

Alunogen, $\text{Al}_2(\text{H}_2\text{O})_{12}(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$: Its atomic arrangement and water content

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Carbondale, Illinois 62901***Abstract**

Alunogen is triclinic, space group $P\bar{1}$ with $a = 7.420(6)\text{\AA}$; $b = 26.97(2)\text{\AA}$; $c = 6.062(5)\text{\AA}$; $\alpha = 89^\circ 57(5)'$; $\beta = 97^\circ 34(5)'$; $\gamma = 91^\circ 53(5)'$; and $Z = 2$. A computer-controlled Buerger-Supper two-circle goniometer (Weissenberg geometry) was utilized for collection of X-ray intensity data. The structure was partially solved by the symbolic addition method and completed by use of Fourier and difference Fourier syntheses. Full-matrix least-squares refinement, with 1675 reflections, led to a final R index of 0.077.

The structure is built of discrete SO_4 and $\text{Al}(\text{Ow})_6$ polyhedra interconnected by a network of hydrogen bonds. Four of the five independent polyhedra are spatially arranged in a manner which gives rise to pseudo-double sheets parallel to (010), thereby accounting for the (010) cleavage and twinning. The fifth polyhedron (an SO_4 group) is situated between pseudo-sheets and is completely surrounded by the five zeolitic water molecules. Mean Al-Ow and S-O distances are 1.887 and 1.467 Å, respectively.

Maximum H_2O content in the alunogen formula was found to be 17 molecules as opposed to the heretofore accepted value of 18. Partial dehydration is accompanied by partial occupancies of zeolitic water sites. That there exists no known aluminum sulfate hydrate other than alunogen is interpreted to be a result of the strong tendency for the Al^{3+} ion to form $\text{Al}(\text{H}_2\text{O})_6^{3+}$ in aqueous solutions.

Introduction

Recent interest in crystalline hydrates has, as one of its major objectives, the revelation of the general rules of solvation, *i.e.*, an attempt via crystal-structure analysis is being made toward unravelling the relationship between polyhedral clustering in crystalline hydrates and the polyhedra which existed in the solution from which the minerals grew. Despite a considerable amount of existing data, there is little real understanding of the behavior of polyhedra in solution or the multiplicity of their phase formation. In this paper, we report the crystal structure of alunogen, a sulfate hydrate with a very high water content. By virtue of its large number of water molecules, alunogen can be thought of as being closely related to solutions. Thus, its crystal structure is of great interest since it may provide a key to these questions. This study will also settle the question of the exact number of water molecules in the alunogen formula and should also yield considerable information concerning the hydration range in which the alunogen structure can exist. In this paper we extend the conclusions reached by us in connection with the structure of kornelite (Robinson and Fang, 1973).

Data collection and reduction

Small, transparent laths of alunogen from Königsberg, Schemnitz district, Hungary (now Nova Bana, Czechoslovakia) were kindly supplied by Professor F. Cesbron of the Laboratoire de Mineralogie et de Cristallographie de la Sorbonne, Paris, France. The crystals are stable while in the sample vial. However, if the crystals are exposed to the atmosphere during periods of low humidity, dehydration begins almost immediately, beginning as small cracks visible only under the optical microscope, progressing to tinges of white on the grain edges, and terminating with the entire grain becoming white, translucent, and crumbly. This occurs within a few hours during unusually cold winter days when indoor humidity is very low. However, crystals exposed to the atmosphere for periods of several weeks during the humid summer months showed no deterioration. In addition to the dehydration problem, alunogen is commonly twinned parallel to (010), so considerable time was spent in finding a suitable crystal.

The unit cell parameters, obtained from precession photographs, are $a = 7.420(6)\text{\AA}$; $b = 26.97(2)\text{\AA}$; $c = 6.062(5)\text{\AA}$; $\alpha = 89^\circ 57(5)'$; $\beta = 97^\circ 34(5)'$; $\gamma =$

TABLE 1. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ALUNOGEN

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
1	0	0	48.83	-49.54	4	-1	-4	35.02	33.85
3	0	0	41.19	42.55	5	-1	-3	18.26	17.34
4	0	0	42.30	37.93	3	-1	-3	22.11	-22.94
5	0	0	13.62	10.26	1	1	3	63.01	-60.51
6	0	1	22.62	20.07	2	1	3	34.35	-37.16
4	0	1	28.23	25.26	3	1	3	34.35	31.89
3	0	1	24.70	-22.47	4	1	3	16.98	-17.42
2	0	1	62.00	59.75	5	1	3	47.79	-44.80
1	0	1	22.15	19.12	6	1	2	22.97	20.78
0	0	1	37.55	-49.04	3	1	2	16.03	-15.16
2	0	-1	71.35	81.96	2	1	2	21.73	-18.04
3	0	-1	26.29	17.00	0	-1	-2	22.63	20.36
4	0	-1	30.43	24.84	3	-1	-2	58.35	-60.43
5	0	-1	38.57	-34.50	4	-1	-2	28.27	27.10
6	0	-1	37.32	32.39	5	-1	-2	18.25	-17.57
7	0	-1	34.80	34.10	5	-1	-1	41.65	44.27
6	0	-2	41.71	-40.79	4	-1	-1	17.66	-21.16
4	0	-2	73.28	78.85	3	-1	-1	56.08	-52.34
3	0	-2	58.90	60.71	2	-1	-1	39.01	39.53
2	0	-2	12.30	-3.19	1	-1	-1	33.84	27.89
1	0	-2	26.09	-28.29	1	1	1	35.00	-35.07
0	0	2	97.07	109.74	2	1	1	43.55	-43.20
1	0	2	12.98	-15.22	3	1	1	48.23	-42.23
2	0	2	42.65	37.55	4	1	1	21.88	-15.84
6	0	2	39.98	-34.53	4	1	0	28.15	-26.65
5	0	3	57.06	-52.20	3	1	0	46.37	43.58
4	0	3	24.90	30.81	2	1	0	43.54	41.95
3	0	3	16.89	13.11	1	1	0	53.15	-55.20
2	0	3	21.05	20.00	1	-1	0	52.01	52.78
2	0	-3	36.69	-35.58	2	-1	0	28.78	-20.97
4	0	-3	31.73	30.94	3	-1	0	27.36	-25.38
6	0	-3	33.44	31.80	4	-1	0	16.35	14.82
6	0	-4	39.71	-35.91	3	-1	1	34.24	29.19
4	0	-4	62.55	58.75	2	-1	1	58.60	59.80
3	0	-4	40.50	37.47	1	-1	1	19.73	18.97
2	0	-4	45.73	-44.94	0	-1	1	9.24	-7.70
0	0	4	60.98	76.54	1	1	-1	37.65	-33.59
2	0	4	54.47	-50.77	2	1	-1	35.99	-41.55
3	0	4	27.23	-21.58	3	1	-1	71.69	63.76
4	0	4	17.90	15.02	5	1	-1	56.30	-55.95
0	0	5	44.22	-40.47	7	1	-1	21.27	18.39
2	0	-5	30.77	26.22	5	1	-2	28.05	25.39
1	-1	-5	22.94	-20.62	4	1	-2	33.90	-35.00
1	1	5	29.45	-24.44	3	1	-2	69.45	68.58
4	1	4	17.93	-13.52	2	-1	2	12.73	5.89
3	1	4	31.61	-28.19	3	-1	2	20.72	23.10
2	1	4	37.60	38.92	5	-1	3	23.20	27.30
0	-1	-4	16.11	-17.20	3	-1	3	26.60	-26.55
2	-1	-4	22.41	-26.74	2	-1	3	15.63	18.79
2	-1	-4	29.02	-25.13	1	-1	3	44.87	43.22

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
2	1	-3	14.72	14.55	2	-2	0	59.94	-62.82
3	1	-3	34.01	39.68	4	-2	0	49.76	53.01
4	1	-3	20.04	-18.04	6	-2	0	23.47	-26.78
5	1	-3	27.63	-28.88	5	-2	1	17.41	-16.31
4	1	-4	43.28	-43.58	2	-2	1	77.53	79.80
3	1	-4	41.30	37.03	1	-2	1	50.64	-52.56
2	1	-4	14.77	17.01	1	2	-1	22.24	-22.06
1	1	-4	13.62	-10.58	2	2	-1	16.37	18.28
2	-1	4	30.61	-31.11	3	2	-1	61.57	60.26
3	-1	4	23.57	20.97	4	2	-1	60.10	-59.86
1	-1	5	17.53	13.63	6	2	-1	30.05	27.22
0	-1	5	23.70	-20.50	4	2	-2	36.75	37.31
1	1	-5	23.72	20.71	1	2	-2	76.80	80.04
1	-2	-5	25.59	24.02	0	-2	2	14.45	15.64
0	-2	-5	22.90	-21.09	1	-2	2	23.49	-20.00
1	2	5	25.21	-19.92	6	-2	2	34.61	-38.26
2	2	5	27.22	27.44	5	-2	3	27.96	-26.40
4	2	4	36.79	35.19	3	-2	3	19.60	23.48
3	2	4	50.36	-44.50	2	-2	3	21.69	23.03
2	2	4	42.66	-41.99	1	-2	3	31.15	-34.79
1	2	4	51.80	49.26	0	-2	3	26.37	27.71
3	-2	-4	19.79	-20.59	1	2	-3	26.12	27.64
4	-2	-4	52.58	47.41	2	2	-3	32.74	-32.69
6	-2	-4	23.32	-23.66	3	2	-3	15.98	18.92
6	-2	-3	40.74	43.75	6	2	-3	27.50	28.38
5	-2	-3	18.10	-19.14	4	2	-4	36.11	33.40
3	-2	-3	21.49	21.09	0	-2	4	25.13	27.74
2	-2	-3	37.48	-37.81	1	-2	4	50.15	50.13
1	-2	-3	12.67	11.45	2	-2	4	57.36	-55.50
0	-2	-3	35.44	33.10	3	-2	4	47.19	-44.02
1	2	3	15.87	-14.63	4	-2	4	40.09	40.13
4	2	3	17.69	-13.49	2	-2	5	33.28	31.67
6	2	2	18.53	-19.28	1	-2	5	30.67	-29.07
3	2	2	15.25	11.29	0	-2	5	23.21	-22.26
1	2	2	33.01	-24.82	1	2	-5	20.59	19.01
0	-2	-2	12.35	-12.39	3	2	-5	17.04	6.06
1	-2	-2	54.33	49.50	1	2	-6	23.04	-21.63
4	-2	-2	51.74	52.65	4	-3	-5	26.09	23.68
6	-2	-2	33.28	-34.42	3	-3	-5	48.84	-44.92
7	-2	-1	21.10	14.21	2	-3	-5	22.90	-23.42
6	-2	-1	31.71	31.48	1	-3	-5	16.76	15.62
5	-2	-1	34.82	-37.05	0	-3	-5	17.81	17.75
4	-2	-1	17.21	-18.03	1	3	5	58.19	-53.53
3	-2	-1	59.84	60.86	2	3	5	24.69	-18.45
1	-2	-1	29.70	-33.44	4	3	4	28.17	-22.53
1	2	1	60.92	-60.33	3	-3	-4	45.30	-48.03
2	2	1	29.45	18.10	4	-3	-4	21.10	16.83
4	2	0	25.68	21.87	6	-3	-4	23.70	-24.26
2	2	0	59.31	-61.58	6	-3	-3	18.03	14.68
1	2	0	40.24	49.14	5	-3	-3	32.88	35.53

TABLE 1--(CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
4	-3	-3	39.23	39.45	5	3	-2	27.65	30.78
3	-3	-3	39.37	-42.78	2	3	-2	11.15	-5.71
2	-3	-3	19.06	-24.12	1	3	-2	47.62	46.25
1	-3	-3	45.76	45.12	0	-3	2	16.62	-23.82
1	3	3	126.81	-129.39	1	-3	2	41.33	-40.53
2	3	3	19.52	24.29	4	-3	2	15.26	15.07
3	3	3	30.94	27.99	5	-3	2	29.54	33.58
5	3	3	43.96	-38.80	6	-3	2	34.87	-39.62
6	3	2	27.48	31.77	7	-3	3	35.11	31.47
3	3	2	17.79	-18.43	3	-3	3	21.83	-20.92
2	3	2	21.27	18.95	1	-3	3	114.44	119.34
1	3	2	60.40	62.76	1	3	-3	25.84	-21.64
0	-1	-2	49.62	-52.41	3	3	-3	46.03	43.24
1	-3	-2	57.16	-58.06	4	3	-3	21.62	-18.85
2	-3	-2	38.60	40.63	5	3	-3	36.82	-34.90
3	-3	-2	15.09	15.06	6	3	-3	19.96	-10.67
5	-3	-2	25.31	-25.37	6	3	-4	24.60	25.50
7	-3	-1	38.92	-36.84	4	3	-4	17.45	-12.12
6	3	-1	21.54	21.50	3	3	-4	44.64	46.92
5	-3	-1	42.63	44.34	4	-3	4	19.91	20.69
4	-3	-1	61.32	65.92	1	-3	5	46.73	47.09
3	-3	-1	74.71	-74.92	3	3	-5	45.32	43.88
2	-3	-1	46.76	-46.58	0	-4	-3	21.62	-18.97
1	3	1	144.22	-152.80	2	-4	-5	36.75	36.84
2	3	1	13.47	-12.19	3	-4	-5	30.75	-28.11
3	3	1	32.21	-31.62	4	-4	-4	37.92	-38.73
5	3	1	19.79	-22.35	0	-4	-4	21.39	-19.62
6	3	1	29.74	-29.14	2	4	4	35.44	32.00
6	3	0	17.81	16.85	3	4	4	19.29	-16.61
4	3	0	22.49	-19.11	5	4	3	17.59	12.93
2	3	0	18.67	-22.45	4	4	3	30.93	-30.14
1	-3	0	20.83	-33.81	2	4	3	17.11	14.11
2	-3	0	13.45	-12.70	1	4	3	12.52	7.78
3	-3	0	41.15	-40.09	0	-4	-3	43.61	-43.52
4	-3	0	23.97	24.37	1	-4	-3	50.98	48.06
6	-3	0	24.77	-27.87	3	-4	-3	28.03	-24.93
7	-3	0	18.95	20.15	4	-4	-2	15.23	-15.21
7	-3	1	23.06	-22.45	3	-4	-2	29.00	30.68
6	-3	1	25.39	27.57	2	-4	-2	48.60	-48.29
3	-3	1	37.85	39.16	1	-4	-2	43.85	44.35
2	-3	1	31.45	-38.87	0	-4	-2	28.36	-23.16
1	-3	1	143.02	157.31	1	4	2	53.76	-57.69
2	3	-1	56.83	56.48	2	4	2	33.74	33.87
3	3	-1	63.23	64.64	3	4	2	20.44	17.86
4	3	-1	78.63	-78.04	4	4	2	29.95	-30.78
5	3	-1	56.43	-56.37	5	4	2	40.57	37.53
6	3	-1	22.65	-18.14	5	4	1	30.79	28.38
7	3	-1	41.09	41.16	4	4	1	33.53	-33.15
7	3	-2	37.71	-34.55	3	4	1	12.12	11.87
					2	4	1	12.78	-6.81

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
1	4	1	45.69	45.36	3	-5	-5	24.34	-24.72
0	-4	-1	75.24	-75.18	0	-5	-5	31.74	29.05
1	-4	-1	38.20	38.75	1	5	5	25.76	-24.07
2	-4	-1	78.16	100.67	2	5	5	43.43	-37.25
3	-4	-1	20.54	14.67	3	5	5	23.08	24.09
4	-4	-1	79.50	-85.72	3	5	4	23.02	-20.94
5	-4	-1	24.10	21.87	1	5	4	28.93	27.05
5	-4	0	32.15	24.51	0	-5	-4	13.97	-17.21
4	-4	0	44.76	-51.21	5	-5	-4	23.25	-18.44
3	-4	0	31.08	37.14	5	-5	-3	42.23	37.95
2	-4	0	13.99	-16.43	4	-5	-3	32.01	-31.77
1	-4	0	21.44	-28.43	3	-5	-3	23.94	-21.67
1	4	0	12.47	-12.67	2	-5	-3	53.35	55.93
4	4	0	38.91	-36.93	0	-5	-3	73.77	-70.96
5	4	0	30.71	35.62	2	5	3	44.00	-45.96
7	4	-1	18.29	-17.05	3	5	3	28.91	29.71
5	4	-1	16.44	15.27	4	5	3	29.72	28.65
4	4	-1	76.21	-74.35	5	5	3	29.73	-27.34
2	4	-1	96.22	96.65	5	5	2	25.04	23.00
1	4	-1	23.52	20.29	4	5	2	18.20	-14.23
0	-4	1	88.27	-89.	3	5	2	20.15	-17.82
1	-4	1	29.33	34.19	2	5	2	22.58	19.21
2	-4	1	62.15	-66.29	0	-5	-2	37.35	-22.90
3	-4	1	38.83	39.55	1	-5	-2	18.30	-15.08
5	-4	2	17.26	22.81	2	-5	-2	10.77	-14.31
4	-4	2	28.59	-29.01	3	-5	-2	31.76	33.65
3	-4	2	24.95	24.13	4	-5	-2	32.37	33.45
2	-4	2	42.81	38.98	5	-5	-2	55.34	-65.75
1	-4	2	51.51	-49.72	6	-5	-2	21.51	-20.64
0	-4	2	60.57	-61.49	7	-5	-2	44.30	44.64
1	4	-2	16.12	8.95	7	-5	-1	19.91	-24.42
2	4	-2	58.50	-57.60	5	-5	-1	56.28	70.54
3	4	-2	19.50	19.55	4	-5	-1	32.25	30.51
4	4	-2	20.35	-20.87	3	-5	-1	17.00	-15.27
3	4	-3	31.58	-33.38	2	-5	-1	65.23	-40.60
2	4	-3	17.15	13.37	1	-5	-1	36.64	42.94
1	4	-3	18.35	14.55	0	-5	-1	23.41	25.64
0	-4	3	23.58	-24.50	1	5	1	34.37	-35.30
1	-4	3	30.62	32.28	3	5	1	13.35	11.49
3	-4	3	19.41	-19.65	5	5	1	15.71	-14.65
4	-4	3	23.37	-18.62	6	5	0	18.31	-22.41
3	-4	4	30.41	-26.77	5	5	0	19.14	16.57
2	-4	4	14.02	12.34	3	5	0	44.43	-43.37
0	-4	4	24.99	-27.59	2	5	0	72.76	74.78
2	4	-4	14.54	19.71	1	5	0	50.76	52.91
3	4	-4	25.22	-31.24	1	-5	0	42.36	-51.01
4	4	-4	53.25	-53.02	2	-5	0	39.86	-39.69
3	4	-5	23.94	-25.47	3	-5	0	54.07	57.18
2	4	-5	35.36	34.24	4	-5	0	32.37	31.26
			20.22	-21.22	7	-5	1	21.27	-17.72

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
5	-5	1	37.62	45.36	4	-6	-2	17.38	-12.43
2	-5	1	59.26	53.92	3	-6	-2	44.65	-46.13
1	-5	1	57.90	59.27	2	-6	-2	37.86	-32.79
1	5	-1	52.45	-52.19	1	-6	-2	25.04	-24.04
2	5	-1	53.65	43.80	0	-6	-2	156.42	-151.53
3	5	-1	24.58	27.61	1	6	2	14.66	17.73
5	5	-1	24.51	-22.09	2	6	2	69.42	61.96
7	5	-2	39.68	-41.04	3	6	2	18.04	-19.87
5	5	-2	74.15	75.14	4	6	2	28.39	-26.56
4	5	-2	30.80	-32.91	6	6	2	21.66	22.22
3	5	-2	54.17	-53.51	6	6	1	18.67	-19.07
1	5	-2	24.82	26.27	5	6	1	22.16	20.42
0	-5	2	104.16	108.90	3	6	1	29.36	-29.26
1	-5	2	34.05	-29.66	2	6	1	62.08	-58.67
2	-5	2	29.63	-32.27	1	6	1	23.64	-22.12
3	-5	2	38.73	42.76	0	-6	-1	49.59	54.82
5	-5	3	48.93	51.16	1	-6	-1	35.55	-33.79
4	-5	3	19.79	-18.30	3	-6	-1	12.93	-12.03
3	-5	3	42.73	-43.54	4	-6	-1	64.66	-64.67
2	-5	3	30.04	32.89	5	-6	-1	28.30	35.79
1	-5	3	30.00	28.96	7	-6	-1	44.93	-48.68
0	-5	3	76.68	79.78	6	-6	0	31.69	29.99
1	5	-3	21.93	-23.15	4	-6	0	26.82	-24.31
2	5	-3	38.26	-32.79	3	-6	0	46.57	-49.23
3	5	-3	22.14	26.45	2	-6	0	13.60	1.38
4	5	-3	24.66	23.41	1	6	0	17.01	17.31
5	5	-3	35.09	-37.05	2	6	0	37.12	-29.81
0	-5	4	20.78	18.64	3	6	0	24.55	-20.90
1	-5	4	22.50	-21.45	4	6	0	45.53	-46.45
3	-5	4	28.14	30.31	5	6	0	18.54	-21.50
3	-5	5	28.79	-31.23	6	6	0	61.23	58.66
2	-5	5	48.56	50.78	7	6	-1	32.31	-33.56
1	-5	5	26.65	33.22	5	6	-1	29.93	35.37
0	-5	5	32.58	-33.99	4	6	-1	43.51	-45.00
1	5	-5	17.21	-16.35	3	6	-1	21.90	-16.74
2	5	-5	22.84	22.57	2	6	-1	17.85	-20.22
3	5	-5	25.78	20.91	1	6	-1	21.92	-17.49
4	-6	-4	35.06	-37.68	0	-6	1	77.44	85.19
3	-6	-4	50.65	-50.91	1	-6	1	10.18	-15.53
2	-6	-4	41.77	42.29	3	-6	1	29.44	-28.86
1	-6	-4	21.50	22.68	4	-6	1	40.19	-42.86
0	-6	-4	85.69	-85.17	5	-6	1	36.68	38.30
2	6	4	46.53	42.33	6	-6	1	17.57	-12.52
3	6	4	25.45	25.91	6	-6	2	24.77	21.54
4	6	3	29.61	-29.08	5	-6	2	30.06	25.82
1	6	3	22.45	23.65	4	-6	2	17.30	-17.37
1	-6	-3	58.83	-57.14	3	-6	2	15.54	-14.31
3	-6	-3	15.04	17.50	2	-6	2	49.69	44.67
4	-6	-3	13.88	-11.10	1	-6	2	21.27	22.25
5	-6	-3	23.78	-18.45	0	-6	2	102.39	-102.32

TABLE 7--(CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
1	6	-2	11.01	-6.58	2	7	0	12.21	-14.36
3	6	-2	43.64	-41.37	1	7	0	77.54	79.82
4	6	-2	17.50	-12.23	1	-7	0	102.08	-105.97
6	6	-3	26.38	-21.15	3	-7	0	60.96	61.54
3	6	-3	27.36	29.81	4	-7	0	31.95	-33.42
1	6	-3	34.05	-33.23	6	-7	0	17.71	10.17
2	-6	3	32.82	36.13	6	-7	1	19.40	22.59
4	-6	3	42.94	-45.53	5	-7	1	31.55	-35.16
5	-6	3	20.66	20.47	4	-7	1	22.46	-22.15
2	-6	4	49.38	48.24	3	-7	1	39.91	40.44
0	-6	4	60.90	-60.36	2	-7	1	9.35	-12.50
2	6	-4	25.21	25.23	1	-7	1	45.89	-47.53
3	6	-4	27.26	-21.86	0	-7	1	23.09	-25.92
4	6	-4	32.13	-38.09	1	7	-1	59.28	-60.09
1	-7	-5	19.26	14.88	2	7	-1	21.07	21.75
1	7	5	34.15	32.40	3	7	-1	38.04	34.91
1	7	4	63.95	63.52	4	7	-1	27.18	25.81
1	-7	-4	60.02	-58.64	6	7	-1	24.44	-25.50
3	-7	-4	46.79	44.88	4	7	-2	22.16	23.34
4	-7	-4	28.18	-24.75	3	7	-2	48.72	-47.09
0	-7	-3	17.57	-22.09	1	7	-2	31.51	-23.47
1	7	3	78.93	77.82	1	-7	2	9.42	-8.11
4	7	3	43.03	40.35	2	-7	2	17.83	16.61
5	7	2	36.92	33.53	3	-7	2	20.65	20.01
4	7	2	20.90	17.54	5	-7	2	35.66	-31.13
3	7	2	38.95	-41.24	4	-7	3	29.55	-29.90
2	7	2	20.73	-19.55	2	-7	3	15.22	17.59
1	7	2	24.29	21.69	1	-7	3	71.85	-72.00
0	-7	-2	43.93	-43.36	0	-7	3	32.43	34.26
1	-7	-2	31.44	25.63	1	7	-3	23.26	21.49
2	-7	-2	12.72	-9.98	2	7	-3	26.82	-27.77
3	-7	-2	55.76	54.67	5	7	-3	18.60	13.99
5	-7	-2	28.56	-30.99	3	7	-4	32.32	-29.74
7	-7	-2	36.55	38.45	1	7	-4	55.01	57.23
6	-7	-1	27.48	35.19	1	-7	4	55.04	-56.16
5	-7	-1	17.89	-25.30	2	-7	4	29.25	31.02
4	-7	-1	18.02	-17.91	2	-7	5	18.13	20.12
3	-7	-1	63.19	-63.26	2	8	5	18.42	-21.75
2	-7	-1	28.38	-27.04	0	-8	-5	29.16	27.49
1	-7	-1	80.35	82.47	2	-8	-5	25.63	-26.83
0	-7	-1	8.42	-10.82	3	-8	-5	22.11	-19.49
1	7	1	45.05	40.71	4	-8	-5	33.89	32.49
2	7	1	15.82	-14.43	4	-8	-4	48.32	-43.60
3	7	1	45.63	-40.67	3	-8	-4	15.83	13.92
4	7	1	32.08	31.85	1	-8	-4	13.35	5.73
5	7	1	40.18	37.26	1	8	4	40.23	-40.37
6	7	0	26.75	-19.45	2	8	4	31.98	30.30
5	7	0	22.38	24.34	3	8	4	24.81	20.75
4	7	0	23.21	24.31	4	8	3	54.49	48.62
3	7	0	94.22	-95.05	3	8	3	18.15	-15.02

TABLE 1--(CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
2	8	3	46.56	-42.68	6	-8	2	27.53	27.96
1	-8	3	25.71	23.08	4	-8	2	16.92	-16.82
0	-8	-3	35.36	33.77	3	-8	2	14.71	-17.67
1	-8	-3	26.18	-26.04	2	-8	2	42.40	45.17
2	-8	-3	11.84	-12.84	1	-8	2	30.49	-31.74
4	-8	-3	26.16	22.12	0	-8	2	33.36	-38.62
5	-8	-3	22.68	-21.22	1	8	-2	33.06	-33.44
6	-8	-3	19.09	-22.50	2	8	-2	17.56	20.23
6	-8	-2	22.27	20.91	3	8	-2	26.98	-29.42
4	-8	-2	22.70	-27.29	4	8	-2	25.84	-28.40
3	-8	-2	23.68	-22.64	6	8	-3	25.92	-29.72
2	-8	-2	18.44	21.01	5	8	-3	28.85	-27.46
1	-8	-2	25.25	-22.58	4	8	-3	34.03	31.75
0	-8	-2	20.49	21.37	2	8	-3	37.19	-41.16
1	8	2	20.79	-21.84	1	8	-3	46.98	-47.03
6	8	1	24.96	-20.96	0	-8	3	52.34	52.41
5	8	1	20.14	-18.08	1	-8	3	30.41	29.47
4	8	1	51.81	53.46	2	-8	3	52.13	-53.65
3	8	1	12.82	-10.07	3	-8	3	20.11	-20.70
2	8	1	16.19	-20.18	4	-8	3	31.25	28.82
1	8	1	31.90	-26.64	4	-8	4	17.68	-17.09
0	-8	-1	40.68	44.84	3	-8	4	36.58	37.12
1	-8	-1	29.70	27.28	2	-8	4	33.24	31.35
2	-8	-1	59.26	-62.30	1	-8	4	40.60	-40.67
3	-8	-1	59.52	-56.22	0	-8	4	16.77	-16.22
4	-8	-1	58.64	57.74	2	8	-4	16.65	18.53
6	-8	-1	31.46	-30.90	4	8	-4	46.10	-42.26
6	-8	0	45.40	48.70	4	8	-5	36.57	35.61
5	-8	0	27.38	-24.42	2	8	-5	26.77	-23.25
4	-8	0	45.26	-46.53	0	-8	5	18.15	14.53
3	-8	0	24.23	24.76	1	-8	5	19.30	20.96
2	-8	0	47.01	45.84	2	-8	5	20.12	-19.24
1	-8	0	75.43	-70.30	1	-9	5	22.50	20.58
1	8	0	115.15	-114.06	0	-9	-5	17.52	14.95
2	8	0	81.83	80.29	2	-9	-5	31.29	29.64
3	8	0	21.95	21.11	3	-9	-5	20.06	19.74
4	8	0	21.82	-23.65	4	-9	-5	24.32	-23.55
5	8	0	41.48	-38.26	4	-9	-4	13.45	15.64
6	8	0	19.72	17.58	2	9	4	16.96	19.58
7	8	0	21.18	15.31	1	9	3	23.29	28.10
6	8	-1	30.94	-29.80	1	-9	-3	53.45	-53.20
4	8	-1	80.20	78.54	2	-9	-3	29.42	32.25
3	8	-1	83.19	-84.97	6	-9	-2	31.42	33.60
2	8	-1	51.86	-51.63	5	-9	-2	16.19	-19.58
1	8	-1	38.09	35.42	3	-9	-2	25.92	25.07
1	-8	1	19.47	-8.93	1	-9	-2	12.44	15.06
2	-8	1	40.32	-53.62	0	-9	-2	43.16	40.95
3	-8	1	24.76	-25.41	1	9	2	35.62	-34.06
4	-8	1	38.30	46.19	2	9	2	12.83	-14.05
6	-8	1	21.90	-21.67	4	9	2	46.01	44.32

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
6	9	2	21.44	-23.42	0	-9	5	18.07	-18.96
5	9	1	45.09	39.07	1	-9	5	29.57	-28.90
4	9	1	23.59	17.92	2	10	5	19.29	-18.43
3	9	-1	20.29	-24.37	0	-10	-5	49.54	47.89
2	9	1	53.16	50.53	1	-10	-5	17.50	-12.58
1	9	1	69.75	71.83	2	-10	-5	67.48	-62.21
0	-9	-1	14.05	-11.20	3	-10	-5	24.60	20.38
2	-9	-1	15.68	15.79	4	-10	-5	25.20	23.64
3	-9	-1	23.90	-25.69	3	-10	-4	15.48	-8.98
4	-9	-1	33.66	-34.89	2	-10	-4	25.21	22.36
6	-9	0	32.54	37.45	0	-10	-4	14.01	12.93
5	-9	0	45.98	-51.85	2	10	4	30.16	-30.55
3	-9	0	78.54	82.07	3	10	4	23.34	23.41
2	-9	0	35.67	-35.68	4	10	3	33.59	31.94
1	-9	0	21.39	19.52	2	10	3	35.20	-33.19
1	9	0	10.97	-5.53	1	10	3	23.73	-25.80
2	9	0	41.51	40.23	0	-10	-3	55.57	65.72
3	9	0	42.22	-39.63	1	-10	-3	24.95	-21.55
5	9	0	26.93	24.79	2	-10	-3	54.39	-55.15
5	9	-1	15.91	11.70	3	-10	-3	13.75	16.94
4	9	-1	18.20	17.04	4	-10	-3	17.36	20.41
3	9	-1	55.71	62.16	5	-10	-3	15.70	-14.94
2	9	-1	30.01	-29.81	5	-10	-2	14.10	-14.36
1	9	-1	27.86	-23.00	3	-10	-2	16.11	-13.40
0	-9	1	46.87	47.54	2	-10	-2	36.62	45.79
1	-9	1	58.58	-58.42	0	-10	-2	31.46	28.85
2	-9	1	25.49	-25.96	2	10	2	37.75	-37.07
4	-9	1	25.24	-23.82	3	10	2	25.29	24.66
5	-9	1	27.41	-22.40	5	10	2	33.91	-36.20
6	-9	2	19.06	19.24	6	10	1	16.40	-19.15
5	-9	2	16.10	-21.70	4	10	1	74.76	71.15
4	-9	2	39.67	-43.25	2	10	1	53.76	-47.95
3	-9	2	23.73	26.36	1	10	1	21.95	-19.91
2	-9	2	15.63	16.57	0	-10	-1	36.72	38.96
1	-9	2	17.69	19.32	2	-10	-1	23.10	-25.98
0	-9	2	32.65	-31.56	3	-10	-1	16.96	-17.44
1	9	-2	17.33	-22.28	4	-10	-1	55.30	53.96
3	9	-2	27.56	-27.55	5	-10	-1	13.35	-12.09
5	9	-2	22.64	26.97	6	-10	-1	21.81	-19.16
6	9	-2	30.87	-33.39	7	-10	0	27.59	32.13
5	9	-3	23.25	21.32	5	-10	0	46.68	-51.09
3	9	-3	19.25	-22.80	3	-10	0	28.74	29.28
1	9	-3	31.25	31.46	2	-10	0	48.11	51.34
0	-9	3	21.21	-22.71	1	-10	0	20.88	-25.59
1	-9	3	89.09	-92.71	1	10	0	43.05	44.77
4	-9	3	32.59	-30.44	2	10	0	17.93	18.06
3	-9	4	27.73	29.68	3	10	0	23.87	23.81
2	-9	4	27.74	-29.73	5	10	0	30.36	-32.84
1	-9	4	16.91	-17.52	5	10	0	16.58	-14.63
0	-9	4	32.57	-31.52	3	10	-1	20.10	-17.37

TABLE I -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
4	10	-1	45.39	43.80	2	11	1	70.60	72.69
3	10	-1	20.17	21.40	1	11	1	17.07	14.87
2	10	-1	22.29	-24.86	0	11	-1	64.78	-65.84
1	10	-1	25.57	-24.74	2	11	-1	9.00	9.52
1	-10	1	41.70	-43.15	3	11	-1	30.81	-34.15
2	-10	1	29.62	-29.60	4	11	-1	17.07	15.18
3	-10	1	13.48	12.62	5	11	-1	40.48	-39.73
4	-10	1	64.47	60.28	6	11	-1	15.11	-9.30
6	-10	1	20.84	-21.63	7	11	0	25.64	-26.99
5	-10	2	23.36	-26.14	6	11	0	15.90	-18.46
4	-10	2	20.70	22.12	5	11	0	29.87	31.19
3	-10	2	23.33	-23.80	4	11	0	19.65	19.99
2	-10	2	44.50	-47.15	3	11	0	35.31	-37.33
0	-10	2	51.93	53.46	2	11	0	35.66	-33.32
2	10	-2	35.06	42.23	1	11	0	23.82	-26.58
3	10	-3	15.65	15.38	2	11	0	13.31	12.81
2	10	-3	39.93	-38.53	3	11	0	54.49	51.75
1	10	-3	11.34	-12.03	4	11	0	22.05	-25.34
0	-10	3	49.97	53.72	5	11	0	44.43	-41.44
2	-10	3	37.29	-38.40	4	11	-1	30.72	31.58
4	-10	3	45.62	44.02	4	11	-1	18.43	-17.89
3	-10	4	20.53	19.94	3	11	-1	10.67	-12.63
2	10	-4	21.39	16.31	1	11	-1	8.68	8.86
3	10	-5	22.29	20.69	0	11	1	14.15	10.77
2	10	-5	62.74	-62.93	1	11	1	29.51	-30.50
0	-10	5	61.88	59.40	2	11	1	60.31	-64.32
2	-10	5	21.88	-20.52	3	11	1	40.76	42.85
2	-11	-5	23.06	22.47	4	11	1	14.46	10.37
5	-11	-4	27.05	25.25	5	11	1	34.97	-35.79
3	-11	-4	43.75	-42.54	5	11	2	40.86	40.67
2	-11	-4	25.76	26.37	4	11	2	40.93	-40.53
1	-11	-4	26.51	25.31	3	11	2	68.96	-72.02
1	11	4	29.00	-28.50	2	11	2	31.55	35.88
3	11	4	27.84	27.77	1	11	2	63.10	65.59
3	11	3	21.79	-21.45	0	11	2	14.00	-13.64
2	11	3	22.93	22.35	1	11	-2	42.53	-43.79
1	-11	-3	22.39	-24.03	2	11	-2	38.30	-41.07
3	-11	-3	19.82	23.54	3	11	-2	58.17	60.29
4	-11	-3	24.80	21.68	4	11	-2	31.00	-31.31
5	-11	-3	53.28	-52.14	5	11	-2	15.85	17.01
3	-11	-2	43.68	-46.75	5	11	-3	33.52	33.74
1	-11	-2	44.09	48.93	4	11	-3	27.10	-24.08
1	11	2	64.47	-62.64	3	11	-3	26.35	-23.46
2	11	2	39.72	-39.85	2	11	-3	18.15	-20.10
3	11	2	73.59	75.17	1	11	-3	36.48	38.20
4	11	2	31.53	31.05	1	-11	3	17.64	-14.49
5	11	2	52.08	-52.95	2	-11	3	36.81	-36.78
6	11	1	20.33	16.02	3	-11	4	15.57	-17.62
4	11	1	44.52	-42.58	1	-11	4	19.22	20.28
					1	11	-4	33.00	-33.87

TABLE 1--(CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
2	11	-4	22.77	-20.23	4	12	-2	17.87	-20.38
3	11	-4	57.91	56.97	5	12	-2	17.84	18.42
4	11	-4	16.62	-21.27	4	12	-3	26.45	26.74
5	11	-4	29.65	-29.03	3	12	-3	16.00	-10.96
1	11	-5	15.79	-12.61	1	12	-3	13.99	13.94
3	-12	-5	17.00	16.30	0	-12	3	17.29	-13.12
3	-12	-4	43.45	43.94	4	-12	3	18.11	19.85
3	12	3	17.40	18.78	3	-12	4	14.96	17.81
1	12	3	17.43	19.37	2	-12	4	15.55	-15.91
0	-12	-3	23.97	-24.40	0	-12	4	12.82	15.05
1	-12	-3	25.27	25.86	1	12	-4	17.84	-17.96
4	-12	-3	32.46	30.52	3	12	-4	38.67	34.88
3	-12	-2	32.07	31.67	1	13	5	25.31	-22.99
2	-12	-2	16.33	12.37	1	-13	-5	20.72	-16.44
0	-12	-2	55.60	59.63	5	-13	-4	16.32	17.51
1	12	2	25.91	29.26	4	-13	-4	24.11	24.37
2	12	2	17.93	-15.91	3	-13	-4	52.04	-52.39
3	12	2	19.88	22.66	2	-13	-4	16.17	-15.41
4	12	2	19.36	-25.03	1	-13	-4	47.96	49.08
4	12	1	17.07	15.29	1	13	4	16.83	-18.16
2	12	1	29.73	-30.41	3	13	4	18.74	17.60
1	12	1	109.87	109.46	4	13	3	30.02	-31.63
0	-12	-1	15.02	-14.31	3	13	3	17.38	-9.99
1	-12	-1	27.48	-29.16	1	-13	-3	26.53	-38.09
2	-12	-1	52.92	-52.90	3	-13	-3	20.09	18.63
3	-12	-1	16.92	17.71	4	-13	-3	12.96	12.83
4	-12	-1	47.63	51.76	5	-13	-3	18.33	16.48
6	-12	0	20.84	-20.24	6	-13	-3	21.21	-21.66
3	-12	0	12.38	8.62	5	-13	-2	23.02	23.64
1	-12	0	61.01	61.61	4	-13	-2	24.89	23.48
1	12	0	17.73	14.32	3	-13	-2	68.71	-74.39
2	12	0	25.30	25.41	2	-13	-2	15.20	-15.71
5	12	0	17.92	19.88	1	-13	-2	94.86	99.54
6	12	0	19.39	-19.12	0	-13	-2	13.20	9.92
4	12	-1	45.81	44.93	1	13	2	71.67	-70.69
2	12	-1	58.25	-57.91	2	13	2	16.59	15.67
0	-12	1	22.44	-26.26	3	13	2	48.93	46.00
1	-12	1	100.36	104.30	5	13	2	26.54	-22.91
2	-12	1	49.21	-48.32	6	13	1	25.21	30.42
3	-12	1	25.28	-22.66	4	13	1	34.38	-32.65
4	-12	1	40.27	39.15	3	13	1	17.56	-15.27
5	-12	1	20.04	-21.93	1	13	1	39.51	-37.60
5	-12	2	19.78	-20.99	0	-13	-1	13.87	13.50
4	-12	2	26.81	-29.18	1	-13	-1	33.65	33.36
3	-12	2	18.26	17.74	2	-13	-1	10.93	-12.02
2	-12	2	19.77	-22.19	3	-13	-1	22.32	23.44
0	-12	2	41.76	43.74	5	-13	0	22.45	19.79
1	12	-2	10.51	11.98	3	-13	0	43.05	-46.62
2	12	-2	18.71	15.75	2	-13	0	9.10	9.31
					1	-13	0	22.65	31.43

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
3	13	0	30.37	31.80	3	14	2	19.71	-16.20
4	13	0	21.16	22.79	4	14	2	14.38	15.96
5	13	0	32.44	-29.17	5	14	2	12.63	8.82
5	13	-1	17.13	-17.38	6	14	1	37.89	35.58
1	13	-1	27.30	-23.25	4	14	1	75.29	-72.84
0-13	1	1	26.72	24.42	3	14	1	26.92	22.00
1-13	1	1	21.35	20.94	2	14	1	69.35	68.89
2-13	1	1	27.77	-27.95	1	14	1	16.58	18.31
3-13	1	1	10.10	7.31	0-14	-1	24.07	-25.84	
4-13	1	1	37.15	36.65	2-14	-1	26.01	25.70	
6-13	1	1	29.57	-33.26	0-14	-5	22.21	-21.30	
5-13	2	1	32.93	35.39	5-14	-1	25.55	25.38	
3-13	2	1	50.09	-54.29	6-14	0	25.76	-29.19	
2-13	2	1	15.15	-14.28	5-14	0	30.32	26.36	
1-13	2	1	69.27	67.65	4-14	0	23.59	27.06	
0-13	2	1	18.65	-21.65	3-14	0	17.42	-18.08	
1	13	-2	93.25	-99.58	2-14	0	11.35	7.03	
2	13	-2	31.28	34.39	1-14	0	51.17	48.38	
3	13	-2	64.86	69.51	1	14	0	71.41	70.75
4	13	-2	13.59	-16.11	3	14	0	15.07	-13.86
5	13	-2	19.41	-18.11	4	14	0	26.82	32.85
5	13	-3	23.40	-25.55	5	14	0	22.25	17.98
3	13	-3	17.96	-21.73	6	14	0	13.62	-12.38
1	13	-3	24.17	25.03	5	14	-1	23.51	23.69
3-13	4	1	27.13	-28.57	4	14	-1	28.14	-29.84
1-13	4	1	33.95	34.68	3	14	-1	19.67	21.07
0-13	4	1	14.85	-12.07	2	14	-1	59.41	59.47
1	13	-4	49.42	-49.44	1	14	-1	24.22	-24.40
2	13	-4	23.68	19.67	0-14	1	23.76	-22.91	
3	13	-4	33.26	33.40	1-14	1	25.93	31.75	
2-14	-5	1	18.65	18.75	2-14	1	45.43	44.37	
5-14	-4	1	17.42	13.11	3-14	1	22.58	20.98	
4-14	-4	1	15.61	14.30	4-14	1	56.60	-55.11	
1-14	-4	1	24.92	-23.13	6-14	1	29.44	27.99	
1	14	4	15.93	18.54	2-14	2	21.65	-19.71	
4	14	3	24.68	-27.46	1-14	2	46.81	51.72	
3	14	3	24.11	22.31	0-14	2	13.03	-15.73	
2	14	3	13.74	13.65	1	14	-2	23.74	22.38
1	14	3	29.71	-29.70	2	14	-2	20.69	22.75
0-14	-3	1	13.41	-16.11	3	14	-2	27.73	-27.99
1-14	+3	1	12.18	14.08	4	14	-2	15.03	10.05
2-14	-3	1	48.45	47.30	5	14	-2	19.62	20.02
4-14	-3	1	44.53	-39.76	5	14	-3	31.08	28.73
5-14	-3	1	28.84	29.67	4	14	-3	54.87	-51.61
6-14	-3	1	12.59	12.24	2	14	-3	53.96	52.22
5-14	-2	1	13.15	13.68	0-14	3	11.13	-13.89	
2-14	-2	1	19.18	21.71	1-14	3	16.08	-14.91	
1-14	-2	1	21.34	21.36	3-14	3	24.07	22.78	
1	14	2	49.06	49.75	4-14	3	17.98	-21.15	
					5-14	4	12.40	-12.11	

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
3-14	4		13.52	-14.18	3-15	2		35.41	-33.92
1-14	4		13.49	12.98	2-15	2		40.94	36.95
0-14	4		12.86	-7.14	2 15	-2		15.28	16.98
4 14	-4		20.45	19.71	3 15	-2		17.63	19.39
2 14	-5		22.80	24.14	4 15	-2		15.20	17.73
1 14	-5		12.23	-12.78	5 15	-2		16.02	-18.39
0-14	5		12.33	-13.31	3 15	-3		21.50	-22.56
2-14	5		17.03	18.13	2 15	-3		19.44	19.90
0-15	-5		23.19	-19.95	1 15	-3		17.46	19.89
1-15	-5		12.79	-9.45	0-15	3		26.70	29.17
2-15	-5		15.90	-19.77	3-15	3		28.18	27.85
5 15	-4		23.91	23.08	4-15	3		20.04	21.07
4 15	-4		11.38	-9.27	5-15	3		13.63	-13.73
2-15	-4		20.19	-16.21	2-15	4		12.20	-16.21
1-15	-4		11.78	11.62	2-15	4		14.61	17.55
2 15	4		18.32	-16.73	1-15	4		13.02	-7.96
4 15	3		14.91	-10.12	1 15	-4		13.16	-14.14
3 15	3		31.83	-34.37	2 15	-4		17.49	18.64
0-15	-3		43.74	-39.47	3 15	-4		13.07	13.42
6-15	-2		15.15	-14.47	3 15	-5		13.73	-15.21
5-15	-2		24.95	27.99	2 15	-5		26.66	27.77
3-15	-2		33.01	-33.99	0-15	5		20.52	20.22
2-15	-2		24.88	-26.35	1-15	5		11.87	8.79
0-15	-2		15.05	18.40	3-15	-5		14.32	-12.46
2 15	2		39.76	-33.77	2-15	-5		41.85	40.20
3 15	2		21.15	20.02	0-15	-5		30.67	-27.65
4 15	2		15.26	-13.72	2 15	4		18.13	12.43
5 15	2		13.20	-15.00	0-15	-4		26.46	26.07
4 15	1		21.64	-18.70	2-15	-4		54.51	-50.60
3 15	1		30.90	-32.13	4-15	-4		13.62	13.70
0-15	-1		7.78	-5.32	6-15	-3		20.78	20.81
3-15	-1		30.00	32.07	5-15	-3		22.19	22.29
4-15	-1		17.15	17.78	4-15	-3		47.87	-47.99
5-15	0		38.84	42.19	3-15	-3		34.31	-33.92
4-15	0		30.11	-32.36	2-15	-3		67.42	65.20
3-15	0		36.68	-30.62	0-15	-3		39.14	-34.77
2-15	0		36.56	36.75	4 15	3		17.91	-13.79
1 15	0		17.41	-18.84	5 15	2		18.49	21.37
2 15	0		37.96	-36.03	4 15	2		26.78	22.97
3 15	0		43.80	37.45	3 15	2		21.75	-22.80
4 15	0		23.03	21.19	1 15	2		14.82	-14.04
5 15	0		25.87	-27.22	2-15	-2		13.73	12.12
3 15	-1		36.62	-34.83	3-15	-2		39.36	-37.91
2 15	-1		22.95	22.93	4-15	-2		14.69	-15.39
0-15	1		7.70	-5.19	5-15	-2		19.28	21.84
1-15	1		37.62	38.11	4-15	-1		23.01	-20.07
3-15	1		30.81	29.08	3-15	-1		12.80	-13.03
4-15	1		36.95	35.89	2-15	-1		63.19	67.20
5-15	1		15.96	-16.81	0-15	-1		59.51	-62.05
5-15	2		21.01	20.94	2 15	1		47.28	53.05

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
3	16	1	13.13	-13.32	3	17	3	12.61	13.27
4	16	1	42.63	-42.32	4	17	3	13.17	7.46
5	16	1	16.42	-18.25	5	17	2	18.26	18.77
6	16	1	30.81	28.51	3	17	2	33.44	-33.43
4	16	0	27.84	27.27	2	17	2	21.17	18.44
3	16	0	16.42	-18.17	1	17	2	14.18	16.95
1	16	0	26.25	-27.19	0-17	-2	15.76	-11.44	
1-16	0	6.86	-13.43		1-17	-2	38.53	-42.03	
4-16	0	23.57	25.16		3-17	-2	51.56	60.83	
6-16	1	25.10	30.20		5-17	-2	25.15	-24.63	
4-16	1	46.20	-46.80		6-17	-2	12.27	12.47	
3-16	1	13.15	-12.86		5-17	-1	11.38	15.50	
2-16	1	67.00	73.48		3-17	-1	14.42	15.28	
0-16	1	59.63	-38.53		2-17	-1	13.58	16.47	
1	16	-1	21.53	18.05	1-17	-1	25.75	-28.10	
2	16	-1	36.27	36.61	1	17	1	32.34	23.70
3	16	-1	14.97	-12.75	2	17	1	23.05	-22.68
5	16	-1	22.70	-23.24	4	17	1	16.14	14.94
4	16	-2	27.63	-29.99	6	17	0	14.76	-14.92
3	16	-2	13.00	-12.02	5	17	0	17.09	18.84
2	16	-2	12.21	11.11	3	17	0	37.84	-39.05
1	16	-2	12.12	-11.84	2	17	0	14.28	13.91
0-16	2	8.90	6.55		1	17	0	28.39	25.32
2-16	2	18.42	-16.35		3-17	0	13.04	14.94	
3-16	2	24.36	-26.45		5-17	0	19.73	20.84	
4-16	2	30.91	30.35		3-17	1	13.55	14.67	
5-16	2	20.76	21.32		2-17	1	34.31	36.21	
4-16	3	21.60	-18.74		1-17	1	51.41	-55.19	
2-16	3	17.04	15.59		0-17	1	12.67	12.71	
0-16	3	45.59	-40.66		1	17	-1	49.85	51.40
1	16	-3	13.68	12.68	2	17	-1	27.60	-30.44
2	16	-3	35.28	35.10	5	17	-1	17.69	-19.96
3	16	-3	22.31	-21.91	6	17	-2	19.42	-22.07
4	16	-3	41.14	-44.37	5	17	-2	32.33	31.83
3	16	-4	12.64	9.95	4	17	-2	17.99	16.88
2	16	-4	45.89	-43.61	3	17	-2	69.16	-69.16
1	16	-4	11.49	-7.71	1	17	-2	52.22	53.33
0-16	4	29.08	29.22		2-17	2	14.89	-14.78	
0-16	5	38.12	-36.65		3-17	2	22.09	21.23	
2	16	-5	39.25	36.96	2-17	3	23.38	23.71	
1-17	-3	15.35	-13.16		1	17	-3	28.73	21.12
1	17	5	16.80	16.90	2	17	-3	20.23	-19.64
3	17	4	28.50	-29.59	3	17	-3	15.09	-16.10
0-17	-4	14.11	-17.94		4	17	-3	26.89	27.70
1-17	-4	11.04	4.27		2	17	-4	14.18	9.32
4-17	-3	28.04	-26.89		1-17	4	19.53	16.59	
3-17	-3	30.10	27.98		3-17	4	12.20	13.23	
1-17	-3	21.59	-18.50		1-17	5	20.68	-19.81	
0-17	-3	14.38	10.44		1	17	-5	25.67	21.96
2	17	3	22.10	-22.70	2	18	4	12.71	-13.07

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
0-18	-4		14.76	10.18	2 18	-2		32.26	-36.02
1-18	-4		29.55	-27.10	1 18	-2		23.61	-24.44
2-18	-4		18.36	-19.84	1-18	2		30.74	25.68
4-18	-4		15.10	14.82	2-18	2		25.05	-26.16
4-18	-3		25.58	-31.16	3-18	2		29.16	-28.08
2-18	-3		24.58	27.30	4-18	2		36.11	38.28
0-18	-3		11.51	-13.31	4-18	3		18.16	-18.51
1 18	3		38.80	-35.72	3-18	3		14.74	13.24
2 18	3		31.52	30.08	2-18	3		14.92	16.75
4 18	3		11.16	-14.08	1-18	3		23.63	-23.90
4 18	2		37.95	37.54	2 18	-3		17.07	18.38
3 18	2		24.49	-22.26	4 18	-3		16.15	-17.74
2 18	2		42.55	-42.30	4 18	-4		22.94	22.52
1 18	2		31.23	27.32	2 18	-4		21.15	-24.89
0-18	-2		21.55	22.62	1 18	-4		14.81	-14.71
1-18	-2		32.34	-37.82	0-19	-4		13.20	10.82
2-18	-2		23.73	-28.66	1-19	-4		41.19	-35.67
3-18	-2		19.29	-22.05	3-19	-4		32.66	30.32
4-18	-2		20.19	19.67	4-19	-4		15.28	-9.47
6-18	-1		12.52	15.09	5-19	-3		18.26	-16.28
5-18	-1		11.69	-13.31	3-19	-3		24.99	-23.92
1-18	-1		9.91	-20.27	1-19	-3		24.58	22.75
0-18	-1		21.63	19.03	0-19	-3		10.02	11.91
1 18	1		22.03	-20.40	1 19	3		14.52	-11.87
2 18	1		29.22	26.75	4 19	3		13.22	13.97
4 18	1		27.05	-26.79	5 19	2		25.19	23.15
5 18	1		27.91	-26.75	4 19	2		25.71	-24.57
6 18	0		22.10	-19.70	3 19	2		23.94	-25.34
4 18	0		40.16	37.32	1 19	2		30.76	32.81
3 18	0		27.33	-29.72	0-19	-2		21.50	18.00
2 18	0		28.90	-26.64	1-19	-2		78.76	-79.37
1 18	0		7.46	-8.88	2-19	-2		15.99	13.07
2-18	0		14.75	-16.78	3-19	-2		52.19	52.58
3-18	0		31.56	-33.79	4-19	-2		18.60	-16.46
4-18	0		43.91	44.10	5-19	-2		11.32	12.41
5-18	0		11.25	9.32	3-19	-1		18.38	-19.72
6-18	0		13.05	-13.09	2-19	-1		14.58	17.86
6-18	1		26.65	30.55	3 19	1		19.47	19.65
5-18	1		24.10	-22.53	4 19	1		17.36	18.97
4-18	1		37.67	-38.28	5 19	0		16.80	17.40
3-18	1		12.59	11.56	3 19	0		17.45	-20.32
2-18	1		21.18	23.68	2 19	0		31.18	-29.51
1-18	1		10.21	-7.88	1 19	0		15.30	15.35
0-18	1		22.11	19.05	2-19	0		24.34	23.78
1 18	-1		30.51	-35.40	3-19	0		40.18	41.71
2 18	-1		10.62	-11.90	4-19	0		19.96	-19.18
4 18	-1		13.84	-15.49	5-19	0		11.42	-14.30
5 18	-2		11.69	-10.00	6-19	0		11.71	8.07
4 18	-2		28.74	28.98	6-19	1		23.66	24.57
3 18	-2		25.34	-26.20	2-19	1		9.99	-3.37

TABLE I -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
1-19	1		10.13	6.32	2-20	1		11.78	-16.89
1 19	-1		7.86	11.69	1 20	-1		16.11	15.68
3 19	-1		21.72	22.73	2 20	-1		42.66	-44.85
5 19	-2		12.70	13.16	4 20	-1		18.14	19.65
3 19	-2		41.14	-40.68	5 20	-1		12.47	-13.41
1 19	-2		75.35	76.21	3 20	-2		25.53	24.62
0-19	2		14.03	-12.88	2 20	-2		54.80	-60.26
1-19	2		40.05	-38.84	1 20	-2		26.32	-25.96
3-19	2		33.90	35.26	0-20	2		74.84	71.28
4-19	2		12.49	12.08	1-20	2		17.98	-14.07
5-19	2		13.80	-13.30	2-20	2		41.30	-42.69
4-19	3		13.41	-11.91	3-20	2		22.63	21.33
1-19	3		27.97	24.72	4-20	2		12.30	10.95
0-19	3		18.23	-16.68	2-20	3		11.29	11.72
1 19	-3		28.46	-23.94	0-20	3		24.42	-19.25
3 19	-3		22.68	21.73	4 20	-3		20.53	18.13
3 19	-4		26.33	-27.50	5 20	-3		20.50	-19.72
1 19	-4		37.72	34.90	3 20	-4		13.66	10.74
3-19	4		26.59	26.25	2 20	-4		20.61	-16.35
2 20	4		16.50	-14.90	1 20	-4		12.60	-11.22
0-20	-4		16.57	14.49	0-20	4		27.14	23.64
2-20	-4		24.57	-21.23	2-20	4		14.61	-14.65
5-20	-3		17.29	-17.06	3-20	4		18.06	19.63
4-20	-3		15.83	12.47	2 21	4		23.44	20.84
1-20	-3		12.60	-7.69	0-21	-4		10.23	-9.64
0-20	-3		22.85	-19.25	3-21	-4		12.20	17.46
1 20	3		14.21	12.68	4-21	-3		14.10	-13.54
2 20	3		11.18	-11.34	3-21	-3		27.80	-33.38
4 20	3		15.56	13.16	1-21	-3		24.36	27.62
3 20	2		21.11	17.42	0-21	-3		32.14	34.12
2 20	2		44.46	-42.87	1 21	3		18.31	-21.40
1 20	2		20.37	-16.60	3 21	3		25.87	28.53
0-20	-2		57.42	55.88	4 21	2		20.27	-21.04
1-20	-2		28.59	-29.60	3 21	2		21.72	-20.65
2-20	-2		52.12	-50.72	2 21	2		29.58	29.57
3-20	-2		19.70	20.19	1 21	2		13.06	12.78
5-20	-2		14.53	-13.28	2-21	-2		17.24	-15.96
4-20	-1		13.07	12.79	3-21	-2		13.45	15.05
3-20	-1		14.02	-12.86	4-21	-2		16.03	16.83
2-20	-1		29.49	-30.56	5-21	-2		16.30	-16.90
2 20	1		38.82	-38.71	5-21	-1		17.56	19.01
4 20	1		20.67	22.64	4-21	-1		19.84	-21.34
5 20	1		17.55	-17.51	3-21	-1		32.91	-34.98
4 20	0		16.96	-13.11	0-21	-1		19.32	24.64
1 20	0		9.72	-10.82	1 21	1		26.42	-29.74
1-20	0		6.63	-13.98	2 21	1		24.47	-22.60
2-20	0		16.93	-21.83	3 21	1		61.95	61.20
6-20	0		11.55	-12.54	5 21	1		33.60	-32.19
5-20	1		22.56	-22.04	2 21	0		17.60	-18.05
4-20	1		12.33	16.29	4-21	0		9.93	7.95

TABLE 1 -- (CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
5-21	0		22.10	-24.24	1-22	1		26.08	-26.49
5-21	1		22.39	25.81	0-22	1		26.09	20.06
4-21	1		23.39	-24.93	1-22	-1		10.24	10.65
3-21	1		53.54	-56.48	2-22	-1		38.29	-36.97
2-21	1		25.88	21.61	4-22	-1		10.35	12.54
1-21	1		14.26	18.09	5-22	-2		13.72	-10.30
0-21	1		26.54	-26.54	4-22	-2		10.05	-8.81
1-21	-1		23.73	-26.01	2-22	-2		17.74	12.82
3-21	-1		34.55	32.15	1-22	-2		12.97	11.92
5-21	-1		17.65	-20.55	0-22	2		13.94	-7.98
4-21	-2		12.97	-16.07	1-22	2		15.63	13.91
3-21	-2		10.98	-13.49	2-22	2		16.53	-21.47
2-21	-2		10.03	8.71	4-22	2		11.14	7.99
0-21	2		15.10	-12.42	0-22	3		13.50	8.90
2-21	2		28.82	-27.64	2-22	-3		27.11	-28.71
3-21	2		22.99	24.22	2-22	-4		14.31	12.49
4-21	2		24.35	24.74	1-22	-4		17.93	17.24
3-21	3		19.75	-22.03	4-23	-3		9.61	5.68
0-21	3		26.95	-30.60	3-23	-3		19.69	-20.52
1-21	-3		19.34	-24.49	2-23	-3		17.43	-18.03
3-21	-3		31.44	33.11	1-23	-3		44.61	43.36
3-21	-4		17.21	-19.00	1-23	3		33.49	-31.97
2-21	4		19.53	-19.63	3-23	3		18.66	17.72
2-22	-4		13.79	13.37	4-23	2		10.59	-9.87
3-22	-3		18.02	11.70	3-23	2		32.55	29.26
2-22	-3		39.05	-37.34	5-23	-2		12.99	12.04
1-22	-3		11.41	8.80	1-23	1		47.37	-46.85
0-22	-3		13.41	11.22	2-23	1		22.12	21.46
3-22	3		9.55	-9.89	3-23	1		34.84	35.17
2-22	2		11.02	-13.04	3-23	0		10.06	11.45
1-22	2		20.88	19.97	1-23	0		9.10	8.69
0-22	-2		9.66	-3.93	3-23	0		10.06	-11.10
1-22	-2		17.85	14.82	5-23	0		10.83	8.23
2-22	-2		10.33	7.99	5-23	1		21.30	20.83
3-22	-1		16.99	16.13	4-23	1		12.12	12.45
2-22	-1		35.31	-37.89	3-23	1		47.60	-51.49
0-22	-1		16.81	13.58	2-23	1		28.74	-27.92
1-22	1		23.08	-24.16	1-23	1		45.71	46.62
2-22	1		17.19	-18.72	1-23	-1		26.87	-24.51
3-22	1		19.48	20.52	2-23	-1		11.03	11.64
4-22	1		12.78	10.69	5-23	-1		16.61	-14.62
4-22	0		12.68	-16.51	1-23	2		22.55	-22.39
3-22	0		20.22	22.21	3-23	2		15.53	-16.10
2-22	0		13.62	15.60	4-23	2		20.47	18.01
2-22	0		14.93	16.59	3-23	3		21.05	-21.93
3-22	0		14.53	16.60	2-23	3		11.88	-10.59
4-22	0		14.29	-17.79	1-23	3		36.95	35.76
4-22	1		17.41	16.89	1-23	-3		52.97	-52.39
3-22	1		36.77	35.02	2-23	-3		16.14	16.87
2-22	1		38.59	-39.03	3-23	-3		10.25	10.34

TABLE I--(CONTINUED)

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
1	23	-4	10.18	-11.84	0	24	4	18.93	-21.10
2	24	-4	15.93	20.57	1	24	-4	14.47	18.47
1	24	-4	21.40	24.23	1	25	-4	16.81	14.77
0	24	-4	23.68	-22.06	0	25	-4	8.81	-8.18
1	24	3	26.05	27.13	2	25	3	13.32	-10.54
1	24	-3	15.96	-13.49	1	25	3	10.25	-10.43
3	24	-3	11.72	-5.97	0	25	-3	13.77	13.98
4	24	-3	13.79	14.97	2	25	-3	8.91	-14.29
4	24	-2	28.56	-26.48	3	25	-3	8.64	9.11
3	24	-2	17.90	16.91	3	25	-2	17.09	-16.67
2	24	-2	27.77	32.21	2	25	-2	11.25	-9.04
0	24	-2	14.14	-18.00	1	25	-2	10.54	10.83
2	24	2	42.80	46.73	1	25	2	9.19	9.86
0	24	-1	10.69	15.24	0	25	-1	16.44	-17.03
2	24	-1	18.80	-20.02	2	25	-1	22.01	21.01
3	24	-1	16.13	-15.80	4	25	-1	10.69	-10.05
4	24	-1	19.51	22.51	5	25	-1	10.80	9.61
5	24	-1	11.66	12.07	5	25	0	9.17	-9.28
4	24	0	32.77	-37.89	4	25	0	14.37	12.18
3	24	0	15.25	14.02	3	25	0	12.77	-13.03
2	24	0	28.36	33.38	2	25	0	14.50	-14.00
2	24	0	39.96	44.14	1	25	0	8.99	-9.30
4	24	0	37.32	-37.35	3	25	0	9.20	7.88
4	24	-1	13.35	16.96	3	25	-1	11.16	-13.22
2	24	-1	11.03	-11.63	2	25	-1	16.59	-16.51
1	24	-1	13.55	16.77	1	25	-1	7.32	6.05
2	24	1	9.12	6.23	0	25	1	14.67	17.44
3	24	1	12.46	-11.07	1	25	1	9.27	-4.87
5	24	1	22.33	22.06	2	25	1	7.80	3.91
4	24	2	26.98	-27.72	3	25	1	9.92	-9.51
2	24	2	27.24	32.29	3	25	2	0.72	-12.27
0	24	2	11.58	-15.15	2	25	2	11.54	-9.25
2	24	-2	32.90	35.52	1	25	-2	12.29	-10.70
4	24	-2	26.73	-24.84	3	25	-2	11.12	8.96
1	24	3	17.73	18.55	0	25	3	11.20	-9.50
3	24	3	16.87	-16.86	2	25	3	15.99	13.37
1	24	4	17.18	-20.10	3	25	3	12.03	-10.38
					1	25	-4	15.47	-14.07