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The crystal structure of sulfoborite, $Mg_3SO_4(B(OH)_4)_2(OH)F$

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Abstract

Sulfoborite, $Mg_3SO_4(B(OH)_4)_2(OH)F$, is orthorhombic, space group *Pnma* with a = 10.132, b = 12.537 and c = 7.775Å (all ±0.001Å). There are four formula units in the unit cell. The crystal structure has been solved using Sayre's equation. All atoms including hydrogens have been located and refined by least squares to an R-value of 0.044. The magnesium ions are of two types; $MgO_2F(OH)_3$ and $MgOF(OH)_4$. The two types of octahedra share an edge and/or corners among themselves. The sulphate tetrahedron shares corners with both types of octahedra and these three units form crude sheets centered about the mirror planes. The sheets are jointed by the boron tetrahedra into a three-dimensional structure. Three hydrogen atoms do not participate in hydrogen bonding, the remaining two form normal hydrogen bonds.

Introduction

The original descriptions of sulfoborite indicated a chemical formula of $Mg_6H_4(BO_3)_4SO_4{\cdot}7H_2O$ (Naupert and Wense, 1893) and orthorhombic symmetry with point group *mm*2 (Bücking, 1893). The mineral has been studied several times since 1893 and no agreement as to the chemical composition was evident. Lobanova (1968) proposed the formula $Mg_6B_4O_{10}(SO_4)_2{\cdot}9H_2O$ even though his published analysis indicated 4.7% fluorine and 0.34% chlorine. Braitsch (1961) suggested $Mg_6SO_4(BO_2OH)_4{\cdot}8H_2O$ as the formula and confirmed by single crystal X-ray diffraction the orthorhombic symmetry. He could not distinguish between the space groups *Pcmn* and $Pc2_1n$. Kondrat'eva (1964) analyzed several samples and confirmed the Lobanova formula. More recently, Ostrovskaya (1967) used infrared spectroscopy to demonstrate the presence of hydroxyl and the absence of water indicating that previous analyses had incorrectly equated OH to H_2O. In addition, it was concluded that the boron was tetrahedrally and not trigonally coordinated.

The major differences between these proposed formulae lie in the amounts of water of hydration, hydroxyl and hydrogen. At the time this work was begun, we were not aware of Ostrovskaya's paper and we felt that a crystal structure determination was the only way to resolve these questions. Since the mineral contains only light elements, it was hoped that the hydrogen atoms could be located and refined. The resulting structure would, in addition to resolving the question of the chemistry of sulfoborite, provide some interesting information about hydrogen bonding and the role of fluorine and hydroxyls in this structure. A preliminary report of the structure analysis was presented by Giese and Penna (1968). Ioryish *et al.* (1976) have published an independent structure determination which differs from that of Giese and Penna in being less accurate, in apparently misidentifying one of the anions and in not locating the hydrogen atoms. For these very important reasons, the structure is reported here.

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H	K	L	FO	FC
0	0	2	9.97	-8.17
0	0	4	137.64	143.10
0	0	6	10.40	9.34
0	0	8	87.94	92.98
0	0	10	5.18	4.37
1	0	1	10.31	8.55
1	0	2	47.15	-45.32
1	0	3	34.74	-35.12
1	0	4	55.52	57.59
1	0	5	30.02	-30.64
1	0	6	29.92	31.26
1	0	7	2.70	11.00
1	0	8	33.28	33.75
1	0	9	12.11	11.92
1	0	10	20.92	21.03
1	0	12	58.34	52.48
2	0	1	50.89	-46.02
2	0	2	72.80	-66.96
2	0	3	15.15	15.06
2	0	4	23.06	19.23
2	0	5	50.12	-50.52
2	0	6	56.75	-57.52
2	0	7	9.45	-9.38
2	0	8	56.30	57.54
2	0	9	52.20	-53.75
2	0	10	5.44	-4.06
3	0	1	170.08	177.74
3	0	2	12.02	10.81
3	0	3	190.31	195.86
3	0	4	2.37	1.65
3	0	5	20.43	20.51
3	0	6	13.15	-12.01
3	0	7	24.80	24.07
3	0	8	2.22	1.28
3	0	9	58.52	59.84
3	0	10	15.26	-14.09
4	0	0	40.21	-37.59
4	0	1	22.95	21.73
4	0	2	45.85	43.29
4	0	3	78.29	78.62
4	0	4	70.38	-69.31
4	0	5	51.23	-49.69
4	0	6	4.58	4.07
4	0	8	69.78	69.70
4	0	9	10.49	10.01
4	0	10	14.79	14.41
4	0	12	21.31	20.35
5	0	1	19.36	19.21
5	0	2	4.17	-3.67
5	0	3	56.40	-54.08
5	0	4	2.[illegible]	1.37
5	0	5	6.29	3.[illegible]
5	0	6	35.59	-36.70
5	0	7	2.16	.39
5	0	8	25.70	-26.15
5	0	9	28.4[illegible]	28.58
5	0	10	12.[illegible]	-13.19
5	0	12	19.68	13.26
6	0	1	31.54	30.06
6	0	2	165.13	1[illegible]-15
6	0	3	61.33	60.13
6	0	4	52.18	-51.77
6	0	5	30.73	-30.80
6	0	6	90.84	90.54
6	0	7	10.49	-9.07
6	0	8	6.63	1.39
6	0	9	12.51	-11.11
7	0	1	7[illegible].27	19.85
7	0	2	19.48	-17.65
7	0	3	17.63	-18.64
7	0	5	33.93	33.42
7	0	6	15.79	-14.75
7	0	8	30.38	30.01
7	0	9	8.52	-4.98
8	0	0	2.67	.61
8	0	1	20.99	21.31
8	0	2	63.41	-69.42
8	0	3	27.23	27.78
8	0	5	48.08	49.01
8	0	6	2.64	-.57
8	0	7	50.66	-47.75
8	0	8	16.98	-17.6[illegible]
8	0	9	19.55	19.30
9	0	1	23.59	-22.91
9	0	2	6.07	-3.06
9	0	3	10.29	-9.98
9	0	4	66.71	64.86
9	0	5	33.68	31.07
9	0	6	27.23	26.[illegible]
9	0	7	15.97	-16.48
9	0	8	6.79	6.70
9	0	9	2.38	.90
9	0	7	10.98	12.08
9	0	8	23.54	-22.97
10	0	0	29.22	[illegible].83
10	0	1	61.56	63.34
10	0	2	3.63	2.99
10	0	3	8.02	-6.76
10	0	4	10.48	-9.39
10	0	5	13.50	11.86
10	0	6	11.26	-9.77
10	0	7	6.65	-6.49
11	0	1	6.96	7.31
11	0	2	2.81	.36
11	0	3	18.84	-17.94
11	0	4	12.61	12.01
11	0	6	10.42	-9.60
11	0	8	22.19	-21.71
12	0	0	60.15	64.02
12	0	1	28.44	28.04
12	0	2	2.96	5.33
12	0	3	6.23	-5.50
12	0	4	24.14	23.98
12	0	5	23.82	23.95
13	0	1	15.88	15.[illegible]
13	0	2	3.[illegible]	-2.[illegible]
13	0	3	5.01	4.06
13	0	4	19.13	19.89
14	0	0	10.77	9.35
14	0	1	25.93	25.58
14	0	2	19.01	-17.72
0	1	1	19.01	16.06
0	1	3	89.08	-95.58
0	1	5	4.03	5.19
0	1	7	16.06	-15.74

H	K	L	FO	FC
0	1	9	4.41	5.45
0	1	11	60.19	58.14
0	1	12	78.82	-83.55
0	1	13	16.35	-15.64
1	1	4	15.10	13.63
1	1	5	34.89	35.24
1	1	6	37.38	38.01
1	1	7	2.57	1.01
1	1	8	15.14	14.67
1	1	9	2.55	.83
1	1	10	7.85	-8.11
1	1	0	23.01	22.39
1	1	1	7.41	6.31
1	1	2	58.63	-55.60
1	1	3	28.96	-29.63
1	1	4	2.94	3.85
1	1	5	23.43	23.20
1	1	6	17.21	-16.76
1	1	7	22.15	21.68
1	1	8	2.37	-.49
1	1	9	28.70	29.37
1	1	10	5.02	-4.17
1	1	1	12.43	-10.17
1	1	7	74.43	-75.08
1	1	3	37.43	-35.75
1	1	4	3[illegible].70	-28.89
1	1	5	[illegible].25	-22.81
1	1	6	7.78	8.62
1	1	7	2.05	-.27
1	1	8	4.07	-2.90
1	1	9	4.82	-3.95
1	1	10	26.10	-25.80
1	1	0	20.46	22.42
1	1	1	17.89	14.41
1	1	2	34.70	33.02
1	1	3	38.31	-37.76
1	1	4	42.32	41.27
1	1	5	17.73	-6.09
1	1	6	24.25	-24.46
1	1	7	34.87	34.50
1	1	8	30.74	30.78
1	1	9	2.84	.41
1	1	10	9.42	-9.02
1	1	1	2.22	1.06
1	1	2	22.90	-23.22
1	1	3	17.44	-17.89
1	1	4	12.12	-10.90
1	1	5	26.67	-24.63
1	1	6	50.33	50.01
1	1	7	7.23	7.44
1	1	8	15.07	14.73
1	1	9	9.90	8.87
1	1	10	2.68	.17
1	2	0	11.22	-10.58
1	2	1	48.55	-48.60
1	2	2	49.38	-52.13
1	2	3	15.96	-13.10
1	2	4	5.94	-3.56
1	2	5	28.35	-26.51
1	2	6	44.27	-44.61
1	2	7	17.27	17.21
1	2	8	3.78	2.42
1	2	9	15.97	-15.63
1	2	1	51.98	50.98
1	2	2	43.48	-44.21
1	2	3	5.72	-5.56
1	2	4	6.24	5.83
1	2	5	8.45	7.82
1	2	6	8.54	8.18
1	2	7	12.51	12.30
1	2	8	9.52	7.91
1	2	9	9.61	9.17
1	2	0	2.07	.62
1	2	1	50.50	-50.29
1	2	2	3.10	-1.53
1	2	3	18.80	19.13
1	2	4	9.71	-8.60
1	2	5	4.49	-2.67
1	2	6	10.14	-9.94
1	2	7	36.43	35.99
1	2	8	5.90	4.37
1	2	9	7.07	6.81
1	2	1	11.38	-11.11
1	2	2	20.11	-20.15
1	2	3	41.37	-43.23
1	2	4	20.82	-19.66
1	2	5	36.41	-35.37
1	2	6	9.81	2.75
1	2	7	3.23	-2.30
1	2	8	4.94	5.41
1	2	0	8.99	9.99
1	2	1	11.82	11.40
1	2	2	34.37	35.46
1	2	3	14.01	-13.93
1	2	4	10.29	-9.59
1	2	5	10.25	-10.01
1	2	6	9.17	8.57
1	2	7	22.08	22.33
1	2	1	16.48	16.09
1	2	2	4.30	-2.73
1	2	3	14.27	-14.73
1	2	4	6.30	-6.03
1	2	5	3.24	-11.77
1	2	6	19.33	18.56
1	2	0	30.13	-33.98
1	2	1	13.16	-12.82
1	2	2	2.99	.28
1	2	3	17.63	-17.47
1	2	4	40.44	-40.90
1	2	5	5.97	4.99
1	2	1	21.54	7.06
1	2	2	12.91	-1.49
1	2	3	3.71	2.97
1	2	4	3.11	-2.21
1	2	0	2.82	.93
1	2	1	2.73	-.64
1	2	2	13.88	14.50
1	2	0	46.19	-37.39
1	2	2	10.20	-7.90
1	2	4	4.16	4.27
1	2	6	19.49	-20.42
1	2	8	22.06	-21.64
1	2	10	27.14	-27.95
1	2	1	58.34	-58.36
1	2	2	65.06	-62.58

H	K	L	FO	FC
1	3	3	8.79	-9.41
1	3	4	8.52	8.04
1	3	5	3.73	3.93
1	3	6	6.41	6.79
1	3	7	26.62	27.49
1	3	8	[illegible]	-3.35
1	3	9	36.86	-37.87
1	3	10	2.76	1.15
2	3	0	99.73	-111.70
2	3	1	23.92	22.22
2	3	2	35.50	-32.59
2	3	3	62.19	-61.15
2	3	4	74.92	76.96
2	3	5	66.13	67.10
2	3	6	9.44	9.76
2	3	7	26.15	-27.07
2	3	8	24.06	-24.54
2	3	9	4.16	-4.42
2	3	10	2.97	-.18
2	3	1	28.34	-28.22
2	3	2	2.97	-1.46
2	3	3	12.28	-13.63
2	3	4	19.25	18.85
2	3	5	20.07	19.90
2	3	6	16.02	-16.49
2	3	7	39.07	-38.57
2	3	8	23.04	23.45
2	3	9	22.33	-22.97
2	3	10	9.43	-9.29
2	3	0	104.14	-112.20
2	3	1	46.02	40.80
2	3	2	21.02	-18.01
2	3	3	57.50	-47.80
2	3	4	16.93	17.65
2	3	5	2.36	1.27
2	3	6	6.55	6.00
2	3	7	3.02	-.77
2	3	8	29.51	-30.47
2	3	9	19.05	18.79
2	3	10	13.23	-13.43
3	3	1	11.17	-9.25
3	3	2	35.95	34.87
3	3	3	8.14	-6.27
3	3	4	23.15	-23.37
3	3	5	45.65	44.48
3	3	6	12.58	-6.07
3	3	7	21.95	20.66
3	3	8	16.09	16.21
3	3	9	13.95	-13.25
3	3	10	15.55	-15.58
3	3	0	35.83	-38.30
3	3	1	16.03	-15.55
3	3	2	3.28	.79
3	3	3	9.25	-9.76
3	3	4	10.36	-10.77
3	3	5	23.62	22.95
3	3	6	4.04	-1.25
3	3	7	18.54	18.83
3	3	8	19.64	-18.39
3	3	9	17.73	-16.48
3	3	1	42.28	-41.19
3	3	2	29.72	-28.89
3	3	3	12.65	-12.43
3	3	4	20.63	-18.54
3	3	5	8.84	8.25
3	3	6	17.79	18.41
3	3	7	20.65	-19.96
3	3	8	4.32	-3.09
3	3	5	13.34	-13.18
3	3	0	33.71	-35.83
3	3	1	67.83	-69.64
3	3	2	3.88	2.44
3	3	3	10.91	9.40
3	3	4	51.98	53.29
3	3	5	5.49	3.08
3	3	6	15.68	14.16
3	3	7	9.27	7.43
3	3	8	3.16	-2.62
3	3	9	24.02	-25.14
3	3	1	7.89	7.57
3	3	2	15.71	15.89
3	3	4	3.46	2.42
3	3	5	2.97	-.25
3	3	6	6.85	5.61
3	3	7	14.06	-14.27
3	3	8	13.85	13.85
3	3	9	16.79	-17.97
3	3	1	13.00	-23.86
3	3	2	29.96	-29.84
3	3	3	11.90	-10.00
3	3	4	3.41	-3.60
3	3	5	14.32	-13.77
3	3	6	4.69	-3.37
3	3	7	21.93	21.98
3	3	8	5.38	-3.51
3	3	9	3.03	-.61
3	3	1	10.20	9.22
3	3	2	21.55	-22.45
3	3	3	24.45	23.86
3	3	4	9.87	8.30
3	3	5	8.79	8.
3	3	6	2.63	-2.44
3	3	7	13.46	-13.09
3	3	8	15.88	-16.46
3	3	9	2.97	-2.72
3	3	1	25.76	26.75
3	3	2	23.97	-25.30
3	3	3	25.29	-25.27
3	3	4	64.44	-60.90
3	3	5	3.75	2.47
3	3	6	4.12	-2.70
3	3	7	21.45	-23.47
3	3	8	6.66	-5.07
3	3	1	86.82	87.36
3	3	2	63.49	-60.54
3	3	3	51.46	54.14
3	3	4	62.63	-65.43
3	3	5	20.37	20.42
3	3	6	53.12	-52.52
3	3	7	73.32	76.89
3	3	8	3.93	.99
3	3	4	7.59	7.69
3	3	5	42.38	-43.94
3	3	6	35.39	-36.05
3	3	7	21.78	-23.34
3	3	8	3.75	-3.50

H	K	L	FO	FC
3	4	9	15.63	-15.29
3	4	10	4.95	3.98
3	4	0	27.73	27.80
3	4	1	80.56	79.48
3	4	2	15.84	15.53
3	4	3	24.23	-20.71
3	4	4	62.41	63.44
3	4	5	36.99	37.38
3	4	6	4.95	-3.54
3	4	7	45.95	-47.55
3	4	8	45.36	46.66
3	4	9	3.55	1.84
3	4	5	5.72	-5.70
3	4	6	12.43	-11.21
3	4	7	30.18	-30.23
3	4	8	2.67	-1.12
3	4	9	25.03	26.48
3	4	10	13.41	-14.32
4	4	0	16.35	17.91
4	4	1	111.56	114.78
4	4	2	29.77	28.71
4	4	3	65.44	-62.77
4	4	4	41.02	-39.73
4	4	5	7.52	7.94
4	4	6	11.18	-10.91
4	4	7	25.15	-25.31
4	4	8	15.77	15.79
4	4	9	35.50	36.58
4	4	10	8.79	7.76
5	4	1	9.09	-7.52
5	4	2	14.79	14.01
5	4	3	72.10	-70.56
5	4	4	26.15	24.78
5	4	5	22.90	-23.40
5	4	6	9.64	-9.33
5	4	7	17.44	-17.33
5	4	8	3.39	-2.85
5	4	9	5.74	4.80
6	4	0	62.12	65.80
6	4	1	12.16	12.53
6	4	2	46.08	-45.58
6	4	3	6.62	-.20
6	4	4	51.63	-50.67
6	4	5	12.24	11.12
6	4	6	25.94	-25.40
6	4	7	20.84	-40.68
6	4	8	12.65	13.[illegible]
6	4	9	8.14	8.
7	4	1	32.02	32.8[illegible]
7	4	2	31.28	-30.53
7	4	3	5.27	-4.94
7	4	4	9.22	8.94
7	4	5	11.44	-10.76
7	4	6	4.54	4.84
7	4	7	2.95	-1.37
7	4	8	18.22	-19.04
7	4	9	17.79	17.50
8	4	0	8.51	-5.50
8	4	1	8.10	8.89
8	4	2	54.35	-53.13
8	4	3	36.00	33.90
8	4	4	7.09	-1.73
8	4	5	17.41	-17.08
8	4	6	55.70	-55.40
8	4	7	8.48	8.19
8	4	8	16.26	15.71
9	4	1	2.50	-2.88
9	4	2	32.93	32.76
9	4	3	10.52	-10.70
9	4	4	14.80	-14.96
9	4	5	33.60	-32.36
9	4	6	3.02	-.97
9	4	7	16.62	-15.30
9	4	8	24.97	-24.73
10	4	0	57.92	61.62
10	4	1	2.50	-4.59
10	4	2	10.12	-10.08
10	4	3	34.76	35.13
10	4	4	16.31	15.38
10	4	5	51.30	-49.75
10	4	6	22.21	-21.56
10	4	7	14.76	14.26
11	4	1	11.38	-10.26
11	4	2	1.63	6.43
11	4	3	36.43	-36.94
11	4	4	20.31	19.92
11	4	5	26.18	-26.26
11	4	6	9.73	-9.02
12	4	0	7.44	3.19
12	4	1	16.71	-18.13
12	4	2	5.89	-3.49
12	4	3	35.63	35.27
12	4	4	24.20	-23.18
13	4	1	21.68	20.71
13	4	2	7.41	-7.35
13	4	3	1.85	7.31
0	5	1	54.53	55.91
0	5	3	3.80	-2.96
0	5	5	42.07	-41.55
0	5	7	34.24	35.82
0	5	9	25.53	-25.57
1	5	1	59.68	59.60
1	5	2	68.20	-69.60
1	5	3	2.94	.85
1	5	4	15.85	15.79
1	5	5	40.17	40.38
1	5	6	30.68	31.42
1	5	7	3.11	1.03
1	5	8	19.30	20.00
1	5	9	10.66	9.97
1	5	10	8.43	-8.28
2	5	0	87.54	-89.24
2	5	1	42.15	-41.87
2	5	2	28.53	28.17
2	5	4	19.95	19.47
2	5	4	66.30	-65.86
2	5	5	18.32	-18.23
2	5	6	30.60	30.86
2	5	7	50.51	51.71
2	5	8	37.79	-37.98
2	5	9	7.83	7.88
2	5	10	24.08	24.50
3	5	1	9.06	8.39
3	5	2	49.54	-49.64

H	K	L	FO	FC
2	4	3	35.27	-36.62
2	4	4	73.49	-74.42
2	4	5	55.03	55.82
2	4	6	14.94	-15.34
2	4	7	31.98	-32.24
2	4	8	2.63	-1.28
2	4	9	8.65	9.42
2	4	10	7.96	7.57
3	4	1	61.12	-56.99
3	4	2	13.41	11.55
3	4	3	16.78	16.49
3	4	4	3.78	1.40
3	4	5	75.54	-74.92
3	4	6	12.43	-11.21
3	4	7	30.18	-30.23
3	4	8	2.67	-1.12
3	4	9	25.03	26.48
3	4	10	13.41	-14.32
4	4	0	16.35	17.91
4	4	1	111.56	114.78
4	4	2	29.77	28.71
4	4	3	65.44	-62.77
4	4	4	41.02	-39.73
4	4	5	7.52	7.94
4	4	6	11.18	-10.91
4	4	7	25.15	-25.31
4	4	8	15.77	15.79
4	4	9	35.50	36.58
4	4	10	8.79	7.76
5	4	1	9.09	-7.52
5	4	2	14.79	14.01
5	4	3	72.10	-70.56
5	4	4	26.15	24.78
5	4	5	22.90	-23.40
5	4	6	9.64	-9.33
5	4	7	17.44	-17.33
5	4	8	3.39	-2.85
5	4	9	5.74	4.80
6	4	0	62.12	65.80
6	4	1	12.16	12.53
6	4	2	46.08	-45.58
6	4	3	6.62	-.20
6	4	4	51.63	-50.67
6	4	5	12.24	11.12
6	4	6	25.94	-25.40
6	4	7	20.84	-40.68
6	4	8	12.65	13.[illegible]
6	4	9	8.14	8.
7	4	1	32.02	32.8[illegible]
7	4	2	31.28	-30.53
7	4	3	5.27	-4.94
7	4	4	9.22	8.94
7	4	5	11.44	-10.76
7	4	6	4.54	4.84
7	4	7	2.95	-1.37
7	4	8	18.22	-19.04
7	4	9	17.79	17.50
8	4	0	8.51	-5.50
8	4	1	8.10	8.89
8	4	2	54.35	-53.13
8	4	3	36.00	33.90
8	4	4	7.09	-1.73
8	4	5	17.41	-17.08
8	4	6	55.70	-55.40
8	4	7	8.48	8.19
8	4	8	16.26	15.71
9	4	1	2.50	-2.88
9	4	2	32.93	32.76
9	4	3	10.52	-10.70
9	4	4	14.80	-14.96
9	4	5	33.60	-32.36
9	4	6	3.02	-.97
9	4	7	16.62	-15.30
9	4	8	24.97	-24.73
10	4	0	57.92	61.62
10	4	1	2.50	-4.59
10	4	2	10.12	-10.08
10	4	3	34.76	35.13
10	4	4	16.31	15.38
10	4	5	51.30	-49.75
10	4	6	22.21	-21.56
10	4	7	14.76	14.26
11	4	1	11.38	-10.26
11	4	2	1.63	6.43
11	4	3	36.43	-36.94
11	4	4	20.31	19.92
11	4	5	26.18	-26.26
11	4	6	9.73	-9.02
12	4	0	7.44	3.19
12	4	1	16.71	-18.13
12	4	2	5.89	-3.49
12	4	3	35.63	35.27
12	4	4	24.20	-23.18
13	4	1	21.68	20.71
13	4	2	7.41	-7.35
13	4	3	1.85	7.31
0	5	1	54.53	55.91
0	5	3	3.80	-2.96
0	5	5	42.07	-41.55
0	5	7	34.24	35.82
0	5	9	25.53	-25.57
1	5	1	59.68	59.60
1	5	2	68.20	-69.60
1	5	3	2.94	.85
1	5	4	15.85	15.79
1	5	5	40.17	40.38
1	5	6	30.68	31.42
1	5	7	3.11	1.03
1	5	8	19.30	20.00
1	5

H	K	L	FO	FC
6	7	2	49.22	30.16
6	7	3	27.62	28.11
6	7	4	9.18	8.42
6	7	5	13.76	12.43
6	7	6	29.56	29.47
6	7	7	8.86	-8.67
6	7	8	3.02	.18
7	7	1	49.74	-49.90
7	7	2	36.70	37.00
7	7	3	4.50	3.44
7	7	4	8.99	-8.61
7	7	5	18.78	-18.66
7	7	6	3.68	-2.62
7	7	7	10.14	-9.24
7	7	8	14.63	-12.89
8	7	0	3.98	2.93
8	7	1	39.04	38.35
8	7	2	21.51	-21.79
8	7	3	15.61	-13.02
8	7	4	12.93	12.50
8	7	5	4.86	-4.48
8	7	6	7.63	-5.89
8	7	7	22.04	-30.86
9	7	1	4.25	4.07
9	7	2	19.12	18.72
9	7	3	34.27	35.19
9	7	4	19.08	18.99
9	7	5	24.54	24.29
9	7	6	8.34	-7.47
9	7	7	8.09	7.31
10	7	0	9.43	-10.16
10	7	1	20.25	19.84
10	7	2	40.61	-41.51
10	7	3	4.41	3.81
10	7	4	4.30	2.89
10	7	5	15.54	15.32
10	7	6	11.89	-13.65
11	7	1	20.85	-20.79
11	7	2	4.14	-2.89
11	7	3	7.09	5.96
11	7	4	2.81	8.07
11	7	5	3.98	4.10
12	7	0	14.89	16.21
12	7	1	18.26	18.63
12	7	2	5.96	4.67
12	7	3	9.32	9.00
12	7	4	29.34	28.46
13	7	1	24.29	-24.45
0	8	0	216.54	228.49
0	8	2	61.79	-62.31
0	8	4	26.39	28.11
0	8	6	22.03	-22.33
0	8	8	50.42	49.02
1	8	1	10.42	11.48
1	8	2	31.63	-31.09
1	8	3	24.21	-24.51
1	8	4	14.27	14.01
1	8	5	20.63	-20.68
1	8	6	9.61	8.06
1	8	7	4.01	-.29
1	8	8	8.75	8.19
1	8	9	10.51	10.33
2	8	0	38.53	38.47
2	8	1	39.85	-41.17
2	8	2	41.52	-41.25
2	8	3	46.39	47.05
2	8	4	4.08	-1.46
2	8	5	29.13	-28.94
2	8	6	44.76	-45.77
2	8	7	10.21	10.71
2	8	8	37.53	36.77
2	8	9	33.25	-32.89
3	8	1	32.13	32.31
3	8	2	11.73	11.12
3	8	3	54.35	55.96
3	8	4	3.67	-3.15
3	8	5	28.12	-27.27
3	8	6	5.45	-4.25
3	8	7	4.72	-3.26
3	8	8	6.91	-5.82
3	8	9	36.04	36.23
4	8	0	11.74	8.87
4	8	1	17.73	-16.65
4	8	2	22.42	22.22
4	8	3	46.47	46.71
4	8	4	40.80	-39.84
4	8	5	56.78	-56.62
4	8	6	3.34	-2.78
4	8	7	43.33	42.43
4	8	8	10.40	10.48

H	K	L	FO	FC
4	8	9	1.85	-1.39
5	8	1	5.79	3.31
5	8	2	9.13	9.06
5	8	3	42.19	-41.48
5	8	4	11.55	11.55
5	8	5	12.56	-13.78
5	8	6	14.25	-13.13
5	8	7	3.02	-2.24
5	8	8	10.61	-10.40
6	8	0	34.33	32.54
6	8	1	26.96	-26.23
6	8	2	61.58	61.01
6	8	3	39.03	38.29
6	8	4	63.15	-61.82
6	8	5	20.73	-20.17
6	8	6	40.73	39.44
6	8	7	2.52	-9.99
6	8	8	9.25	-7.41
7	8	1	22.20	21.78
7	8	2	20.70	-20.38
7	8	3	6.62	-5.60
7	8	4	14.93	15.41
7	8	5	12.78	-12.37
7	8	6	7.41	6.71
7	8	7	1.77	-.13
7	8	8	7.49	-6.86
8	8	0	52.98	-54.94
8	8	1	33.24	33.42
8	8	2	27.92	28.51
8	8	3	2.42	1.34
8	8	4	45.59	-45.00
8	8	5	1.66	1.13
8	8	6	7.67	6.23
8	8	7	15.18	-14.61
9	8	1	24.01	22.54
9	8	2	26.28	26.28
9	8	3	10.64	9.76
9	8	4	8.36	-8.34
9	8	5	11.29	-11.16
9	8	6	5.19	-4.51
9	8	0	23.31	24.61
9	8	1	47.55	47.96
9	8	2	13.42	13.53
9	8	3	13.97	-13.55
9	8	4	11.29	-10.97
10	8	5	2.64	1.53
10	8	6	2.74	-2.41
11	8	1	1.73	2.07
11	8	2	4.92	4.46
11	8	3	23.07	-23.67
11	8	4	15.02	14.41
12	8	0	32.09	31.96
12	8	1	19.77	18.36
12	8	2	6.44	-5.95
12	8	3	2.69	-.76
12	9	1	39.56	40.25
0	9	3	59.24	-61.94
0	9	5	36.48	36.47
0	9	7	6.05	-5.01
0	9	9	14.16	14.68
1	9	1	27.19	25.87
1	9	2	53.05	-54.26
1	9	3	4.19	-.39
1	9	4	5.07	3.53
1	9	5	29.09	29.68
1	9	6	14.15	14.09
1	9	7	5.23	4.95
1	9	8	12.51	12.90
1	9	9	19.73	18.73
2	9	0	6.33	-5.73
2	9	1	12.03	11.94
2	9	2	24.98	-24.36
2	9	3	40.57	-41.37
2	9	4	12.07	-11.94
2	9	5	12.78	11.87
2	9	6	17.87	-17.71
2	9	7	7.71	7.22
2	9	8	15.80	-15.68
2	9	9	18.60	18.47
3	9	1	9.18	8.62
3	9	2	27.32	-28.05
3	9	3	16.91	-16.19
3	9	4	5.97	-6.09
3	9	5	1.48	-.86
3	9	6	21.41	21.11
3	9	7	2.43	-1.17
3	9	8	1.73	8.68
3	9	9	7.15	7.04
4	9	0	3.65	12.24
4	9	1	13.99	-12.85

H	K	L	FO	FC
4	9	2	14.47	14.78
4	9	3	14.45	-14.68
4	9	4	18.53	18.09
4	9	5	13.63	-14.20
4	9	6	7.96	-7.65
4	9	7	27.05	26.63
4	9	8	28.64	27.86
5	9	1	2.63	.31
5	9	2	24.45	-24.47
5	9	3	20.18	-20.18
5	9	4	21.84	-22.08
5	9	5	22.69	-22.43
5	9	6	34.63	34.30
5	9	7	5.63	-5.16
5	9	8	4.75	-3.74
6	9	0	16.95	17.57
6	9	1	44.76	-43.92
6	9	2	21.08	-21.09
6	9	3	14.31	12.23
6	9	4	13.67	13.73
6	9	5	14.15	-13.28
6	9	6	25.59	-25.08
6	9	7	29.60	28.76
6	9	8	1.86	11.24
7	9	1	22.10	20.49
7	9	2	29.72	-29.75
7	9	3	5.59	-5.65
7	9	4	4.50	-4.27
7	9	5	4.16	-4.15
7	9	6	9.51	9.53
7	9	7	9.81	13.93
8	9	0	9.71	10.37
8	9	1	39.33	-38.86
8	9	2	10.85	-10.21
8	9	3	6.41	4.91
8	9	4	4.25	-3.25
8	9	5	14.03	-13.55
8	9	6	19.62	-19.70
9	9	1	22.32	21.64
9	9	2	8.84	8.70
9	9	3	10.14	-9.97
9	9	4	15.53	-14.80
10	9	0	5.83	-4.87
10	9	1	19.23	-18.38
10	9	2	11.64	10.56
10	9	3	4.36	1.62
10	9	4	3.98	-3.57
11	9	1	12.46	11.64
11	9	2	18.48	-17.91
11	9	3	14.60	-14.13
0	9	5	2.68	-1.76
0	9	7	14.75	14.03
0	9	9	12.02	-11.63
1	9	0	12.22	-11.95
1	9	1	7.93	-7.34
1	9	2	17.30	-17.25
1	9	3	3.77	-2.77
1	9	4	18.02	17.54
1	9	5	46.76	-45.07
1	9	6	16.05	16.22
1	9	7	3.93	-2.63
1	9	8	3.10	1.64
2	9	0	23.63	-23.73
2	9	1	47.32	-47.04
2	9	2	20.09	-19.60
2	9	3	21.30	-23.69
2	9	4	4.37	3.45
2	9	5	2.52	1.30
2	9	6	15.15	14.76
2	9	7	2.82	-.53
2	9	8	2.60	.81
2	9	9	72.77	-73.41
3	9	1	6.10	-5.78
3	9	2	21.39	-21.61
3	9	3	15.68	-16.33
3	9	4	26.23	25.12
3	9	5	20.98	21.05
3	9	6	3.65	2.78
3	9	7	19.39	-19.36
3	9	8	28.01	-27.87
4	9	0	13.00	-13.49
4	9	1	3.90	2.86
4	9	2	5.58	1.02
4	9	3	5.46	4.43
4	9	4	13.89	14.15
4	9	5	3.82	-2.94
4	9	6	26.40	-24.47
4	9	7	10.44	9.94
4	9	8	64.41	-66.87
5	9	1	5.37	5.22

H	K	L	FO	FC
5	9	2	39.70	-41.00
5	9	3	18.13	-17.27
5	9	4	5.66	4.48
5	9	5	4.28	1.22
5	9	6	15.18	-14.45
5	9	7	10.98	10.04
5	9	8	28.83	-28.15
6	9	1	22.68	-22.74
6	9	2	11.80	11.49
6	9	3	6.14	-5.79
6	9	4	18.26	-18.50
6	9	5	18.91	17.20
6	9	6	7.76	-7.93
6	9	7	16.44	15.57
6	9	8	4.71	4.71
7	9	1	8.53	[illegible]
7	9	2	4.55	-4.17
7	9	3	9.29	-10.29
7	9	4	11.70	-11.76
7	9	5	10.05	10.07
7	9	6	20.44	19.94
7	9	7	10.82	10.77
8	9	1	45.87	-45.78
8	9	2	20.77	-20.76
8	9	3	20.08	-19.47
8	9	4	7.50	-5.86
8	9	5	9.63	-8.32
8	9	6	14.08	14.00
8	9	7	22.10	-21.41
9	9	1	31.15	-32.15
9	9	2	32.82	-32.06
9	9	3	9.27	-8.11
9	9	4	14.19	-7.29
9	9	5	33.79	33.26
10	9	1	5.15	4.28
10	9	2	8.58	6.39
10	9	3	13.89	-14.79
10	9	4	4.41	3.41
10	9	5	12.46	12.20
11	9	1	5.32	4.35
11	9	2	3.43	2.84
11	9	3	32.92	-33.69
11	9	4	15.87	-14.11
12	9	1	25.31	-24.92
12	9	2	9.39	-8.19
12	9	3	19.18	-19.35
12	9	4	7.13	-6.80
12	9	5	3.88	-3.33
12	9	6	3.10	.49
12	9	7	55.86	56.38
12	9	8	14.59	-14.75
0	11	1	44.42	46.21
0	11	5	38.48	-38.47
0	11	7	30.00	-30.25
1	11	1	28.52	29.29
1	11	2	6.49	-6.81
1	11	3	5.29	5.73
1	11	5	5.68	-21.28
1	11	6	31.11	-31.18
1	11	7	16.03	-15.79
1	11	8	4.08	-3.16
2	11	0	18.36	18.44
2	11	1	39.47	39.60
2	11	2	17.50	16.93
2	11	3	14.64	-13.57
2	11	4	30.08	30.05
2	11	5	12.64	13.59
2	11	6	4.27	1.68
2	11	7	35.06	-35.08
2	11	8	23.45	23.14
3	11	1	2.95	1.29
3	11	2	42.02	41.11
3	11	3	4.88	4.23
3	11	4	9.60	10.09
3	11	5	18.53	18.97
3	11	6	11.34	-9.76
3	11	7	10.31	-10.35
3	11	8	3.68	-2.22
4	11	0	15.25	14.34
4	11	1	16.28	-15.21
4	11	2	47.94	-47.16
4	11	3	32.94	33.32
4	11	4	2.91	1.54
4	11	5	12.80	-11.58
4	11	6	14.98	-14.27
4	11	7	13.60	-13.88
5	11	1	9.70	9.06
5	11	2	17.41	17.88
5	11	3	17.21	17.19

H	K	L	FO	FC
5	11	4	4.0[illegible]	2.99
5	11	5	26.87	26.32
5	11	6	21.84	-20.72
5	11	7	4.49	2.18
6	11	0	17.35	16.36
6	11	1	23.24	-22.64
6	11	2	6.22	-5.11
6	11	3	52.28	52.72
6	11	4	22.21	21.28
6	11	5	21.69	-21.13
6	11	6	4.34	3.86
6	11	7	3.15	10.60
7	11	1	28.14	-27.96
7	11	2	29.81	29.02
7	11	3	10.87	10.45
7	11	4	6.35	-5.55
7	11	5	11.35	-10.13
7	11	6	2.65	-3.23
8	11	0	5.87	5.32
8	11	1	3.97	-2.20
8	11	2	6.18	5.68
8	11	3	22.97	23.48
8	11	4	16.14	14.55
8	11	5	27.06	-25.97
9	11	1	4.25	-3.67
9	11	2	15.62	14.31
9	11	3	20.92	20.54
9	11	4	12.94	13.13
9	11	5	15.25	15.12
10	11	0	20.51	-20.76
10	11	1	5.81	5.38
10	11	2	2.80	2.51
10	11	3	12.89	12.35
11	11	1	7.05	-7.27
0	12	0	92.35	92.62
0	12	2	65.66	67.58
0	12	4	31.25	-30.14
0	12	6	45.78	47.86
0	12	8	5.48	5.50
1	12	1	4.67	5.28
1	12	2	12.34	-11.17
1	12	3	22.56	-22.88
1	12	4	17.08	17.68
1	12	5	1[illegible].54	-14.14
1	12	6	18.0[illegible]	17.91
1	12	7	3.17	-2.91
2	12	0	26.87	-24.64
2	12	1	15.79	13.62
2	12	2	15.93	15.49
2	12	3	17.52	-16.72
2	12	4	42.67	-43.65
2	12	5	6.45	5.03
2	12	6	3.95	.29
2	12	7	32.15	-30.87
3	12	1	53.27	53.02
3	12	2	9.92	9.52
3	12	3	53.83	55.54
3	12	4	3.77	-3.89
3	12	5	8.69	-7.31
3	12	6	2.73	-.27
3	12	7	7.28	7.10
4	12	0	20.52	20.47
4	12	1	48.92	47.81
4	12	2	5.98	-4.78
4	12	3	13.92	-12.14
4	12	4	20.18	-19.91
4	12	5	14.44	13.42
4	12	6	13.47	-13.87
4	12	7	7.05	5.34
5	12	1	2.39	1.12
5	12	2	4.29	3.22
5	12	3	27.78	-27.27
5	12	4	2.41	-.52
5	12	5	11.69	-13.01
5	12	6	18.97	-17.60
5	12	7	7.09	6.84
6	12	0	99.17	100.13
6	12	1	15.93	14.91
6	12	2	11.20	9.81
6	12	3	1.65	-.87
6	12	4	13.20	13.34
6	12	5	9.99	9.73
6	12	6	4.89	.51
7	12	1	12.09	11.89
7	12	2	10.89	-9.98
7	12	3	7.00	-6.14
7	12	4	19.55	20.22
7	12	5	15.98	-15.53
8	12	0	6.00	5.23
8	12	1	13.92	13.34

H	K	L	FO	FC
8	12	2	24.74	-22.95
8	12	3	6.61	5.52
8	12	4	7.40	6.62
8	12	5	13.32	-12.99
9	12	1	32.33	31.48
9	12	2	16.88	19.69
9	12	3	17.04	16.[illegible]1
9	12	4	4.81	-4.20
9	12	0	26.53	26.98
10	12	1	4.16	4.64
10	12	2	5.20	-3.01
0	13	1	29.01	-29.30
0	13	3	2.44	-7.14
0	13	5	21.13	-22.45
0	13	7	16.82	16.80
1	13	1	21.56	22.09
1	13	2	32.21	-31.74
1	13	3	2.26	1.48
1	13	4	7.70	6.85
1	13	5	12.84	13.34
2	13	3	22.23	20.97
2	13	4	9.77	-8.28
2	13	5	39.69	-39.20
3	13	1	21.76	-21.69
3	13	2	19.34	18.25
3	13	3	5.83	-4.84
3	13	4	29.72	-30.78
3	13	5	5.49	-5.22
4	13	3	22.42	21.63
4	13	4	36.00	35.7[illegible]
4	13	5	3.94	-.77
5	13	1	27.09	-27.35
5	13	2	19.59	-19.[illegible]6
5	13	3	14.84	-14.[illegible]5
5	13	4	6.88	-6.[illegible]5
5	13	5	6.37	5.78
5	13	6	6.55	-6.34
6	13	0	5.62	-1[illegible].16
6	13	1	3.33	-.58
6	13	2	57.42	[illegible].18
6	13	3	15.38	-15.61
6	13	4	23.85	-22.44
6	13	5	3.10	1.99
6	13	6	21.26	20.75
7	13	1	2.31	2.57
7	13	2	15.18	-14.89
7	13	3	10.49	-10.50
7	13	4	5.35	-5.13
7	13	5	6.13	-5.63
7	13	6	36.96	36.10
8	13	1	22.81	-22.61
8	13	2	3.50	-.80
8	13	3	8.82	-7.97
8	13	4	30.12	-30.47
8	13	5	19.62	-19.50
8	13	6	8.92	8.34
9	13	1	27.87	27.84
9	13	2	20.89	-20.43
9	13	3	5.68	5.43
9	13	4	2.81	-.70
9	13	5	3.11	-.74
10	13	1	19.56	18.93
10	13	2	6.11	5.53
10	13	3	13.79	-13.55
10	13	4	19.04	-18.63
10	13	5	12.34	10.57
10	13	6	8.62	-7.75
11	13	2	12.04	-12.01
11	13	3	44.44	-44.67
11	13	4	3.38	-2.54
11	13	5	10.87	-10.72
11	13	6	5.29	-2.62
11	13	4	5.25	4.60
12	13	1	19.17	-18.16
12	13	2	19.09	17.77
12	13	4	11.30	-11.06
12	13	5	31.30	31.60
12	13	6	2.86	1.62
0	14	1	18.13	-17.84
0	14	2	9.78	-9.76
0	14	3	14.73	14.91
0	14	4	8.04	6.80
0	14	5	44.94	45.20
1	14	1	10.05	19.28
1	14	2	21.89	21.50
1	14	3	22.33	-23.16
1	14	4	3.85	3.37
1	14	5	8.08	-6.85
2	14	1	2.[illegible]	-.65
2	14	2	4.11	3.92

H	K	L	FO	FC
3	14	6	3.11	2.55
4	14	0	6.11	-6.24
4	14	1	10.61	-9.27
4	14	2	5.94	4.09
4	14	3	13.07	-11.87
4	14	4	37.96	37.77
4	14	5	15.57	-15.58
5	14	1	4.73	4.19
5	14	2	13.32	12.84
5	14	3	19.05	18.22
5	14	4	4.92	-4.75
5	14	5	28.27	27.25
6	14	0	13.52	-11.[illegible]
6	14	1	3.64	-3.48
6	14	2	15.20	-15.99
6	14	3	8.25	-8.15
6	14	4	3.21	3.77
7	14	1	2.94	-2.60
7	14	2	20.76	-20.45
7	14	3	10.85	14.77
8	14	0	13.89	-13.39
8	14	1	15.8[illegible]	-14.93
8	14	2	9.55	9.55
0	15	1	2.76	-.55
0	15	3	19.05	19.13
0	15	5	4.[illegible]2	-3.85
1	15	1	11.12	-10.47
1	15	2	21.77	22.34
1	15	3	3.36	2.08
1	15	4	6.48	6.93
1	15	5	13.28	-12.76
2	15	0	13.10	-20.73
2	15	1	7.15	6.88
2	15	2	23.81	22.02
2	15	3	14.53	14.54
2	15	4	5.62	-4.28
2	15	5	7.53	-6.39
3	15	1	3.58	-2.33
3	15	2	26.33	25.29
3	15	3	2.91	1.15
3	15	4	1.81	-.18
3	15	5	10.17	10.20
4	15	0	11.93	-12.00
4	15	1	1.73	-.80
4	15	2	2.90	.71
4	15	3	19.74	19.09
4	15	4	22.04	-20.48
5	15	1	5.45	-6.08
5	15	2	13.32	13.72
5	15	3	4.11	4.02
5	15	4	6.15	5.60
6	15	0	10.91	-10.63
6	15	1	7.52	7.35
6	15	2	7.15	6.72
6	15	3	10.52	10.22
7	15	1	15.85	-15.93
7	15	2	22.06	22.28
0	16	0	51.28	50.27
0	16	2	42.08	-41.03
0	16	4	25.93	-27.05
1	16	1	9.42	9.29
1	16	2	16.45	-16.00
1	16	3	14.12	-14.55
1	16	4	4.82	-3.33
2	16	0	13.63	12.99
2	16	1	24.03	-24.22
2	16	2	16.62	-15.58
2	16	3	34.25	34.50