

The crystal chemistry and petrogenesis of a magnesian rhodonite¹

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Abstract

Rhodonite with unusually high magnesium and low iron contents, $Mn_{3.73}Mg_{0.73}Ca_{0.51}Fe_{0.03}Si_5O_{15}$, occurs in a metamorphosed sedimentary evaporite sequence at Balmat, New York. It coexists with an unusual pyroxene having average composition close to $MnMgSi_2O_6$, talc, calcite, and a number of other minerals. Refinement of the crystal structure using single-crystal X-ray diffraction data shows that Mg has a marked preference for the M4 site ($Mg_{0.47}Mn_{0.53}$), and that M1, M2, and M3 have nearly equal Mg occupancies of slightly more than 0.1. Relations with coexisting phases indicate that both the Mg content and degree of ordering of Mg in M4 are near the maximum to be expected for naturally occurring rhodonite.

Introduction

Two samples of rhodonite were found by miners in different areas of the Balmat Mine No. 4, and saved only because of their attractive appearance and uniqueness. Portions of each sample were kindly made available to us by Dr. Dill of the mine staff, and we refer to them simply as samples 1 and 2, respectively. The rhodonite of sample 1 occurs with a pyroxene of approximate composition $MnMgSi_2O_6$ which is currently under investigation, and fine-grained talc and quartz. The second sample also has both rhodonite and the pyroxene, but also contains barite, anhydrite, manganese calcite, apatite, quartz, hauerite, and a phase tentatively identified as datolite. These two samples were recovered from interlayered metasediments (evaporites) consisting largely of talc, tremolite, calcite, and anhydrite, which are the host rocks for the ore body. The deposit has been regionally metamorphosed with estimated conditions of $P = 6.5 \pm 0.5$ kbar, $T = 625 \pm 25^\circ\text{C}$ (Brown *et al.*, 1978). The conditions for equilibration of rhodonite and its coexisting phases are thus reasonably well-defined.

Preliminary energy-dispersive analyses using the electron microprobe revealed that the rhodonite was unusually rich in Mg and poor in Fe. Quantitative

spectrometer analyses were therefore obtained for rhodonite from both samples, and the results are presented in Table 1. Single-crystal X-ray diffraction confirmed that the analyzed material had the rhodonite structure. Because this rhodonite has a Mg content greater than that of most other rhodonites, and because the iron content is exceptionally low, we concluded that a structure refinement would provide definitive data regarding the occupancy of Mg over the octahedral sites.

X-ray diffraction data

Unit-cell parameters were determined by least-squares refinement, with data for nineteen reflections obtained from a powder diffractometer pattern as corrected with quartz as an internal standard. The parameters are $a = 9.797(3)$, $b = 10.497(3)$, $c = 12.185(4)\text{\AA}$, $\alpha = 108.55(4)$, $\beta = 103.02(4)$, $\gamma = 82.49(4)^\circ$. The space group is $C\bar{1}$. We use this setting, recommended by Ohashi and Finger (1975), as well as the atom nomenclature of those authors, because it provides a more direct means of comparing pyroxenoid structures. Powder diffractometer data are listed in Table 2.

Intensity data were obtained from a cleavage fragment measuring approximately $0.15 \times 0.20 \times 0.40$ mm, mounted for rotation about the c axis on the Weissenberg-geometry diffractometer. MoK α radiation, monochromated with a flat graphite crystal and detected with a scintillation counter, was used. The Supper-Pace automated system was used, employing

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	-12	0	26.6	24.9	4	0	0	88.7	99.8
1	-11	0	9.7	10.0	6	0	0	208.2	209.0
3	-11	0	17.3	19.2	8	0	0	143.8	143.3
5	-11	0	3.6 *	2.9	10	0	0	155.1	146.1
2	-10	0	40.9	38.1	12	0	0	28.6	23.7
4	-10	0	6.7	5.6	3	1	0	186.4	191.9
6	-10	0	52.8	53.1	5	1	0	161.1	164.1
1	-9	0	111.7	113.3	7	1	0	107.4	106.5
3	-9	0	17.9	16.5	9	1	0	3.1 *	0.1
5	-9	0	59.6	57.5	11	1	0	49.9	50.2
7	-9	0	42.5	42.9	2	2	0	145.1	149.8
2	-8	0	35.3	35.1	4	2	0	32.0	29.7
4	-8	0	98.5	98.6	6	2	0	28.7	28.3
6	-8	0	22.3	23.4	8	2	0	46.8	45.4
8	-8	0	38.7	35.6	10	2	0	12.5	12.2
1	-7	0	12.4	12.0	12	2	0	11.9	11.0
3	-7	0	35.5	34.8	1	3	0	2.6 *	2.3
5	-7	0	42.9	42.0	3	3	0	95.4	96.6
7	-7	0	36.5	37.8	5	3	0	71.3	69.2
9	-7	0	3.4 *	5.0	7	3	0	47.0	47.4
2	-6	0	43.2	44.4	9	3	0	54.2	52.3
4	-6	0	42.2	40.5	11	3	0	22.0	25.5
6	-6	0	84.1	85.3	0	4	0	18.5	19.0
8	-6	0	24.5	25.4	2	4	0	13.0	12.4
10	-6	0	108.3	105.9	4	4	0	48.3	48.9
1	-5	0	57.8	55.2	6	4	0	9.0	9.0
3	-5	0	108.8	109.2	8	4	0	40.2	39.6
5	-5	0	24.3	23.4	10	4	0	26.9	23.3
7	-5	0	103.9	104.3	1	5	0	31.9	36.5
9	-5	0	33.1	32.8	3	5	0	9.1	6.8
11	-5	0	6.8	6.8	5	5	0	12.5	8.6
2	-4	0	22.5	22.9	7	5	0	12.4	11.7
4	-4	0	7.0	7.1	9	5	0	25.8	27.2
6	-4	0	76.2	74.7	11	5	0	33.3	30.3
8	-4	0	78.6	77.5	0	6	0	48.3	54.7
10	-4	0	45.7	43.7	2	6	0	32.1	34.1
1	-3	0	49.3	48.9	4	6	0	72.8	75.2
3	-3	0	32.6	33.7	6	6	0	29.9	30.1
5	-3	0	63.6	64.1	8	6	0	82.6	80.2
7	-3	0	5.5	9.1	10	6	0	9.5	8.0
9	-3	0	17.1	19.6	1	7	0	15.1	20.7
11	-3	0	18.3	18.1	3	7	0	3.0 *	1.1
2	-2	0	143.1	142.9	5	7	0	25.6	23.4
4	-2	0	11.2	11.4	7	7	0	52.3	52.1
6	-2	0	58.9	59.4	9	7	0	36.0	35.6
8	-2	0	41.7	43.7	0	8	0	20.1	24.5
10	-2	0	59.6	59.2	2	8	0	69.0	79.6
12	-2	0	23.7	24.8	4	8	0	13.0	14.2
3	-1	0	324.2	349.5	6	8	0	43.8	48.3
5	-1	0	29.2	28.2	8	8	0	7.4	8.1
7	-1	0	176.9	181.2	10	8	0	28.2	26.1
9	-1	0	68.4	69.1	1	9	0	46.6	57.0
11	-1	0	73.6	72.9	3	9	0	47.4	55.8

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	9	0	45.4	49.3	6	-8	1	9.7	6.4
7	9	0	70.5	75.8	8	-8	1	31.7	34.2
9	9	0	56.1	56.1	-11	-7	1	28.4	26.7
10	10	0	14.7	21.7	-9	-7	1	14.6	14.3
10	10	0	10.7	17.1	-7	-7	1	8.7	6.0
10	10	0	18.4	20.5	-5	-7	1	79.7	81.4
10	10	0	16.0	14.6	-3	-7	1	106.3	106.2
10	10	0	8.2	4.4	-1	-7	1	16.9	18.8
11	11	0	19.8	26.1	1	-7	1	8.0	4.8
11	11	0	28.1	38.2	3	-7	1	8.9	8.5
11	11	0	20.7	26.1	5	-7	1	55.1	55.4
11	11	0	36.7	36.9	7	-7	1	42.8	43.9
12	12	0	39.8	62.2	9	-7	1	14.0	14.2
12	12	0	44.0	55.3	-10	-6	1	59.6	60.7
12	12	0	48.6	58.3	-8	-6	1	20.1	21.4
-1	-13	1	8.7	4.9	-6	-6	1	57.0	56.2
-4	-12	1	16.1	17.8	-4	-6	1	52.3	52.5
-2	-12	1	82.3	81.1	-2	-6	1	2.8 *	2.6
0	-12	1	29.2	29.3	0	-6	1	22.0	21.1
2	-12	1	65.5	64.4	2	-6	1	132.2	133.8
4	-12	1	34.3	34.4	4	-6	1	35.4	35.9
-7	-11	1	16.0	17.3	6	-6	1	25.8	24.9
-5	-11	1	23.4	23.1	8	-6	1	50.1	52.0
-3	-11	1	45.3	43.4	10	-6	1	31.5	32.0
-1	-11	1	3.4 *	3.3	-11	-5	1	58.0	56.6
1	-11	1	3.5 *	7.4	-9	-5	1	23.0	25.9
3	-11	1	11.9	9.1	-7	-5	1	16.5	12.4
5	-11	1	22.5	21.7	-5	-5	1	131.8	135.4
-8	-10	1	3.7 *	3.8	-3	-5	1	74.2	74.0
-6	-10	1	68.8	69.0	-1	-5	1	162.7	168.7
-4	-10	1	22.7	20.2	1	-5	1	155.3	156.3
-2	-10	1	3.4 *	2.4	3	-5	1	8.9	10.2
0	-10	1	47.6	51.7	5	-5	1	65.3	67.7
2	-10	1	35.8	36.3	7	-5	1	100.1	98.3
4	-10	1	52.6	48.7	9	-5	1	27.9	26.7
6	-10	1	23.5	28.1	-12	-4	1	42.2	40.4
-9	-9	1	55.2	52.7	-10	-4	1	90.5	91.1
-7	-9	1	16.6	16.7	-8	-4	1	51.4	57.6
-5	-9	1	28.4	27.0	-6	-4	1	337.7	357.0
-3	-9	1	60.5	64.8	-4	-4	1	151.1	149.0
-1	-9	1	21.7	21.6	-2	-4	1	72.6	78.9
1	-9	1	74.6	74.2	0	-4	1	257.2	267.0
3	-9	1	113.3	112.0	2	-4	1	363.8	382.9
5	-9	1	65.6	62.8	4	-4	1	358.3	382.1
7	-9	1	71.9	69.9	6	-4	1	71.9	74.4
-10	-8	1	39.4	38.1	8	-4	1	156.4	153.6
-8	-8	1	13.1	7.4	10	-4	1	87.4	82.8
-6	-8	1	3.3 *	3.3	-11	-3	1	22.0	19.3
-4	-8	1	33.9	36.7	-9	-3	1	113.0	114.6
-2	-8	1	29.0	27.6	-7	-3	1	215.7	226.5
0	-8	1	38.6	38.3	-5	-3	1	136.4	141.9
2	-8	1	3.2 *	7.3	-3	-3	1	242.9	258.4
4	-8	1	12.7	12.2	-1	-3	1	95.9	91.0

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
1	-3	1	275.0	297.4	2	2	1	182.4	183.7
3	-3	1	126.1	119.8	4	2	1	53.9	52.1
5	-3	1	91.9	89.8	6	2	1	63.5	65.1
7	-3	1	41.9	40.8	8	2	1	67.9	70.0
9	-3	1	28.6	30.3	10	2	1	7.5	7.5
11	-3	1	114.9	109.7	12	2	1	42.7	38.9
-12	-2	1	13.7	18.4	-11	3	1	25.8	28.3
-10	-2	1	98.8	102.1	-9	3	1	38.5	37.8
-8	-2	1	29.5	34.8	-7	3	1	13.8	13.3
-6	-2	1	80.5	86.6	-5	3	1	34.7	37.6
-4	-2	1	48.3	49.3	-3	3	1	142.6	142.4
-2	-2	1	68.0	69.9	-1	3	1	57.0	57.6
2	-2	1	125.2	125.1	1	3	1	24.9	24.9
4	-2	1	42.8	41.0	3	3	1	34.0	32.6
6	-2	1	30.7	31.1	5	3	1	29.9	28.7
8	-2	1	9.5	12.2	7	3	1	32.0	30.7
10	-2	1	20.7	18.3	9	3	1	39.7	40.2
-11	-1	1	25.1	25.4	11	3	1	55.5	54.4
-9	-1	1	9.4	11.3	-10	4	1	30.3	25.1
-7	-1	1	42.5	38.3	-8	4	1	18.5	21.7
-5	-1	1	57.8	62.3	-6	4	1	62.5	62.5
-3	-1	1	5.3	5.5	-4	4	1	93.3	96.9
3	-1	1	114.2	114.8	-2	4	1	11.0	11.7
5	-1	1	25.3	24.9	0	4	1	22.2	24.4
7	-1	1	53.1	53.3	2	4	1	29.1	28.5
9	-1	1	30.1	27.3	4	4	1	21.7	0.9
11	-1	1	11.1	13.6	6	4	1	41.2	41.3
-12	0	1	60.2	59.2	8	4	1	39.2	38.5
-10	0	1	68.4	71.3	10	4	1	16.2	10.4
-8	0	1	102.2	105.3	-11	5	1	23.1	18.3
-6	0	1	66.5	67.3	-9	5	1	3.4 *	3.3
-4	0	1	74.6	76.7	-7	5	1	111.4	115.2
4	0	1	44.8	43.1	-5	5	1	11.6	13.3
6	0	1	30.1	29.2	-3	5	1	77.8	76.8
8	0	1	22.0	22.3	-1	5	1	98.7	97.9
10	0	1	3.4 *	2.4	1	5	1	74.9	75.6
12	0	1	7.1	2.6	3	5	1	14.1	15.6
-11	1	1	34.4	34.2	5	5	1	12.3	11.9
-9	1	1	3.1 *	3.1	7	5	1	131.8	132.0
-7	1	1	40.4	37.1	9	5	1	54.9	53.6
-5	1	1	107.3	113.0	11	5	1	87.2	87.7
-3	1	1	25.0	25.3	-10	6	1	8.2	7.0
3	1	1	118.3	120.7	-8	6	1	3.3 *	1.3
5	1	1	28.1	28.5	-6	6	1	27.7	30.9
7	1	1	69.9	72.1	-4	6	1	26.7	28.1
9	1	1	9.8	11.6	-2	6	1	41.4	40.3
11	1	1	7.2	3.9	0	6	1	43.9	43.7
-12	2	1	47.0	48.4	2	6	1	23.5	20.9
-10	2	1	70.0	71.9	4	6	1	30.2	29.7
-8	2	1	138.4	142.2	6	6	1	26.1	28.0
-6	2	1	47.0	47.7	8	6	1	49.2	49.7
-4	2	1	63.0	63.6	10	6	1	13.1	13.9
-2	2	1	155.0	157.7	-9	7	1	3.7 *	4.6

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-7	7	1	41.7	42.3	-5	-11	2	8.7	5.2
-5	7	1	10.7	9.7	-3	-11	2	72.2	68.4
-3	7	1	66.6	66.1	-1	-11	2	32.7	29.9
-1	7	1	20.7	21.3	1	-11	2	13.8	11.9
1	7	1	27.8	27.7	3	-11	2	33.3	35.4
3	7	1	48.2	50.4	5	-11	2	3.7 *	9.8
5	7	1	18.5	17.3	-8	-10	2	18.4	18.6
7	7	1	91.5	90.3	-6	-10	2	85.5	83.6
9	7	1	49.4	50.4	-4	-10	2	49.0	52.0
-8	8	1	21.4	22.2	-2	-10	2	51.3	54.9
-6	8	1	38.8	36.3	0	-10	2	48.9	51.4
-4	8	1	35.2	33.3	2	-10	2	3.3 *	0.1
-2	8	1	8.0	1.0	4	-10	2	8.9	8.0
0	8	1	131.4	132.3	6	-10	2	33.5	34.2
2	8	1	22.3	18.1	-9	-9	2	50.3	48.3
4	8	1	83.5	78.4	-7	-9	2	103.7	106.9
6	8	1	119.1	119.0	-5	-9	2	19.0	24.2
8	8	1	70.5	66.1	-3	-9	2	88.9	90.5
-7	9	1	49.7	51.5	-1	-9	2	91.1	91.8
-5	9	1	61.3	61.5	1	-9	2	60.8	60.6
-3	9	1	151.6	152.3	3	-9	2	72.9	77.2
-1	9	1	203.0	207.6	5	-9	2	96.4	95.2
1	9	1	56.6	54.7	7	-9	2	34.0	29.8
3	9	1	165.7	167.4	-10	-8	2	20.2	30.4
5	9	1	82.9	82.2	-8	-8	2	3.6 *	4.2
7	9	1	124.3	121.1	-6	-8	2	40.0	38.9
-6	10	1	53.0	53.6	-4	-8	2	64.3	63.9
-4	10	1	135.3	135.9	-2	-8	2	263.0	269.2
-2	10	1	27.5	23.7	0	-8	2	36.8	40.8
0	10	1	43.7	42.8	2	-8	2	144.3	138.6
2	10	1	11.7	12.7	4	-8	2	167.8	161.3
4	10	1	31.6	31.3	6	-8	2	100.2	97.1
6	10	1	74.4	73.8	8	-8	2	56.1	54.4
-5	11	1	11.5	13.0	-11	-7	2	38.8	35.1
-3	11	1	72.3	73.1	-9	-7	2	63.5	65.6
-1	11	1	25.3	20.9	-7	-7	2	87.2	88.4
1	11	1	104.0	103.5	-5	-7	2	236.9	242.3
3	11	1	24.9	22.1	-3	-7	2	218.1	218.0
5	11	1	93.9	92.7	-1	-7	2	143.4	141.3
-2	12	1	51.4	46.8	1	-7	2	163.2	165.9
0	12	1	17.3	16.5	3	-7	2	91.7	88.4
2	12	1	21.9	21.3	5	-7	2	165.2	163.9
4	12	1	38.3	39.7	7	-7	2	67.5	60.8
-3	-13	2	33.1	33.9	9	-7	2	45.6	45.8
-1	-13	2	37.6	38.3	-10	-6	2	89.3	94.6
1	-13	2	33.7	32.9	-8	-6	2	33.2	36.2
-6	-12	2	7.4	4.4	-6	-6	2	106.0	107.9
-4	-12	2	15.5	14.1	-4	-6	2	59.8	59.7
-2	-12	2	6.9	5.2	-2	-6	2	24.5	25.0
0	-12	2	47.2	42.0	0	-6	2	21.4	20.4
2	-12	2	42.1	37.3	2	-6	2	6.7	7.4
4	-12	2	26.0	20.9	4	-6	2	16.2	16.5
-7	-11	2	9.3	6.9	6	-6	2	35.7	35.3

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
8	-6	2	41.5	42.3	7	-1	2	7.9	8.6
10	-6	2	30.8	32.1	9	-1	2	26.0	28.1
-11	-5	2	27.1	27.2	11	-1	2	44.6	44.3
-9	-5	2	34.0	35.0	-10	0	2	16.4	17.9
-7	-5	2	31.6	31.4	-8	0	2	75.2	79.5
-5	-5	2	23.6	26.3	-6	0	2	23.3	26.9
-3	-5	2	26.8	27.2	-4	0	2	67.3	68.1
-1	-5	2	29.4	27.9	2	0	2	97.3	98.8
1	-5	2	30.3	27.9	4	0	2	70.7	76.9
3	-5	2	2.7 *	2.8	6	0	2	110.3	114.6
5	-5	2	32.8	31.1	8	0	2	28.6	33.9
7	-5	2	42.6	42.5	10	0	2	73.6	76.1
9	-5	2	17.4	18.0	-11	1	2	3.4 *	2.2
-12	-4	2	3.8 *	4.5	-9	1	2	32.3	29.4
-10	-4	2	50.4	53.2	-7	1	2	52.8	53.6
-8	-4	2	63.1	68.3	-5	1	2	85.9	88.3
-6	-4	2	128.8	132.0	-3	1	2	70.6	73.5
-4	-4	2	29.1	29.1	3	1	2	6.1	6.3
-2	-4	2	22.4	22.5	5	1	2	66.5	63.5
0	-4	2	44.9	44.2	7	1	2	7.2	3.0
2	-4	2	88.4	88.4	9	1	2	78.1	75.7
4	-4	2	43.9	43.4	11	1	2	91.1	88.9
6	-4	2	3.0 *	1.2	-12	2	2	12.1	9.8
8	-4	2	35.4	37.5	-10	2	2	8.3	8.4
10	-4	2	15.8	11.3	-8	2	2	16.1	18.7
-11	-3	2	24.9	26.3	-6	2	2	41.2	41.3
-9	-3	2	64.6	61.7	-4	2	2	2.6 *	5.9
-7	-3	2	44.8	42.2	-2	2	2	58.5	59.7
-5	-3	2	45.5	42.8	0	2	2	51.8	49.9
-3	-3	2	124.3	125.2	2	2	2	69.1	67.1
-1	-3	2	138.4	142.3	4	2	2	19.3	16.7
1	-3	2	219.4	229.3	6	2	2	92.1	91.4
3	-3	2	76.6	72.5	8	2	2	39.5	41.6
5	-3	2	69.0	66.9	10	2	2	9.1	11.9
7	-3	2	60.8	57.5	-11	3	2	16.7	14.7
9	-3	2	10.6	11.8	-9	3	2	31.1	33.4
-12	-2	2	26.9	26.4	-7	3	2	25.3	26.4
-10	-2	2	34.0	31.7	-5	3	2	45.4	44.9
-8	-2	2	121.1	124.8	-3	3	2	62.9	62.8
-6	-2	2	34.8	35.2	-1	3	2	17.1	17.7
-4	-2	2	129.8	135.8	1	3	2	76.8	76.9
2	-2	2	91.6	91.7	3	3	2	73.8	72.7
4	-2	2	34.8	34.9	5	3	2	5.3	3.3
6	-2	2	129.4	129.5	7	3	2	93.6	93.0
8	-2	2	3.1 *	0.5	9	3	2	25.4	25.7
10	-2	2	48.3	47.3	11	3	2	86.1	84.4
-11	-1	2	24.8	26.9	-10	4	2	44.7	49.9
-9	-1	2	7.4	8.4	-8	4	2	10.2	9.3
-7	-1	2	16.9	16.9	-5	4	2	14.1	12.5
-5	-1	2	36.7	38.9	-4	4	2	21.5	20.6
-3	-1	2	19.8	19.8	-2	4	2	29.0	30.2
3	-1	2	43.3	45.6	0	4	2	44.5	41.7
5	-1	2	8.7	6.4	2	4	2	51.5	48.0

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	4	-2	147.9	147.3	-6	10	2	13.3	10.8
6	4	2	26.8	24.4	-4	10	2	53.1	50.3
8	4	2	100.0	101.0	2	10	2	47.9	45.2
10	4	2	98.4	94.7	0	10	2	22.5	18.4
-11	5	2	71.9	70.0	2	10	2	32.9	28.1
-9	5	2	59.5	53.6	4	10	2	8.5	11.8
-7	5	2	211.1	213.5	6	10	2	3.7 *	5.6
-5	5	2	22.8	24.6	-3	11	2	52.7	55.4
-3	5	2	159.9	158.0	-1	11	2	45.8	48.2
-1	5	2	260.4	261.9	1	11	2	46.3	48.9
1	5	2	293.5	299.3	3	11	2	11.8	14.1
3	5	2	223.3	223.6	5	11	2	37.2	37.9
5	5	2	35.4	34.9	0	12	2	9.0	6.1
7	5	2	200.2	204.4	2	12	2	10.6	6.5
9	5	2	50.6	49.4	-3	-13	3	90.9	89.4
-10	6	2	127.0	127.7	-1	-13	3	18.5	17.6
-8	6	2	73.8	73.0	1	-13	3	79.2	77.5
-6	6	2	84.3	83.2	-6	-12	3	37.4	34.9
-4	6	2	124.7	121.1	-4	-12	3	13.4	7.5
-2	6	2	41.6	43.3	-2	-12	3	46.1	41.7
0	6	2	344.7	364.3	0	-12	3	55.5	51.7
2	6	2	35.3	35.4	2	-12	3	67.3	64.4
4	6	2	58.2	59.4	4	-12	3	30.9	28.7
6	6	2	26.2	25.2	-7	-11	3	25.6	27.6
8	6	2	39.7	39.5	-5	-11	3	99.8	97.7
10	6	2	66.9	63.1	-3	-11	3	143.9	138.6
-9	7	2	27.9	26.6	-1	-11	3	168.9	163.9
-7	7	2	92.6	90.8	1	-11	3	97.3	94.5
-5	7	2	61.1	61.4	3	-11	3	50.8	53.4
-3	7	2	69.3	69.9	5	-11	3	84.9	86.5
-1	7	2	119.7	123.8	-8	-10	3	55.4	57.5
1	7	2	81.3	80.8	-6	-10	3	84.8	83.3
3	7	2	10.0	7.2	-2	-10	3	79.8	77.9
5	7	2	116.6	117.4	0	-10	3	9.2	7.3
7	7	2	30.0	29.1	4	-10	3	28.3	29.1
9	7	2	67.1	63.9	6	-10	3	13.2	13.6
-8	8	2	13.5	11.7	-9	-9	3	38.6	38.3
-5	8	2	3.5 *	6.7	-7	-9	3	21.4	21.6
-4	8	2	17.8	14.4	-5	-9	3	6.8	6.5
-2	8	2	44.9	42.9	-3	-9	3	15.1	9.7
0	8	2	9.6	11.1	-1	-9	3	7.8	9.5
2	8	2	35.2	35.2	1	-9	3	3.2 *	0.4
4	8	2	64.9	65.3	3	-9	3	38.6	37.2
6	8	2	34.2	34.4	5	-9	3	3.3 *	4.7
8	8	2	25.1	25.1	7	-9	3	3.5 *	5.8
-7	9	2	35.1	36.1	-10	-8	3	13.4	8.0
-5	9	2	29.0	27.6	-8	-8	3	6.7	5.6
-3	9	2	7.8	3.5	-6	-8	3	78.3	81.7
-1	9	2	50.5	44.9	-4	-8	3	21.5	20.1
1	9	2	29.3	26.5	-2	-8	3	64.4	66.9
3	9	2	16.2	11.0	0	-8	3	101.3	102.2
5	9	2	45.1	42.6	2	-8	3	19.6	21.0
7	9	2	15.6	17.4	4	-8	3	9.3	8.4

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	-8	3	13.6	14.4	3	-3	3	10.6	10.3
8	-3	3	44.2	41.7	5	-3	3	13.4	15.9
-11	-7	3	64.6	64.1	7	-3	3	27.4	26.1
-9	-7	3	126.1	126.9	9	-3	3	42.0	40.4
-7	-7	3	41.8	48.5	11	-3	3	3.6 *	0.3
-5	-7	3	138.6	140.1	-12	-2	3	31.2	29.7
-3	-7	3	51.1	48.5	-10	-2	3	19.8	21.4
-1	-7	3	51.7	51.6	-8	-2	3	18.0	21.4
1	-7	3	107.3	106.3	-6	-2	3	10.3	9.6
3	-7	3	8.0	4.7	-4	-2	3	14.5	14.2
5	-7	3	166.3	169.6	2	-2	3	16.7	13.6
7	-7	3	12.3	13.0	4	-2	3	50.5	51.4
9	-7	3	47.9	45.2	6	-2	3	104.6	104.4
-10	-6	3	36.9	38.7	8	-2	3	49.7	50.9
-8	-6	3	8.5	8.9	10	-2	3	66.9	69.3
-6	-6	3	35.5	38.1	-11	-1	3	16.1	12.9
-4	-6	3	69.1	68.6	-9	-1	3	43.4	43.9
-2	-6	3	119.8	118.9	-7	-1	3	38.7	39.8
0	-6	3	39.3	39.5	-5	-1	3	94.4	98.1
2	-6	3	53.8	54.0	-3	-1	3	57.9	58.3
4	-6	3	12.5	13.2	3	-1	3	14.4	16.9
6	-6	3	10.7	10.6	5	-1	3	2.6 *	4.9
8	-6	3	3.5 *	1.9	7	-1	3	13.4	14.8
10	-6	3	45.7	44.5	9	-1	3	57.1	56.1
-11	-5	3	22.6	23.6	11	-1	3	59.2	56.6
-9	-5	3	30.4	30.0	-12	0	3	24.5	18.1
-7	-5	3	7.7	4.5	-10	0	3	55.4	62.3
-5	-5	3	13.2	16.1	-8	0	3	35.4	31.9
-3	-5	3	16.8	13.5	-6	0	3	26.2	26.5
-1	-5	3	24.9	24.7	-4	0	3	94.5	100.1
1	-5	3	13.0	14.1	2	0	3	47.7	49.2
3	-5	3	56.8	57.4	4	0	3	132.8	135.2
5	-5	3	29.0	26.3	6	0	3	39.0	40.1
7	-5	3	3.3 *	2.1	8	0	3	90.3	94.6
9	-5	3	7.9	6.4	10	0	3	37.9	37.3
-12	-4	3	3.7 *	2.4	-11	1	3	27.1	24.8
-10	-4	3	59.8	60.1	-9	1	3	66.8	64.4
-8	-4	3	44.0	42.8	-7	1	3	130.7	132.3
-6	-4	3	79.2	78.3	-5	1	3	98.8	96.4
-4	-4	3	86.5	84.4	-3	1	3	217.2	227.2
-2	-4	3	39.4	36.8	3	1	3	26.2.1	264.9
0	-4	3	39.1	41.6	5	1	3	179.3	186.5
2	-4	3	28.3	26.8	7	1	3	102.1	103.7
4	-4	3	167.3	167.0	9	1	3	15.8	17.6
6	-4	3	65.6	66.0	11	1	3	139.0	133.5
8	-4	3	79.1	80.9	-12	2	3	35.8	33.5
10	-4	3	76.2	72.9	-10	2	3	101.0	97.5
-11	-3	3	13.1	10.9	-8	2	3	3.2 *	3.0
-9	-3	3	13.3	8.4	-6	2	3	394.4	413.6
-7	-3	3	21.6	21.3	-4	2	3	163.7	161.4
-5	-3	3	44.4	46.1	-2	2	3	122.2	130.3
-3	-3	3	32.2	28.7	0	2	3	254.3	264.3
1	-3	3	71.1	72.1	2	2	3	322.5	325.2

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	2	3	273.5	281.2	1	7	3	34.5	37.5
6	2	3	105.7	107.7	3	7	3	36.5	41.3
8	2	3	147.4	153.0	5	7	3	71.4	69.5
10	2	3	54.4	52.4	7	7	3	16.4	15.8
-11	3	3	32.0	29.7	9	7	3	63.1	61.6
-9	3	3	84.4	89.5	-8	8	3	64.2	61.5
-7	3	3	71.6	76.6	-6	8	3	16.1	16.9
-5	3	3	14.0	13.0	-4	8	3	23.7	24.5
-3	3	3	123.2	121.8	-2	8	3	49.7	49.7
-1	3	3	47.0	54.5	0	8	3	16.1	14.1
1	3	3	34.8	29.1	2	8	3	61.3	61.6
3	3	3	142.2	140.6	4	8	3	3.3 *	1.6
5	3	3	32.3	30.7	6	8	3	57.6	57.6
7	3	3	19.5	22.9	8	8	3	36.3	34.0
9	3	3	38.0	37.6	-7	9	3	18.2	20.9
11	3	3	37.2	40.5	-5	9	3	6.9	15.0
-10	4	3	55.2	55.8	-3	9	3	29.8	27.8
-8	4	3	33.9	34.0	-1	9	3	42.1	39.1
-6	4	3	11.6	9.0	1	9	3	14.1	13.8
-4	4	3	15.8	16.2	3	9	3	3.5 *	7.2
-2	4	3	86.8	85.7	5	9	3	3.6 *	4.2
0	4	3	18.5	16.0	7	9	3	19.6	21.3
2	4	3	22.3	20.8	-6	10	3	3.7 *	10.6
4	4	3	36.8	38.1	-4	10	3	80.7	80.0
6	4	3	47.1	45.0	-2	10	3	26.8	25.7
8	4	3	39.0	41.0	0	10	3	68.7	73.3
10	4	3	25.6	20.5	2	10	3	21.0	26.3
-9	5	3	31.6	34.2	4	10	3	15.3	20.8
-7	5	3	12.2	15.1	6	10	3	22.9	26.5
-5	5	3	92.7	95.2	-3	11	3	7.2	7.9
-3	5	3	10.7	8.6	-1	11	3	14.5	13.8
-1	5	3	64.1	63.9	1	11	3	12.9	11.6
1	5	3	11.8	8.1	3	11	3	3.9 *	8.9
3	5	3	102.0	99.1	-3	-13	4	35.1	38.4
5	5	3	3.3 *	10.1	-1	-13	4	26.1	24.0
7	5	3	3.4 *	0.5	1	-13	4	3.7 *	2.9
9	5	3	49.1	50.8	-6	-12	4	60.5	61.1
-10	6	3	28.8	32.8	-4	-12	4	29.9	29.4
-8	6	3	37.6	36.0	-2	-12	4	17.6	19.4
-6	6	3	26.1	25.4	0	-12	4	59.7	58.8
-4	6	3	10.2	3.2	2	-12	4	35.6	32.4
-2	6	3	2.9 *	0.4	4	-12	4	71.2	68.9
0	6	3	46.9	46.3	-7	-11	4	35.6	38.4
2	6	3	12.9	12.0	-5	-11	4	61.0	57.4
4	6	3	63.1	65.1	-3	-11	4	37.6	36.2
6	6	3	12.9	11.3	-1	-11	4	142.1	144.3
8	6	3	27.5	27.0	1	-11	4	8.2	5.0
10	6	3	14.5	14.4	3	-11	4	58.8	54.8
-9	7	3	97.6	97.1	5	-11	4	55.2	53.2
-7	7	3	48.3	49.0	-8	-10	4	42.1	40.6
-5	7	3	121.2	122.2	-6	-10	4	3.5 *	4.4
-3	7	3	63.9	66.1	-4	-10	4	32.6	34.5
-1	7	3	28.3	30.4	-2	-10	4	34.3	32.8

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	-10	4	52.8	52.4	7	-5	4	52.6	52.0
2	-10	4	87.4	86.7	9	-5	4	7.5	6.7
4	-10	4	19.6	19.5	-12	-4	4	39.6	39.8
6	-10	4	46.8	43.5	-10	-4	4	19.3	14.0
-9	-9	4	3.7 *	8.5	-8	-4	4	18.1	17.0
-7	-9	4	26.2	22.2	-6	-4	4	98.9	103.9
-5	-9	4	6.9	6.8	-4	-4	4	125.3	128.6
-3	-9	4	3.1 *	2.5	-2	-4	4	57.5	51.4
-1	-9	4	20.7	16.5	0	-4	4	60.7	64.2
1	-9	4	11.1	9.7	2	-4	4	57.0	57.5
3	-9	4	55.6	54.5	4	-4	4	16.8	17.3
5	-9	4	10.0	10.5	6	-4	4	39.7	39.3
7	-9	4	28.1	28.1	8	-4	4	110.0	109.2
-10	-8	4	27.1	25.9	10	-4	4	19.6	13.5
-8	-8	4	32.3	31.2	-11	-3	4	21.0	21.3
-6	-8	4	72.4	71.3	-9	-3	4	125.8	126.0
-4	-8	4	19.6	16.0	-7	-3	4	130.6	138.2
-2	-8	4	85.9	84.4	-5	-3	4	108.6	116.1
0	-8	4	3.1 *	4.2	-3	-3	4	156.6	149.3
2	-8	4	32.1	30.7	1	-3	4	93.1	97.3
4	-8	4	57.9	54.0	3	-3	4	81.0	75.4
6	-8	4	64.7	62.1	5	-3	4	293.0	304.8
8	-8	4	104.6	102.6	7	-3	4	14.0	3.1
-11	-7	4	21.1	19.9	9	-3	4	81.1	79.4
-9	-7	4	21.0	21.3	-12	-2	4	174.2	164.4
-7	-7	4	17.4	18.2	-10	-2	4	62.2	57.6
-5	-7	4	3.2 *	3.4	-8	-2	4	43.2	36.9
-3	-7	4	19.0	18.2	-6	-2	4	209.7	216.9
-1	-7	4	45.0	47.2	-4	-2	4	309.3	330.0
1	-7	4	42.7	41.0	2	-2	4	258.9	274.4
3	-7	4	55.6	54.7	4	-2	4	242.0	248.7
5	-7	4	101.2	102.8	6	-2	4	181.4	183.4
7	-7	4	11.2	11.4	8	-2	4	81.9	80.4
9	-7	4	29.7	30.2	10	-2	4	16.8	14.1
-10	-6	4	7.2	8.1	-11	-1	4	22.0	18.4
-8	-6	4	14.7	13.8	-9	-1	4	93.5	97.5
-6	-6	4	30.0	28.4	-7	-1	4	65.4	71.5
-4	-6	4	11.2	11.7	-5	-1	4	176.1	188.7
-2	-6	4	11.0	10.7	3	-1	4	23.7	25.0
0	-6	4	47.1	47.6	5	-1	4	32.2	30.5
2	-6	4	14.3	15.1	7	-1	4	12.6	14.7
4	-6	4	78.4	82.8	9	-1	4	55.9	54.8
6	-6	4	40.2	38.7	11	-1	4	10.0	9.7
8	-6	4	48.3	46.8	-12	0	4	26.0	27.9
-11	-5	4	13.5	10.3	-10	0	4	71.3	76.6
-9	-5	4	74.8	74.1	-8	0	4	24.6	16.3
-7	-5	4	46.8	45.7	-6	0	4	11.5	10.8
-5	-5	4	35.8	34.4	-4	0	4	68.2	72.2
-3	-5	4	123.3	119.9	2	0	4	52.4	53.9
-1	-5	4	47.0	46.3	4	0	4	38.4	38.6
1	-5	4	63.2	62.5	6	0	4	21.8	23.6
3	-5	4	8.9	9.1	8	0	4	11.4	11.6
5	-5	4	24.3	22.2	10	0	4	23.7	20.6

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-11	1	4	20.9	21.1	9	5	4	30.2	30.6
-9	1	4	36.6	37.8	-10	6	4	13.6	8.0
-7	1	4	21.8	25.9	-8	6	4	10.9	10.7
-5	1	4	54.2	59.0	-6	6	4	43.4	44.3
-3	1	4	36.8	35.3	-4	6	4	5.8	5.9
3	1	4	90.0	88.8	-2	6	4	81.1	82.5
5	1	4	27.3	27.7	0	6	4	43.3	42.9
7	1	4	35.2	37.3	2	6	4	13.4	10.8
9	1	4	24.4	22.7	4	6	4	48.8	52.2
11	1	4	26.6	27.0	6	6	4	27.3	26.3
-12	2	4	38.5	38.7	8	6	4	16.5	17.1
-10	2	4	72.9	75.9	-9	7	4	10.0	11.6
-8	2	4	49.2	51.0	-7	7	4	30.5	28.6
-6	2	4	88.0	86.2	-5	7	4	69.0	71.7
-4	2	4	43.0	45.6	-3	7	4	3.3 *	0.2
-2	2	4	39.8	43.2	-1	7	4	31.5	32.3
0	2	4	50.5	49.8	1	7	4	77.4	82.7
2	2	4	42.4	40.2	3	7	4	16.0	13.2
4	2	4	67.8	66.9	5	7	4	48.9	49.6
6	2	4	25.7	25.6	7	7	4	35.8	39.6
8	2	4	45.2	44.1	-8	8	4	15.1	14.1
10	2	4	15.8	15.7	-6	8	4	63.1	64.3
-11	3	4	52.9	53.2	-4	8	4	23.6	26.2
-9	3	4	37.8	38.1	-2	8	4	17.4	17.5
-7	3	4	73.2	73.2	0	8	4	78.9	80.9
-5	3	4	88.4	90.7	2	8	4	3.5 *	1.2
-3	3	4	6.1	5.1	4	8	4	11.2	8.8
-1	3	4	172.6	176.2	6	8	4	3.6 *	4.6
1	3	4	120.2	117.9	-7	9	4	12.4	11.8
3	3	4	20.6	21.0	-5	9	4	9.9	9.5
5	3	4	30.0	32.9	-3	9	4	52.2	51.6
7	3	4	21.3	22.1	-1	9	4	34.5	34.0
9	3	4	37.1	35.3	1	9	4	46.8	41.4
-10	4	4	26.7	28.3	3	9	4	28.5	28.1
-8	4	4	100.5	102.9	5	9	4	39.7	37.1
-6	4	4	21.0	17.7	-4	10	4	21.9	18.2
-4	4	4	102.9	102.4	-2	10	4	29.2	26.2
-2	4	4	37.3	35.1	0	10	4	114.8	115.0
0	4	4	53.9	55.9	2	10	4	78.2	72.9
2	4	4	100.1	102.9	4	10	4	98.8	92.8
4	4	4	3.1 *	1.3	-1	11	4	86.4	87.9
6	4	4	106.0	107.9	1	11	4	86.8	87.2
8	4	4	3.5 *	1.0	-5	-13	5	35.9	32.9
10	4	4	50.3	47.2	-3	-13	5	12.1	11.2
-9	5	4	44.6	43.4	-1	-13	5	32.7	29.3
-7	5	4	25.0	25.1	1	-13	5	30.9	32.4
-5	5	4	49.0	48.2	-6	-12	5	20.6	18.4
-3	5	4	27.9	30.5	-4	-12	5	24.2	23.4
-1	5	4	8.2	12.2	-2	-12	5	3.7 *	6.6
1	5	4	3.1 *	4.3	0	-12	5	17.4	13.4
3	5	4	12.9	8.0	2	-12	5	45.5	45.7
5	5	4	62.4	64.6	4	-12	5	34.4	31.4
7	5	4	12.3	13.9	-7	-11	5	31.9	29.5

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-5	-11	5	7.7	5.4	-11	-5	5	83.8	80.5
-1	-11	5	30.6	26.3	-9	-5	5	122.1	126.9
-1	-11	5	61.1	58.8	-7	-5	5	71.1	73.1
1	-11	5	50.1	47.9	-5	-5	5	166.3	169.9
3	-11	5	69.7	68.3	-3	-5	5	183.2	181.9
5	-11	5	69.3	66.9	-1	-5	5	183.6	183.0
-8	-10	5	29.0	28.3	1	-5	5	78.7	81.2
-6	-10	5	14.5	13.6	3	-5	5	42.5	44.4
-4	-10	5	3.5 *	6.2	5	-5	5	59.6	61.5
-2	-10	5	3.2 *	5.4	7	-5	5	58.3	56.3
0	-10	5	30.2	27.8	9	-5	5	41.4	38.2
2	-10	5	24.9	23.0	-12	-4	5	59.6	61.1
4	-10	5	7.4	0.5	-10	-4	5	27.6	31.3
6	-10	5	35.3	33.3	-8	-4	5	54.9	60.3
-9	-9	5	54.2	53.4	-6	-4	5	55.0	59.8
-7	-9	5	41.9	40.6	-4	-4	5	55.0	53.1
-5	-9	5	69.7	67.7	-2	-4	5	39.8	37.6
-3	-9	5	14.5	6.5	0	-4	5	95.7	95.6
-1	-9	5	53.2	52.4	2	-4	5	26.8	26.9
1	-9	5	7.9	7.5	4	-4	5	38.7	36.9
3	-9	5	55.6	57.1	6	-4	5	64.7	66.0
5	-9	5	3.3 *	3.3	8	-4	5	6.9	1.1
7	-9	5	28.2	29.8	10	-4	5	3.7 *	5.3
-10	-8	5	26.2	26.9	-11	-3	5	46.6	44.0
-8	-8	5	58.6	62.0	-9	-3	5	18.5	21.9
-6	-8	5	34.4	35.1	-7	-3	5	28.0	35.1
-4	-8	5	36.3	36.5	-5	-3	5	7.6	10.5
-2	-8	5	3.2 *	4.6	-3	-3	5	43.9	42.7
0	-8	5	124.9	127.7	-1	-3	5	39.8	39.3
2	-8	5	62.3	63.6	1	-3	5	83.9	81.3
4	-8	5	41.5	42.4	3	-3	5	40.4	39.3
6	-8	5	52.3	51.8	5	-3	5	6.4	4.1
8	-8	5	28.1	25.9	7	-3	5	56.8	55.3
-11	-7	5	27.4	30.6	9	-3	5	41.0	39.8
-9	-7	5	7.3	1.0	-12	-2	5	128.5	126.2
-7	-7	5	49.1	51.2	-10	-2	5	55.1	56.8
-5	-7	5	14.1	16.1	-8	-2	5	31.1	30.9
-3	-7	5	129.1	128.9	-6	-2	5	154.5	160.6
-1	-7	5	168.4	172.7	-4	-2	5	5.8	1.3
1	-7	5	29.3	29.7	2	-2	5	126.5	128.2
3	-7	5	44.6	41.6	4	-2	5	36.2	39.1
5	-7	5	89.8	88.8	6	-2	5	40.4	40.0
7	-7	5	28.4	27.2	8	-2	5	72.5	71.5
9	-7	5	76.6	75.4	10	-2	5	46.0	45.5
-10	-6	5	68.3	60.2	-11	-1	5	24.6	25.0
-8	-6	5	167.4	167.7	-9	-1	5	105.7	106.0
-6	-6	5	7.1	0.4	-7	-1	5	133.5	145.6
-4	-6	5	166.1	160.1	-5	-1	5	10.1	10.0
-2	-6	5	303.8	313.7	-3	-1	5	49.7	45.0
2	-6	5	186.5	186.5	1	-1	5	22.1	17.3
4	-6	5	22.4	18.1	3	-1	5	17.8	14.4
6	-6	5	186.8	186.0	5	-1	5	173.9	177.3
8	-6	5	97.0	94.3	7	-1	5	111.6	115.3

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	
9	-1	5	36.7	35.7	4	4	5	11.8	7.9	
-12	0	5	22.8	23.4	6	4	5	63.0	60.9	
-11	0	5	119.6	123.5	8	4	5	24.5	25.1	
-3	0	5	54.3	55.9	-9	5	5	43.0	45.5	
-5	0	5	21.9	21.3	-7	5	5	16.7	17.8	
-4	0	5	138.4	141.9	-5	5	5	43.1	42.1	
-2	0	5	30.9	26.9	-3	5	5	10.1	8.1	
0	0	5	57.4	63.7	-1	5	5	2.9	*	
2	0	5	5.2	0.3	1	5	5	29.4	29.7	
4	0	5	159.0	162.2	3	5	5	3.1	*	
6	0	5	18.8	19.1	5	5	5	97.1	97.7	
8	0	5	11.7	11.3	7	5	5	24.4	25.0	
10	0	5	88.9	85.5	9	5	5	63.6	65.5	
-11	1	5	3.5	*	4.7	-8	6	5	3.4	*
-9	1	5	28.6	30.2	-6	6	5	88.4	81.2	
-7	1	5	27.4	29.3	-4	6	5	25.1	21.3	
-5	1	5	44.8	46.1	-2	6	5	56.6	56.0	
-3	1	5	65.8	64.9	0	6	5	37.0	31.4	
-1	1	5	8.6	12.5	2	6	5	101.1	100.5	
1	1	5	49.9	45.0	4	6	5	160.3	156.2	
3	1	5	35.9	36.4	6	6	5	54.3	49.9	
5	1	5	35.2	36.3	8	6	5	76.7	75.6	
7	1	5	13.0	15.4	-7	7	5	117.1	110.6	
9	1	5	59.2	62.1	-5	7	5	114.4	114.5	
-10	2	5	30.2	33.3	-3	7	5	158.2	161.4	
-8	2	5	3.1	*	5.3	-1	7	5	15.9	14.9
-6	2	5	3.1	*	7.5	1	7	254.9	257.5	
-4	2	5	2.7	*	3.2	3	7	109.9	108.6	
-2	2	5	45.3	46.7	5	7	5	81.1	86.4	
0	2	5	39.9	40.1	7	7	5	45.2	50.8	
2	2	5	20.0	16.2	-6	8	5	140.7	134.6	
4	2	5	57.4	56.9	-4	8	5	21.7	27.5	
6	2	5	32.6	32.9	-2	8	5	57.8	59.0	
8	2	5	19.9	23.6	0	8	5	16.8	12.9	
10	2	5	3.7	*	9.4	2	8	5	28.1	26.3
-11	3	5	25.0	25.1	4	8	5	48.1	50.4	
-9	3	5	21.9	23.6	6	8	5	112.5	110.7	
-7	3	5	38.1	38.6	-5	9	5	30.8	26.7	
-5	3	5	74.8	78.3	-3	9	5	6.2	1.0	
-3	3	5	39.7	41.0	-1	9	5	81.7	85.2	
-1	3	5	36.7	37.8	1	9	5	10.2	3.9	
1	3	5	19.8	14.8	3	9	5	100.4	101.0	
3	3	5	53.8	56.8	5	9	5	17.4	11.0	
5	3	5	73.5	73.9	-4	10	5	29.7	27.0	
7	3	5	56.4	57.9	-2	10	5	8.9	12.2	
9	3	5	73.8	74.3	0	10	5	9.2	9.2	
-10	4	5	9.0	5.2	2	10	5	40.8	42.2	
-8	4	5	15.5	15.6	4	10	5	29.4	30.2	
-6	4	5	47.4	49.2	-5	-13	6	65.1	64.9	
-4	4	5	38.3	41.5	-3	-13	6	3.8	*	
-2	4	5	63.2	64.5	-1	-13	6	29.7	29.8	
0	4	5	9.3	6.0	1	-13	6	12.3	12.1	
2	4	5	57.6	58.7	-6	-12	6	35.3	36.4	

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-4	-12	6	52.1	51.6	0	-6	6	63.3	63.2
-2	-12	6	24.3	24.5	2	-6	6	98.6	100.5
0	-12	6	3.5 *	3.9	4	-6	6	63.2	65.9
2	-12	6	33.0	32.8	6	-6	6	104.3	103.1
-7	-11	6	13.7	14.3	8	-6	5	24.8	24.8
-5	-11	6	46.4	47.9	-11	-5	6	82.0	78.0
-3	-11	6	64.2	64.0	-9	-5	6	44.5	41.5
-1	-11	6	3.5 *	5.0	-7	-5	6	48.2	44.2
1	-11	6	3.5 *	7.0	-5	-5	6	64.0	58.6
3	-11	6	44.9	43.4	-3	-5	6	100.2	103.2
5	-11	6	34.7	31.8	-1	-5	6	254.8	260.1
-8	-10	6	86.6	82.4	1	-5	6	10.8	12.3
-6	-10	6	42.6	40.0	3	-5	6	77.6	74.8
-4	-10	6	79.6	75.8	5	-5	6	74.1	71.0
-2	-10	6	56.4	52.7	7	-5	6	8.2	6.5
0	-10	6	137.9	135.7	9	-5	6	69.7	66.2
2	-10	6	134.0	136.4	-12	-4	6	23.1	23.0
4	-10	6	89.9	89.0	-10	-4	6	80.9	84.2
6	-10	6	3.6 *	0.7	-8	-4	6	32.0	32.4
-9	-9	6	89.8	85.5	-6	-4	6	86.8	87.3
-7	-9	6	136.7	137.9	-4	-4	6	31.4	35.2
-5	-9	6	149.1	148.0	-2	-4	6	70.0	69.8
-3	-9	6	69.3	65.6	0	-4	6	51.0	51.7
-1	-9	6	165.2	166.5	2	-4	6	47.1	45.5
1	-9	6	152.0	154.7	4	-4	6	117.6	119.5
3	-9	6	41.4	38.7	6	-4	6	3.1 *	3.1
5	-9	6	59.0	63.1	8	-4	6	41.1	41.1
7	-9	6	68.0	70.1	-11	-3	6	31.4	31.3
-10	-8	6	51.9	59.4	-9	-3	6	18.9	14.8
-8	-8	6	65.0	67.6	-7	-3	6	3.1 *	11.5
-6	-8	6	10.6	13.6	-5	-3	6	23.5	25.0
-4	-8	6	35.9	40.9	-3	-3	6	24.1	23.7
-2	-8	6	24.5	28.4	1	-3	6	32.1	31.1
0	-8	6	74.1	75.1	3	-3	6	50.6	50.6
2	-8	6	16.2	12.6	5	-3	6	30.3	30.9
4	-8	6	31.2	30.6	7	-3	6	17.0	15.4
6	-8	6	9.3	10.4	9	-3	6	35.5	35.4
8	-8	6	14.4	15.8	-12	-2	6	42.1	44.3
-11	-7	6	17.0	14.0	-10	-2	6	27.2	30.4
-9	-7	6	6.9	7.8	-8	-2	6	31.0	30.4
-7	-7	6	22.0	21.0	-6	-2	6	44.9	43.5
-5	-7	6	51.1	55.5	-4	-2	6	9.7	12.0
-3	-7	6	21.0	21.4	2	-2	6	62.4	65.1
-1	-7	6	54.1	53.5	4	-2	6	88.0	89.4
1	-7	6	38.9	39.4	6	-2	6	49.1	49.8
3	-7	6	7.9	7.1	8	-2	6	95.2	94.4
5	-7	6	24.1	23.7	10	-2	6	7.4	1.3
7	-7	6	24.9	22.0	-11	-1	6	3.5 *	7.4
-10	-6	6	25.9	28.1	-9	-1	6	24.5	24.8
-8	-6	6	141.6	145.5	-7	-1	6	70.8	74.4
-6	-6	6	46.2	49.2	-5	-1	6	15.7	13.0
-4	-6	6	92.2	92.3	-3	-1	6	81.9	84.1
-2	-6	6	38.8	38.3	1	-1	6	31.2	28.3

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	-1	6	35.3	37.4	0	4	6	74.4	75.0
5	-1	6	2.9 *	0.7	2	4	6	124.2	123.3
7	-1	6	80.5	79.8	4	4	6	46.0	48.9
9	-1	6	53.6	51.8	6	4	6	9.1	11.5
-12	0	6	3.5 *	5.0	8	4	6	22.2	23.9
-10	0	6	3.5 *	6.3	-9	5	6	46.0	45.8
-8	0	6	66.3	67.9	-7	5	6	7.2	7.7
-6	0	6	16.2	19.0	-5	5	6	19.0	19.7
-4	0	6	59.6	64.3	-3	5	6	94.5	98.9
-2	0	6	86.1	87.1	-1	5	6	34.6	38.2
0	0	6	37.3	34.7	1	5	6	27.9	25.8
2	0	6	4.6	0.8	3	5	6	104.0	102.7
4	0	6	27.7	27.7	5	5	6	39.2	39.1
6	0	6	32.9	31.4	7	5	6	22.0	27.5
8	0	6	52.4	52.8	-8	6	6	7.3	4.6
10	0	6	23.7	22.9	-6	6	6	27.7	26.0
-11	1	6	31.3	30.1	-4	6	6	34.1	32.5
-9	1	6	11.3	12.7	-2	6	6	38.4	32.4
-7	1	5	35.6	38.2	0	6	6	3.3 *	6.9
-5	1	6	134.5	108.4	2	6	6	11.4	13.0
-3	1	6	10.2	11.9	4	6	6	47.7	48.9
-1	1	6	4.9	4.2	6	6	6	20.7	21.6
1	1	6	12.3	12.4	8	6	6	3.7 *	0.3
3	1	6	7.8	0.4	-7	7	6	7.7	11.9
5	1	6	67.7	68.0	-5	7	6	6.1	5.2
7	1	6	55.3	54.7	-3	7	6	9.8	4.1
9	1	6	54.9	56.6	-1	7	6	9.8	4.0
-10	2	6	7.6	10.0	1	7	6	35.0	34.5
-8	2	6	24.6	25.8	3	7	6	62.4	60.1
-6	2	6	13.0	10.8	5	7	6	17.8	17.7
-4	2	6	38.0	39.9	7	7	6	25.4	30.9
-2	2	6	142.3	141.6	-6	8	6	3.7 *	7.1
0	2	6	50.9	53.8	-4	8	6	78.2	72.8
2	2	6	93.5	87.3	-2	8	6	37.5	31.0
4	2	6	111.5	106.9	0	8	6	20.7	15.3
6	2	6	92.4	91.4	2	8	6	3.5 *	2.7
8	2	6	105.5	104.4	4	8	6	10.7	10.7
-11	3	6	63.4	59.7	6	8	6	19.1	14.7
-9	3	6	118.8	115.5	-5	9	6	72.9	71.0
-7	3	6	47.6	53.0	-3	9	6	13.5	17.1
-5	3	6	253.4	258.5	-1	9	6	87.0	91.2
-3	3	6	200.6	202.0	1	9	6	25.8	21.0
-1	3	6	171.4	172.1	3	9	6	54.1	57.3
1	3	6	202.1	201.4	-2	10	6	50.6	49.9
3	3	6	82.9	80.9	0	10	6	29.1	27.2
5	3	6	267.9	274.2	2	10	6	51.1	47.3
7	3	6	28.2	30.2	-5	-13	7	126.5	119.5
9	3	6	48.2	51.8	-3	-13	7	92.7	87.0
-10	4	6	18.6	16.4	-1	-13	7	63.5	62.6
-8	4	6	56.5	56.2	1	-13	7	82.5	79.3
-6	4	6	109.9	110.0	-6	-12	7	58.2	58.2
-4	4	6	113.6	110.2	-4	-12	7	9.0	9.3
-2	4	6	244.1	245.1	-2	-12	7	41.5	42.1

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	-12	7	3.6 *	10.4	8	-6	7	78.8	76.4
2	-12	7	3.6 *	2.1	-11	-5	7	3.7 *	4.6
-7	-11	7	31.5	29.9	-9	-5	7	38.1	36.9
-5	-11	7	8.4	10.6	-7	-5	7	7.2	9.2
-3	-11	7	3.3 *	3.8	-5	-5	7	32.9	30.7
-1	-11	7	37.3	38.0	-3	-5	7	52.1	49.7
1	-11	7	56.3	55.4	-1	-5	7	44.8	47.3
3	-11	7	61.8	62.8	1	-5	7	21.5	22.1
5	-11	7	41.8	42.9	3	-5	7	22.5	22.1
-3	-10	7	87.5	91.4	5	-5	7	27.7	28.4
-6	-10	7	27.1	25.4	7	-5	7	19.7	16.2
-4	-10	7	80.0	80.0	9	-5	7	18.6	18.9
0	-10	7	79.5	82.6	-12	-4	7	12.1	15.2
2	-10	7	30.8	27.4	-10	-4	7	11.4	7.1
4	-10	7	3.6 *	7.7	-8	-4	7	3.3 *	2.9
6	-10	7	66.5	62.5	-6	-4	7	27.7	27.8
-9	-9	7	16.6	20.9	-4	-4	7	38.5	41.1
-7	-9	7	128.5	129.2	-2	-4	7	14.0	13.6
-5	-9	7	44.9	40.9	0	-4	7	13.7	11.3
-3	-9	7	26.4	23.5	2	-4	7	24.9	24.9
-1	-9	7	74.2	71.9	4	-4	7	47.2	45.9
1	-9	7	45.8	43.9	6	-4	7	60.5	61.0
3	-9	7	152.6	152.5	8	-4	7	38.2	36.6
5	-9	7	35.8	34.2	-11	-3	7	32.3	30.1
7	-9	7	72.4	69.3	-9	-3	7	56.4	57.9
-10	-8	7	21.5	19.9	-7	-3	7	37.2	38.3
-8	-8	7	8.0	9.0	-5	-3	7	75.0	77.2
-6	-8	7	58.8	58.7	1	-3	7	19.6	20.0
-4	-8	7	52.9	57.1	3	-3	7	40.2	39.5
-2	-8	7	9.6	9.7	5	-3	7	42.1	44.7
0	-8	7	14.0	12.3	7	-3	7	40.9	39.4
2	-8	7	6.5	9.1	9	-3	7	41.8	40.2
4	-8	7	3.4 *	0.2	-12	-2	7	48.3	54.2
6	-8	7	10.6	9.8	-10	-2	7	49.6	43.9
-11	-7	7	3.9 *	4.1	-8	-2	7	63.7	66.5
-9	-7	7	37.4	34.9	-6	-2	7	69.1	71.6
-7	-7	7	3.4 *	2.5	-4	-2	7	2.7 *	2.6
-5	-7	7	55.6	55.2	2	-2	7	121.4	125.1
-3	-7	7	74.9	76.2	4	-2	7	9.7	8.5
-1	-7	7	30.6	32.0	6	-2	7	101.4	100.4
1	-7	7	20.0	19.6	8	-2	7	72.9	71.3
3	-7	7	53.8	55.3	-11	-1	7	107.1	102.4
5	-7	7	3.1 *	2.2	-9	-1	7	97.4	95.0
7	-7	7	16.4	15.7	-7	-1	7	32.4	29.5
-10	-6	7	41.5	39.8	-5	-1	7	97.7	97.9
-8	-6	7	98.6	97.2	-3	-1	7	31.9	31.5
-6	-6	7	10.9	14.5	1	-1	7	127.9	128.9
-4	-6	7	47.1	44.5	3	-1	7	114.2	114.1
-2	-6	7	63.5	59.3	5	-1	7	138.9	140.1
0	-6	7	11.5	11.7	7	-1	7	85.7	87.4
2	-6	7	120.2	124.4	9	-1	7	109.7	106.6
4	-6	7	30.1	29.9	-10	0	7	85.0	81.5
6	-6	7	87.7	85.2	-8	0	7	185.4	191.1

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-6	0	7	30.7	27.6	-1	5	7	35.0	39.8
-4	0	7	215.2	218.9	1	5	7	17.0	22.0
-2	0	7	275.3	278.7	3	5	7	85.0	86.5
0	0	7	206.7	208.6	5	5	7	55.9	52.5
2	0	7	132.9	137.8	7	5	7	108.3	105.1
4	0	7	10.0	4.3	-8	6	7	16.8	14.2
6	0	7	144.5	145.3	-6	6	7	9.0	6.7
8	0	7	44.9	44.8	-4	6	7	49.1	49.7
11	1	7	26.3	28.6	-2	6	7	44.8	44.9
-9	1	7	38.8	42.1	0	6	7	58.6	58.7
-7	1	7	41.6	44.1	2	6	7	17.9	14.4
-5	1	7	46.4	47.7	4	6	7	92.1	86.3
-3	1	7	17.8	17.0	6	6	7	3.7	*
-1	1	7	58.9	58.4	-7	7	7	3.7	*
1	1	7	77.0	76.9	-5	7	7	31.6	30.9
3	1	7	9.3	8.2	-3	7	7	6.6	6.7
5	1	7	36.2	35.7	-1	7	7	10.3	13.1
7	1	7	31.2	32.0	1	7	7	15.9	9.4
9	1	7	16.8	17.1	3	7	7	3.6	*
10	2	7	6.5	8.5	5	7	7	21.1	21.6
-8	2	7	25.7	24.9	-6	8	7	44.4	44.7
-6	2	7	19.9	20.7	-4	8	7	40.0	43.6
-4	2	7	65.9	66.3	-2	8	7	44.5	48.7
-2	2	7	79.8	80.7	0	8	7	25.0	30.4
0	2	7	26.5	22.5	2	8	7	11.0	13.9
2	2	7	17.9	15.3	4	8	7	8.1	4.9
4	2	7	46.7	44.7	-3	9	7	3.8	*
6	2	7	24.0	23.5	-1	9	7	40.8	2.8
8	2	7	24.0	24.1	1	9	7	12.9	37.2
-9	3	7	39.0	41.1	3	9	7	94.1	12.0
-7	3	7	55.3	56.7	-3	-13	8	3.8	*
-5	3	7	59.0	59.8	-1	-13	8	6.9	6.2
-3	3	7	64.2	66.4	-6	-12	8	64.0	65.0
-1	3	7	6.7	4.2	-4	-12	8	15.3	14.3
1	3	7	14.0	13.8	-2	-12	8	64.5	62.2
3	3	7	42.5	42.5	0	-12	8	23.1	21.8
5	3	7	20.3	22.7	2	-12	8	14.9	21.9
7	3	7	30.1	31.9	-7	-11	8	9.7	11.1
9	3	7	39.2	31.6	-5	-11	8	6.8	5.6
-10	4	7	6.6	9.3	-3	-11	8	11.8	14.8
-8	4	7	10.3	8.3	-1	-11	8	64.9	65.8
-6	4	7	3.3	*	1	-11	8	19.5	15.1
-4	4	7	48.6	47.1	3	-11	8	49.7	44.2
-2	4	7	34.2	38.3	-8	-10	8	42.6	38.5
0	4	7	89.2	85.5	-6	-10	8	49.6	48.6
2	4	7	74.2	74.6	-4	-10	8	21.6	23.8
4	4	7	9.5	9.2	-2	-10	8	35.8	34.1
6	4	7	24.1	20.2	0	-10	8	65.8	65.4
8	4	7	18.1	19.5	2	-10	8	36.0	35.5
-9	5	7	20.1	23.3	4	-10	8	8.5	3.6
-7	5	7	148.8	148.4	-9	-9	8	3.5	*
-5	5	7	3.3	*	-7	-9	8	11.4	1.0
-3	5	7	84.9	87.8	-5	-9	8	13.0	

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-3	-9	8	9.0	8.2	8	-4	8	92.4	81.7
-1	-9	8	28.9	30.5	-11	-3	8	48.2	51.3
1	-9	8	54.1	53.1	-9	-3	8	80.9	88.3
3	-9	8	44.4	44.9	-7	-3	8	61.4	67.0
5	-9	8	59.9	58.9	-5	-3	8	81.0	88.6
-10	-8	8	20.5	14.6	-3	-3	8	55.6	59.0
-8	-8	8	20.5	16.6	1	-3	8	6.6	4.0
-6	-8	8	8.3	5.8	3	-3	8	47.9	48.8
-4	-8	8	22.7	24.7	5	-3	8	35.9	37.7
-2	-8	8	39.1	40.4	7	-3	8	22.3	20.9
0	-8	8	31.3	32.7	9	-3	8	14.4	14.0
2	-8	8	17.3	17.8	-12	-2	8	49.2	51.3
4	-8	8	46.2	47.1	-10	-2	8	13.1	16.9
6	-8	8	50.9	49.8	-8	-2	8	10.4	9.0
-11	-7	8	41.5	38.8	-6	-2	8	18.7	20.2
-9	-7	8	30.7	26.4	-4	-2	8	41.1	41.9
-7	-7	8	76.0	78.1	0	-2	8	123.5	129.5
-5	-7	8	60.1	60.8	2	-2	8	35.8	37.1
-3	-7	8	5.3	0.0	4	-2	8	30.9	28.7
-1	-7	8	66.0	66.2	6	-2	8	28.9	31.0
1	-7	8	24.0	25.8	8	-2	8	17.5	13.0
3	-7	8	14.4	14.1	-11	-1	8	45.5	47.7
5	-7	8	3.3 *	7.0	-9	-1	8	18.5	23.1
7	-7	8	9.1	6.8	-7	-1	8	31.2	33.5
-10	-6	8	22.4	24.5	-5	-1	8	82.7	88.3
-8	-6	8	27.7	31.4	-3	-1	8	25.8	26.2
-6	-6	8	72.4	74.9	1	-1	8	90.6	93.5
-4	-6	8	41.1	42.2	3	-1	8	31.2	31.9
-2	-6	8	101.2	99.5	5	-1	8	23.1	25.5
0	-6	8	33.1	34.8	7	-1	8	28.1	29.1
2	-6	8	12.2	13.1	9	-1	8	28.2	23.6
4	-6	8	12.3	11.3	-10	0	8	13.9	13.9
6	-6	8	71.0	70.9	-8	0	8	128.9	131.5
8	-6	8	22.2	21.8	-6	0	8	65.8	70.6
-11	-5	8	35.6	37.7	-4	0	8	72.1	74.7
-9	-5	8	32.3	35.2	-2	0	8	19.3	19.9
-7	-5	8	123.9	127.9	0	0	8	106.3	108.1
-5	-5	8	3.0 *	3.2	2	0	8	49.6	50.8
-3	-5	8	21.7	17.1	4	0	8	115.6	113.5
-1	-5	8	104.2	106.4	6	0	8	18.8	21.3
1	-5	8	124.1	128.1	8	0	8	3.5 *	0.3
3	-5	8	198.0	200.9	-11	1	8	73.3	77.4
5	-5	8	5.6	1.3	-9	1	8	54.5	57.0
7	-5	8	80.8	79.5	-7	1	8	17.0	18.7
-10	-4	8	61.9	57.4	-5	1	8	157.2	159.6
-8	-4	8	168.0	172.8	-3	1	8	155.3	158.0
-6	-4	8	186.7	196.1	-1	1	8	104.3	108.6
-4	-4	8	165.8	165.3	1	1	8	3.1 *	6.4
-2	-4	8	121.7	122.2	3	1	8	3.2 *	0.1
0	-4	8	292.5	302.4	5	1	8	40.1	40.7
2	-4	8	185.5	191.5	7	1	8	73.6	75.9
4	-4	8	104.6	106.9	-10	2	8	24.5	24.4
6	-4	8	33.0	34.6	-8	2	8		

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-6	2	8	82.1	80.9	-6	-12	9	36.4	32.3
-4	2	8	59.0	59.5	-4	-12	9	27.8	25.0
-2	2	8	83.3	86.8	-2	-12	9	23.0	22.1
0	2	8	65.2	66.7	0	-12	9	9.8	10.7
2	2	8	35.4	34.5	2	-12	9	19.5	17.7
4	2	8	120.5	122.5	-7	-11	9	56.5	51.4
6	2	8	13.6	13.3	-5	-11	9	37.7	35.6
8	2	8	25.6	27.6	-3	-11	9	36.1	37.7
-9	3	8	30.6	34.1	-1	-11	9	8.1	3.0
-7	3	8	57.2	57.8	1	-11	9	3.5 *	11.3
-5	3	8	9.9	4.2	3	-11	9	3.6 *	2.4
-3	3	8	10.0	13.1	-8	-10	9	3.6 *	3.1
-1	3	8	50.0	53.7	-6	-10	9	28.8	29.8
1	3	8	19.6	13.9	-4	-10	9	31.1	31.5
3	3	8	3.2 *	11.8	-2	-10	9	31.7	34.7
5	3	8	56.0	60.7	0	-10	9	7.6	11.0
7	3	8	18.2	20.5	2	-10	9	25.7	28.5
-8	4	8	31.8	35.1	4	-10	9	58.3	52.8
-6	4	8	8.5	6.2	-9	-9	9	30.6	25.4
-4	4	8	39.4	38.4	-7	-9	9	20.5	19.0
-2	4	8	37.4	39.4	-5	-9	9	9.3	5.5
0	4	8	31.4	31.2	-3	-9	9	56.2	53.3
2	4	8	30.9	27.1	-1	-9	9	48.3	49.8
4	4	8	3.3 *	0.4	1	-9	9	74.9	73.5
6	4	8	26.0	28.6	3	-9	9	47.7	47.3
-9	5	8	7.8	7.1	5	-9	9	71.1	65.7
-7	5	8	26.0	26.5	-10	-8	9	29.6	23.7
-5	5	8	3.2 *	0.6	-8	-8	9	57.0	50.8
-3	5	8	11.9	8.6	-6	-8	9	144.8	147.4
-1	5	8	3.2 *	0.9	-4	-8	9	170.0	168.2
1	5	8	23.1	27.9	-2	-8	9	154.3	151.7
3	5	8	21.3	22.6	0	-8	9	87.2	83.5
5	5	8	14.9	10.6	2	-8	9	130.0	130.0
7	5	8	84.1	84.4	4	-8	9	151.9	153.0
-8	6	8	45.4	46.9	6	-8	9	45.3	45.4
-6	6	8	19.5	24.7	-9	-7	9	54.7	59.0
-4	6	8	68.7	69.9	-7	-7	9	95.3	96.8
-2	6	8	35.4	36.3	-5	-7	9	150.5	152.3
0	6	8	3.3 *	5.3	-3	-7	9	65.5	65.5
2	6	8	31.6	36.5	-1	-7	9	52.4	55.1
4	6	8	12.7	5.9	1	-7	9	71.0	74.6
6	6	8	45.5	52.1	3	-7	9	21.9	24.1
-5	7	8	37.7	32.4	5	-7	9	26.9	26.8
-3	7	8	9.5	0.1	7	-7	9	33.0	32.0
-1	7	8	41.2	37.9	-10	-6	9	24.3	28.6
1	7	8	3.5 *	2.2	-8	-6	9	47.1	51.5
3	7	8	35.0	31.3	-6	-6	9	24.3	23.0
5	7	8	74.0	68.2	-4	-6	9	92.5	93.5
-4	8	8	43.8	44.4	-2	-6	9	38.3	42.3
-2	8	8	125.4	119.8	0	-6	9	53.6	53.6
0	8	8	33.8	28.5	2	-6	9	61.4	62.7
2	8	8	88.3	83.6	4	-6	9	22.1	23.3
-3	-13	9	12.3	6.4	6	-6	9	7.5	6.3

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-11	-5	9	22.0	30.6	0	0	9	37.4	35.0
-9	-5	9	21.8	16.0	2	0	9	81.0	81.0
-7	-5	9	101.9	107.9	4	0	9	11.6	12.3
-5	-5	9	39.0	37.3	6	0	9	33.8	36.0
-3	-5	9	33.3	35.2	8	0	9	20.4	21.9
-1	-5	9	62.6	66.7	-9	1	9	50.0	51.7
1	-5	9	125.3	126.9	-7	1	9	3.2 *	1.6
3	-5	9	53.4	55.6	-5	1	9	24.0	26.4
5	-5	9	31.5	30.9	-3	1	9	37.8	38.0
7	-5	9	22.3	20.6	-1	1	9	32.3	31.5
-10	-4	9	83.8	83.3	1	1	9	30.3	33.1
-8	-4	9	85.0	88.2	3	1	9	44.9	50.0
-6	-4	9	3.1 *	6.6	5	1	9	22.4	24.1
-4	-4	9	143.5	146.8	7	1	9	43.6	44.4
-2	-4	9	137.5	140.6	-10	2	9	40.8	38.2
0	-4	9	146.2	151.4	-8	2	9	21.5	21.9
2	-4	9	17.3	14.2	-6	2	9	33.6	36.7
4	-4	9	3.2 *	6.2	-4	2	9	74.6	77.2
6	-4	9	88.1	85.0	-2	2	9	40.3	41.8
8	-4	9	18.7	21.0	0	2	9	32.1	35.1
-11	-3	9	48.2	47.6	2	2	9	15.3	13.1
-9	-3	9	86.8	93.7	4	2	9	7.4	4.5
-7	-3	9	82.3	83.5	6	2	9	3.6 *	3.5
-5	-3	9	67.2	71.7	-9	3	9	35.0	34.9
-3	-3	9	10.7	8.9	-7	3	9	13.8	13.8
1	-3	9	23.5	23.7	-5	3	9	19.9	17.3
3	-3	9	137.3	139.3	-3	3	9	9.7	9.2
5	-3	9	85.3	87.8	-1	3	9	32.6	31.4
7	-3	9	30.2	30.0	1	3	9	25.4	23.6
-10	-2	9	43.6	41.3	3	3	9	24.9	24.2
-8	-2	9	54.1	53.7	5	3	9	46.7	46.8
-6	-2	9	84.7	88.0	7	3	9	78.0	75.9
-4	-2	9	18.0	21.8	-8	4	9	103.4	96.7
0	-2	9	18.5	20.1	-6	4	9	8.4	10.6
2	-2	9	63.0	66.6	-4	4	9	13.6	11.5
4	-2	9	49.6	49.9	-2	4	9	89.3	87.2
6	-2	9	33.5	33.2	0	4	9	86.0	84.3
8	-2	9	47.8	47.5	2	4	9	123.2	116.7
-11	-1	9	23.3	21.1	4	4	9	35.9	33.0
-9	-1	9	13.7	14.3	6	4	9	92.5	91.7
-7	-1	9	37.5	40.5	-7	5	9	29.0	30.3
-5	-1	9	58.7	58.8	-5	5	9	122.9	122.7
-3	-1	9	34.7	35.1	-3	5	9	68.1	67.8
-1	-1	9	38.8	40.5	-1	5	9	220.9	221.7
1	-1	9	13.6	16.8	1	5	9	72.3	75.5
3	-1	9	6.1	2.2	3	5	9	70.6	76.4
5	-1	9	46.1	48.9	5	5	9	58.8	63.3
7	-1	9	22.1	24.2	-6	6	9	19.8	18.3
-10	0	9	11.5	12.3	-4	6	9	48.9	44.7
-8	0	9	39.4	39.9	-2	6	9	36.7	35.2
-6	0	9	41.5	45.4	0	6	9	16.2	17.0
-4	0	9	3.1 *	5.9	2	6	9	22.5	22.7
-2	0	9	19.4	18.9	4	6	9	38.9	34.7

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-5	7	9	7.0	3.9	2	-6	10	46.7	47.6
-1	7	9	56.2	54.1	4	-6	10	22.7	23.9
-1	7	9	84.3	79.7	6	-6	10	28.2	26.5
1	7	9	22.1	23.7	-11	-5	10	29.8	29.3
3	7	9	3.8 *	7.4	-9	-5	10	19.1	18.1
-2	8	9	24.7	27.2	-7	-5	10	30.8	34.0
0	8	9	20.3	24.3	-5	-5	10	34.9	32.2
-4	-12	10	73.2	74.3	-3	-5	10	13.3	11.5
-2	-12	10	129.4	124.4	-1	-5	10	5.4	3.9
0	-12	10	66.5	61.5	1	-5	10	37.3	37.9
-7	-11	10	66.3	65.6	3	-5	10	41.8	42.9
-5	-11	10	109.2	107.0	5	-5	10	11.5	6.7
-3	-11	10	108.7	105.1	7	-5	10	22.4	21.3
-1	-11	10	74.6	76.2	-10	-4	10	12.7	7.6
1	-11	10	45.2	45.1	-8	-4	10	57.3	55.2
3	-11	10	52.4	55.1	-6	-4	10	17.7	16.3
-8	-10	10	50.0	54.7	-4	-4	10	15.6	14.3
-6	-10	10	75.0	28.0	0	-4	10	48.5	50.1
-4	-10	10	33.5	29.5	2	-4	10	49.2	52.3
-2	-10	10	18.9	16.6	4	-4	10	57.2	57.9
0	-10	10	26.5	26.3	6	-4	10	75.2	75.6
2	-10	10	30.7	34.4	-11	-3	10	3.5 *	4.1
4	-10	10	45.5	44.4	-9	-3	10	32.6	33.8
-2	-9	10	41.7	35.6	-7	-3	10	59.0	61.8
-7	-9	10	82.7	89.4	-5	-3	10	19.4	19.9
-5	-9	10	44.3	44.4	1	-3	10	45.2	45.2
-3	-9	10	81.6	83.5	3	-3	10	22.0	24.3
-1	-9	10	43.1	42.8	5	-3	10	48.3	47.9
1	-9	10	18.7	20.3	7	-3	10	27.8	27.9
3	-9	10	10.7	4.5	-10	-2	10	11.7	7.2
5	-9	10	27.5	24.7	-8	-2	10	55.0	55.7
-10	-8	10	123.5	124.2	-6	-2	10	36.3	36.6
-8	-8	10	34.4	37.0	-4	-2	10	5.2	0.5
-6	-8	10	91.4	95.2	0	-2	10	15.0	13.7
-4	-8	10	47.8	45.7	2	-2	10	19.0	16.6
-2	-8	10	30.2	32.3	4	-2	10	12.9	9.9
0	-8	10	67.1	70.1	6	-2	10	47.2	46.1
2	-8	10	43.2	44.0	-11	-1	10	46.6	47.5
4	-8	10	116.7	115.2	-9	-1	10	17.4	21.3
-9	-7	10	10.8	8.0	-7	-1	10	46.0	48.0
-7	-7	10	59.7	55.2	-5	-1	10	59.5	61.6
-5	-7	10	23.1	23.6	-3	-1	10	38.7	39.8
-3	-7	10	126.6	125.6	-1	-1	10	19.7	21.0
-1	-7	10	9.1	11.5	1	-1	10	49.3	53.4
1	-7	10	78.5	74.7	3	-1	10	18.3	19.2
3	-7	10	60.3	60.2	5	-1	10	24.7	27.6
5	-7	10	30.4	30.3	7	-1	10	60.4	59.6
-10	-6	10	27.7	24.0	-10	0	10	10.0	11.2
-8	-6	10	39.5	37.4	-8	0	10	57.3	56.2
-6	-6	10	38.8	35.0	-6	0	10	27.3	27.6
-4	-6	10	10.0	6.9	-4	0	10	62.3	57.7
-2	-6	10	28.5	28.3	-2	0	10	30.3	32.3
0	-6	10	5.9	1.6	0	0	10	77.6	75.7

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	10	91.7	91.7	-8	-10	11	15.6	13.5
4	0	10	96.2	93.9	-6	-10	11	3.6 *	2.8
6	0	10	66.0	63.4	-4	-10	11	8.4	8.4
-9	1	10	27.6	22.2	-2	-10	11	20.0	19.2
-7	1	10	194.0	189.9	0	-10	11	20.0	18.5
-5	1	10	90.7	90.7	2	-10	11	24.2	25.0
-3	1	10	93.9	94.5	-9	-9	11	18.9	18.9
-1	1	10	162.7	159.7	-7	-9	11	26.4	28.1
1	1	10	173.7	175.8	-5	-9	11	14.4	14.1
3	1	10	171.9	177.8	-3	-9	11	17.1	14.6
5	1	10	9.8	1.6	-1	-9	11	26.0	26.3
7	1	10	87.2	90.2	1	-9	11	29.7	28.6
-8	2	10	94.2	89.4	3	-9	11	7.0	5.7
-6	2	10	91.5	93.8	-8	-8	11	20.0	12.5
-4	2	10	76.3	73.7	-6	-8	11	25.3	21.8
-2	2	10	43.6	44.3	-4	-8	11	50.3	48.6
0	2	10	106.0	108.1	-2	-8	11	28.2	27.6
2	2	10	6.3	4.9	0	-8	11	25.9	23.3
4	2	10	16.1	21.3	2	-8	11	50.5	51.2
6	2	10	3.7 *	0.4	4	-8	11	68.2	69.0
-9	3	10	19.7	22.0	-9	-7	11	6.4	6.3
-7	3	10	48.9	47.6	-7	-7	11	48.2	48.8
-5	3	10	8.4	9.1	-5	-7	11	8.4	10.2
-3	3	10	9.0	8.2	-3	-7	11	15.4	15.9
-1	3	10	95.8	94.9	-1	-7	11	53.6	57.3
1	3	10	57.3	58.4	1	-7	11	3.3 *	0.1
3	3	10	64.2	66.5	3	-7	11	21.9	20.6
5	3	10	10.9	3.0	5	-7	11	11.9	12.4
-8	4	10	21.0	19.1	-10	-6	11	20.0	20.3
-6	4	10	14.7	10.1	-8	-6	11	46.9	50.1
-4	4	10	74.9	67.5	-6	-6	11	3.5 *	6.3
-2	4	10	29.7	33.0	-4	-6	11	37.5	37.9
0	4	10	17.0	12.9	-2	-6	11	19.0	16.1
2	4	10	17.3	18.2	0	-6	11	7.5	4.8
4	4	10	32.1	31.7	2	-6	11	11.9	12.4
-7	5	10	26.2	25.5	4	-6	11	72.8	69.3
-5	5	10	28.7	27.9	6	-6	11	14.6	11.9
-3	5	10	37.6	34.7	-9	-5	11	24.9	21.6
-1	5	10	3.4 *	0.8	-7	-5	11	62.2	63.2
1	5	10	70.9	65.2	-5	-5	11	45.0	48.2
3	5	10	30.5	27.7	-3	-5	11	30.8	29.3
-4	6	10	8.9	5.9	-1	-5	11	18.1	18.0
-2	6	10	19.8	14.5	1	-5	11	7.7	4.9
0	6	10	26.9	24.8	3	-5	11	49.3	50.7
2	6	10	21.0	19.6	5	-5	11	13.2	14.7
-3	7	10	96.9	96.5	-10	-4	11	31.6	34.5
-1	7	10	45.8	34.3	-8	-4	11	39.0	34.6
-4	-12	11	55.8	50.3	-6	-4	11	21.4	22.4
-2	-12	11	89.4	93.4	-4	-4	11	12.1	11.9
-5	-11	11	49.0	41.4	0	-4	11	36.7	38.3
-3	-11	11	61.0	58.7	2	-4	11	3.3 *	1.8
-1	-11	11	35.5	37.2	4	-4	11	111.4	109.1
1	-11	11	98.9	95.8	6	-4	11	44.6	44.6

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	
-9	-3	11	12.6	8.6	-6	4	11	24.2	19.5	
-7	-3	11	64.1	61.1	-4	4	11	33.8	29.6	
-5	-3	11	112.4	117.9	-2	4	11	29.7	31.0	
1	-3	11	144.1	144.5	0	4	11	8.2	5.1	
3	-3	11	118.9	120.9	2	4	11	54.7	52.1	
5	-3	11	114.9	115.7	4	4	11	10.4	7.9	
-10	-2	11	57.7	53.2	-5	5	11	30.5	30.1	
-8	-2	11	63.7	64.1	-3	5	11	16.8	8.5	
-6	-2	11	159.0	163.2	-1	5	11	3.5	* 0.5	
-4	-2	11	150.8	156.5	1	5	11	20.7	20.9	
2	-2	11	60.1	61.8	-2	6	11	14.6	9.6	
4	-2	11	104.5	110.7	0	6	11	38.1	38.6	
6	-2	11	62.7	67.4	-5	-11	12	20.4	18.6	
-9	-1	11	3.6	*	10.3	-3	-11	12	3.6	*
-9	-1	11	44.1	49.2	-1	-11	12	68.0	67.5	
-7	-1	11	15.0	18.7	-6	-10	12	3.7	*	
-5	-1	11	15.7	16.0	-4	-10	12	56.5	57.1	
-3	-1	11	56.3	57.8	-2	-10	12	33.1	33.7	
-1	-1	11	17.6	17.8	0	-10	12	21.9	24.1	
1	-1	11	60.1	57.8	2	-10	12	13.9	13.8	
3	-1	11	79.2	79.8	-7	-9	12	44.8	41.2	
5	-1	11	8.9	3.3	-5	-9	12	26.4	20.3	
-10	0	11	3.6	*	2.2	-3	-9	12	48.0	48.0
-8	0	11	17.6	17.3	-1	-9	12	7.4	5.0	
-6	0	11	38.4	39.9	1	-9	12	25.8	25.8	
-4	0	11	60.6	57.4	3	-9	12	7.7	3.7	
-2	0	11	17.9	16.8	-8	-8	12	29.4	24.7	
0	0	11	42.0	40.3	-6	-8	12	13.7	15.9	
2	0	11	38.7	37.1	-4	-8	12	39.0	38.8	
4	0	11	36.6	36.7	-2	-8	12	14.0	16.0	
6	0	11	17.0	15.6	0	-8	12	24.2	23.3	
-9	1	11	7.2	3.8	2	-8	12	40.3	38.9	
-7	1	11	72.7	68.3	4	-8	12	19.2	17.8	
-5	1	11	14.4	15.4	-9	-7	12	63.8	58.9	
-3	1	11	16.1	17.5	-7	-7	12	34.1	35.1	
-1	1	11	11.2	2.2	-5	-7	12	34.6	31.7	
1	1	11	64.6	63.9	-3	-7	12	80.5	80.3	
3	1	11	25.7	21.9	-1	-7	12	119.6	120.5	
5	1	11	42.8	44.5	1	-7	12	62.0	58.1	
-8	2	11	35.4	31.8	3	-7	12	30.6	29.2	
-6	2	11	64.8	61.3	-8	-6	12	81.3	80.3	
-4	2	11	48.8	49.1	-6	-6	12	86.5	83.4	
-2	2	11	104.1	98.9	-4	-6	12	167.7	164.2	
0	2	11	95.9	96.6	-2	-6	12	171.5	168.8	
2	2	11	12.6	11.0	0	-6	12	94.5	97.5	
4	2	11	3.7	*	9.4	2	-6	12	83.6	83.6
-7	3	11	9.8	2.6	4	-6	12	45.7	48.5	
-5	3	11	94.8	92.9	-9	-5	12	29.1	33.6	
-3	3	11	29.0	29.9	-7	-5	12	55.8	63.5	
-1	3	11	21.1	21.2	-5	-5	12	46.4	48.1	
1	3	11	55.3	58.2	-3	-5	12	14.5	12.5	
3	3	11	42.2	38.1	-1	-5	12	5.5	2.2	
5	3	11	110.2	109.5	1	-5	12	21.7	19.5	

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	-5	12	22.1	25.1	1	3	12	8.4	11.0
5	-5	12	25.8	25.4	3	3	12	19.9	20.3
-10	-4	12	23.9	21.6	-4	4	12	3.6 *	12.0
-8	-4	12	23.7	26.2	-2	4	12	44.0	47.6
-6	-4	12	39.6	41.2	0	4	12	11.0	15.9
-4	-4	12	54.8	57.6	2	4	12	19.2	26.9
0	-4	12	39.1	38.5	-1	5	12	14.9	10.8
2	-4	12	25.1	22.4	-6	-10	13	83.5	77.4
4	-4	12	52.1	53.8	-4	-10	13	73.9	70.6
-9	-3	12	14.7	18.9	-2	-10	13	99.9	94.5
-7	-3	12	97.7	100.4	0	-10	13	136.7	134.8
-5	-3	12	48.6	50.8	-7	-9	13	47.7	52.9
1	-3	12	32.7	33.0	-5	-9	13	65.1	61.1
3	-3	12	20.5	21.4	-3	-9	13	60.5	58.9
5	-3	12	28.4	31.6	-1	-9	13	24.0	24.7
-8	-2	12	52.3	56.6	1	-9	13	3.6 *	0.2
-6	-2	12	76.1	76.1	-8	-8	13	25.3	22.9
-4	-2	12	17.5	15.4	-6	-8	13	43.7	43.6
0	-2	12	67.5	68.5	-4	-8	13	8.0	15.7
2	-2	12	30.2	30.5	-2	-8	13	78.3	77.8
4	-2	12	127.3	123.9	0	-8	13	31.6	33.5
-9	-1	12	56.1	55.4	2	-8	13	15.5	13.6
-7	-1	12	9.1	8.8	-7	-7	13	13.2	9.3
-5	-1	12	84.3	84.2	-5	-7	13	30.9	32.7
-3	-1	12	52.0	51.2	-3	-7	13	43.7	43.3
-1	-1	12	72.4	73.8	-1	-7	13	58.4	59.3
1	-1	12	24.2	19.4	1	-7	13	59.4	63.5
3	-1	12	11.8	15.7	3	-7	13	59.9	56.6
5	-1	12	14.8	12.1	-8	-6	13	3.8 *	2.7
-8	0	12	40.2	38.6	-6	-6	13	86.3	84.2
-6	0	12	21.8	17.8	-4	-6	13	50.1	51.2
-4	0	12	8.0	10.3	-2	-6	13	110.6	111.1
-2	0	12	28.3	30.7	0	-6	13	21.5	21.0
0	0	12	25.9	26.3	2	-6	13	31.8	28.3
2	0	12	47.9	44.9	4	-6	13	67.3	62.9
4	0	12	32.6	31.7	-9	-5	13	30.9	28.9
-7	1	12	43.0	43.5	-7	-5	13	35.2	39.2
-5	1	12	21.0	20.7	-5	-5	13	8.6	3.3
-3	1	12	6.5	1.5	-3	-5	13	32.0	30.4
-1	1	12	36.6	41.7	-1	-5	13	11.4	10.0
1	1	12	21.8	15.0	1	-5	13	53.1	48.3
3	1	12	41.1	44.2	3	-5	13	36.1	36.5
-8	2	12	8.5	9.5	-8	-4	13	46.8	43.9
-6	2	12	25.0	24.5	-6	-4	13	18.5	15.9
-4	2	12	3.6 *	6.4	-4	-4	13	20.2	19.3
-2	2	12	32.1	32.7	0	-4	13	23.3	25.7
0	2	12	18.4	15.9	2	-4	13	51.9	52.1
2	2	12	30.8	26.5	4	-4	13	31.1	28.8
4	2	12	27.1	30.4	-9	-3	13	7.2	7.6
-7	3	12	3.7 *	7.4	-7	-3	13	45.7	44.5
-5	3	12	7.4	0.4	-5	-3	13	8.2	0.1
-3	3	12	15.8	9.9	-1	-3	13	6.7	6.5
-1	3	12	7.3	2.6	1	-3	13	7.4	1.3

H	K	L	F(OBS)	F(CALC)
3	-3	13	41.5	43.3
-8	-2	13	8.7	8.9
-6	-2	13	6.5	8.6
-4	-2	13	15.8	17.4
-2	-2	13	6.8	0.2
0	-2	13	22.3	21.3
2	-2	13	31.5	33.4
4	-2	13	35.9	36.3
-7	-1	13	32.1	32.0
-5	-1	13	11.7	14.6
-3	-1	13	16.9	18.6
-1	-1	13	25.8	20.7
1	-1	13	24.7	25.7
3	-1	13	3.7 *	6.2
-2	-	13	52.5	53.1
-6	-	13	49.1	55.5
-4	-	13	46.7	48.3
-2	-	13	17.7	18.2
-	-	13	7.3	4.5
0	-	13	29.6	34.2
-7	1	13	10.8	12.8
-5	1	13	28.2	27.8
-3	1	13	35.4	32.5
-1	1	13	12.5	10.2
1	1	13	3.9 *	3.6
3	1	13	80.4	76.9
-2	2	13	64.1	55.4
-4	2	13	45.7	42.7
-2	2	13	61.2	57.1
2	2	13	88.5	78.4
2	2	13	27.3	23.6
-5	3	13	117.4	112.6
-3	3	13	135.8	134.0
-1	3	13	14.2	16.2
1	3	13	113.3	111.6