-92.8
1	0	-10*	5.0	-6.9
1	0	-8	44.3	42.9
1	0	-6	13.6	-14.1
1	0	-4	51.3	55.0
1	0	-2	31.5	32.8
1	0	0	9.0	-6.8
1	0	2	27.6	-25.9
1	0	4	27.3	-28.8
1	0	6	25.1	25.1
1	0	8	109.4	-125.5
1	0	10	45.0	-45.1
1	0	12	9.4	-10.6
1	0	14	16.9	-15.7
1	0	16	32.7	31.4
1	0	18	48.8	47.1
1	0	20	36.6	-33.0
1	0	22	31.1	29.5
1	0	24*	6.6	-6.8
1	0	26	13.5	-14.4
2	0	-24	42.8	-37.9
2	0	-22	34.2	32.0
2	0	-20*	7.8	-5.0
2	0	-18	19.6	-14.8
2	0	-16	12.7	-10.3
2	0	-14	76.5	78.1
2	0	-12	67.2	-71.2
2	0	-10	90.4	100.1
2	0	-8	83.8	89.0
2	0	-6	138.6	-173.6
2	0	-4	19.4	-19.5
2	0	-2	22.4	22.2
2	0	0	19.9	20.1
2	0	2	61.1	64.3
2	0	4	53.3	53.8
2	0	6	144.6	-176.3
2	0	8	40.5	-34.6
2	0	10	121.1	-132.8
2	0	12	57.2	58.9
2	0	14*	6.7	5.7
2	0	16	16.1	-11.9
2	0	18*	7.7	-2.8
2	0	20	20.2	-17.7
2	0	22*	7.3	-1.1
2	0	24	16.7	-13.3
3	0	-24*	6.6	-1.9
3	0	-22	32.9	-29.5
3	0	-20	56.4	-53.7
3	0	-18	41.3	-39.6
3	0	-16	32.8	32.9
3	0	-14	18.6	19.2
3	0	-12	19.0	19.0
3	0	-10	14.1	-10.8
3	0	-8	64.6	-67.7
3	0	-6	21.8	21.0
3	0	-4	10.6	-10.5
3	0	-2	16.7	-14.5
3	0	0	43.8	-39.9
3	0	2	29.5	-25.5
3	0	4	27.6	26.4
3	0	6	27.0	25.2
3	0	8	51.1	52.1
3	0	10	25.0	-23.2
3	0	12	15.2	-14.4
3	0	14	71.7	70.7
3	0	16*	7.4	1.1
3	0	18	35.0	33.0
3	0	20*	7.7	-3.6
3	0	22	34.0	-30.0
3	0	24	30.5	-27.9
4	0	-24	22.3	-17.8
4	0	-22	11.7	-10.4
4	0	-20	18.9	-17.2
4	0	-18	14.7	15.8
4	0	-16	35.3	33.2
4	0	-14	81.0	86.4
4	0	-12*	6.3	-3.0
4	0	-10	92.6	101.7
4	0	-8	82.8	-88.4
4	0	-6	60.5	-60.6
4	0	-4	90.8	-102.6
4	0	-2	7.8	-9.2
4	0	0*	4.1	-2.6
4	0	2	99.5	-101.0
4	0	4	42.1	40.4
4	0	6	79.6	-81.8
4	0	8	30.2	-26.2
4	0	10	46.6	43.9
4	0	12	58.9	57.7
4	0	14	91.6	-94.3
4	0	16	15.9	14.1
4	0	18	48.7	-45.3
4	0	20	31.6	-28.0
4	0	22	21.5	15.6
4	0	24	14.6	11.1
5	0	-24	30.1	27.7
5	0	-22	34.6	-32.0
5	0	-20*	7.7	6.0
5	0	-18	45.2	-43.8
5	0	-16	34.1	-34.7
5	0	-14	23.6	23.7
5	0	-12	15.3	15.2
5	0	-10	28.5	-29.5
5	0	-8	38.1	-36.4
5	0	-6	63.1	-63.2
5	0	-4	51.4	-50.7
5	0	-2	24.3	-22.2
5	0	0	8.5	9.5
5	0	2	12.6	12.7
5	0	4	58.3	58.5
5	0	6	55.7	55.7
5	0	8	18.1	17.4
5	0	10*	6.5	-2.1
5	0	12*	7.0	-9.9
5	0	14	42.0	-43.0
5	0	16	27.5	25.0
5	0	18	31.9	29.9
5	0	20	28.2	-26.7
5	0	22	20.8	17.9
6	0	-24	14.9	-15.1
6	0	-22	21.5	-15.9
6	0	-20	22.8	19.1
6	0	-18	28.5	-25.0
6	0	-16	30.5	-28.5
6	0	-14	57.2	51.0
6	0	-12	47.5	-44.7
6	0	-10	38.4	35.8
6	0	-8	36.3	-33.7
6	0	-6	61.0	-58.6
6	0	-4	92.4	-99.2
6	0	-2	62.7	51.6
6	0	0	36.9	38.3
6	0	2	127.1	137.8
6	0	4	28.0	-22.3
6	0	6	48.1	-44.2
6	0	8	28.0	23.1
6	0	10	23.4	-20.9
6	0	12	88.4	90.1
6	0	14	37.4	35.1
6	0	16*	7.8	.5
6	0	18	44.1	-43.2
6	0	20	19.1	18.0
6	0	22	10.2	10.1
7	0	-22	24.8	21.5
7	0	-20*	7.2	.7
7	0	-18	12.9	-12.3
7	0	-16	38.8	38.2
7	0	-14	26.2	-25.7
7	0	-12	17.7	16.1
7	0	-10	20.3	20.4
7	0	-8	14.6	14.3
7	0	-6	52.5	51.4
7	0	-4	68.1	67.3
7	0	-2	50.9	46.8
7	0	0	40.6	37.7
7	0	2	32.0	29.1
7	0	4	48.8	47.4
7	0	6*	6.7	7.5
7	0	8*	7.0	3.3
7	0	10	39.2	-37.9
7	0	12	40.9	-41.2
7	0	14	34.5	-32.3
7	0	16	29.0	27.8
7	0	18*	7.2	-7.0
7	0	20*	6.3	4.8
7	0	22	13.1	12.9
8	0	-22*	5.2	-6.0
8	0	-20*	6.7	4.4
8	0	-18	32.5	-30.1
8	0	-16	27.0	24.9
8	0	-14	16.6	-13.8
8	0	-12	51.6	-51.5
8	0	-10	64.4	67.0
8	0	-8*	7.2	-3.3
8	0	-6*	7.0	5.5
8	0	-4*	6.8	-1.6
8	0	-2*	6.7	.6
8	0	0	50.5	-47.9
8	0	2	90.3	90.8
8	0	4	81.7	-82.5
8	0	6*	7.2	4.0
8	0	8	32.6	-28.3
8	0	10	73.5	-76.4
8	0	12	55.0	57.2
8	0	14	54.5	52.6
8	0	16	16.1	-15.9
8	0	18	26.0	21.1
8	0	20	18.2	17.2
9	0	-20	16.6	-15.5
9	0	-18	21.2	-19.0
9	0	-16*	7.4	8.6
9	0	-14	30.4	29.9
9	0	-12	36.6	35.5
9	0	-10*	7.7	-8.9
9	0	-8*	7.6	.2
9	0	-6	24.6	-21.4
9	0	-4*	7.3	4.8
9	0	-2	22.5	18.3
9	0	0	15.5	-11.2
9	0	2	38.0	-33.0
9	0	4	39.0	-34.3
9	0	6*	7.6	-1.2
9	0	8	14.3	12.2
9	0	10	33.7	-32.8
9	0	12*	7.7	6.1
9	0	14	17.9	-16.4
9	0	16*	6.8	-2.7
9	0	18	10.5	8.4
10	0	-18	23.0	-21.5
10	0	-16	47.1	44.6
10	0	-14	23.4	-18.7
10	0	-12	17.9	-16.8
10	0	-10	39.0	37.5
10	0	-8*	7.8	8.1
10	0	-6	47.9	-49.0
10	0	-4	30.6	28.4
10	0	-2	43.2	41.2
10	0	0	83.9	-86.4
10	0	2	51.5	48.9
10	0	4*	7.8	-4.1
10	0	6	16.2	-16.7
10	0	8	16.1	-13.9
10	0	10	49.9	48.6
10	0	12*	7.3	-1.1
10	0	14*	6.7	1.7
10	0	16	16.0	-13.2
11	0	-16	26.0	-25.3
11	0	-14	22.9	20.7
11	0	-12	43.8	42.5
11	0	-10*	7.5	1.7
11	0	-8*	7.7	-10.0
11	0	-6	52.3	-51.0
11	0	-4	60.0	-59.3
11	0	-2	30.3	-27.4
11	0	0	14.7	-13.2
11	0	2*	7.8	-2.9
11	0	4*	7.7	-.8
11	0	6*	7.6	.9
11	0	8*	7.4	2.2
11	0	10*	7.1	4.3
11	0	12*	6.5	-3.0
11	0	14	16.5	-13.3
12	0	-14	12.3	-12.7
12	0	-12	38.1	35.0
12	0	-10	61.5	-61.1
12	0	-8	14.9	12.9
12	0	-6*	7.3	-8.1
12	0	-4	22.5	-19.5
12	0	-2	17.1	16.3
12	0	0*	7.4	8.5
12	0	2	39.2	35.3
12	0	4	20.1	17.4
12	0	6*	7.0	2.8
12	0	8	22.3	-22.4
12	0	10	30.1	28.3
12	0	12	9.0	-8.7
13	0	-12	11.0	8.3
13	0	-10	14.1	14.0
13	0	-8*	6.1	-4.4
13	0	-6*	6.4	3.0
13	0	-4*	6.6	3.5
13	0	-2*	6.7	-6.1
13	0	0*	6.7	.1
13	0	2	20.6	18.5
13	0	4*	6.2	6.6
13	0	6	20.8	18.2
13	0	8	14.7	13.4
14	0	-6	38.0	38.5
14	0	-4	8.5	11.5
14	0	-2	14.0	-13.5
14	0	0	34.9	35.5
14	0	2	18.5	-15.6
0	1	2	29.6	26.9
0	1	3	8.3	-6.2
0	1	4	30.6	29.8
0	1	5	7.9	6.3
0	1	6*	2.9	2.7
0	1	7	47.7	49.7
0	1	8	32.8	-34.3
0	1	9*	3.7	2.7
0	1	10	54.7	57.4
0	1	11	100.7	118.0
0	1	12	30.5	30.9
0	1	13	34.7	-34.2
0	1	14	37.9	38.2
0	1	15	34.6	33.9
0	1	16*	3.8	.7
0	1	17	11.2	-11.8
0	1	18	19.0	-18.0
0	1	19*	6.1	-3.4
0	1	20	26.3	-25.9
0	1	21*	6.0	-5.3
0	1	22	27.5	27.4
0	1	23*	5.6	.6
0	1	24*	5.2	3.0
0	1	25	8.9	-7.5
0	1	26	7.5	7.6
1	1	-26	17.4	17.8
1	1	-25	28.3	27.7
1	1	-24*	5.2	-2.0
1	1	-23	22.8	-21.4
1	1	-22*	5.9	6.0
1	1	-21	13.5	13.3
1	1	-20	32.4	31.6
1	1	-19*	6.1	3.4
1	1	-18	11.3	8.9
1	1	-17*	5.8	-1.8
1	1	-16	24.5	-22.5
1	1	-15	35.3	34.7
1	1	-14	50.3	53.1
1	1	-13	68.4	72.2
1	1	-12	23.4	19.1
1	1	-11*	4.2	-.3
1	1	-10	32.6	31.0
1	1	-9	14.8	10.9
1	1	-8	7.8	-7.6
1	1	-7	38.0	39.1
1	1	-6	45.8	48.7
1	1	-5	40.2	-42.6
1	1	-4*	2.4	-2.4
1	1	-3	31.7	-30.7
1	1	-2	82.6	-82.9
1	1	0	35.2	-29.9
1	1	1	28.4	24.4
1	1	2	67.3	63.7
1	1	3	4.8	-2.2
1	1	4	43.3	-43.8
1	1	5	43.0	45.6
1	1	6	18.3	14.8
1	1	7	52.3	58.2
1	1	8	44.4	-47.5
1	1	9	49.0	-50.8
1	1	10	83.4	-92.5
1	1	11	9.2	8.7
1	1	12	54.2	-55.9
1	1	13*	4.9	-5.8
1	1	14	22.8	-21.1
1	1	15*	5.4	-4.7
1	1	16	16.8	15.2
1	1	17	12.5	-11.6
1	1	18	9.7	-7.8
1	1	19	35.3	-34.2
1	1	20	16.5	-15.5
1	1	21	13.7	-12.9
1	1	22	16.0	-15.4
1	1	23	24.3	-21.1
1	1	24	11.2	-9.3
1	1	25	9.0	9.0
1	1	26	15.7	-16.3
2	1	-26	16.1	16.8
2	1	-25	20.0	17.6
2	1	-24	24.3	-22.0
2	1	-23*	5.6	-.8
2	1	-22*	5.8	-2.6
2	1	-21	12.9	-11.3
2	1	-20	11.8	8.4
2	1	-19	33.9	32.9
2	1	-18	33.4	-32.0
2	1	-17	13.0	-8.4
2	1	-16	29.0	29.8
2	1	-15*	5.4	-6.8
2	1	-14	15.0	-15.1
2	1	-13	53.4	52.3
2	1	-12	67.5	-74.5
2	1	-11*	4.3	-2.1
2	1	-10	46.0	-47.7
2	1	-9	93.2	-109.0
2	1	-8	33.0	33.9
2	1	-7	67.9	72.2
2	1	-6	38.7	-37.7
2	1	-5	143.7	-170.9
2	1	-4	65.7	70.9
2	1	-3	23.6	22.5
2	1	-2	12.6	11.0
2	1	-1	56.4	55.6
2	1	0	42.1	-39.9
2	1	1	8.8	7.2
2	1	2	20.3	-19.0
2	1	3	42.4	-41.1
2	1	4	12.6	10.8
2	1	5*	3.0	-2.5
2	1	6	53.0	-58.0
2	1	7	29.7	-26.5
2	1	8	16.2	-16.7
2	1	9	6.3	4.8
2	1	10	15.9	-15.0
2	1	11	60.5	64.7
2	1	12	43.1	-44.1
2	1	13	30.9	-29.9
2	1	14	24.7	26.2
2	1	15*	5.5	3.0
2	1	16*	5.7	-1.4
2	1	17	57.7	-58.3
2	1	18	21.4	-21.1
2	1	19*	6.1	-8.7
2	1	20	10.2	-9.0
2	1	21*	5.9	-3.2
2	1	22	10.9	9.3
2	1	23	24.6	23.0
2	1	24	16.0	-13.4
3	1	-26	11.0	8.1
3	1	-25	15.9	-13.3
3	1	-24*	5.0	.9
3	1	-23	13.5	11.6
3	1	-22	14.0	12.6
3	1	-21	33.4	32.9
3	1	-20*	6.1	5.7
3	1	-19	44.8	-44.1
3	1	-18	65.3	-68.9
3	1	-17	46.0	47.5
3	1	-16	30.4	-29.3
3	1	-15*	5.5	-3.0
3	1	-14	41.0	42.0
3	1	-13	40.7	-42.2
3	1	-12	42.2	-45.0
3	1	-11*	4.5	1.1
3	1	-10	23.6	22.3
3	1	-9	26.2	-26.6
3	1	-8	45.5	-46.9
3	1	-7	31.3	-30.4
3	1	-6	87.6	-95.2
3	1	-5	44.3	46.9
3	1	-4	23.7	-21.5
3	1	-3*	2.9	4.1
3	1	-2*	2.8	-3.4
3	1	-1*	2.8	-2.9
3	1	0	35.9	-34.7
3	1	1	5.2	5.5
3	1	2	12.9	-10.4
3	1	3	19.7	-16.5
3	1	4	129.1	-149.1
3	1	5	47.4	50.4
3	1	6	23.6	21.3
3	1	7	20.5	21.6
3	1	8	32.1	32.9
3	1	9	51.9	-53.3
3	1	10	34.0	-32.3
3	1	11*	4.7	6.3
3	1	12	47.0	48.9
3	1	13	52.7	-56.2
3	1	14	20.2	19.8
3	1	15	20.5	-18.0
3	1	16*	5.9	-6.6
3	1	17*	6.0	5.3
3	1	18	44.8	45.0
3	1	19*	6.1	.5
3	1	20	33.8	33.5
3	1	21	14.6	-12.8
3	1	22	18.1	-18.4
3	1	23	12.1	9.9
3	1	24*	4.5	2.0
3	1	25	8.9	9.0
4	1	-25	19.5	19.1
4	1	-24	8.6	8.3
4	1	-23	16.3	-16.1
4	1	-22	24.3	-21.0
4	1	-21	30.1	30.9
4	1	-20*	6.0	-5.7
4	1	-19	23.1	-20.8
4	1	-18	30.9	30.5
4	1	-17	30.3	-31.4
4	1	-16	26.7	-26.8
4	1	-15	28.8	-28.8
4	1	-14	10.0	-10.5
4	1	-13*	5.2	-7.2
4	1	-12*	5.0	4.1
4	1	-11*	4.8	-.1
4	1	-10	27.2	-28.1
4	1	-9	22.0	-20.7
4	1	-8	78.1	85.8
4	1	-7	52.9	58.1
4	1	-6	27.0	28.7
4	1	-5	67.0	-68.6
4	1	-4	48.5	50.1
4	1	-3	12.2	12.3
4	1	-2	57.4	57.6
4	1	-1	52.3	48.8
4	1	0	48.2	51.7
4	1	1	86.7	95.9
4	1	2	16.4	12.6
4	1	3	82.3	-90.7
4	1	4	57.5	56.9
4	1	5	34.4	33.5
4	1	6*	3.9	2.2
4	1	7	95.0	-106.6
4	1	8*	4.3	-4.5
4	1	9	46.3	-47.8
4	1	10*	4.8	-7.0
4	1	11	27.7	25.7
4	1	12	46.9	50.5
4	1	13	8.6	8.1
4	1	14*	5.7	-4.6
4	1	15	27.5	26.7
4	1	16*	6.0	-.7
4	1	17	17.8	-16.3
4	1	18	17.7	16.3
4	1	19*	6.0	-1.8
4	1	20	24.5	-22.7
4	1	21*	5.6	-2.5
4	1	22*	5.3	6.7
4	1	23	12.4	12.0
4	1	24*	4.0	6.1
5	1	-25	8.2	8.7
5	1	-24	26.1	24.6
5	1	-23	11.7	-9.5
5	1	-22*	5.5	1.9
5	1	-21*	5.8	-2.2
5	1	-20	17.5	15.4
5	1	-19	28.3	-28.9
5	1	-18	10.9	-10.2
5	1	-17	19.7	-18.0
5	1	-16	43.0	-43.6
5	1	-15	19.9	19.0
5	1	-14	16.9	15.2
5	1	-13*	5.5	-5.1
5	1	-12	38.8	38.6
5	1	-11	42.0	-44.5
5	1	-10	20.2	21.1
5	1	-9	31.0	32.0
5	1	-8	46.7	45.2
5	1	-7	44.0	-45.6
5	1	-6	59.5	-60.5
5	1	-5	32.6	32.2
5	1	-4	71.1	-73.8
5	1	-3	69.1	72.9
5	1	-2	85.5	89.4
5	1	-1	46.2	-46.4
5	1	0	37.5	-33.7
5	1	1	19.5	-20.3
5	1	2	66.7	68.3
5	1	3	63.2	-69.6
5	1	4	29.1	24.7
5	1	5	64.2	-66.8
5	1	6	76.3	-84.3
5	1	7	9.5	8.9
5	1	9	12.4	-12.2
5	1	10	30.9	31.5
5	1	11	25.0	22.6
5	1	12*	5.5	-3.5
5	1	13	19.5	18.5
5	1	14	61.1	61.8
5	1	15	20.5	21.1
5	1	16	10.7	11.7
5	1	17*	6.1	4.0
5	1	18*	6.0	8.6
5	1	19	21.9	19.5
5	1	20*	5.7	5.3
5	1	21	18.7	-17.3
5	1	22	25.3	-19.2
5	1	23	13.6	12.3
6	1	-24	22.2	-24.0
6	1	-23	11.2	-10.3
6	1	-22	17.6	15.2
6	1	-21	15.3	12.5
6	1	-20*	5.8	-1.2
6	1	-19	33.1	-32.2
6	1	-18	42.7	42.1
6	1	-17*	6.1	7.5
6	1	-16	58.7	62.6
6	1	-15	13.2	-13.2
6	1	-14	19.7	-19.4
6	1	-13	18.5	-17.7
6	1	-12	25.8	-26.8
6	1	-11	20.9	-19.2
6	1	-10	17.9	16.8
6	1	-9	84.2	93.0
6	1	-8	39.1	-38.2
6	1	-7	10.5	-8.9
6	1	-6	35.9	35.9
6	1	-5	15.5	-12.4
6	1	-4	50.9	52.6
6	1	-3	86.9	93.9
6	1	-2	70.3	-77.2
6	1	-1	74.9	-78.9
6	1	0	15.0	-13.4
6	1	1	30.7	28.7
6	1	2	7.5	7.1
6	1	3*	4.4	6.1
6	1	4	30.4	30.3
6	1	5*	4.7	-3.3
6	1	6	8.8	-8.9
6	1	7	45.0	-44.2
6	1	8	9.0	8.5
6	1	9	58.9	60.8
6	1	10	44.1	-43.7
6	1	11*	5.6	-2.8
6	1	12	15.6	-15.2
6	1	13	50.8	51.7
6	1	14*	6.0	2.7
6	1	15	22.3	20.3
6	1	16*	6.1	1.8
6	1	17*	6.0	.0
6	1	18	11.6	-11.5
6	1	19*	5.7	5.1
6	1	20*	5.4	-1.0
6	1	21	16.1	-13.4
6	1	22	18.8	-16.0
7	1	-22	8.9	-6.8
7	1	-21	8.7	-7.0
7	1	-20	16.3	15.7
7	1	-19*	5.9	-7.4
7	1	-18	19.2	-17.5
7	1	-17*	6.1	-6.0
7	1	-16	20.1	-18.2
7	1	-15	12.8	12.8
7	1	-14*	6.1	-1.1
7	1	-13	47.1	50.9
7	1	-12	12.3	10.4
7	1	-11	18.2	15.6
7	1	-10*	5.6	1.5
7	1	-9*	5.4	3.9
7	1	-8	12.5	-9.7
7	1	-7*	5.2	-2.9
7	1	-6	23.5	-21.8
7	1	-5*	5.0	-1.3
7	1	-4	17.9	15.8
7	1	-3	12.7	-12.2
7	1	-2	9.3	-6.6
7	1	-1	23.4	22.0
7	1	0	37.4	36.2
7	1	1	16.2	13.9
7	1	2	87.2	95.7
7	1	3	43.2	-42.3
7	1	4	10.0	-8.1
7	1	5	9.2	10.6
7	1	6	12.2	9.7
7	1	7	18.5	17.9
7	1	8	21.2	20.1
7	1	9*	5.7	.9
7	1	10	19.1	-16.8
7	1	11	27.8	25.0
7	1	12	42.1	-45.8
7	1	13	32.8	30.9
7	1	14	38.6	38.2
7	1	15	12.2	10.7
7	1	16*	5.8	-4.4
7	1	17*	6.0	8.3
7	1	18*	5.6	-5.8
7	1	19*	5.3	5.4
7	1	20	21.7	19.5
7	1	21	32.4	-30.2
8	1	-21	11.4	10.4
8	1	-20*	5.1	-8.2
8	1	-19	10.1	8.9
8	1	-18	34.3	34.2
8	1	-17	31.0	30.2
8	1	-16	12.7	12.0
8	1	-15	14.3	13.0
8	1	-14	38.8	40.9
8	1	-13	28.8	29.5
8	1	-12*	6.0	-2.3
8	1	-11	42.7	-45.4
8	1	-10	26.9	-26.3
8	1	-9	36.1	36.1
8	1	-8	23.5	-21.9
8	1	-7	41.9	-42.6
8	1	-6*	5.5	-1.2
8	1	-5	27.3	-27.7
8	1	-4	11.0	8.5
8	1	-3	28.4	29.5
8	1	-2	21.3	-20.4
8	1	-1*	5.3	3.9
8	1	0	31.9	-32.2
8	1	1*	5.3	-3.0
8	1	2*	5.4	1.6
8	1	3	30.8	30.3
8	1	4	23.2	-24.0
8	1	5*	5.6	1.2
8	1	6*	5.7	-.5
8	1	7	53.0	-55.9
8	1	8	22.9	22.2
8	1	9	54.3	56.9
8	1	10	56.7	-58.2
8	1	11	25.6	-24.8
8	1	12	17.9	-15.9
8	1	14	22.8	-20.4
8	1	15	10.5	-10.4
8	1	16*	5.7	-4.2
8	1	17	27.9	-24.4
8	1	18*	5.1	3.2
8	1	19	22.0	-21.2
9	1	-21	5.2	-5.4
9	1	-20*	4.4	4.9
9	1	-19	8.2	7.8
9	1	-18	9.1	-8.6
9	1	-17*	5.5	1.2
9	1	-16	38.1	-38.4
9	1	-15*	5.9	1.4
9	1	-14*	6.3	5.0
9	1	-13	10.4	-9.9
9	1	-12	44.1	43.5
9	1	-11	17.0	-14.6
9	1	-10	54.5	-58.6
9	1	-9*	6.0	-1.6
9	1	-8	35.2	34.5
9	1	-7	37.9	-37.5
9	1	-6	23.9	-22.7
9	1	-5	22.3	-19.8
9	1	-4	86.1	-93.2
9	1	-3	32.0	30.5
9	1	-2	58.3	60.3
9	1	-1*	5.7	6.5
9	1	0	51.8	54.2
9	1	1*	5.8	-2.3
9	1	2	34.2	-31.9
9	1	3	37.3	36.5
9	1	4	19.6	16.1
9	1	5*	5.9	5.7
9	1	6	17.6	-15.8
9	1	7	23.5	-22.5
9	1	8	35.7	-34.5
9	1	9	24.4	23.5
9	1	10*	6.1	-6.2
9	1	12*	6.0	-7.5
9	1	13	12.4	-12.2
9	1	14*	5.7	1.5
9	1	15*	5.5	5.3
9	1	16	33.6	-31.5
9	1	17	9.8	-7.1
9	1	18	12.1	9.0
9	1	19	13.1	13.8
10	1	-19	9.7	-9.8
10	1	-18	13.8	-13.3
10	1	-17	38.1	38.4
10	1	-16	15.2	-14.5
10	1	-15	24.8	-23.8
10	1	-14*	5.7	-1.6
10	1	-13*	5.8	-.1
10	1	-12*	6.0	-9.0
10	1	-11	17.9	17.0
10	1	-10*	6.1	-4.2
10	1	-9	32.2	-30.4
10	1	-8*	6.1	-5.4
10	1	-7	40.7	-40.2
10	1	-6	26.2	23.4
10	1	-5	60.4	62.2
10	1	-4	48.2	-48.6
10	1	-3	71.0	-76.6
10	1	-2*	6.0	-5.1
10	1	-1	46.4	45.5
10	1	0	14.7	-13.5
10	1	1	63.2	65.7
10	1	2	32.0	-31.3
10	1	3	36.6	-36.5
10	1	4	33.3	31.9
10	1	5*	6.1	5.8
10	1	6	20.3	19.0
10	1	7*	6.1	-7.7
10	1	8*	6.0	-5.0
10	1	9	59.2	-59.6
10	1	10	23.7	22.6
10	1	11	10.2	-10.8
10	1	12*	5.6	1.8
10	1	13	33.4	33.5
10	1	14*	5.2	5.6
10	1	15	30.9	-29.6
10	1	16	26.9	27.5
10	1	17	15.3	14.1
11	1	-18	15.6	-16.7
11	1	-17	11.6	-11.3
11	1	-16	20.9	20.5
11	1	-15*	4.9	5.4
11	1	-14*	5.2	-.3
11	1	-13	8.6	-8.3
11	1	-12*	5.6	5.6
11	1	-11*	5.7	-7.2
11	1	-10	47.4	47.9
11	1	-9*	5.9	-7.6
11	1	-8	29.3	30.1
11	1	-7	21.1	-20.9
11	1	-6	32.9	-31.4
11	1	-5*	6.0	5.6
11	1	-4*	6.1	-8.2
11	1	-3	27.7	26.9
11	1	-2*	6.1	-3.6
11	1	-1	20.4	17.3
11	1	0	30.6	28.5
11	1	1*	6.1	-1.6
11	1	2	12.9	9.8
11	1	3	14.9	-11.6
11	1	4	26.9	26.6
11	1	5	14.1	-12.8
11	1	6*	5.9	-3.3
11	1	7	25.5	-24.1
11	1	8	31.7	-31.9
11	1	9*	5.6	-3.4
11	1	10*	5.5	-.6
11	1	11*	5.3	-2.8
11	1	12	15.6	14.1
11	1	13*	4.6	.7
11	1	14	9.5	6.9
11	1	15	12.5	-12.3
12	1	-12*	4.9	-2.2
12	1	-11	13.7	-11.8
12	1	-10*	5.3	-4.6
12	1	-9	26.5	25.6
12	1	-8*	5.5	2.3
12	1	-7	17.3	-16.5
12	1	-6	28.7	28.8
12	1	-5	9.6	8.0
12	1	-4	11.4	10.0
12	1	-3	9.7	-8.8
12	1	-2	11.1	-10.4
12	1	-1*	5.8	-4.1
12	1	0	31.2	-30.1
12	1	1	27.4	-25.5
12	1	2*	5.7	-1.4
12	1	3	28.4	26.2
12	1	4*	5.6	-4.2
12	1	5	23.3	-21.8
12	1	6	38.2	38.6
12	1	7*	5.3	2.6
12	1	8	16.4	15.6
12	1	9*	4.8	-4.7
12	1	10	8.8	-6.4
12	1	11*	4.1	.6
12	1	12	7.7	6.9
13	1	-12	25.8	30.1
13	1	-11	13.1	13.8
13	1	-10*	4.1	.0
13	1	-9*	4.4	3.8
13	1	-8*	4.6	1.5
13	1	-7*	4.8	-1.3
13	1	-6*	4.9	-5.2
13	1	-5	16.5	-15.7
13	1	-4	25.6	-22.9
13	1	-3*	5.1	6.0
13	1	-2*	5.1	.8
13	1	-1	13.3	11.2
13	1	0*	5.1	-.4
13	1	1*	5.1	3.5
13	1	2	13.3	-11.2
13	1	3	14.7	13.7
13	1	4	34.9	33.5
13	1	5	19.1	-17.6
13	1	6	17.7	-17.1
13	1	7*	4.0	.8
13	1	8	12.3	-11.6
13	1	9	19.1	20.3
14	1	-6	7.3	8.3
14	1	-5*	3.3	.7
14	1	-4	14.8	17.1
14	1	-3	11.4	-10.1
14	1	-2	23.4	24.0
14	1	-1	16.5	16.6
14	1	0	5.8	-5.4
14	1	1	25.7	-29.3
0	2	2	61.8	-63.2
0	2	3	111.1	101.3
0	2	4	44.3	39.3
0	2	5	25.7	-25.5
0	2	6	35.2	-34.6
0	2	7*	3.3	4.5
0	2	8	17.1	-15.1
0	2	9	66.7	-67.7
0	2	10	33.5	-34.7
0	2	11	28.0	-25.2
0	2	12	25.0	-25.1
0	2	13	20.4	-18.9
0	2	14	8.8	-7.7
0	2	15	13.0	10.9
0	2	16*	5.7	6.1
0	2	17	12.5	12.0
0	2	18	30.2	32.8
0	2	19	21.4	-22.5
0	2	20	22.7	-22.8
0	2	21*	5.9	2.7
0	2	22	16.2	14.4
0	2	23	14.5	14.8
0	2	24*	4.8	2.9
0	2	25	9.0	-7.5
1	2	-25	18.6	19.3
1	2	-24*	4.8	-4.4
1	2	-23*	5.4	-3.0
1	2	-22*	5.7	6.3
1	2	-21*	5.9	4.7
1	2	-20	28.4	-30.5
1	2	-19	44.3	-45.8
1	2	-18*	6.0	-5.2
1	2	-17	40.5	-39.9
1	2	-16	12.9	-13.5
1	2	-15	10.6	10.7
1	2	-14*	5.2	.7
1	2	-13	43.9	43.9
1	2	-12	14.8	-14.4
1	2	-11	47.1	50.3
1	2	-10*	4.1	4.7
1	2	-9	30.7	30.6
1	2	-8	44.7	-44.6
1	2	-7	15.4	-13.0
1	2	-6	8.9	8.9
1	2	-5	73.0	-66.2
1	2	-4	100.1	86.9
1	2	-3	38.7	31.2
1	2	-2	74.2	59.1
1	2	-1	10.7	-10.9
1	2	0	70.9	63.6
1	2	1	17.7	14.9
1	2	2	9.0	5.6
1	2	3	27.6	-26.6
1	2	4	5.4	-5.7
1	2	5	44.4	40.9
1	2	6	78.0	-77.9
1	2	7	35.4	-34.4
1	2	8	36.5	37.3
1	2	9	32.6	34.9
1	2	10*	4.2	.5
1	2	11	18.4	-16.6
1	2	12	15.0	-15.0
1	2	13	15.4	-15.9
1	2	14	17.7	18.5
1	2	15	15.4	-17.9
1	2	16	24.1	-24.5
1	2	17	12.6	15.0
1	2	18	16.9	18.7
1	2	19*	6.0	5.2
1	2	20*	6.0	-3.6
1	2	21*	5.8	-7.5
1	2	22*	5.6	6.8
1	2	23	14.1	-11.5
1	2	24*	4.7	.1
1	2	25	12.6	-13.8
2	2	-24	24.5	23.6
2	2	-23	23.3	-24.6
2	2	-22	16.2	-16.4
2	2	-21*	5.9	-8.4
2	2	-20*	6.0	-5.2
2	2	-19	36.7	39.0
2	2	-18*	6.0	8.0
2	2	-17	30.3	-32.2
2	2	-16	70.6	-73.1
2	2	-15	28.2	29.1
2	2	-14	14.9	14.9
2	2	-13*	5.0	6.6
2	2	-12*	4.8	2.8
2	2	-11	16.0	-16.3
2	2	-10*	4.2	2.3
2	2	-9	58.2	58.3
2	2	-8	13.0	12.5
2	2	-7	30.4	29.3
2	2	-6	52.9	51.3
2	2	-5	61.1	-58.7
2	2	-4	21.6	19.1
2	2	-3	145.2	-123.1
2	2	-2	23.4	-19.7
2	2	-1	141.5	-109.8
2	2	0	9.7	6.1
2	2	1	120.9	-101.6
2	2	2	74.5	-67.4
2	2	3	16.5	16.1
2	2	4	27.5	24.5
2	2	5	20.7	-20.0
2	2	6	47.2	-48.3
2	2	7	27.9	26.5
2	2	8	44.5	43.5
2	2	9	50.5	-51.6
2	2	10	7.1	6.5
2	2	11	9.0	9.0
2	2	12*	4.9	5.3
2	2	13	21.0	-19.5
2	2	14	14.8	13.8
2	2	15*	5.6	8.3
2	2	16	28.9	30.8
2	2	17	23.8	-26.1
2	2	18	29.4	33.1
2	2	19	9.6	-8.9
2	2	20*	5.9	.2
2	2	21	10.0	-10.9
2	2	22*	5.5	-1.4
2	2	23	10.0	8.8
2	2	24*	4.4	-5.2
2	2	25	5.6	6.9
3	2	-25	13.4	12.7
3	2	-24*	4.6	-7.3

TABLE 2, Continued

h	k	l	F_{obs}	F_{calc}
3	2	-23*	5.2	5.0
3	2	-22*	5.6	-2.7
3	2	-21*	5.8	6.3
3	2	-20	15.7	15.8
3	2	-19	28.0	-31.3
3	2	-18	13.9	-14.5
3	2	-17	36.0	-38.4
3	2	-16	20.1	-21.2
3	2	-15	48.8	-52.6
3	2	-14	62.7	70.2
3	2	-13	20.9	23.2
3	2	-12	16.6	17.4
3	2	-11	20.5	21.5
3	2	-10	40.3	45.3
3	2	-9	24.4	26.0
3	2	-8*	4.0	-.2
3	2	-7	59.8	-62.0
3	2	-6	18.1	-15.1
3	2	-5	56.1	-53.4
3	2	-4	51.2	-49.1
3	2	-3	50.2	-47.0
3	2	-2	26.4	-23.3
3	2	-1	91.6	-77.9
3	2	0	100.6	93.4
3	2	1	52.7	49.4
3	2	2	9.4	-10.6
3	2	3	48.7	43.7
3	2	4	102.9	-97.4
3	2	5	32.7	32.0
3	2	6	55.2	-54.1
3	2	7*	3.9	8.2
3	2	8*	4.1	-3.9
3	2	9	56.7	51.3
3	2	10	40.5	-41.3
3	2	11	31.8	-31.7
3	2	12	72.9	77.6
3	2	13	16.0	-17.3
3	2	14	21.3	23.6
3	2	15	11.7	10.1
3	2	16	36.8	-36.9
3	2	17	30.1	31.1
3	2	18	14.5	-16.8
3	2	19	25.0	-26.3
3	2	20	17.5	-18.6
3	2	21	22.2	22.1
3	2	22*	5.3	3.6
3	2	23*	4.8	-.8
4	2	-24*	4.3	2.2
4	2	-23*	5.0	.8
4	2	-22	15.8	-16.6
4	2	-21	7.9	-8.9
4	2	-20*	6.0	.7
4	2	-19*	6.1	-6.5
4	2	-18	20.8	20.4
4	2	-17	22.8	-24.5
4	2	-16	41.6	-44.3
4	2	-15	40.3	44.7
4	2	-14	22.1	25.0
4	2	-13	49.5	-55.1
4	2	-12	27.4	-30.2
4	2	-11	18.1	-18.8
4	2	-10	28.6	-29.2
4	2	-9	48.9	53.4
4	2	-8	48.2	48.0
4	2	-7	7.1	-4.7
4	2	-6	21.1	19.4
4	2	-5	16.4	-14.8
4	2	-4	68.5	-67.3
4	2	-3	72.5	66.3
4	2	-2	69.7	56.9
4	2	-1	111.6	-107.5
4	2	0	65.0	-61.0
4	2	1	26.2	24.4
4	2	2	19.9	-17.3
4	2	3	123.0	117.1
4	2	4	109.9	108.7
4	2	5	48.6	-45.7
4	2	6	31.4	-30.4
4	2	7	92.6	93.7
4	2	8	61.0	65.2
4	2	9	12.8	11.4
4	2	10	12.1	12.5
4	2	11	27.9	-29.4
4	2	12*	5.3	-5.5
4	2	13	49.1	51.9
4	2	14	13.6	13.5
4	2	15	32.4	34.6
4	2	16	27.6	27.0
4	2	17	37.7	-36.3
4	2	18	19.4	-19.6
4	2	19	33.2	34.3
4	2	20	8.5	8.7
4	2	21	19.6	-20.7
4	2	22*	5.0	3.8
4	2	23*	4.3	5.3
4	2	24	16.9	-19.3
5	2	-24	6.4	6.7
5	2	-23	26.0	25.0
5	2	-22*	5.3	5.0
5	2	-21	21.1	21.2
5	2	-20*	5.9	.4
5	2	-19*	6.0	1.4
5	2	-18	19.2	21.0
5	2	-17*	6.1	5.6
5	2	-16	28.1	32.3
5	2	-15	45.3	-51.8
5	2	-14	21.2	23.2
5	2	-13	41.6	47.4
5	2	-12*	5.4	-4.0
5	2	-11	23.1	24.7
5	2	-10*	5.0	9.8
5	2	-9*	4.8	3.9
5	2	-8*	4.7	3.6
5	2	-7	38.5	37.7
5	2	-6	17.0	-16.3
5	2	-5	39.8	39.6
5	2	-4	97.5	-85.3
5	2	-3	42.9	-40.1
5	2	-2	43.7	42.2
5	2	-1	74.8	74.3
5	2	0	22.2	-21.0
5	2	1	25.6	23.0
5	2	2*	4.0	1.3
5	2	3	14.7	-13.0
5	2	4	75.8	75.4
5	2	5	25.3	22.0
5	2	6	35.0	-34.6
5	2	7	19.9	19.8
5	2	8*	4.8	6.7
5	2	9*	5.0	6.1
5	2	10	21.6	-23.0
5	2	11	39.2	-42.8
5	2	12*	5.6	4.2
5	2	13*	5.8	-7.3
5	2	14	17.0	16.4
5	2	15	30.9	-33.7
5	2	16*	6.0	-11.6
5	2	17*	6.0	4.6
5	2	18	22.7	-24.3
5	2	19	12.5	13.0
5	2	20	10.2	9.3
5	2	21	13.5	13.9
5	2	22	18.7	-18.2
5	2	23	10.6	-11.0
6	2	-23*	4.1	-1.8
6	2	-22	9.3	8.9
6	2	-21*	5.4	1.0
6	2	-20	8.8	-11.5
6	2	-19	14.9	14.9
6	2	-18*	6.1	4.7
6	2	-17	36.8	-41.1
6	2	-16	24.3	24.2
6	2	-15*	6.1	-1.8
6	2	-14*	6.0	-2.4
6	2	-13	22.4	-22.9
6	2	-12*	5.7	-5.2
6	2	-11*	5.6	-6.3
6	2	-10*	5.4	3.1
6	2	-9*	5.3	-.9
6	2	-8	59.1	-63.2
6	2	-7	68.2	70.4
6	2	-6	47.4	40.2
6	2	-5	9.2	-8.7
6	2	-4	11.5	-10.5
6	2	-3	21.3	21.3
6	2	-2	42.3	42.1
6	2	-1	30.1	-30.5
6	2	0	8.7	8.0
6	2	1	10.1	-9.6
6	2	2*	4.5	1.3
6	2	3	32.5	33.4
6	2	4	37.5	37.0
6	2	5	17.1	17.4
6	2	6	12.1	10.1
6	2	7	30.1	-30.8
6	2	8*	5.2	-2.2
6	2	9*	5.4	7.2
6	2	10	24.6	-25.6
6	2	11	27.9	-30.9
6	2	12	39.8	-39.6
6	2	13	12.7	-13.0
6	2	14	34.0	-37.2
6	2	15	62.9	66.7
6	2	16	14.4	15.2
6	2	17*	5.9	-6.0
6	2	18	21.9	-21.5
6	2	19*	5.4	7.7
6	2	20	20.2	20.1
6	2	21	6.7	5.5
6	2	22	6.7	-7.5
7	2	-23	12.0	15.4
7	2	-22*	4.2	-.8
7	2	-21	27.3	29.1
7	2	-20	18.1	-17.2
7	2	-19	18.2	-17.7
7	2	-18	10.6	-11.0
7	2	-17	22.0	-19.7
7	2	-16	29.4	27.9
7	2	-15	13.9	12.4
7	2	-14	29.7	-30.3
7	2	-13	11.7	11.8
7	2	-12	13.8	-13.2
7	2	-11	13.1	14.3
7	2	-10*	6.6	3.2
7	2	-9	73.4	68.1
7	2	-8	64.7	-56.0
7	2	-7	36.8	-36.6
7	2	-6*	5.2	-5.6
7	2	-5*	5.1	2.0
7	2	-4	10.7	-10.5
7	2	-3	14.1	-14.9
7	2	-2	26.6	27.9
7	2	-1	31.7	31.1
7	2	0	8.1	7.8
7	2	1	11.0	9.1
7	2	2	28.4	-29.4
7	2	3	20.0	-20.2
7	2	4	10.3	-10.9
7	2	5	31.6	-32.6
7	2	6*	5.4	2.7
7	2	7*	5.5	4.2
7	2	8	44.6	-46.4
7	2	9	22.7	-23.2
7	2	10	26.8	28.8
7	2	11	16.5	17.6
7	2	12	39.8	44.6
7	2	13	13.0	11.8
7	2	14	56.1	-58.4
7	2	15	22.9	-22.0
7	2	16	30.9	32.4
7	2	17*	5.6	-4.0
7	2	18	14.3	12.6
7	2	19*	5.0	-.1
7	2	20	11.3	-11.2
7	2	21*	3.5	7.1
8	2	-21	15.8	-14.6
8	2	-20	13.7	16.1
8	2	-19	10.0	10.5
8	2	-18	22.0	-25.0
8	2	-17	16.0	16.8
8	2	-16	12.8	-16.4
8	2	-15	17.9	-18.9
8	2	-14*	5.9	-1.1
8	2	-13*	6.0	-2.5
8	2	-12	15.8	17.5
8	2	-11*	5.9	4.5
8	2	-10	22.9	25.4
8	2	-9	17.1	-16.5
8	2	-8*	5.7	3.0
8	2	-7	51.9	58.2
8	2	-6	13.3	15.5
8	2	-5	14.9	15.2
8	2	-4*	5.5	-4.8
8	2	-3*	5.4	-5.6
8	2	-2	29.2	30.6
8	2	-1	60.1	-63.9
8	2	0	19.9	-20.3
8	2	1	13.3	12.3
8	2	2	43.0	45.0
8	2	3	33.3	-34.1
8	2	4	13.3	-13.4
8	2	5	12.4	13.2
8	2	6	18.2	-19.3
8	2	7	31.9	33.5
8	2	8*	5.9	1.1
8	2	9	26.6	-27.6
8	2	10*	6.0	-7.2
8	2	11	41.6	-45.5
8	2	14*	5.9	-9.7
8	2	15	17.6	-17.6
8	2	16	20.7	20.2
8	2	17*	5.2	-7.1
8	2	18	11.2	-9.1
8	2	19	19.7	19.3
9	2	-19*	4.5	3.6
9	2	-18	14.4	-15.1
9	2	-17	11.4	-12.2
9	2	-16*	5.5	-.0
9	2	-15	23.6	-26.7
9	2	-14	10.8	-11.6
9	2	-13	10.3	11.1
9	2	-12	13.3	14.1
9	2	-11	20.2	19.1
9	2	-10*	6.0	11.7
9	2	-9*	6.0	6.3
9	2	-8*	5.9	3.6
9	2	-7	17.6	-20.1
9	2	-6*	5.9	2.7
9	2	-5	47.2	-51.1
9	2	-4*	5.8	.4
9	2	-3	58.8	-62.1
9	2	-2*	5.8	8.8
9	2	-1	12.2	-15.1
9	2	0	14.2	-13.6
9	2	1	23.3	-26.0
9	2	2	30.3	33.8
9	2	3	27.9	29.6
9	2	4	34.3	-36.1
9	2	5	35.6	-38.7
9	2	6	31.0	-33.8
9	2	7*	6.0	6.8
9	2	8	9.9	9.4
9	2	12	24.8	25.7
9	2	13	15.4	15.4
9	2	14	35.2	38.8
9	2	15	7.8	8.0
9	2	16*	4.9	.3
9	2	17	15.0	-14.6
9	2	18	24.6	-27.3
10	2	-19	12.0	-12.8
10	2	-18*	4.0	-.7
10	2	-17	10.8	10.5
10	2	-16	15.8	17.0
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10	2	-14	22.0	-23.4
10	2	-13	10.0	10.8
10	2	-12	24.9	27.0
10	2	-11	24.0	-27.0
10	2	-10	10.3	9.8
10	2	-9	36.2	-37.7
10	2	-8	14.8	-14.4
10	2	-7	38.1	39.5
10	2	-6	33.1	36.1
10	2	-5	17.5	-18.3
10	2	-4	21.6	-23.6
10	2	-3	12.6	-11.5
10	2	-2	53.0	-56.5
10	2	-1	36.8	37.9
10	2	0*	6.0	-1.3
10	2	1	27.4	-28.7
10	2	2*	6.0	-3.2
10	2	3	18.8	-18.1
10	2	4	42.2	-43.5
10	2	5	74.2	81.9
10	2	6	52.1	56.0
10	2	7	16.7	-15.7
10	2	8	11.2	-11.9
10	2	9	14.7	13.7
10	2	10	12.1	-12.5
10	2	11*	5.6	.2
10	2	12	13.6	12.1
10	2	13	10.8	-12.0
10	2	14*	4.8	-1.9
10	2	15*	4.3	-5.8
11	2	-14*	4.8	6.8
11	2	-13	10.9	-12.1
11	2	-12	7.6	6.2
11	2	-11	11.0	11.5
11	2	-10	22.3	-24.3
11	2	-9	15.5	14.7
11	2	-8	20.9	22.7
11	2	-7	10.9	11.4
11	2	-6*	5.9	1.2
11	2	-5*	5.9	-1.9
11	2	-4*	5.9	-4.8
11	2	-3	15.3	-16.5
11	2	-2	18.9	21.3
11	2	-1	17.6	18.3
11	2	0*	6.0	-5.7
11	2	1	8.0	9.5
11	2	2	13.5	13.4
11	2	3*	5.9	8.0
11	2	4	11.5	11.2
11	2	5	13.4	12.5
11	2	6	14.3	14.9
11	2	7*	5.6	7.1
11	2	8*	5.5	-3.0
11	2	9*	5.4	-5.9
11	2	10	12.0	11.1
11	2	11	28.1	27.5
11	2	12*	4.6	-2.0
11	2	13	12.2	-12.2
11	2	14	8.9	10.1
12	2	-13	8.3	9.9
12	2	-12	13.4	13.6
12	2	-11	11.7	-12.4
12	2	-10	12.1	-14.3
12	2	-9	18.2	20.1
12	2	-8*	5.3	-.3
12	2	-7*	5.4	2.1
12	2	-6	16.1	-17.5
12	2	-5*	5.5	-1.2
12	2	-4	13.2	-14.9
12	2	-3	21.4	19.7
12	2	-2	11.9	11.0
12	2	-1*	5.6	.8
12	2	0*	5.6	2.6
12	2	1	12.0	-12.9
12	2	2	8.8	-10.1
12	2	3*	5.4	7.8
12	2	4*	5.4	-3.4
12	2	5	13.0	14.1
12	2	6	18.7	20.4
12	2	7	14.9	-15.3
12	2	8	7.6	-7.9
12	2	9*	4.4	6.8
12	2	10	7.1	7.1
12	2	11	11.1	-12.5
13	2	-10	4.6	4.1
13	2	-9	13.5	16.5
13	2	-8	16.7	-19.6
13	2	-7	14.3	17.0
13	2	-6	9.5	-9.9
13	2	-5	7.6	-7.8
13	2	-4	21.9	25.4
13	2	-3	14.3	14.6
13	2	-2*	4.8	9.0
13	2	-1	10.9	12.2
13	2	0	10.6	11.2
13	2	1	11.8	12.6
13	2	2*	4.6	-.8
13	2	3*	4.5	-3.0
13	2	4*	4.3	-.4
13	2	5	13.4	-12.8
0	3	2	69.4	-79.9
0	3	3	41.2	-40.9
0	3	4	94.2	78.3
0	3	5*	2.6	-1.8
0	3	6	20.2	17.5
0	3	7	55.8	55.1
0	3	8	65.6	-65.2
0	3	9	64.6	-66.5
0	3	10	54.1	53.6
0	3	11	9.9	-9.8
0	3	12	32.5	-33.4
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0	3	14	25.8	-26.1
0	3	15	34.0	-33.5
0	3	16	12.4	-13.6
0	3	17	20.3	20.6
0	3	18*	5.3	4.5
0	3	19*	5.3	-3.9
0	3	20	30.3	-30.9
0	3	21	23.7	-23.8
0	3	22*	4.7	2.4
0	3	23*	4.3	3.1
0	3	24	9.0	-8.9
1	3	-23	12.7	-15.0
1	3	-22	22.6	22.7
1	3	-21	13.6	-11.9
1	3	-20*	5.3	3.2
1	3	-19	9.7	10.2
1	3	-18*	5.4	4.1
1	3	-17	39.1	-41.0
1	3	-16	16.2	-17.6
1	3	-15	24.6	-23.4
1	3	-14	19.9	-18.3
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1	3	-12	30.0	-30.2
1	3	-11	8.9	6.5
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1	3	-9	27.7	-25.3
1	3	-8	54.5	-55.4
1	3	-7	46.1	44.6
1	3	-6	10.0	6.7
1	3	-5	196.4	-163.1
1	3	-4	24.4	-20.7
1	3	-3	33.0	28.7
1	3	-2	31.6	32.0
1	3	0	23.6	24.3
1	3	1	68.5	-58.7
1	3	2	18.0	-16.1
1	3	3	113.1	92.5
1	3	4	28.7	25.7
1	3	5	67.9	-54.3
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1	3	8	17.9	-15.9
1	3	9	80.5	80.3
1	3	10	17.2	16.2
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1	3	12	6.3	-7.8
1	3	13	12.1	12.6
1	3	14	46.5	-47.2
1	3	15	66.9	59.0
1	3	16	16.4	16.0
1	3	17	53.3	-53.5
1	3	18*	5.3	-7.7
1	3	19	27.9	29.4
1	3	20*	5.2	11.1
1	3	21*	5.0	3.6
1	3	22*	4.7	1.7
1	3	23	9.5	-8.5
2	3	-24	14.1	13.2
2	3	-23	8.1	-6.2
2	3	-22	7.6	8.0
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2	3	-20	21.7	22.5
2	3	-19	16.5	-16.2
2	3	-18	16.1	-16.0
2	3	-17	35.3	37.9
2	3	-16	17.4	-16.7
2	3	-15	23.8	24.9
2	3	-14	34.9	-35.3
2	3	-13	14.3	-14.5
2	3	-12	16.0	15.0
2	3	-11*	4.3	-3.6
2	3	-10	15.5	15.0
2	3	-9	10.5	-10.5
2	3	-8	19.5	20.0
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2	3	-6	80.3	-76.4
2	3	-5	40.2	37.1
2	3	-4	18.5	14.7
2	3	-3	54.9	46.9
2	3	-2	57.9	-47.4
2	3	-1	7.3	-5.6
2	3	0	5.7	9.4
2	3	1	12.1	-10.6
2	3	2	101.9	83.4
2	3	3	55.3	49.8
2	3	4	31.0	27.7
2	3	5	65.1	59.6
2	3	6	105.8	-97.6
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2	3	9*	3.9	4.9
2	3	10	22.8	-21.6
2	3	11	28.4	-29.1
2	3	12	35.0	-38.5
2	3	13	42.5	-44.4
2	3	14	40.7	40.2
2	3	15	27.3	29.3
2	3	16	26.8	30.5
2	3	17	16.3	-17.3
2	3	18	10.9	-9.6
2	3	19	9.4	9.3
2	3	20	12.6	-14.8
2	3	21*	4.9	.0
2	3	22	17.6	17.7
2	3	23	25.0	-25.0
2	3	24	11.8	-11.0
3	3	-24	7.2	-6.6
3	3	-23	6.3	5.7
3	3	-22*	4.7	2.6
3	3	-21*	5.0	1.3
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3	3	-15	34.3	-37.6
3	3	-14	21.0	-22.2
3	3	-13	18.4	-21.0
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3	3	-10*	4.2	5.2
3	3	-9	40.1	-41.3
3	3	-8	12.3	-12.0
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3	3	-6	52.5	51.3
3	3	-5	29.0	-26.7
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3	3	-3	12.7	13.3
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3	3	2	24.0	19.0
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3	3	8	18.1	-18.7
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3	3	10	7.1	-6.0
3	3	11	44.2	43.4
3	3	12	12.6	12.1
3	3	13	19.6	-19.3
3	3	14*	5.1	-3.4
3	3	15	24.9	26.3
3	3	16*	5.3	1.4
3	3	17*	5.3	4.8
3	3	18	14.2	14.0
3	3	19*	5.2	12.0
3	3	20*	5.0	4.1
3	3	21	9.3	9.9
3	3	22	7.4	-7.3
3	3	23	13.7	14.7
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4	3	-23*	3.8	5.7
4	3	-22*	4.5	-1.2
4	3	-21*	4.9	1.9
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4	3	-19*	5.3	-1.3
4	3	-18*	5.4	-5.9
4	3	-17	19.7	20.2
4	3	-16	19.3	-20.1
4	3	-15*	5.3	-.6
4	3	-14	21.6	-22.7
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4	3	-8	27.2	27.1
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4	3	-6	30.5	28.2
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4	3	1*	3.3	-1.9
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4	3	3*	3.4	3.4
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4	3	5	28.9	28.7
4	3	6	36.4	-35.5
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4	3	9	17.0	-18.1
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4	3	17	37.4	37.3
4	3	18*	5.2	-3.9
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4	3	22*	3.8	3.7
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5	3	-23*	3.4	-1.2
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5	3	-20*	5.1	-1.1
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5	3	4	17.1	-18.1
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5	3	6	7.6	8.7
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5	3	8*	4.6	-4.1
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5	3	11	20.4	-21.1
5	3	12	20.6	-22.6
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5	3	21	10.1	-8.8
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6	3	-21	13.2	12.6
6	3	-20*	4.8	-6.6
6	3	-19*	5.2	-2.3
6	3	-18	21.0	-20.6
6	3	-17*	5.6	-.7
6	3	-16	15.5	15.5
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6	3	-12	13.4	-13.2
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6	3	-2	27.6	-25.4
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6	3	5	8.6	-8.9
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6	3	9	9.2	10.8
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6	3	11	37.5	-40.2
6	3	12	41.1	43.4
6	3	13	19.2	-21.0
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6	3	15	9.2	10.5
6	3	16	17.0	-17.1
6	3	17	16.5	-17.2
6	3	18*	4.8	3.3
6	3	19	24.1	24.7
6	3	20	14.4	15.9
6	3	21	8.3	-9.3
7	3	-21*	3.6	-5.9
7	3	-20	21.1	23.0
7	3	-19*	4.6	-3.2
7	3	-18	17.0	17.0
7	3	-17	16.0	18.0
7	3	-16*	5.7	-.7
7	3	-15	33.9	-35.2
7	3	-14	17.1	-17.5
7	3	-13	18.4	17.5
7	3	-12	25.5	26.8
7	3	-11*	6.1	-6.4
7	3	-10*	6.1	3.0
7	3	-9*	6.0	1.8
7	3	-8*	5.7	-6.4
7	3	-7*	5.1	-4.2
7	3	-6	13.9	-13.7
7	3	-5	23.7	-23.3
7	3	-4	31.0	-31.1
7	3	-3	58.2	-62.2
7	3	-2	21.5	-20.5
7	3	-1	12.7	-11.3
7	3	0*	4.6	6.2
7	3	1	22.4	22.2
7	3	2	30.9	-32.0
7	3	3	12.1	-12.0
7	3	4*	4.8	-5.3
7	3	5	44.2	45.6
7	3	6	15.3	15.2
7	3	7	52.7	-56.9
7	3	8	14.7	-13.3
7	3	9	19.0	20.8
7	3	10	10.1	-8.8
7	3	11*	5.3	-2.7
7	3	12	20.6	-23.6
7	3	13	10.3	-10.5
7	3	14*	5.2	-5.4
7	3	15*	5.1	5.3
7	3	16	20.1	-22.4
7	3	17	14.2	-16.2
7	3	18*	4.3	2.3
7	3	19	30.1	-31.9
7	3	20*	2.9	1.1
8	3	-20	16.1	-17.8
8	3	-19	13.7	-14.2
8	3	-18*	4.5	-5.8
8	3	-17	8.8	-8.6
8	3	-16*	4.9	-7.8
8	3	-15	11.0	-9.8
8	3	-14*	5.2	-2.3
8	3	-13	13.8	16.1
8	3	-12	10.6	-10.8
8	3	-11*	5.3	-3.9
8	3	-10	11.8	13.8
8	3	-9*	5.2	-4.1
8	3	-8	15.5	-15.8
8	3	-7	10.7	-11.8
8	3	-6*	5.1	-3.3
8	3	-5*	5.1	.6
8	3	-4	33.3	-36.1
8	3	-3	12.8	-12.0
8	3	-2*	5.0	2.8
8	3	-1	22.3	-22.7
8	3	0	52.5	56.7
8	3	1	10.8	-11.2
8	3	2	13.0	13.9
8	3	3*	5.1	-10.2
8	3	4	26.8	29.5
8	3	5	26.1	28.5
8	3	6	9.5	11.1
8	3	7	40.4	42.5
8	3	8	44.1	-49.2
8	3	9	28.5	31.4
8	3	10	43.0	-44.7
8	3	11	12.5	-12.5
8	3	12	26.5	28.0
8	3	13*	5.1	6.6
8	3	14	10.7	-10.5
8	3	15*	4.8	-1.1
8	3	16	7.7	8.6
8	3	17*	4.1	-.5
8	3	18*	3.5	3.1
9	3	-19*	3.1	7.9
9	3	-18*	3.8	4.5
9	3	-17	29.3	32.2
9	3	-16*	4.6	6.7
9	3	-15	21.2	-23.7
9	3	-14	22.1	-24.9
9	3	-13	22.8	27.6
9	3	-12	10.3	-10.3
9	3	-11*	5.2	-.8
9	3	-10	12.1	-12.4
9	3	-9*	5.3	-3.8
9	3	-8*	5.3	4.7
9	3	-7	15.9	17.8
9	3	-6*	5.2	.8
9	3	-5	13.8	14.2
9	3	-4	15.9	16.8
9	3	-3	53.3	-57.8
9	3	-2	18.8	-20.6
9	3	-1	23.3	27.7
9	3	0*	5.2	-4.2
9	3	1*	5.2	-6.4
9	3	2*	5.3	-4.6
9	3	3*	5.3	-6.4
9	3	4*	5.3	-5.2
9	3	5	44.8	49.1
9	3	6	10.7	10.4
9	3	7	26.5	-28.4
9	3	8	15.3	-15.0
9	3	9	9.6	10.0
9	3	10	10.2	-9.0
9	3	11*	5.1	1.2
9	3	12*	5.0	-6.2
9	3	13	12.0	-12.0
9	3	14*	4.5	-2.9
9	3	15	12.3	-12.1
9	3	16*	3.7	-1.6
10	3	-17	26.6	-29.3
10	3	-16	14.4	-16.5
10	3	-15*	4.2	2.8
10	3	-14*	4.5	-1.4
10	3	-13	12.7	-14.5
10	3	-12	11.0	10.4
10	3	-11*	5.0	2.2
10	3	-10	17.7	19.5
10	3	-9	11.0	10.0
10	3	-8	11.6	-11.4
10	3	-7	15.5	-16.8
10	3	-6	25.2	28.5
10	3	-5	13.5	16.5
10	3	-4*	5.3	-2.3
10	3	-3	13.7	14.2
10	3	-2*	5.3	-12.1
10	3	-1	12.8	13.3
10	3	0*	5.3	-3.0
10	3	1*	5.3	-.8
10	3	2	17.0	18.5
10	3	3	7.7	-6.6
10	3	4*	5.3	-3.5
10	3	5	10.6	11.1
10	3	6	6.8	6.2
10	3	7*	5.2	1.4
10	3	8	11.1	-10.6
10	3	9	19.7	22.1
10	3	10	26.4	-29.1
10	3	11*	4.7	1.8
10	3	12	9.3	-10.6
10	3	13*	4.1	-8.4
10	3	14*	3.6	-.1
10	3	15*	2.9	3.1
11	3	-15	9.4	10.7
11	3	-14	9.8	11.8
11	3	-13	12.7	-12.6
11	3	-12*	4.3	7.6
11	3	-11*	4.5	-3.8
11	3	-10*	4.7	-2.4
11	3	-9	24.2	25.3
11	3	-8	14.4	13.7
11	3	-7*	5.0	-3.2
11	3	-6	15.1	-16.2
11	3	-5	31.1	34.0
11	3	-4*	5.1	-1.4
11	3	-3	16.1	-19.1
11	3	-2	9.7	-11.4
11	3	-1	10.2	11.5
11	3	0*	5.1	4.7
11	3	1*	5.1	-4.1
11	3	2	8.1	-8.9
11	3	3*	5.0	-2.3
11	3	4*	5.0	-3.4
11	3	5*	4.9	-1.2
11	3	6*	4.9	-.3
11	3	7*	4.7	-1.1
11	3	8	13.5	16.5
11	3	9*	4.4	-3.0
11	3	10*	4.1	6.0
11	3	11	11.2	11.5
11	3	12	8.0	8.4
12	3	-12*	3.0	-2.5
12	3	-11	15.3	15.6
12	3	-10*	3.8	6.1
12	3	-9*	4.0	5.8
12	3	-8	14.4	16.6
12	3	-7	13.6	15.4
12	3	-6*	4.5	-9.4
12	3	-5	19.4	20.9
12	3	-4	35.0	-36.3
12	3	-3*	4.6	1.9
12	3	-2	23.2	25.9
12	3	-1	16.4	17.0
12	3	0*	4.6	-3.6
12	3	1*	4.6	3.4
12	3	2	14.8	-14.2
12	3	3	6.4	-6.1
12	3	4	9.9	10.2
12	3	5	11.9	-10.5
12	3	6	17.0	17.7
12	3	7	5.1	-5.7
12	3	8	15.9	-16.9
12	3	9*	3.0	-1.5
13	3	-6*	3.1	-7.0
13	3	-5	27.2	31.3
13	3	-4*	3.4	-8.1
13	3	-3	31.7	-35.5
13	3	-2	18.2	-22.0
13	3	-1	15.9	-19.2
13	3	0	8.0	8.0
13	3	1*	3.4	1.0
13	3	2	14.3	15.2
13	3	3	19.2	-20.6
13	3	4	14.9	17.6
0	4	3	27.7	31.2
0	4	4*	2.1	-3.0
0	4	5*	2.4	-2.0
0	4	6*	2.5	3.0
0	4	7	54.6	-52.7
0	4	8	6.6	-3.5
0	4	9*	3.3	.1
0	4	10	13.6	13.9
0	4	11	14.6	-15.1
0	4	12	31.7	-31.6
0	4	13	25.2	-24.7
0	4	14	7.1	7.1
0	4	15	67.0	71.5
0	4	16	7.7	-6.8
0	4	17	28.0	29.1
0	4	18	12.5	-11.5
0	4	19*	4.2	-.3
0	4	20	7.9	-7.2
0	4	21	12.4	12.8
0	4	22	12.3	10.9
0	4	23	22.7	-24.0
1	4	-23	11.0	-11.0
1	4	-22	32.1	32.8
1	4	-21	6.3	6.7
1	4	-20	5.8	-4.4
1	4	-19	9.6	-13.1
1	4	-18*	4.4	2.0
1	4	-17	13.6	11.4
1	4	-16	34.7	-32.9
1	4	-15	25.7	24.7
1	4	-14	40.5	-40.8
1	4	-13	12.1	-10.6
1	4	-12	39.6	-39.5
1	4	-11*	3.7	2.9
1	4	-10	36.4	37.0
1	4	-9	18.8	16.6
1	4	-8	18.7	18.6
1	4	-7	10.4	11.1
1	4	-6	24.8	-23.9
1	4	-5*	2.4	-.6
1	4	-4	14.0	11.8
1	4	-3	17.1	-18.3
1	4	-2	66.4	-74.2
1	4	-1	23.9	-31.8
1	4	0	26.8	25.5
1	4	1	15.4	-20.0
1	4	2	40.3	-45.0
1	4	3	33.2	-33.9
1	4	4	21.6	20.4
1	4	5	14.9	-12.1
1	4	6	32.3	-31.6
1	4	7	41.3	-39.8
1	4	8	35.8	36.5
1	4	9	11.7	-11.3
1	4	10	20.1	-18.1
1	4	11	19.9	19.6
1	4	12	43.1	41.4
1	4	13	19.8	19.2
1	4	14*	4.2	-1.9
1	4	15	18.9	19.1
1	4	16	24.1	-23.4
1	4	17*	4.3	5.7
1	4	18	19.0	18.7
1	4	19	17.9	-18.4
1	4	20*	4.0	3.9
1	4	21*	3.7	.9

TABLE 2, Continued

h	k	l	F_{obs}	F_{calc}
1	4	22	14.1	13.4
1	4	23*	2.4	4.8
2	4	-23	7.9	9.1
2	4	-22	9.1	-9.3
2	4	-21*	3.8	-1.6
2	4	-20	13.2	-15.4
2	4	-19	8.5	-8.8
2	4	-18*	4.4	1.7
2	4	-17	18.7	-17.7
2	4	-16*	4.5	2.9
2	4	-15*	4.4	.3
2	4	-14	8.1	-8.5
2	4	-13	7.3	8.1
2	4	-12	26.6	-27.0
2	4	-11	10.5	-9.0
2	4	-10	7.7	7.2
2	4	-9	20.5	18.9
2	4	-8	7.5	5.9
2	4	-7	14.7	16.2
2	4	-6	50.9	45.7
2	4	-5	17.3	-16.0
2	4	-4	48.2	42.1
2	4	-3	35.9	30.0
2	4	-2*	2.2	.7
2	4	-1	31.7	27.0
2	4	0	38.9	-34.7
2	4	1	38.4	-35.5
2	4	2	17.2	-14.8
2	4	3	60.3	53.3
2	4	4*	2.5	-.4
2	4	5	31.9	33.8
2	4	6	16.0	14.6
2	4	7	25.0	23.3
2	4	8	19.9	21.0
2	4	9	41.1	44.1
2	4	10	9.2	-8.6
2	4	11*	3.8	3.4
2	4	12*	4.0	-4.9
2	4	13	30.8	-31.0
2	4	14	34.7	38.0
2	4	15	35.7	34.5
2	4	16	16.0	-14.8
2	4	17	7.1	7.0
2	4	18	15.6	16.8
2	4	19	11.6	10.9
2	4	20	10.7	-9.8
2	4	21	13.5	13.5
2	4	22	11.9	-12.3
3	4	-22	22.2	22.1
3	4	-21*	3.6	3.0
3	4	-20	11.2	-11.9
3	4	-19	16.0	15.1
3	4	-18	19.0	20.5
3	4	-17	31.6	31.4
3	4	-16*	4.5	-5.0
3	4	-15*	4.5	5.3
3	4	-14	32.5	-34.3
3	4	-13	23.6	24.9
3	4	-12	47.5	-52.5
3	4	-11	25.0	28.7
3	4	-10	75.7	83.8
3	4	-9	13.1	-10.2
3	4	-8	24.9	-23.7
3	4	-7*	3.3	5.8
3	4	-6	26.2	24.5
3	4	-5	8.8	-8.5
3	4	-4	72.0	66.4
3	4	-3	59.5	-53.6
3	4	-2	61.3	-47.5
3	4	-1	35.6	-29.7
3	4	0	30.2	-24.6
3	4	1	10.8	10.1
3	4	2	8.5	-7.3
3	4	3	20.4	19.9
3	4	4	41.2	37.0
3	4	5	18.4	16.8
3	4	6	24.9	-22.5
3	4	7	8.7	7.5
3	4	8	54.2	54.0
3	4	9	4.8	5.0
3	4	10*	3.8	3.2
3	4	11	21.4	-24.1
3	4	12	34.8	35.0
3	4	13*	4.2	5.5
3	4	14	33.4	-33.5
3	4	15*	4.3	2.8
3	4	16	21.8	21.4
3	4	17	11.2	-11.5
3	4	18	12.0	12.2
3	4	19	9.0	-8.0
3	4	20*	3.7	-3.8
3	4	21	6.1	-6.2
3	4	22*	2.5	3.3
4	4	-22	16.4	-20.7
4	4	-21	20.7	22.4
4	4	-20	15.0	16.8
4	4	-19	6.1	-7.0
4	4	-18*	4.4	-2.2
4	4	-17	8.7	-8.4
4	4	-16*	4.6	-2.5
4	4	-15	21.1	20.8
4	4	-14	28.1	31.0
4	4	-13	8.1	7.1
4	4	-12*	4.3	4.1
4	4	-11	18.9	20.0
4	4	-10	19.9	-22.4
4	4	-9	30.0	-27.7
4	4	-8	7.2	8.1
4	4	-7	26.0	-24.8
4	4	-6	16.2	15.9
4	4	-5	53.3	-49.9
4	4	-4	33.3	29.3
4	4	-3	35.8	-30.5
4	4	-2	51.2	41.9
4	4	-1	86.4	77.3
4	4	0	24.1	-21.6
4	4	1	9.6	8.1
4	4	2	37.5	-35.2
4	4	3	6.5	-5.9
4	4	4	8.8	8.1
4	4	5	49.5	49.3
4	4	6*	3.5	3.4
4	4	7	39.6	-43.2
4	4	8	20.6	20.0
4	4	9	23.5	-24.7
4	4	10	17.3	17.9
4	4	11	18.8	18.5
4	4	12	9.8	-10.0
4	4	13	56.4	-60.1
4	4	14	10.4	-10.1
4	4	15	16.4	-17.3
4	4	16	5.6	5.7
4	4	17	11.9	-11.8
4	4	18	11.5	10.5
4	4	19	10.6	-11.2
4	4	20	11.1	-11.6
4	4	21	5.1	5.8
5	4	-22	11.2	-13.8
5	4	-21*	3.1	3.5
5	4	-20	26.9	28.6
5	4	-19*	4.0	-2.6
5	4	-18	34.6	37.5
5	4	-17*	4.5	-1.7
5	4	-16	49.2	-51.9
5	4	-15	8.1	-8.9
5	4	-14	18.0	17.2
5	4	-13	41.3	-42.6
5	4	-12	4.8	-4.3
5	4	-11	30.9	-30.5
5	4	-10	22.5	19.9
5	4	-9*	4.3	5.0
5	4	-8*	4.3	-.8
5	4	-7	13.1	-11.7
5	4	-6	42.7	37.3
5	4	-5	22.2	17.2
5	4	-4	23.9	-17.2
5	4	-3	14.4	-13.2
5	4	-2	28.1	26.3
5	4	-1	28.3	-28.4
5	4	0	34.3	-34.5
5	4	1*	3.4	.1
5	4	2	47.2	45.4
5	4	3	16.9	15.2
5	4	4	15.7	14.1
5	4	5	28.9	29.0
5	4	6	62.4	-64.4
5	4	7*	3.9	.5
5	4	8	53.5	56.7
5	4	9*	4.1	-1.7
5	4	10*	4.2	.5
5	4	11*	4.2	.1
5	4	12	11.4	-11.6
5	4	13	15.1	-15.1
5	4	14	18.8	-19.3
5	4	15	15.7	16.5
5	4	16	11.2	13.0
5	4	17	11.3	10.2
5	4	18	36.0	-36.7
5	4	19*	3.5	-5.0
5	4	20	4.6	5.6
6	4	-21*	2.5	2.4
6	4	-20*	3.2	-2.2
6	4	-19	15.7	-17.4
6	4	-18	8.7	10.1
6	4	-17*	4.3	6.5
6	4	-16	21.9	23.5
6	4	-15	12.6	-13.0
6	4	-14	29.3	-30.4
6	4	-13	24.4	-23.4
6	4	-12	23.0	22.9
6	4	-11	77.6	77.9
6	4	-10	21.2	-19.3
6	4	-9	18.2	16.7
6	4	-8	42.5	-40.0
6	4	-7	40.7	-33.8
6	4	-6	22.6	20.6
6	4	-5	45.6	39.5
6	4	-4*	4.1	-5.2
6	4	-3	13.9	-13.8
6	4	-2	8.1	-8.2
6	4	-1	52.6	-52.0
6	4	0	8.3	7.9
6	4	1	88.2	88.8
6	4	2	28.8	-27.6
6	4	3*	3.8	2.3
6	4	4	15.7	-16.0
6	4	5	43.4	-42.6
6	4	6	16.6	-17.8
6	4	7	31.9	30.1
6	4	8	7.9	8.8
6	4	9	37.5	-40.7
6	4	10	12.1	-12.9
6	4	11	35.7	-36.0
6	4	12	10.2	-10.8
6	4	13	18.0	16.5
6	4	14	7.6	-7.9
6	4	15	7.4	-7.5
6	4	16	6.9	-7.2
6	4	17*	3.8	1.0
6	4	18*	3.4	-5.2
6	4	19	7.9	6.4
7	4	-20	14.8	18.1
7	4	-19	11.3	-13.2
7	4	-18	13.4	14.3
7	4	-17*	3.9	-4.9
7	4	-16	11.5	-10.9
7	4	-15	12.9	-11.8
7	4	-14	40.3	-40.7
7	4	-13*	4.8	3.0
7	4	-12*	4.9	1.6
7	4	-11	22.5	-21.1
7	4	-10	7.5	6.4
7	4	-9*	4.9	-5.4
7	4	-8	50.4	-48.0
7	4	-7	42.6	41.8
7	4	-6	93.8	101.8
7	4	-5	16.8	16.1
7	4	-4	63.2	-65.4
7	4	-3*	4.0	.4
7	4	-2	51.9	-54.9
7	4	-1*	4.0	9.5
7	4	0	44.9	47.5
7	4	1	43.7	-44.0
7	4	2	8.7	6.2
7	4	3	15.4	-15.3
7	4	4	47.8	-51.3
7	4	5*	4.2	-.7
7	4	6	56.0	59.2
7	4	7*	4.2	-1.8
7	4	8	35.8	-35.9
7	4	9*	4.3	-.4
7	4	10	41.4	-44.4
7	4	11*	4.3	.4
7	4	12	33.9	34.6
7	4	13	17.9	18.6
7	4	14	15.9	-16.5
7	4	15	10.1	10.7
7	4	16	9.3	7.3
7	4	17*	3.2	2.2
7	4	18	5.7	-5.4
8	4	-19	13.8	-16.2
8	4	-18	13.8	-13.0
8	4	-17	6.2	-6.8
8	4	-16*	3.7	.9
8	4	-15*	3.9	.5
8	4	-14	6.2	9.2
8	4	-13	12.2	-13.8
8	4	-12	18.3	-20.4
8	4	-11	39.1	44.9
8	4	-10	29.2	-30.8
8	4	-9*	4.4	-.0
8	4	-8*	4.3	-.0
8	4	-7*	4.3	-3.2
8	4	-6	9.1	-9.8
8	4	-5*	4.2	8.7
8	4	-4	18.2	17.8
8	4	-3	43.0	-44.2
8	4	-2	19.2	17.5
8	4	-1	16.6	-20.9
8	4	0	7.6	-8.1
8	4	1*	4.2	1.8
8	4	2	22.3	-24.1
8	4	3	42.5	-42.0
8	4	4*	4.3	-4.4
8	4	5	21.9	17.6
8	4	6	9.4	10.8
8	4	7*	4.3	5.3
8	4	8	9.6	9.4
8	4	9	9.7	10.4
8	4	10*	4.3	2.9
8	4	11	24.7	25.2
8	4	12	12.2	13.2
8	4	13*	3.9	1.2
8	4	14	16.6	-18.2
8	4	15	5.3	6.2
8	4	16	17.7	18.7
8	4	17	17.0	18.5
9	4	-17	14.4	-17.3
9	4	-16*	3.1	.6
9	4	-15	13.9	13.9
9	4	-14	14.3	15.1
9	4	-13*	3.9	3.2
9	4	-12	34.3	-37.5
9	4	-11*	4.1	-1.8
9	4	-10*	4.2	-.5
9	4	-9	19.9	22.9
9	4	-8	41.5	44.8
9	4	-7*	4.3	3.9
9	4	-6	11.1	-9.6
9	4	-5	18.9	19.1
9	4	-4*	4.3	-.3
9	4	-3	6.6	5.6
9	4	-2	34.1	34.0
9	4	-1*	4.3	.5
9	4	0	63.4	-71.2
9	4	1	13.1	14.8
9	4	2	37.1	39.3
9	4	3	11.1	10.7
9	4	4	9.9	-8.3
9	4	5	16.0	15.9
9	4	6*	4.3	.4
9	4	7	14.8	16.2
9	4	8	10.5	10.3
9	4	9*	4.1	-2.3
9	4	10*	4.0	-1.3
9	4	11*	3.9	3.0
9	4	12	15.3	-17.2
9	4	13	9.0	-8.2
9	4	14	16.7	16.4
9	4	15	9.5	9.2
10	4	-15	9.7	10.5
10	4	-14	6.3	-5.8
10	4	-13	9.3	9.1
10	4	-12	16.7	19.3
10	4	-11	4.9	-4.5
10	4	-10*	3.9	-3.1
10	4	-9	15.3	13.6
10	4	-8	10.4	-11.8
10	4	-7	11.0	-11.7
10	4	-6*	4.1	2.0
10	4	-5	30.6	-32.5
10	4	-4	13.3	12.9
10	4	-3*	4.2	-6.8
10	4	-2	19.9	20.5
10	4	-1*	4.2	.8
10	4	0	9.8	8.3
10	4	1	21.5	22.2
10	4	2	7.9	-10.1
10	4	3	21.0	-21.3
10	4	4	7.8	-8.7
10	4	5*	4.1	-1.2
10	4	6*	4.1	4.9
10	4	7	9.1	8.4
10	4	8	16.3	18.6
10	4	9	25.4	-27.0
10	4	10	14.8	17.3
10	4	11	16.9	19.1
10	4	12	12.7	15.2
11	4	-12	11.3	13.1
11	4	-11	8.6	-10.4
11	4	-10	10.3	-11.8
11	4	-9	14.1	-15.0
11	4	-8	20.5	22.9
11	4	-7*	3.7	4.7
11	4	-6*	3.8	8.7
11	4	-5	7.0	7.5
11	4	-4	11.7	-12.5
11	4	-3*	3.9	-.9
11	4	-2	7.8	7.5
11	4	-1	7.5	-7.9
11	4	0	12.1	-12.1
11	4	2	17.8	17.7
11	4	3	13.3	14.7
11	4	4*	3.7	3.4
11	4	5	4.8	4.6
11	4	6*	3.5	3.4
11	4	7	12.6	13.3
11	4	8	13.0	-13.3
11	4	9	17.2	-19.7
11	4	10	16.3	20.9
12	4	-7	6.5	6.7
12	4	-6*	2.9	2.2
12	4	-5	8.6	-9.3
12	4	-4	5.5	5.6
12	4	-3	7.2	-7.6
12	4	-2	5.1	4.9
12	4	-1	18.7	20.4
12	4	0*	3.1	1.6
12	4	1	12.0	14.5
12	4	2*	3.0	2.3
12	4	3	11.3	11.6
12	4	4*	2.7	-7.1
12	4	5	8.6	8.9
0	5	3	7.8	-6.6
0	5	4	13.4	-13.4
0	5	5	5.3	5.6
0	5	6	24.2	25.4
0	5	7	16.2	-17.9
0	5	8	32.3	30.8
0	5	9	10.1	-7.9
0	5	10*	3.1	-2.2
0	5	11	12.5	12.4
0	5	12	11.9	13.4
0	5	13	9.8	-10.4
0	5	14	15.5	-16.4
0	5	15	15.1	16.8
0	5	16	15.9	-16.3
0	5	17	12.1	13.3
0	5	18*	3.3	5.2
0	5	19	13.6	-13.8
0	5	20*	2.7	3.6
0	5	21	15.2	17.3
1	5	-20	6.2	5.7
1	5	-19	15.4	17.8
1	5	-18	22.5	23.9
1	5	-17*	3.6	1.6
1	5	-16*	3.7	-2.9
1	5	-15	29.6	27.3
1	5	-14	42.7	-43.2
1	5	-13	39.1	-36.3
1	5	-12*	3.5	2.3
1	5	-11	10.3	10.0
1	5	-10	20.1	-21.4
1	5	-9	13.9	-12.9
1	5	-8	8.0	7.1
1	5	-7	12.7	12.3
1	5	-6	26.3	26.0
1	5	-5*	2.3	2.1
1	5	-4	7.2	-8.6
1	5	-3	63.3	63.5
1	5	-2	45.4	-51.0
1	5	-1	36.7	-43.3
1	5	0	10.5	13.0
1	5	1*	1.5	-3.5
1	5	2	44.1	52.8
1	5	3	19.7	20.5
1	5	4	25.0	27.5
1	5	5*	2.3	2.7
1	5	6	18.6	18.6
1	5	7	15.1	13.6
1	5	8	6.6	-6.5
1	5	9	11.8	-10.5
1	5	10	35.8	-37.4
1	5	11	8.0	8.2
1	5	12	18.6	-18.1
1	5	13	77.2	-78.1
1	5	14	27.5	25.1
1	5	15*	3.5	1.1
1	5	16	8.9	9.5
1	5	17	4.6	4.1
1	5	18	11.5	13.0
1	5	19*	3.0	-2.6
1	5	20*	2.6	-1.3
1	5	21	7.0	7.3
2	5	-20	5.3	4.6
2	5	-19	13.7	-13.3
2	5	-17*	3.6	3.5
2	5	-18	8.4	-7.6
2	5	-16	18.6	-18.5
2	5	-15	19.0	-18.4
2	5	-14	32.5	31.1
2	5	-13	10.6	9.7
2	5	-12	11.5	10.8
2	5	-11	12.5	-13.0
2	5	-10	38.5	-37.3
2	5	-9*	3.2	3.5
2	5	-8	13.5	13.2
2	5	-7	23.8	-22.7
2	5	-6*	2.7	5.9
2	5	-5	43.1	-38.7
2	5	-4	21.5	-19.6
2	5	-3	18.0	14.4
2	5	-2	106.6	85.9
2	5	-1	24.6	-22.0
2	5	0	34.6	30.4
2	5	1	20.1	-20.4
2	5	2	23.1	-21.4
2	5	3	37.2	35.6
2	5	4	27.0	29.2
2	5	5	27.0	-26.5
2	5	6	10.2	9.2
2	5	7*	2.8	-2.6
2	5	8	6.1	5.2
2	5	9	15.4	16.3
2	5	10	10.7	11.1
2	5	11*	3.3	2.1
2	5	12	7.4	-8.4
2	5	13	5.9	-6.2
2	5	14	13.6	-13.6
2	5	15	16.8	16.7
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2	5	17	10.8	11.1
2	5	18	11.2	11.5
2	5	19	13.9	13.6
2	5	20	11.2	13.1
3	5	-20*	2.5	4.1
3	5	-19	8.1	-9.7
3	5	-18*	3.3	-3.1
3	5	-17	30.2	30.1
3	5	-16	14.7	16.9
3	5	-15	7.7	-7.1
3	5	-14*	3.8	2.8
3	5	-13*	3.8	-8.5
3	5	-12*	3.7	-2.5
3	5	-11	68.0	67.4
3	5	-10	16.6	-14.5
3	5	-9	54.4	-50.4
3	5	-8	43.8	39.6
3	5	-7	35.6	29.8
3	5	-6	30.3	27.5
3	5	-5	22.0	20.9
3	5	-4	14.6	-11.3
3	5	-3	38.4	-33.0
3	5	-2	36.8	30.6
3	5	-1	28.2	-23.2
3	5	0	31.3	27.0
3	5	1	85.2	74.1
3	5	2	50.9	-46.2
3	5	3	55.0	-51.4
3	5	4	46.9	46.8
3	5	5	42.5	37.3
3	5	6	7.3	-7.3
3	5	7	28.5	29.7
3	5	8	52.2	-53.9
3	5	9	22.2	-21.8
3	5	10	8.8	9.4
3	5	11*	3.4	1.5
3	5	12	16.5	-17.5
3	5	13	9.7	-9.3
3	5	14	17.0	-16.8
3	5	15*	3.5	-4.7
3	5	16	16.1	18.5
3	5	17	15.5	-17.3
3	5	18*	3.0	-7.4
3	5	19	14.2	15.3
3	5	20	4.8	-5.4
4	5	-19	6.7	-6.3
4	5	-18	29.5	-31.8
4	5	-17	21.4	22.6
4	5	-16	24.4	26.7
4	5	-15	13.7	-15.7
4	5	-14	12.0	-13.3
4	5	-13	14.0	-14.2
4	5	-12	14.3	-14.2
4	5	-11	22.9	23.9
4	5	-10	78.3	81.0
4	5	-9*	3.7	-4.0
4	5	-8	11.7	-14.1
4	5	-7	25.9	-21.5
4	5	-6	57.0	-49.1
4	5	-5	62.5	55.2
4	5	-4	52.4	46.2
4	5	-3	27.8	-24.1
4	5	-2	21.2	-17.9
4	5	-1	7.4	-6.6
4	5	0	55.3	-49.8
4	5	1	45.7	42.4
4	5	2	16.7	14.8
4	5	3	21.1	-21.2
4	5	4	49.8	-47.7
4	5	5	12.3	12.6
4	5	6	28.1	-27.5
4	5	7	18.6	19.6
4	5	8	23.7	22.5
4	5	9	22.4	-23.4
4	5	10*	3.4	-1.0
4	5	11	33.2	34.9
4	5	12*	3.5	-6.6
4	5	13	16.8	-17.0
4	5	14*	3.5	-4.2
4	5	15*	3.5	-2.9
4	5	16	22.7	-22.6
4	5	17	9.1	9.4
4	5	18	5.4	4.5
4	5	19	6.7	-7.1
5	5	-19	7.2	7.1
5	5	-18	8.6	10.0
5	5	-17*	3.2	-4.4
5	5	-16*	3.4	-3.1
5	5	-15	8.1	8.2
5	5	-14	14.2	-13.1
5	5	-13	7.8	-7.6
5	5	-12	15.3	17.2
5	5	-11	19.2	-17.8
5	5	-10	7.9	6.9
5	5	-9	39.4	38.2
5	5	-8	8.4	-6.7
5	5	-7*	3.8	-5.0
5	5	-6	9.4	7.1
5	5	-5	23.6	-19.7
5	5	-4	30.0	-29.1
5	5	-3	19.3	14.8
5	5	-2	80.1	-70.2
5	5	-1	101.0	-99.2
5	5	0	14.0	14.3
5	5	1	24.3	22.7
5	5	2	4.9	-4.8
5	5	3	22.7	-22.5
5	5	4*	3.1	2.1
5	5	5	17.0	15.8
5	5	6	27.4	29.8
5	5	7	18.1	20.5
5	5	8	15.3	-17.5
5	5	9	7.7	-8.1
5	5	10	20.3	-21.9
5	5	11	32.0	-32.4
5	5	12	34.5	37.8
5	5	13	11.3	11.7
5	5	14*	3.4	.1
5	5	15	17.0	-18.0
5	5	16*	3.1	-.0
5	5	17	9.2	10.2
6	5	-18	11.1	13.3
6	5	-17*	2.9	-2.7
6	5	-16	11.4	-12.4
6	5	-15	7.3	-7.2
6	5	-14*	3.6	-2.8
6	5	-13	5.9	5.0
6	5	-12	10.1	11.4
6	5	-11	11.9	-11.5
6	5	-10*	3.9	-.3
6	5	-9*	4.0	-.3
6	5	-8	15.4	13.0
6	5	-7	11.5	-9.6
6	5	-6	24.6	-23.0
6	5	-5	22.0	21.9
6	5	-4*	3.8	-4.3
6	5	-3	20.5	21.8
6	5	-2	9.6	10.5
6	5	-1	6.9	-7.5
6	5	0	48.6	-46.3
6	5	1	27.0	27.9
6	5	2*	3.3	-2.2
6	5	3	11.0	12.2
6	5	4	8.5	6.9
6	5	5	24.1	-27.0
6	5	6	10.0	-9.6
6	5	7	26.0	27.9
6	5	8	19.4	20.2
6	5	9	6.0	6.9
6	5	10	28.8	33.3
6	5	11	16.8	-19.4
6	5	12*	3.5	-1.2
6	5	13	7.4	7.6
6	5	14	19.3	-21.2
6	5	15*	3.0	4.4
6	5	16	10.3	-11.6
6	5	17	20.5	-24.3
7	5	-17	10.7	12.6
7	5	-16*	2.8	2.6
7	5	-15	18.0	-18.5
7	5	-14	6.9	-7.4
7	5	-13*	3.5	1.5
7	5	-12*	3.6	-1.7
7	5	-11	6.3	-6.2
7	5	-10	9.0	-6.4
7	5	-9	15.3	14.9
7	5	-8	9.8	-9.8
7	5	-7*	3.8	-3.7
7	5	-6	19.0	17.1
7	5	-5	18.8	17.3
7	5	-4	7.7	-8.6
7	5	-3*	3.5	1.8
7	5	-2	29.6	-32.4
7	5	-1	32.2	-31.8
7	5	0	18.4	-20.5
7	5	1	10.8	-11.0
7	5	3	22.1	-21.9
7	5	4	33.8	35.7
7	5	5	28.1	29.3
7	5	6	11.2	11.1
7	5	7	11.0	-11.3
7	5	8	17.0	18.0
7	5	9	26.8	29.1
7	5	10	6.8	-6.2
7	5	11	11.4	-11.1
7	5	12	17.6	-18.2
7	5	13	6.8	-6.6
7	5	14*	2.8	2.4
7	5	15	13.2	-14.2
7	5	16	17.7	23.3
8	5	-16	10.4	-10.6
8	5	-15*	2.5	-3.1
8	5	-14	20.9	-22.4
8	5	-13	26.8	30.7
8	5	-12	13.5	14.2
8	5	-11	17.8	-20.5
8	5	-10	5.9	-4.9
8	5	-9*	3.5	.1
8	5	-8	22.4	-24.8
8	5	-7	18.5	20.6
8	5	-6	16.8	15.9
8	5	-5	18.5	-18.2
8	5	-4	7.1	7.3
8	5	-3	10.0	-10.0
8	5	-2*	3.5	1.4
8	5	-1	18.7	19.9
8	5	0	37.9	41.0
8	5	1	6.9	-5.9
8	5	2*	3.5	1.6
8	5	3	10.1	-10.4
8	5	4	17.1	-16.8
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8	5	7	16.1	-18.6
8	5	8	6.3	5.3
8	5	9	6.8	-7.4
8	5	10	17.6	19.2
8	5	11*	3.1	3.8
8	5	12*	2.9	.1
8	5	13	19.1	-20.7
9	5	-14	16.6	20.0
9	5	-13	24.0	26.5
9	5	-12	29.7	-34.0
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9	5	-10	15.2	18.3
9	5	-9	18.5	19.1
9	5	-8	13.8	15.1
9	5	-7	5.2	4.1
9	5	-6	7.1	7.7
9	5	-5*	3.4	-1.3
9	5	-4	34.8	37.9
9	5	-3	10.4	-11.2
9	5	-2	15.7	17.3
9	5	-1*	3.4	-3.2
9	5	0*	3.4	.0
9	5	1*	3.4	-.7
9	5	2*	3.4	2.9
9	5	3	13.6	12.5
9	5	4	11.3	-11.9
9	5	5*	3.4	1.2
9	5	6	7.6	7.0
9	5	7	4.6	5.8
9	5	8	4.7	4.3
9	5	9	20.7	22.4
9	5	10	13.4	-13.5
9	5	11	20.2	-23.4
9	5	12	8.7	10.3
10	5	-11	10.6	11.6
10	5	-10*	2.5	6.1
10	5	-9*	2.7	-8.0
10	5	-8	14.8	14.1
10	5	-7*	3.0	5.8
10	5	-6	9.8	9.8
10	5	-5	9.1	11.6
10	5	-4*	3.2	3.6
10	5	-3	8.8	-12.7
10	5	-2*	3.2	-7.3
10	5	-1*	3.2	-5.7
10	5	0	13.2	13.9
10	5	1*	3.2	.6
10	5	2	5.0	4.6
10	5	3*	3.1	-5.0
10	5	4	17.2	-19.5
10	5	5	9.2	10.2
10	5	6	10.4	-11.2
10	5	7*	2.6	2.8
10	5	8	12.5	-13.2
10	5	9	8.4	8.4
11	5	-7	4.7	5.8
11	5	-6*	2.3	4.0
11	5	-5	18.2	20.5
11	5	-4	8.5	-9.6
11	5	-3	21.7	-23.0
11	5	-2	7.6	8.3
11	5	-1	6.8	7.3
11	5	0	10.2	-8.6
11	5	1	4.9	-5.8
11	5	2	14.7	-16.7
11	5	3	7.5	9.7
11	5	4	7.5	-10.9
11	5	5	7.6	8.2

Description of the Structure

The platy habit of crystals and the perfect {001} cleavage, as well as the optical properties, are consistent with the sheet structure of biringuccite. The arrangement of sheets in the cell, and of atoms within one sheet, are shown in Figures 2 and 3, respectively. The thick sheets, parallel to the *ab* plane, are the result of polymerization of $[B_{10}O_{13}(OH)_8]^{4-}$ units, not yet found as discrete monomers, which can be considered in turn as a dimeric form of the $[B_5O_6(OH)_5]^{2-}$ group. As can be seen in Figures 2 and 3, the repeat unit $[B_{10}O_{16}(OH)_2]^{4-}$ in the sheet of biringuccite is made by two almost equivalent halves—B(1) through B(5) and B(6) through

B(10)—related by a pseudosymmetry element. This is an axial glide plane parallel to *ac*, at $y/b \simeq 0.57$, with translation of $a/2$ along [100]. Each half of the repeat unit in the biringuccite sheet is built by two B-O tetrahedra and three B-O triangles; the tetrahedra and triangles are bound to each other in the same way as ezcurrite (Cannillo, Dal Negro, and Ungaretti, 1973), in $K_2[B_5O_8(OH)]\cdot 2H_2O$ (Marezio, 1969), in veatchite (Clark and Christ, 1971), in p-veatchite (Rumanova and Gandymov, 1971), and in gowerite (Konnert, Clark, and Christ, 1972). But while in ezcurrite the pentaboric groups are interconnected to make chains with $[B_5O_7(OH)_3]^{2-}$ as the repeat unit, in the three latter compounds polymerization leads to the formation of sheets with the repeat unit $[B_5O_8(OH)]^{2-}$. The structures which most closely resemble biringuccite are those of veatchite and p-veatchite; these also have sheets which are "non-smooth" only on the side of farther approach.

In agreement with the third rule of Christ (1960), oxygens linked to one boron will have an attached proton; they are OH(9) and OH(17), at the ends of two hexagonal rings protruding from the sheet on the side of the farther adjacent sheet (Fig. 2).

The B-O and B-B distances in biringuccite polyanions are listed in Table 5, the average overall distance being 1.474 Å for tetrahedral B-O and 1.368 Å for triangular B-O. The O-B-O angles in the polyanion are given in Table 6; the O-B-O and B-O-B angles within the rings, in Table 7. All angles indicate fairly regular boron-oxygen rings, which are roughly planar according to the displacements reported in Table 8. This same table also gives the tilt angles between the ring planes, as well as angle between triangles and rings. The tilt angles between triangles and the rings to which they are attached range from 2.6 to 15.2°. Unlike veatchite, in birin-

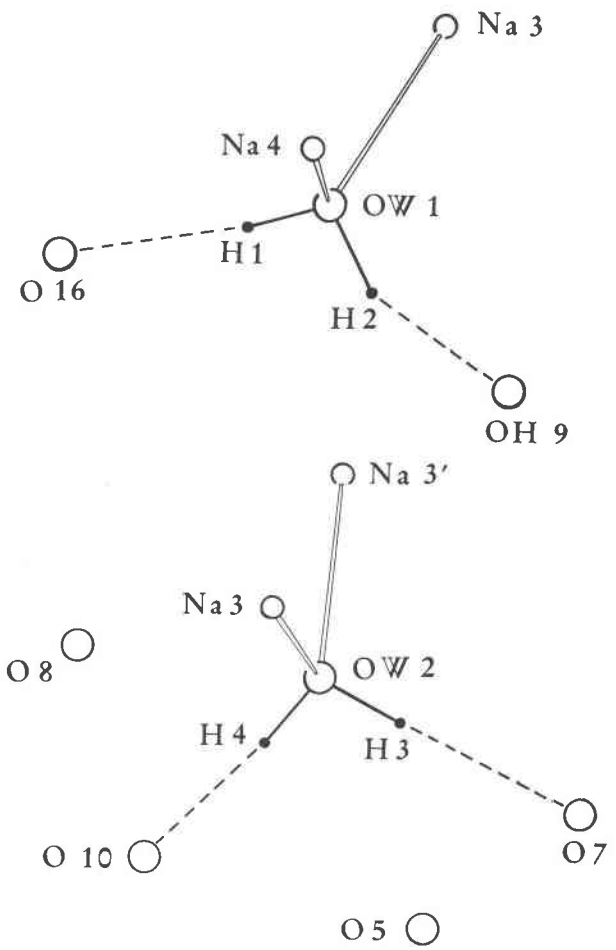

FIG. 1. Environment of water molecules.

TABLE 3. Angles and Distances Involving Possible Hydrogen Bonding*

Oxygen-oxygen distance less than 3.2 Å				
Ow(1)-O(16,2)	2.829 Å	O(16,2)-Ow(1)-OH(9,2)		122.4°
Ow(1)-OH(9,2)	2.764			
Ow(2)-O(7)	3.148	O(7)	-Ow(2)-O(10)	104.2
Ow(2)-O(10)	2.912	O(7)	O(5)	44.4
Ow(2)-O(5)	3.136	O(7)	O(8)	147.5
Ow(2)-O(8)	2.882	O(10)	O(5)	76.9
		O(10)	O(8)	49.0
OH(9)-O(7,2)	2.703	O(5)	O(8)	124.3
OH(17)-O(8,2)	2.841			
Tetrahedral environment of Ow(1)				
Na(3) - Ow(1) - Na(4)		111.9°		
Na(3)		OH(9,2)	94.5	
Na(3)		O(16,2)	126.8	
Na(4)		OH(9,2)	116.3	
Na(4)		O(16,2)	86.4	
OH(9,2)		O(16,2)	122.4	
Tetrahedral environments of Ow(2)				
Na(3)-Ow(2)-Na(3,2)	100.6°	Na(3)-Ow(2)-Na(3,2)		100.6°
Na(3) O(7)	110.1	Na(3)	O(5)	91.0
Na(3) O(10)	114.5	Na(3)	O(8)	99.4
Na(3,2) O(7)	108.9	Na(3,2)	O(5)	153.2
Na(3,2) O(10)	118.5	Na(3,2)	O(8)	77.8
O(7) O(10)	104.2	O(5)	O(8)	124.3

*The second number in parentheses denotes the asymmetric unit -x,-y,-z.

TABLE 4. Distances and Angles Related to Hydrogen Bonds*

Donor atom (D)		Acceptor atom (A)	Distances (Å) D-A	D-H	H-A	Angles (°) DHA	HDH	ADA
Ow(1)	H(1)	O(16,2)	2.829	0.88	1.96	173	100	122.4
Ow(1)	H(2)	OH(9,2)	2.764	1.01	1.87	145		
Ow(2)	H(3)	O(7)	3.148	0.99	2.16	178	100	104.2
Ow(2)	H(4)	O(10)	2.912	0.92	2.04	158		
OH(9)	H(5)	O(7,2)	2.703	0.97	1.75	171		
OH(17)	H(6)	O(8,2)	2.841	0.81	2.06	164		

* The second number in parentheses denotes the asymmetric unit -x,-y,-z.

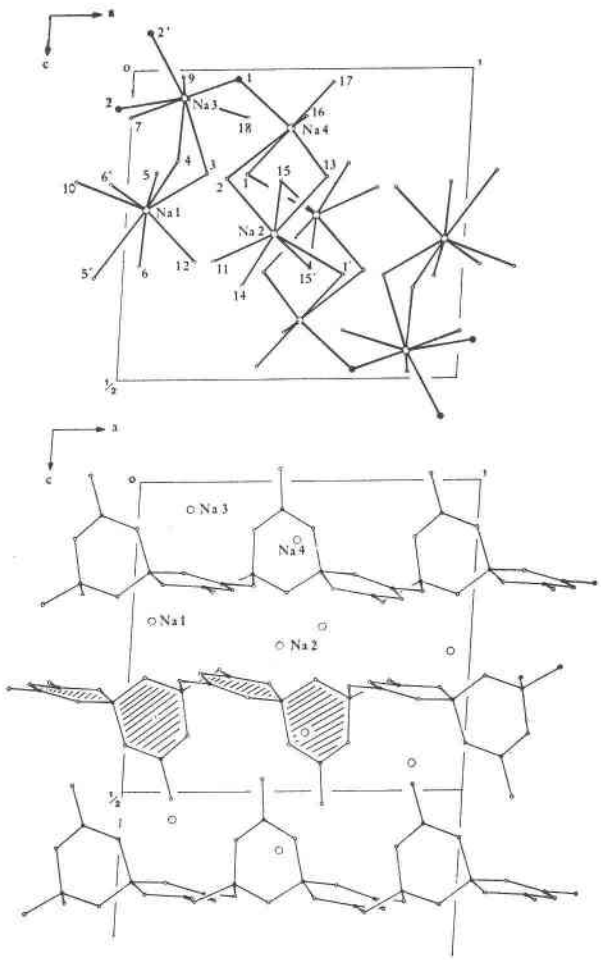

FIG. 2. Sodium-oxygen coordination polyhedra (top) and boron-oxygen sheets (bottom). Atoms with numbers only are oxygens. Blackened circles refer to water oxygens in the upper figure and to boron atoms in the lower figure; hatched areas point out the asymmetric unit in the sheet.

guccite the triangles having the hydroxyl groups are not the most tilted ones; their angles correspond to either the minimum or intermediate (8.0°) values. Among the four other triangles which take part in building the sheet, two are noticeably tilted out of planarity with their rings (15.2 and 12.4°); the remaining two triangles show average tilt angles.

Each sheet has two adjacent symmetrical neighbors related by the 2_1 axes and by the symmetry centers, respectively. Without considering the appendages containing the OH groups, the distance between the mean planes of two sheets related by the 2_1 axes is about 3.4 Å; the distance between the planes of the centrosymmetrical pair of sheets is 7.0 Å. Inside the gaps between the B-O sheets, the Na-O polyhedra are found, with their own three-dimensional arrangement.

In biringuccite there are four independent Na atoms. Na(1) and Na(2) are surrounded by oxygen atoms belonging to the B-O sheets, while Na(3) and Na(4) are bound also to hydroxyl groups and water molecules. An upper limit of 3 Å was chosen for Na-O bond lengths, according to the considerations reported by Brown and Shannon (1973). Moreover, the Na-O distances are distributed into two distinct ranges, the boundary being at about 2.7 Å (see Table 9). Since Na-O distances vary over a very wide range, it is impossible to give a simple geometrical description of the coordination polyhedra. The coordination of Na(1) is eight-fold, including

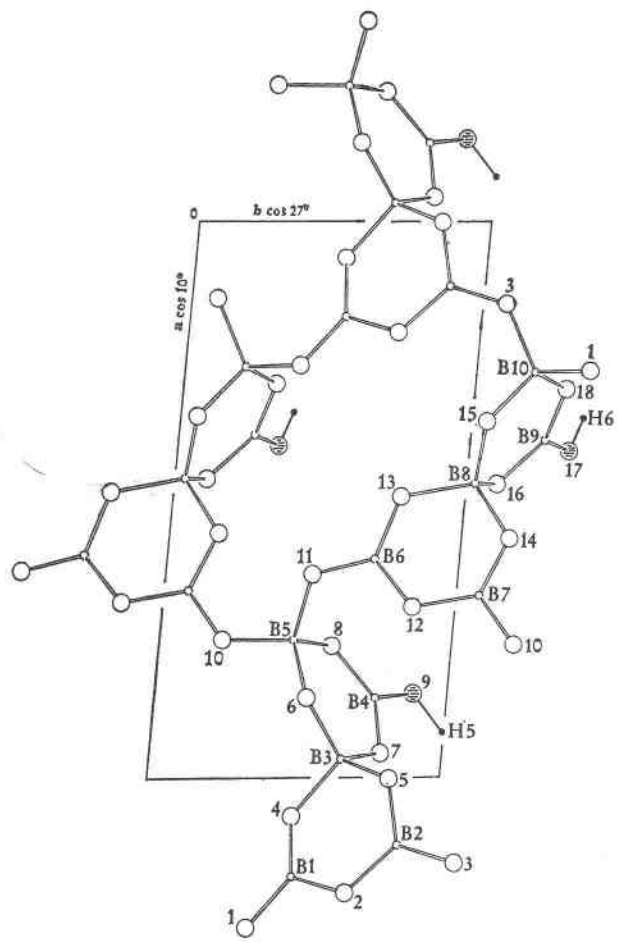

FIG. 3. Perspective view of the polyanion sheet. Hatched circles mark OH groups. The drawing is rotated 27° around *b* (horizontal) and 10° around *a* (down the page). Two asymmetric units are represented, of which only one has labelled atoms (oxygens with numbering only).

TABLE 5. B-O and B-B Distances with their Standard Deviations

B(1)-O(1)	1.346	(10) Å	B(6)-O(11)	1.359	(12) Å
O(2)	1.389	(12)	O(12)	1.393	(10)
O(4)	1.357	(9)	O(13)	1.366	(9)
ave.	1.364		ave.	1.373	
B(2)-O(2)	1.413	(10)	B(7)-O(10)	1.364	(10)
O(3)	1.343	(12)	O(12)	1.387	(12)
O(5)	1.374	(9)	O(14)	1.353	(10)
ave.	1.377		ave.	1.368	
B(3)-O(4)	1.501	(10)	B(8)-O(13)	1.513	(11)
O(5)	1.476	(11)	O(14)	1.471	(10)
O(6)	1.421	(10)	O(15)	1.426	(10)
O(7)	1.489	(9)	O(16)	1.479	(9)
ave.	1.472		ave.	1.472	
B(4)-O(7)	1.353	(10)	B(9)-O(16)	1.368	(10)
O(8)	1.363	(10)	O(18)	1.359	(10)
OH(9)	1.365	(10)	OH(17)	1.370	(10)
ave.	1.360		ave.	1.366	
B(5)-O(6)	1.455	(10)	B(10)-O(1)	1.505	(11)
O(8)	1.498	(9)	O(3)	1.483	(10)
O(10)	1.473	(12)	O(15)	1.442	(10)
O(11)	1.477	(10)	O(18)	1.477	(9)
ave.	1.476		ave.	1.477	
Ring 1			Ring 2		
B(1)-B(2)	2.431	(14) Å	B(3)-B(4)	2.489	(14) Å
B(1)-B(3)	2.526	(12)	B(3)-B(5)	2.577	(12)
B(2)-B(3)	2.503	(13)	B(4)-B(5)	2.509	(12)
ave.	2.489		ave.	2.525	
Ring 3			Ring 4		
B(6)-B(7)	2.406	(14)	B(8)-B(9)	2.469	(13)
B(6)-B(8)	2.512	(13)	B(8)-B(10)	2.533	(12)
B(7)-B(8)	2.498	(12)	B(9)-B(10)	2.491	(12)
ave.	2.472		ave.	2.498	
Between rings					
B(5)-B(6)	2.503	(13) Å			
B(5)-B(7)	2.538	(14)			
B(2)-B(10)	2.536	(13)			
B(1)-B(10)	2.552	(14)			
ave.	2.532				

TABLE 6. O-B-O Angles in Triangles and Tetrahedra*

O(1)-B(1)-O(2)	115.5°	O(11)-B(6)-O(12)	120.5°
O(1) O(4)	124.4	O(11) O(13)	119.1
O(2) O(4)	119.9	O(12) O(13)	120.4
O(2)-B(2)-O(3)	121.7	O(10)-B(7)-O(12)	117.1
O(2) O(5)	119.0	O(10) O(14)	122.1
O(3) O(5)	119.4	O(12) O(14)	120.8
O(4)-B(3)-O(5)	110.5	O(13)-B(8)-O(14)	110.5
O(4) O(6)	109.7	O(13) O(15)	108.9
O(4) O(7)	106.0	O(13) O(16)	105.4
O(5) O(6)	111.6	O(14) O(15)	108.9
O(5) O(7)	106.3	O(14) O(16)	109.3
O(6) O(7)	112.5	O(15) O(16)	113.9
O(7)-B(4)-O(8)	122.4	O(16)-B(9)-O(18)	121.3
O(7) OH(9)	120.6	O(16) OH(17)	116.2
O(8) OH(9)	117.0	O(18) OH(17)	122.5
O(6)-B(5)-O(8)	111.3	O(1)-B(10)-O(3)	109.0
O(6) O(10)	108.2	O(1) O(15)	108.1
O(6) O(11)	113.0	O(1) O(18)	106.6
O(8) O(10)	107.9	O(3) O(15)	112.9
O(8) O(11)	106.6	O(3) O(18)	106.8
O(10) O(11)	109.8	O(15) O(18)	113.2

* The average standard deviation for O-B-O angles is 0.7°.

two long bonds, while Na(2) coordinates seven oxygens in an irregular way, with all distances below 2.7 Å. Na(3) exhibits a very irregular eight-fold coordination with three long distances; Na(4) has a coordination close to an octahedron, but one bond falls outside 2.7 Å. Of the two water molecules, each one is attached to two Na atoms, Ow(1) being shared by Na(3) and Na(4) and Ow(2) by two Na(3)'s.

The pseudosymmetry pointed out for the B-O sheets is still evident for Na(1) and Na(2) not only with respect to their positions, but also to their way of coordinating. Na(3) and Na(4), however, lie well outside pseudosymmetrical positions, and as a consequence there is a less even distribution of these atoms in the structure, leaving a narrow channel approximately along ¼, *y*, ⅜.

The Na polyhedra make up a three-dimensional framework in the following way: each Na(1) and Na(2) forms a chain with its screw-axis symmetrically equivalent, by the sharing of the O(5)-O(6) edge and the O(15) corner respectively. Na(3) centrosymmetric pairs—common edge Ow(2)-Ow(2′)—bridge the Na(1) chains in the *c* direction, sharing the O(3)-O(4) edge; as a consequence the Na(1) and Na(3) polyhedra form a two-dimensional network in the *bc* plane; Na(4) provides the connections between the Na(1)-Na(3) sheets and the Na(2) chains in the *a* direction, through the sharing of the Ow(1) corner with the former and the O(2)-O(13) edge with the latter.

The Na polyhedra occur between the boron-oxygen sheets. In particular, Na(1) and Na(2) fill the space left between the "smooth" surfaces of the sheets, on the side with mean inter-layer distance of 3.4 Å. These two sodium atoms lie approximately midway in this space, tightly connecting the sheets. Na(3) and Na(4) are placed in the other intersheet space but close to one sheet; each of them makes

TABLE 7. O-B-O and B-O-B Angles within the Rings

Ring 1		Ring 3	
B(1)-O(2)-B(2)	120.3°	B(6)-O(12)-B(7)	119.9°
O(2)-B(2)-O(5)	119.0	O(12)-B(7) -O(14)	120.8
B(2)-O(5)-B(3)	122.8	B(7)-O(14)-B(8)	124.4
O(5)-B(3)-O(4)	110.5	O(14)-B(8) -O(13)	110.5
B(3)-O(4)-B(1)	124.1	B(8)-O(13)-B(6)	121.4
O(4)-B(1)-O(2)	119.9	O(13)-B(6) -O(12)	120.4
ave.	119.4	ave.	119.6
Ring 2		Ring 4	
B(3)-O(7)-B(4)	122.2°	B(8)-O(16)-B(9)	120.3°
O(7)-B(4)-O(8)	122.4	O(16)-B(9) -O(18)	121.3
B(4)-O(8)-B(5)	122.4	B(9)-O(18)-B(10)	122.8
O(8)-B(5)-O(6)	113.2	O(18)-B(10)-O(15)	113.2
B(5)-O(6)-B(3)	127.3	B(10)-O(15)-B(8)	124.1
O(6)-B(3)-O(7)	112.5	O(15)-B(8) -O(16)	113.9
ave.	119.7	ave.	119.3

TABLE 8. Displacements of Other Atoms from Planes of Ring Oxygens, Inter-Ring and Triangle-Ring Angles

	Ring 1	Ring 2	Ring 4	Ring 3
Ring oxygen atoms	O(2), O(4), O(5)	O(6), O(7), O(8)	O(15), O(16), O(18)	O(12), O(13), O(14)
Associated atoms	B(1) 0.12 Å B(2) -0.19 B(3) -0.08 O(1) 0.24 O(3) -0.54	B(3) -0.16 Å B(4) 0.10 B(5) -0.03 OH(9) 0.28	B(8) -0.28 Å B(9) 0.02 B(10) 0.09 OH(17) 0.09	B(6) 0.15 Å B(7) -0.07 B(8) 0.12 O(10) -0.20 O(11) 0.44
Angle between contacting rings	1, 2 88.5°		3, 4 88.3°	
Angles between non-contacting rings	2, 3 88.5 1, 3 5.7		1, 4 87.6 2, 4 7.3	
Oxygen atoms of triangle Triangle-ring angle	O(1), O(2), O(4) 6.9°	O(7), O(8), OH(9) 8.0°	O(16), OH(17), O(18) 2.6°	O(10), O(12), O(14) 5.5°
Oxygen atoms of triangle Triangle-ring angle	O(2), O(3), O(5) 15.2°			O(11), O(12), O(13) 12.4°

several bonds with the neighboring sheet, but only one with a hydroxyl group of the farther sheet (interlayer distance 7.0 Å). This disposition of Na atoms is quite different from the cation distribution in similar borates, especially of Sr in veatchite and p-veatchite; in these minerals in fact the Sr atoms lie in the sheet itself, and the intersheet connection on the "loose" side is provided only by hydrogen bonds.

While no hydrogen bonds take place between the "smooth" sides of B-O sheets, as in veatchite and p-veatchite, such bonds do occur between the other "non-smooth" side of the sheets.

A high cohesion in the *ab* plane produces the sheet structure; pairs of sheets are strongly connected on the side of the closer approach, but along the sides of farther approach, the relatively few Na-O bonds and hydrogen bridges result in minimum cohesion, and thus {001} cleavage.

An electrostatic valence balance was computed according to the method by Brown and Shannon (1973). Data from their Table 1 were chosen. For hydrogen bonds the curve by the same authors, reported by Donnay and Donnay (1973), was used. In Table 10 the contribution of different atoms and the bond strength sums (v.u.) are reported. The balances that result are not fully satisfactory for oxygens related to the controversial hydrogens H(3) and H(4).

TABLE 9. Na-O Distances with Their Standard Deviations*

Na(1)-O(3)	2.570 (8) Å	Na(3)-Ow(1)	2.600 (9) Å
O(4)	2.478 (7)	Ow(2)	2.500 (8)
O(5)	2.990 (7)	Ow(2,2)	2.500 (10)
O(5,3)	2.930 (9)	O (3)	2.976 (8)
O(6)	2.471 (7)	O (4)	2.446 (6)
O(6,3)	2.287 (6)	O (7)	2.986 (7)
O(10)	2.459 (8)	O (18)	2.340 (7)
O(12,3)	2.566 (10)	OH(9,2)	2.775 (8)
Na(2)-O(1,3)	2.654 (9)	Na(4)-Ow(1)	2.385 (11)
O(2)	2.546 (10)	O (1)	2.467 (8)
O(11,3)	2.539 (7)	O (2)	2.858 (9)
O(13)	2.618 (9)	O (13)	2.406 (8)
O(14,3)	2.457 (7)	O (16)	2.512 (7)
O(15)	2.298 (6)	OH(17,2)	2.294 (8)
O(15,3)	2.454 (7)		

* The second numbering in parentheses denotes the following asymmetric units:

2	$-x$	$-y$	$-z$
3	$-x$	$1/2+y$	$1/2-z$

TABLE 10. Electrostatic Valence Balance

Atom	B△	B▽	Na(1)	Na(2)	Na(3)	Na(4)	H—	..H	Sums
O(1)	1.07	0.70	-	0.10	-	0.16	-	-	2.03
O(2)	0.91 0.91	-	-	0.13	-	0.07	-	-	2.02
O(3)	1.09	0.73	0.12	-	0.06	-	-	-	2.00
O(4)	1.02	0.70	0.14	-	0.17	-	-	-	2.03
O(5)	1.00	0.74	0.05 0.06	-	-	-	-	-	1.85
O(6)	-	0.85 0.80	0.22 0.14	-	-	-	-	-	2.01
O(7)	1.02	0.71	-	-	0.05	-	-	0.21 0.13	2.12
O(8)	0.99	0.71	-	-	-	-	-	0.18	1.88
OH(9)	0.99	-	-	-	0.08	-	0.79	0.20	2.06
O(10)	1.02	0.75	0.15	-	-	-	-	0.16	2.08
O(11)	1.03	0.74	-	0.13	-	-	-	-	1.90
O(12)	0.95 0.93	-	0.12	-	-	-	-	-	2.00
O(13)	1.02	0.67	-	0.11	-	0.19	-	-	1.99
O(14)	1.05	0.76	-	0.16	-	-	-	-	1.97
O(15)	-	0.84 0.82	-	0.22 0.15	-	-	-	-	2.03
O(16)	1.00	0.73	-	-	-	0.15	-	0.17	2.05
OH(17)	0.98	-	-	-	-	0.24	0.82	-	2.04
O(18)	1.02	0.75	-	-	0.22	-	-	-	1.99
Ow(1)	-	-	-	-	0.12	0.19	0.83 0.80	-	1.94
Ow(2)	-	-	-	-	0.15 0.15	-	0.87 0.84	-	2.01
Sums	18.00	12.00	1.00	1.00	1.00	1.00	4.95	1.05	40.00

References

BROWN, J. D., AND R. D. SHANNON (1973) Empirical bond-strength-bond-length curves for oxides. *Acta Crystallogr.* **A 29,** 266–282.

CANNILLO, E., A. DAL NEGRO, AND L. UNGARETTI (1973) The crystal structure of ezcurrite. *Am. Mineral.* **58,** 110–115.

CHRIST, C. L. (1960) Crystal chemistry and systematic classification of hydrated borate minerals. *Am. Mineral.* **45,** 334–340.

CIPRIANI, C., AND P. VANNUCCINI (1961) Hoeferite e nasinite: due nuovi borati fra i prodotti di Larderello. Parte I. *Acc. Naz. Lincei,* **30,** 74–83.

——— (1961a) Hoeferite e nasinite: due nuovi borati fra i prodotti di Larderello. Parte II. *Acc. Naz. Lincei,* **30,** 235–245.

——— (1961b) A proposito del nome del borato naturale $2Na_2O \cdot 5B_2O_5 \cdot 4H_2O$ di Larderello. *Acc. Naz. Lincei,* **31,** 141–142.

CLARK, JOAN R., AND C. L. CHRIST (1971) Veatchite: crystal structure and correlation with p-veatchite. *Am. Mineral.* **56,** 1934–1954.

CROMER, DON T., AND J. T. WABER (1965) Scattering factors computed from relativistic Dirac-Slater wave function. *Acta Crystallogr.* **18,** 104–109.

DONNAY, G., AND J. D. H. DONNAY (1973) Bond-valence summation for borates. *Acta Crystallogr.* **B 29,** 1417–1425.

FERRARIS, G., AND M. FRANCHINI-ANGELA (1972) Survey of the geometry and environment of water molecules in crystalline hydrates studied by neutron diffraction. *Acta Crystallogr.* **B 28,** 3572–3583.

GERMAIN, G., P. MAIN, AND M. M. WOOLFSON (1971) The application of phase relationship to complex structures, III. The optimum use of phase relationship. *Acta Crystallogr.* **A 27,** 368–376.

HAMILTON, W. C. (1959) On the isotropic temperature factor equivalent to a given anisotropic temperature factor. *Acta Crystallogr.* **12,** 609–610.

KONNERT, JUDITH A., JOAN R. CLARK, AND C. L. CHRIST (1972) Gowerite, $CaB_5O_8(OH) \cdot B(OH)_3 \cdot 3H_2O$: crystal structure and comparison with related borates. *Am. Mineral.* **57,** 381–396.

MACGILLAVRY, C. H., AND G. D. RIECK, Editors (1962) *International Tables for X-ray Crystallography,* Vol. 3. The Kynoch Press, Birmingham, England.

MAREZIO, M. (1969) The crystal structure of $K_2B_5O_8(OH) \cdot 2H_2O$. *Acta Crystallogr.* **B 25,** 1787–1795.

RUMANOVA, I. M., AND O. GANDYMOV (1971) The crystal structure of the natural strontium borate, p-veatchite, $Sr_2B_5O_8(OH)_2 \cdot B(OH)_3 \cdot H_2O$. *Sov. Phys. Crystallogr.* **16,** 75–81.

TENNYSON, C. (1963) Eine Systematik der Borate auf Kristallchemischer Grundlage. *Fortschr. Mineral.* **41,** 64–91.

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