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The crystal structures and the phase transformation of Zn–Li silicates

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Abstract

The room-temperature form (α) of colorless transparent synthetic $Zn(Zn_{0.1}Li_{0.6}Si_{0.3})SiO_4$ has monoclinic symmetry with a = 6.340(1), b = 10.516(2), c = 5.011(1)A, β = 90.50(2)°, space group $P2_1/n$, and Z = 4. It transforms at about 400°C to a high-temperature form (β) which is orthorhombic with a = 6.406(3), b = 10.520(8), c = 5.043(2)A, space group $Pmnb$, and Z = 4. The crystal structures for both forms were determined by 3-dimensional Patterson analysis from X-ray intensity data collected at room temperature and at 450°C. The structures were refined by the least-squares methods to a final weighted R = 0.068 (unweighted R = 0.068) and 0.064 (unweighted R = 0.070) for the room-temperature and the high-temperature form respectively.

The high-temperature structure is a tetrahedral framework structure with a sharing coefficient of 3. There are two different tetrahedral sites: T1, an 8-fold site, and T2, a 4-fold site. The T1 site contains all Zn and Li and some Si; the T2 site is all Si. The T1 tetrahedra form puckered layers parallel to (010) and are composed of corner-shared tetrahedral chains. These chains are parallel to [100]. Unlike pyroxenes, all tetrahedra lie on the same side of the chain axis. The layers stack in antiparallel arrangement and are cross-linked by the T2 tetrahedra to constitute the framework structure.

Below the transition temperature, the 8-fold T1 site splits into two symmetry-independent 4-fold positions T1(o) and T1(m) sites, and the symmetry degenerates from $Pmnb$ to $P2_1/n$. Zn atoms are completely ordered on T1(o). At the transition, Zn atoms may concentrate in either of the two T1 positions. This option results in a domain structure with the two related by reflection across (100). The order–disorder transformation also produces twin (α') structure which has monoclinic symmetry with space group $B2_1$ and a = 13.01, b = 10.41, c = 10.07A, and $\beta \approx 90°$.

Introduction

During exploratory studies of willemite crystal growth from a polymolybdate flux with methods previously developed for BeO (Austerman, 1964), a new non-hexagonal crystal form was obtained. The crystal-growth experiments were made with Li_2MoO_4–MoO_3 as the flux composition, over the range of 10 percent to 35 percent MoO_3 by weight, at temperatures between 900° and 1100°C. At all flux compositions with greater than 20±1 percent MoO_3, willemite invariably formed. However, with the MoO_3 component ≤20 percent, only the new type of crystal, with good crystal faces, was grown. The flux composition boundary between the willemite and the new structure regions was found to be independent of temperature within a range of ±1 percent MoO_3. In some experiments Mn was added in small amounts, but this Mn did not appear to influence the formation of the new type of crystal.

The preliminary electron microprobe chemical

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h	k	l	F_{obs}	F_{calc}
0	0	4	5.7	0.4
0	0	6	51.4	52.4
0	1	1	12.4	13.6
0	1	2	56.7	56.3
0	1	3	36.1	31.9
0	1	4	65.9	65.3
0	1	5	30.9	28.0
0	1	6	29.6	28.9
0	1	7	17.4	15.9
0	2	0	27.4	33.4
0	2	2	22.6	24.8
0	2	3	3.1	3.7
0	2	4	3.6	3.5
0	2	5	22.9	20.4
0	2	6	10.0	8.5
0	2	7	15.9	12.6
0	3	1	51.8	53.1
0	3	2	17.0	19.4
0	3	3	93.7	94.8
0	3	4	32.4	34.5
0	3	5	64.5	62.4
0	3	6	22.4	22.8
0	3	7	22.5	20.1
0	4	1	50.4	46.7
0	4	2	75.9	75.1
0	4	3	20.2	16.5
0	4	4	4.7	4.5
0	4	5	23.1	23.9
0	4	6	30.4	30.2
0	4	7	35.6	33.3
0	5	1	40.5	40.7
0	5	2	38.0	37.1
0	5	3	63.0	65.2
0	5	4	35.1	32.9
0	5	5	35.4	35.0
0	5	6	10.1	7.4
0	5	7	3.9	4.7
0	6	1	7.3	2.9
0	6	2	48.4	52.5
0	6	3	8.4	8.3
0	6	4	10.3	11.2
0	6	5	7.6	7.0
0	6	6	16.5	14.8
0	6	7	5.2	1.1
0	7	1	36.0	38.0
0	7	2	30.4	31.2
0	7	3	64.5	68.7
0	7	4	23.3	23.1
0	7	5	41.5	43.1
0	7	6	5.8	4.1
0	8	0	44.0	42.5
0	8	1	66.3	68.9
0	8	2	30.1	28.8
0	8	3	26.1	24.9
0	8	4	4.9	5.0
0	8	5	18.9	19.9
0	8	6	10.9	9.0
0	9	1	37.4	38.9
0	9	2	2.1	0.2
0	9	3	70.7	73.9
0	9	4	6.9	6.8
0	9	5	52.3	51.0
0	9	6	7.7	9.2
0	10	0	39.0	42.1
0	10	1	18.8	19.9
0	10	2	30.2	32.5
0	10	3	4.8	4.3
0	10	4	10.2	11.6
0	10	5	7.5	6.6
0	11	1	9.5	9.4
0	11	2	32.1	34.1
0	11	3	13.5	15.5
0	11	4	32.9	34.5
0	11	5	5.9	6.3
0	12	0	72.5	72.7
0	12	1	18.5	20.2
0	12	2	47.3	46.0
0	12	3	10.0	9.4
0	12	4	4.9	1.3
0	13	1	11.1	11.2
0	13	2	17.0	15.8
0	13	3	24.0	23.5
0	13	4	21.0	20.7
0	14	0	8.6	2.8
0	14	1	10.4	9.0
0	14	2	1.3	0.6
0	14	3	3.6	3.0
0	15	1	7.6	7.3
0	15	2	11.9	11.8
1	0	1	27.2	28.6
1	0	3	20.8	17.5
1	0	5	31.2	36.1
1	0	7	26.9	29.1
1	1	0	43.8	41.9
1	1	1	81.0	79.3
1	1	2	31.8	33.4
1	1	3	42.9	43.3
1	1	4	10.9	8.4
1	1	5	1.7	1.7
1	1	6	18.2	19.2

h	k	l	F_{obs}	F_{calc}
1	1	7	16.5	20.5
1	2	0	53.8	56.1
1	2	1	34.1	34.8
1	2	2	55.4	59.3
1	2	3	35.9	38.2
1	2	4	24.8	28.3
1	2	5	15.7	17.5
1	2	6	5.2	5.2
1	2	7	3.7	0.9
1	3	0	75.4	75.4
1	3	1	38.9	34.5
1	3	2	50.6	50.1
1	3	3	48.5	47.1
1	3	4	1.6	2.7
1	3	5	22.4	21.5
1	3	6	18.5	20.6
1	3	7	3.6	1.1
1	4	0	8.8	12.8
1	4	1	3.2	0.4
1	4	2	38.4	34.8
1	4	3	14.1	12.1
1	4	4	47.9	49.8
1	4	5	18.3	18.9
1	4	6	29.0	31.3
1	4	7	15.5	16.2
1	5	0	29.2	29.8
1	5	1	39.7	39.7
1	5	2	27.3	26.6
1	5	3	5.0	0.9
1	5	4	21.6	20.8
1	5	5	22.5	22.4
1	5	6	10.0	7.2
1	5	7	21.4	24.0
1	6	0	28.4	27.2
1	6	1	35.8	40.1
1	6	2	17.2	15.5
1	6	3	51.7	55.8
1	6	4	3.4	2.1
1	6	5	27.5	29.1
1	6	6	5.8	1.0
1	7	0	30.9	29.1
1	7	1	26.1	27.0
1	7	2	28.9	26.7
1	7	3	8.0	6.3
1	7	4	15.4	14.4
1	7	5	16.6	16.5
1	7	6	6.2	0.9
1	8	0	31.2	35.0
1	8	1	8.8	9.7
1	8	3	7.6	7.6
1	8	4	36.5	38.2
1	8	5	10.0	11.1
1	8	6	28.0	29.9
1	9	0	42.6	43.5
1	9	1	10.5	10.4
1	9	2	32.9	35.4
1	9	3	21.4	21.3
1	9	4	12.6	13.7
1	9	5	14.3	12.2
1	9	6	3.3	4.0
1	10	0	13.1	15.9
1	10	1	9.0	8.5
1	10	2	26.1	29.7
1	10	3	19.3	19.2
1	10	4	18.8	20.9
1	10	5	11.4	12.2
1	11	0	14.1	15.2
1	11	1	30.3	30.0
1	11	2	3.1	0.3
1	11	3	14.1	13.8
1	11	4	16.3	16.3
1	11	5	1.6	3.4
1	12	0	17.2	16.5
1	12	1	1.5	1.4
1	12	2	7.8	7.3
1	12	3	17.8	17.4
1	12	4	6.1	5.3
1	13	0	17.0	17.3
1	13	1	25.7	27.2
1	13	2	7.0	7.3
1	13	3	16.7	17.8
1	13	4	3.9	4.4
1	14	0	24.4	25.3
1	14	1	3.4	6.8
1	14	2	30.0	31.3
1	14	3	7.8	7.5
1	15	0	22.3	22.9
1	15	1	8.4	8.3
1	15	2	14.5	14.0
2	0	2	56.9	59.7
2	0	4	10.7	11.7
2	0	6	18.4	17.1
2	1	0	2.4	2.7
2	1	1	51.9	49.6
2	1	2	46.0	42.8
2	1	3	75.8	77.5
2	1	4	35.7	33.4
2	1	5	41.9	41.8
2	1	6	8.1	7.0
2	1	7	3.1	6.4
2	2	0	115.8	112.8
2	2	1	72.0	66.0
2	2	2	70.4	64.5
2	2	3	31.4	28.4

h	k	l	F_{obs}	F_{calc}
2	2	4	4.8	2.6
2	2	5	22.8	23.0
2	2	6	20.1	20.2
2	2	7	36.6	37.4
2	3	0	4.0	1.8
2	3	1	59.6	57.5
2	3	2	5.3	8.1
2	3	3	97.9	99.9
2	3	4	20.9	22.8
2	3	5	64.3	63.8
2	3	6	17.7	19.2
2	3	7	20.6	19.6
2	4	0	52.6	54.4
2	4	1	52.5	56.0
2	4	2	39.3	40.1
2	4	3	8.9	11.0
2	4	4	10.6	10.7
2	4	5	13.6	12.3
2	4	6	9.2	8.6
2	4	7	10.4	10.2
2	5	0	5.1	4.6
2	5	1	4.3	5.3
2	5	2	52.8	55.1
2	5	3	1.6	1.9
2	5	4	55.8	58.0
2	5	5	9.1	6.9
2	5	6	24.5	25.7
2	5	7	9.1	8.1
2	6	1	22.4	23.2
2	6	2	97.1	96.0
2	6	3	11.4	12.1
2	6	6	38.9	39.2
2	7	0	3.6	2.9
2	7	1	16.0	15.3
2	7	2	31.7	32.3
2	7	3	33.8	32.2
2	7	4	40.1	40.6
2	7	5	27.9	26.8
2	7	6	21.1	21.3
2	8	0	6.1	6.9
2	8	1	27.8	30.6
2	8	2	2.8	2.9
2	8	3	3.8	0.8
2	8	4	3.1	2.9
2	8	5	15.3	14.3
2	8	6	4.4	5.0
2	9	0	3.6	2.4
2	9	1	19.7	18.9
2	9	2	16.3	17.9
2	9	3	40.1	40.5
2	9	4	22.2	24.3
2	9	5	33.7	33.2
2	9	6	14.7	14.4
2	10	0	69.0	69.4
2	10	1	38.2	36.1
2	10	2	42.0	41.1
2	10	3	13.4	12.1
2	10	4	4.9	5.2
2	10	5	12.7	11.7
2	11	0	2.1	2.0
2	11	1	15.8	15.3
2	11	2	21.9	21.0
2	11	3	27.8	28.9
2	11	4	24.6	23.1
2	11	5	17.3	17.9
2	12	0	32.2	33.3
2	12	1	2.3	2.2
2	12	2	24.1	24.6
2	12	3	4.1	4.8
2	12	4	7.4	6.4
2	13	0	4.4	0.1
2	13	1	17.5	17.4
2	13	2	9.9	10.9
2	13	3	35.1	36.9
2	13	4	12.4	9.1
2	14	0	5.6	2.6
2	14	1	39.0	39.3
2	14	2	6.0	3.2
2	14	3	17.7	16.9
2	15	0	4.9	0.8
2	15	1	16.9	16.5
3	0	1	30.8	34.4
3	0	3	59.1	59.9
3	0	5	32.3	32.5
3	0	7	3.9	0.9
3	1	0	35.1	32.3
3	1	1	29.8	29.2
3	1	2	32.0	27.9
3	1	3	14.1	11.5
3	1	4	23.3	20.1
3	1	5	26.1	24.6
3	1	6	6.9	5.1
3	1	7	19.7	21.4
3	2	0	11.2	14.2
3	2	1	19.9	19.5
3	2	2	37.4	32.1
3	2	3	5.1	4.4
3	2	4	19.3	48.9
3	2	5	13.3	14.2
3	2	6	29.4	30.7
3	2	7	11.4	12.3
3	3	0	63.6	62.0
3	3	1	26.2	23.5
3	3	2	51.6	52.0

h	k	l	F_{obs}	F_{calc}
3	3	3	39.9	37.1
3	3	4	18.1	18.0
3	3	5	20.5	18.8
3	3	6	6.1	5.8
3	3	7	5.4	3.0
3	4	0	31.3	34.6
3	4	1	5.9	7.6
3	4	2	42.5	45.2
3	4	3	24.6	25.2
3	4	4	23.1	24.6
3	4	5	15.4	15.4
3	4	6	5.3	4.7
3	5	0	27.5	27.9
3	5	1	47.4	45.2
3	5	2	11.5	13.3
3	5	3	23.8	22.5
3	5	4	14.9	12.7
3	5	5	3.8	4.4
3	5	6	18.5	18.6
3	6	0	18.9	17.5
3	6	1	17.3	19.7
3	6	2	7.7	8.5
3	6	3	15.1	12.8
3	6	5	25.8	27.3
3	6	6	5.9	4.5
3	7	0	27.5	26.7
3	7	1	42.5	42.6
3	7	2	16.4	17.3
3	7	3	23.7	23.5
3	7	4	3.0	1.4
3	7	5	7.7	6.8
3	7	6	10.5	10.1
3	8	0	40.9	44.1
3	8	1	16.7	17.5
3	8	2	45.4	47.7
3	8	3	18.5	18.7
3	8	4	23.2	24.0
3	8	5	9.9	9.9
3	8	6	3.3	4.0
3	9	0	40.0	40.3
3	9	1	14.9	13.0
3	9	2	28.7	27.9
3	9	3	22.3	20.6
3	9	4	3.1	0.3
3	9	5	11.4	9.4
3	10	0	6.1	6.2
3	10	1	3.6	3.2
3	10	2	17.4	15.9
3	10	3	8.7	7.6
3	10	4	24.8	24.9
3	10	5	14.1	14.5
3	11	0	11.2	11.5
3	11	1	22.5	23.7
3	11	2	16.7	17.1
3	11	3	1.4	3.2
3	11	4	17.0	15.5
3	12	0	17.9	17.6
3	12	1	11.8	12.9
3	12	2	12.9	12.3
3	12	3	22.8	23.5
3	12	4	2.6	2.9
3	13	0	16.3	16.2
3	13	1	10.4	11.2
3	13	2	20.2	19.4
3	13	3	7.2	5.7
3	14	0	15.8	15.7
3	14	1	4.6	0.2
3	14	2	6.6	5.3
3	15	0	19.6	20.1
4	0	0	155.9	163.2
4	0	2	100.6	97.0
4	0	4	6.2	0.2
4	0	6	37.8	37.6
4	1	0	7.5	7.0
4	1	1	7.0	4.6
4	1	2	45.3	45.3
4	1	3	19.2	16.6
4	1	4	55.0	54.0
4	1	5	20.3	18.2
4	1	6	27.6	27.7
4	2	0	15.3	17.5
4	2	1	51.7	54.3
4	2	2	12.5	12.8
4	2	3	8.6	10.3
4	2	4	2.6	1.4
4	2	5	14.6	12.8
4	2	6	4.7	6.4
4	3	0	7.0	4.8
4	3	1	29.8	28.8
4	3	2	12.0	14.4
4	3	3	59.6	59.0
4	3	4	25.1	26.3
4	3	5	44.3	42.4
4	3	6	18.0	19.1
4	4	0	82.4	80.4
4	4	1	58.9	55.4
4	4	2	49.7	47.0
4	4	3	22.5	21.3
4	4	4	2.0	3.2
4	4	5	16.2	15.5
4	4	6	22.0	21.9
4	5	0	1.7	3.8
4	5	1	24.4	25.0
4	5	2	32.9	30.0

h	k	l	F_{obs}	F_{calc}
4	5	3	43.3	43.7
4	5	4	31.5	29.7
4	5	5	24.7	24.5
4	5	6	12.0	10.3
4	6	0	39.0	40.8
4	6	1	3.5	0.5
4	6	2	28.5	30.4
4	6	3	6.0	4.7
4	6	4	7.0	6.7
4	6	5	6.7	4.7
4	6	6	12.2	11.4
4	7	0	3.1	0.6
4	7	1	23.9	24.2
4	7	2	25.6	24.5
4	7	3	46.3	47.5
4	7	4	20.8	20.6
4	7	5	30.8	31.2
4	7	6	6.2	6.0
4	8	0	31.7	27.9
4	8	1	61.7	60.9
4	8	2	22.7	19.7
4	8	3	26.8	26.6
4	8	4	6.4	3.8
4	8	5	12.5	12.2
4	9	0	3.9	0.2
4	9	1	26.1	25.3
4	9	2	3.1	0.1
4	9	3	52.1	51.1
4	9	4	3.9	5.1
4	9	5	38.2	36.5
4	10	0	28.4	27.1
4	10	1	19.3	19.5
4	10	2	22.3	22.3
4	10	3	8.1	6.2
4	10	4	9.9	8.7
4	11	0	4.1	2.9
4	11	1	6.5	7.0
4	11	2	25.9	26.7
4	11	3	12.1	12.6
4	11	4	29.1	30.0
4	12	0	55.5	52.7
4	12	1	17.1	17.7
4	12	2	35.6	33.7
4	12	3	10.4	10.3
4	13	0	4.6	1.5
4	13	1	9.4	7.6
4	13	2	14.0	13.3
4	13	3	17.6	16.8
4	14	0	3.9	1.9
4	14	1	10.4	11.2
5	0	1	25.3	26.1
5	0	3	8.0	6.5
5	0	5	22.6	24.1
5	1	0	25.5	27.0
5	1	1	39.9	39.5
5	1	2	16.6	18.5
5	1	3	21.7	20.3
5	1	4	5.0	3.0
5	1	5	6.6	6.4
5	1	6	11.0	11.5
5	2	0	35.1	39.2
5	2	1	13.9	14.8
5	2	2	40.7	43.1
5	2	3	21.6	21.6
5	2	4	20.5	21.3
5	2	5	12.8	12.6
5	2	6	3.9	3.6
5	3	0	46.8	47.3
5	3	1	18.0	15.8
5	3	2	38.3	37.3
5	3	3	29.3	26.6
5	3	4	11.1	9.2
5	3	5	15.3	13.3
5	3	6	8.8	9.8
5	4	0	2.4	4.8
5	4	1	8.1	9.2
5	4	2	24.4	23.2
5	4	3	5.7	4.2
5	4	4	33.9	33.6
5	4	5	13.1	13.0
5	4	6	19.5	20.9
5	5	0	18.3	16.6
5	5	1	22.4	22.8
5	5	2	21.2	19.7
5	5	3	6.9	5.0
5	5	4	17.7	16.8
5	5	5	21.0	20.3
5	6	0	15.5	15.9
5	6	1	16.5	19.1
5	6	2	10.5	10.1
5	6	3	32.8	34.4
5	6	4	2.5	2.1
5	6	5	21.1	22.1
5	7	0	20.8	20.1
5	7	1	15.0	15.8
5	7	2	23.6	22.4
5	7	3	7.9	7.2
5	7	4	15.9	14.8
5	7	5	14.2	14.5
5	8	0	15.4	16.1
5	8	1	8.4	7.2
5	8	2	11.8	11.2
5	8	3	3.0	4.3
5	8	4	26.3	27.9

h	k	l	F_{obs}	F_{calc}
5	8	5	8.3	7.6
5	9	0	29.0	30.0
5	9	1	6.5	6.8
5	9	2	27.1	28.2
5	9	3	16.5	15.5
5	9	4	15.6	15.1
5	10	0	13.6	14.5
5	10	2	22.4	23.4
5	10	3	10.4	12.8
5	10	4	15.2	16.1
5	11	0	12.7	11.7
5	11	1	19.4	18.8
5	11	2	3.6	1.1
5	11	3	6.2	6.0
5	12	0	10.5	9.8
5	12	1	8.4	5.5
5	12	2	3.3	3.5
5	12	3	10.5	10.2
5	13	0	14.9	14.6
6	0	0	23.7	25.8
6	0	2	19.4	21.0
6	0	4	3.5	4.9
6	1	0	2.9	1.7
6	1	1	17.3	19.4
6	1	2	28.7	27.1
6	1	3	36.0	37.0
6	1	4	26.4	25.4
6	1	5	23.0	21.6
6	2	0	46.2	43.3
6	2	1	57.6	56.3
6	2	2	30.5	27.8
6	2	3	25.3	25.1
6	2	5	13.3	11.4
6	3	0	6.3	2.7
6	3	1	21.4	20.7
6	3	2	3.9	4.5
6	3	3	46.5	44.9
6	3	4	13.0	13.2
6	3	5	35.5	32.5
6	4	0	18.8	18.4
6	4	1	34.7	35.8
6	4	2	15.7	15.8
6	4	3	10.9	10.8
6	4	4	5.9	5.5
6	4	5	7.0	6.7
6	5	0	5.2	4.9
6	5	1	2.6	4.3
6	5	2	33.2	33.6
6	5	3	4.5	3.8
6	5	4	40.2	40.2
6	5	5	4.2	2.6
6	6	0	77.5	74.1
6	6	1	14.3	14.2
6	6	2	50.7	46.9
6	6	3	8.0	8.7
6	6	5	3.9	0.2
6	7	0	4.3	3.8
6	7	1	7.0	4.7
6	7	2	21.1	21.6
6	7	3	16.4	14.1
6	7	4	30.3	30.1
6	8	1	23.0	25.2
6	8	2	3.4	0.2
6	9	0	4.9	3.6
6	9	1	8.5	7.5
6	9	2	8.5	9.8
6	9	3	21.7	19.7
6	9	4	15.8	16.0
6	10	0	38.4	37.0
6	10	1	28.1	27.4
6	10	2	23.7	22.1
6	10	3	12.0	11.1
6	11	0	5.7	2.6
6	11	1	8.5	8.9
6	11	2	17.1	15.6
6	12	0	17.4	16.0
6	12	1	4.7	2.8
7	0	1	16.2	18.1
7	0	3	29.6	31.8
7	0	5	20.1	20.8
7	1	0	15.6	15.1
7	1	1	15.2	15.6
7	1	2	17.3	16.1
7	1	3	7.3	5.1
7	1	4	11.2	12.3
7	1	5	15.0	14.4
7	2	0	7.7	9.6
7	2	1	8.9	8.0
7	2	2	14.1	14.2
7	2	3	4.3	2.5
7	2	4	24.9	26.7
7	2	5	6.1	8.1
7	3	0	29.3	31.4
7	3	1	9.6	9.5
7	3	2	26.3	27.3
7	3	3	19.1	18.1
7	3	4	12.1	11.5
7	4	0	15.1	16.9
7	4	1	2.6	5.3
7	4	2	22.0	23.6
7	4	3	13.0	14.5
7	4	4	15.2	14.3
7	5	0	14.0	15.6
7	5	1	22.2	22.2

h	k	l	F_{obs}	F_{calc}
7	5	2	6.6	7.2
7	5	3	12.1	10.9
7	5	4	8.1	7.0
7	6	0	7.6	7.4
7	6	1	11.6	11.0
7	6	2	3.6	3.3
7	6	4	4.9	1.8
7	7	0	15.5	16.6
7	7	1	20.6	22.6
7	7	2	10.9	11.8
7	7	3	13.4	12.6
7	8	0	23.1	23.6
7	8	1	8.9	9.2
7	8	2	25.9	27.0
7	8	3	9.7	10.6
7	9	0	23.8	25.3
7	9	1	8.4	6.7
7	9	2	18.7	18.7
7	10	0	5.9	3.5
7	10	1	3.7	3.0
7	10	2	9.2	9.5
8	0	0	59.2	57.6
8	0	2	39.8	37.1
8	0	4	3.3	0.1
8	1	0	5.2	4.1
8	1	1	3.5	0.9
8	1	2	22.6	22.9
8	1	3	6.9	4.0
8	1	4	31.1	31.2
8	2	0	4.1	4.4
8	2	1	27.5	28.6
8	2	2	4.8	3.7
8	2	3	10.0	8.1
8	2	4	3.9	0.4
8	3	0	5.2	3.6
8	3	1	9.5	7.7
8	3	2	4.9	5.8
8	3	3	22.4	21.6
8	4	0	31.4	30.2
8	4	1	32.1	32.0
8	4	2	20.4	18.7
8	4	3	14.4	14.6
8	5	0	4.9	1.7
8	5	1	7.6	10.0
8	5	2	19.8	17.5
8	5	3	19.2	19.1
8	6	0	13.5	11.8
8	6	1	7.5	1.3
8	6	2	9.7	10.6
8	7	0	7.7	0.4
8	7	1	9.1	8.5
8	8	0	13.2	12.1
8	8	1	35.8	35.6
9	0	1	9.0	7.9
9	1	0	12.2	13.2
9	1	1	17.9	18.5
9	1	2	7.7	8.8
9	2	0	12.5	13.3
9	2	1	5.1	7.3
9	2	2	16.1	17.5
9	3	0	19.2	22.5
9	3	1	6.7	6.5
9	3	2	15.8	17.1
9	4	0	3.9	5.2
9	4	1	2.5	2.9
9	5	0	7.9	6.8
9	5	1	11.0	12.6
1	0	-7	6.2	4.9
1	0	-5	35.4	37.8
1	0	-3	83.9	86.6
1	0	-1	79.9	83.9
1	1	-7	17.0	18.2
1	1	-6	4.1	1.4
1	1	-5	19.4	18.3
1	1	-4	14.3	12.1
1	1	-3	4.3	0.2
1	1	-2	21.3	18.6
1	1	-1	45.6	44.4
1	2	-7	13.1	12.0
1	2	-6	37.8	38.3
1	2	-5	17.7	17.7
1	2	-4	56.2	54.3
1	2	-3	15.4	12.8
1	2	-2	25.5	19.0
1	2	-1	5.5	7.3
1	3	-7	1.8	2.0
1	3	-6	17.8	18.1
1	3	-5	24.5	21.2
1	3	-4	2.7	4.2
1	3	-3	48.8	45.8
1	3	-2	45.3	45.5
1	3	-1	35.6	32.3
1	4	-7	3.9	3.0
1	4	-6	4.3	6.4
1	4	-5	17.7	18.0
1	4	-4	21.8	24.1
1	4	-3	36.7	36.3
1	4	-2	32.4	36.3
1	4	-1	23.8	24.0
1	5	-7	11.3	13.3
1	5	-6	24.9	23.8
1	5	-5	7.6	5.1
1	5	-4	21.1	19.0
1	5	-3	42.2	40.7

h	k	l	F_{obs}	F_{calc}
1	5	-2	9.9	11.4
1	5	-1	65.3	64.6
1	6	-6	6.2	6.0
1	6	-5	33.3	33.5
1	6	-4	4.6	2.5
1	6	-3	31.8	28.3
1	6	-2	13.6	13.8
1	6	-1	8.3	2.8
1	7	-6	17.6	17.4
1	7	-5	2.6	0.3
1	7	-4	12.3	9.9
1	7	-3	36.2	36.7
1	7	-2	12.6	12.7
1	7	-1	54.6	55.3
1	8	-6	6.5	5.0
1	8	-5	10.4	10.9
1	8	-4	21.0	23.2
1	8	-3	22.3	23.9
1	8	-2	41.8	43.9
1	8	-1	23.1	25.9
1	9	-6	23.5	25.7
1	9	-5	14.0	13.0
1	9	-4	10.4	9.9
1	9	-3	28.1	26.9
1	9	-2	22.3	22.5
1	9	-1	18.6	17.4
1	10	-5	16.2	17.3
1	10	-4	27.1	26.5
1	10	-3	16.0	15.5
1	10	-2	13.7	12.1
1	10	-1	8.9	7.5
1	11	-5	10.5	9.6
1	11	-4	16.5	15.7
1	11	-3	8.2	10.7
1	11	-2	18.3	19.5
1	11	-1	28.2	29.6
1	12	-4	1.0	1.7
1	12	-3	30.1	31.0
1	12	-2	12.7	11.2
1	12	-1	22.5	24.1
1	13	-4	8.7	6.9
1	13	-3	3.3	3.0
1	13	-2	17.6	17.1
1	13	-1	14.3	14.2
1	14	-3	5.9	6.8
1	14	-2	3.9	0.2
1	14	-1	2.0	0.3
1	15	-2	16.3	17.0
1	15	-1	5.1	0.2
2	0	-6	17.4	16.3
2	0	-4	10.4	12.1
2	0	-2	55.7	59.0
2	1	-7	6.5	5.5
2	1	-6	8.0	6.7
2	1	-5	43.9	42.3
2	1	-4	38.7	35.4
2	1	-3	78.5	79.3
2	1	-2	48.9	47.2
2	1	-1	52.3	49.3
2	2	-7	40.8	39.6
2	2	-6	23.1	21.5
2	2	-5	26.8	27.6
2	2	-4	3.3	1.3
2	2	-3	27.2	21.2
2	2	-2	70.9	64.4
2	2	-1	67.7	61.2
2	3	-7	21.1	19.5
2	3	-6	18.4	18.6
2	3	-5	68.6	64.7
2	3	-4	20.6	22.2
2	3	-3	102.1	102.0
2	3	-2	9.2	9.3
2	3	-1	60.9	59.1
2	4	-7	14.2	12.1
2	4	-6	9.1	8.0
2	4	-5	16.0	14.9
2	4	-4	10.4	10.7
2	4	-3	8.2	8.9
2	4	-2	39.6	39.2
2	4	-1	52.6	55.4
2	5	-7	9.2	9.2
2	5	-6	25.5	24.9
2	5	-5	8.5	7.0
2	5	-4	59.2	60.0
2	5	-3	1.2	2.5
2	5	-2	60.0	61.6
2	5	-1	5.7	4.9
2	6	-6	42.4	41.6
2	6	-5	2.1	3.0
2	6	-4	3.5	2.6
2	6	-3	10.3	9.5
2	6	-2	97.9	95.4
2	6	-1	21.1	21.6
2	7	-6	21.4	20.2
2	7	-5	28.9	26.8
2	7	-4	42.2	40.9
2	7	-3	34.5	32.4
2	7	-2	36.3	35.8
2	7	-1	16.0	16.2
2	8	-6	6.4	5.1
2	8	-5	17.7	16.9
2	8	-4	4.0	2.5
2	8	-3	3.5	1.0
2	8	-2	4.6	3.6

h	k	l	F_{obs}	F_{calc}
2	8	-1	28.1	30.1
2	9	-6	12.9	13.7
2	9	-5	34.4	33.2
2	9	-4	24.2	24.8
2	9	-3	42.1	40.5
2	9	-2	19.2	21.0
2	9	-1	19.2	19.5
2	10	-5	14.7	13.4
2	10	-4	4.7	6.3
2	10	-3	12.2	10.4
2	10	-2	41.9	40.7
2	10	-1	38.0	35.4
2	11	-5	19.8	18.8
2	11	-4	26.8	23.7
2	11	-3	29.8	30.2
2	11	-2	24.7	23.8
2	11	-1	16.7	16.2
2	12	-4	6.7	6.7
2	12	-3	6.1	5.3
2	12	-2	24.1	24.9
2	12	-1	3.1	2.1
2	13	-4	10.0	9.9
2	13	-3	36.3	37.1
2	13	-2	12.1	11.3
2	13	-1	17.9	18.2
2	14	-3	14.8	13.9
2	14	-2	6.3	3.1
2	14	-1	37.4	37.9
2	15	-2	5.4	3.7
2	15	-1	17.1	17.2
3	0	-7	22.0	23.1
3	0	-5	34.5	36.6
3	0	-3	38.9	36.0
3	0	-1	23.6	16.5
3	1	-7	10.3	14.6
3	1	-6	23.4	22.8
3	1	-5	9.0	7.6
3	1	-4	17.2	15.2
3	1	-3	50.1	49.9
3	1	-2	15.0	15.2
3	1	-1	71.4	70.3
3	2	-7	1.5	2.4
3	2	-6	3.9	5.1
3	2	-5	14.6	16.4
3	2	-4	17.8	19.9
3	2	-3	36.6	37.5
3	2	-2	29.7	33.1
3	2	-1	40.9	40.9
3	3	-7	3.0	0.5
3	3	-6	29.5	29.8
3	3	-5	21.6	20.2
3	3	-4	12.5	11.8
3	3	-3	43.6	42.0
3	3	-2	28.9	28.7
3	3	-1	29.9	27.7
3	4	-6	29.5	30.4
3	4	-5	19.3	19.5
3	4	-4	41.5	40.3
3	4	-3	23.1	21.0
3	4	-2	17.4	13.2
3	4	-1	20.3	16.0
3	5	-6	5.4	1.9
3	5	-5	13.8	11.6
3	5	-4	13.4	12.8
3	5	-3	8.5	9.7
3	5	-2	21.1	21.3
3	5	-1	39.7	38.2
3	6	-6	4.8	1.6
3	6	-5	27.0	28.1
3	6	-4	2.1	0.6
3	6	-3	55.1	58.0
3	6	-2	11.8	10.3
3	6	-1	52.1	54.3
3	7	-6	7.7	7.9
3	7	-5	10.3	8.9
3	7	-4	6.0	4.9
3	7	-3	4.0	1.0
3	7	-2	19.1	18.7
3	7	-1	26.7	26.6
3	8	-6	28.9	29.5
3	8	-5	11.7	10.9
3	8	-4	31.9	31.7
3	8	-3	10.0	9.5
3	8	-2	4.1	1.6
3	8	-1	1.7	3.4
3	9	-5	9.7	9.4
3	9	-4	2.4	2.6
3	9	-3	20.3	17.9
3	9	-2	25.4	25.6
3	9	-1	9.0	9.1
3	10	-5	12.3	12.9
3	10	-4	14.5	16.7
3	10	-3	22.5	22.4
3	10	-2	18.2	20.3
3	10	-1	16.5	16.5
3	11	-4	16.6	15.8
3	11	-3	19.9	18.6
3	11	-2	5.4	2.3
3	11	-1	29.9	29.7
3	12	-4	2.6	4.3
3	12	-3	22.4	22.9
3	12	-2	9.4	8.7
3	12	-1	10.4	8.7
3	13	-3	20.4	19.9

h	k	l	F_{obs}	F_{calc}
3	13	-2	4.1	3.5
3	13	-1	26.4	25.9
3	14	-2	21.2	22.6
3	14	-1	6.5	6.9
4	0	-6	42.9	43.4
4	0	-4	4.2	5.8
4	0	-2	98.0	94.9
4	1	-6	26.4	26.2
4	1	-5	20.4	18.1
4	1	-4	56.5	56.1
4	1	-3	18.6	16.6
4	1	-2	54.4	54.5
4	1	-1	6.9	7.6
4	2	-6	7.4	6.2
4	2	-5	19.8	17.6
4	2	-4	3.8	1.4
4	2	-3	7.7	7.6
4	2	-2	11.0	12.3
4	2	-1	51.6	54.0
4	3	-6	16.4	17.8
4	3	-5	45.2	42.7
4	3	-4	26.4	26.2
4	3	-3	62.2	61.2
4	3	-2	19.3	19.5
4	3	-1	33.0	33.2
4	4	-6	25.0	25.1
4	4	-5	20.7	20.7
4	4	-4	1.6	6.5
4	4	-3	18.4	14.6
4	4	-2	48.7	45.8
4	4	-1	56.5	51.8
4	5	-6	13.6	9.5
4	5	-5	26.7	26.0
4	5	-4	34.1	31.6
4	5	-3	47.4	47.0
4	5	-2	36.0	35.7
4	5	-1	28.3	26.9
4	6	-6	13.5	10.8
4	6	-5	6.1	6.0
4	6	-4	6.3	6.4
4	6	-3	3.5	5.2
4	6	-2	28.1	29.1
4	7	-6	8.3	6.6
4	7	-5	32.2	31.1
4	7	-4	24.6	23.3
4	7	-3	50.3	49.4
4	7	-2	28.5	26.9
4	7	-1	27.2	27.2
4	8	-5	19.2	18.3
4	8	-4	6.5	2.8
4	8	-3	21.8	18.7
4	8	-2	21.2	19.0
4	8	-1	59.9	56.9
4	9	-5	40.9	38.0
4	9	-4	5.3	4.0
4	9	-3	55.2	54.4
4	9	-2	3.4	0.9
4	9	-1	29.5	28.8
4	10	-5	7.2	6.3
4	10	-4	8.3	8.0
4	10	-3	4.3	5.1
4	10	-2	21.6	20.7
4	10	-1	19.2	19.2
4	11	-4	32.9	32.7
4	11	-3	13.8	13.5
4	11	-2	31.4	31.7
4	11	-1	9.0	8.2
4	12	-3	7.3	6.1
4	12	-2	36.0	32.6
4	12	-1	15.1	15.6
4	13	-3	18.7	17.4
4	13	-2	16.2	15.1
4	13	-1	7.6	8.5
4	14	-1	10.7	10.9
5	0	-5	26.0	29.6
5	0	-3	54.7	59.6
5	0	-1	54.2	57.5
5	1	-6	6.2	6.0
5	1	-5	8.1	8.9
5	1	-4	6.5	4.2
5	1	-3	4.2	4.4
5	1	-2	15.3	16.1
5	1	-1	28.0	28.6
5	2	-6	27.6	29.2
5	2	-5	13.2	14.4
5	2	-4	33.2	34.1
5	2	-3	14.6	14.0
5	2	-2	7.7	2.8
5	2	-1	4.4	3.0
5	3	-6	19.9	21.3
5	3	-5	16.3	14.5
5	3	-4	6.0	4.8
5	3	-3	29.8	28.8
5	3	-2	24.0	25.2
5	3	-1	17.4	17.1
5	4	-6	6.1	4.8
5	4	-5	15.4	15.1
5	4	-4	12.6	14.7
5	4	-3	26.5	27.9
5	4	-2	17.0	20.3
5	4	-1	22.8	23.7
5	5	-6	18.7	19.4
5	5	-5	8.5	7.2
5	5	-4	15.1	14.7

h	k	l	F_{obs}	F_{calc}
5	5	-3	31.6	30.8
5	5	-2	5.0	3.0
5	5	-1	40.7	40.9
5	6	-5	26.7	27.9
5	6	-3	29.9	28.8
5	6	-2	9.2	9.1
5	6	-1	13.4	11.5
5	7	-5	3.3	2.6
5	7	-4	12.7	10.9
5	7	-3	27.9	28.6
5	7	-2	4.6	6.0
5	7	-1	36.1	36.7
5	8	-5	7.7	8.1
5	8	-4	12.3	14.0
5	8	-3	15.1	17.4
5	8	-2	22.9	24.6
5	8	-1	17.8	18.0
5	9	-4	12.3	11.9
5	9	-3	21.6	20.2
5	9	-2	13.1	13.0
5	9	-1	12.6	12.6
5	10	-4	20.6	18.9
5	10	-3	17.9	17.3
5	10	-2	6.8	6.0
5	10	-1	12.8	11.9
5	11	-3	10.2	10.8
5	11	-2	12.3	13.6
5	11	-1	21.1	21.7
5	12	-3	26.3	27.1
5	12	-2	7.7	6.7
5	12	-1	21.8	22.4
5	13	-1	11.4	11.1
6	0	-2	16.9	17.4
6	1	-5	22.4	22.5
6	1	-4	29.8	28.7
6	1	-3	40.7	40.8
6	1	-2	31.1	31.0
6	1	-1	24.0	23.6
6	2	-5	17.2	17.7
6	2	-3	20.0	16.3
6	2	-2	28.6	26.0
6	2	-1	54.1	51.7
6	3	-5	35.2	33.6
6	3	-4	12.1	12.1
6	3	-3	50.2	49.7
6	3	-2	8.3	7.0
6	3	-1	27.2	27.8
6	4	-5	10.9	10.0
6	4	-4	5.7	3.8
6	4	-3	9.3	9.7
6	4	-2	14.3	13.0
6	4	-1	35.1	35.9
6	5	-5	3.6	2.4
6	5	-4	43.6	43.5
6	5	-3	5.9	4.6
6	5	-2	42.0	41.2
6	5	-1	4.4	3.3
6	6	-5	4.7	2.1
6	6	-4	6.2	7.0
6	6	-3	5.7	5.0
6	6	-2	46.8	43.6
6	6	-1	12.1	12.1
6	7	-4	31.9	30.5
6	7	-3	16.5	15.4
6	7	-2	27.5	26.5
6	7	-1	8.7	8.3
6	8	-4	3.6	2.1
6	8	-3	2.7	3.9
6	8	-2	3.8	0.9
6	8	-1	24.5	25.4
6	9	-4	17.1	16.5
6	9	-3	22.8	20.7
6	9	-2	13.6	14.4
6	9	-1	11.5	10.8
6	10	-3	9.5	9.0
6	10	-2	22.7	20.4
6	10	-1	27.2	26.5
6	11	-2	19.6	19.3
6	11	-1	11.4	10.3
6	12	-1	3.9	3.1
7	0	-5	22.1	24.7
7	0	-3	23.8	24.8
7	0	-1	10.9	9.0
7	1	-5	4.4	3.7
7	1	-4	9.0	8.7
7	1	-3	23.4	25.2
7	1	-2	4.0	5.7
7	1	-1	30.3	32.1
7	2	-5	9.2	10.8
7	2	-4	6.5	11.0
7	2	-3	18.2	19.8
7	2	-2	15.1	18.8
7	2	-1	17.1	18.2
7	3	-5	11.8	11.5
7	3	-4	8.2	7.9
7	3	-3	22.4	22.2
7	3	-2	14.0	15.9
7	3	-1	13.5	12.9
7	4	-4	21.6	23.3
7	4	-3	14.1	14.9

h	k	l	F_{obs}	F_{calc}
7	4	-2	8.6	6.5
7	4	-1	9.7	8.6
7	5	-4	7.1	5.9
7	5	-3	4.9	5.2
7	5	-2	12.5	12.5
7	5	-1	18.5	19.2
7	6	-4	2.0	0.1
7	6	-3	30.4	34.5
7	6	-2	4.1	4.9
7	6	-1	28.4	29.3
7	7	-3	4.2	0.2
7	7	-2	10.6	11.1
7	7	-1	14.6	14.2
7	8	-3	4.2	5.9
7	8	-2	4.8	0.4
7	8	-1	1.9	1.5
7	9	-2	14.6	15.5
7	9	-1	6.8	5.2
7	10	-2	9.7	11.8
7	10	-1	9.8	11.4
8	0	-4	7.8	8.4
8	0	-2	35.5	32.8
8	1	-4	32.9	32.7
8	1	-3	5.7	4.8
8	1	-2	28.3	28.7
8	1	-1	5.8	3.0
8	2	-4	4.0	0.7
8	2	-3	9.0	8.3
8	2	-2	2.4	2.5
8	2	-1	29.1	29.5
8	3	-4	12.6	12.6
8	3	-3	26.2	25.0
8	3	-2	9.7	9.8
8	3	-1	15.2	14.7
8	4	-3	11.4	10.1
8	4	-2	18.2	16.3
8	4	-1	30.8	29.7
8	5	-3	21.1	22.5
8	5	-2	19.5	20.4
8	5	-1	12.4	12.4
8	6	-3	5.2	1.6
8	6	-2	7.8	7.5
8	6	-1	2.3	1.8
8	7	-2	16.7	16.3
8	7	-1	13.6	13.5
8	8	-1	32.7	32.5
9	0	-1	20.1	21.7
9	1	-2	8.2	8.5
9	1	-1	9.9	12.3
9	2	-2	5.5	4.7
9	2	-1	1.0	1.3
9	3	-2	11.7	13.8
9	3	-1	7.8	7.3
9	4	-1	9.9	9.7
9	5	-1	17.1	19.0

h	k	l	F_{obs}	F_{calc}
0	0	2	157.3	161.8
0	0	4	1.7	3.0
0	0	6	42.2	41.9
0	1	1	10.8	12.1
0	1	2	55.5	53.6
0	1	3	29.9	26.6
0	1	4	56.7	57.2
0	1	5	21.5	20.0
0	1	6	19.6	21.2
0	1	7	9.1	9.3
0	2	0	28.9	32.7
0	2	1	58.0	63.1
0	2	2	21.3	23.0
0	2	3	1.9	3.2
0	2	4	2.5	2.8
0	2	5	17.2	16.0
0	2	6	5.6	5.8
0	2	7	6.5	6.2
0	3	1	54.5	51.7
0	3	2	17.9	18.6
0	3	3	89.1	87.1
0	3	4	29.7	30.2
0	3	5	49.7	50.2
0	3	6	16.4	16.4
0	3	7	11.1	12.7
0	4	0	137.6	138.8
0	4	1	53.1	45.7
0	4	2	79.7	73.3
0	4	3	15.9	14.1
0	4	4	2.9	5.1
0	4	5	21.7	20.8
0	4	6	24.0	24.1
0	4	7	22.9	23.7
0	5	1	42.1	39.7
0	5	2	39.0	35.6
0	5	3	60.4	59.7
0	5	4	31.4	30.1
0	5	5	27.8	27.5
0	5	6	6.6	7.0
0	5	7	1.3	1.6
0	6	0	66.7	69.2
0	6	1	2.6	1.2
0	6	2	45.2	46.3
0	6	3	8.5	7.5
0	6	4	8.0	8.2
0	6	5	6.6	6.5
0	6	6	9.4	9.5
0	7	1	36.3	36.4
0	7	2	25.7	26.4
0	7	3	61.7	63.1
0	7	4	15.9	16.0
0	7	5	34.6	36.0
0	7	6	2.2	0.5
0	8	0	38.5	34.1
0	8	1	67.4	64.7
0	8	2	25.6	22.6
0	8	3	22.3	20.3
0	8	4	4.8	3.7
0	8	5	17.2	17.8
0	8	6	4.5	5.4
0	9	1	35.0	35.0
0	9	2	1.2	0.2
0	9	3	61.1	61.2
0	9	4	4.4	4.9
0	9	5	35.8	35.1
0	9	6	4.7	5.7
0	10	0	36.5	37.4
0	10	1	13.6	15.1
0	10	2	27.4	27.6
0	10	3	3.9	4.5
0	10	4	9.1	9.0
0	10	5	1.7	1.9
0	11	1	8.9	9.4
0	11	2	26.0	28.1
0	11	3	15.3	16.1
0	11	4	23.3	24.9
0	11	5	7.2	7.7
0	12	0	61.5	58.5
0	12	1	19.8	19.8
0	12	2	37.7	36.0
0	12	3	7.9	8.3
0	12	5	2.1	3.6
0	13	1	8.5	9.1
0	13	2	13.5	13.4
0	13	3	17.0	17.4
0	13	4	15.3	15.5
0	14	1	4.4	4.0
0	14	2	2.2	2.1
0	14	3	3.1	2.4
0	15	1	3.9	4.7
0	15	2	10.4	11.4
1	0	1	54.3	56.3
1	0	3	30.7	31.4
1	0	5	2.4	0.8

h	k	l	F_{obs}	F_{calc}
1	0	7	11.8	13.4
1	1	1	18.9	16.6
1	1	2	2.0	4.6
1	1	3	22.0	19.4
1	1	4	14.5	12.3
1	1	5	6.9	6.1
1	1	6	9.5	9.1
1	1	7	2.9	1.7
1	2	0	54.7	56.8
1	2	1	20.0	20.9
1	2	2	16.4	19.4
1	2	3	10.7	11.0
1	2	4	14.8	13.4
1	2	5	2.2	0.8
1	2	6	14.9	15.0
1	2	7	5.3	4.8
1	3	1	36.7	31.8
1	3	2	5.8	3.9
1	3	3	45.6	41.9
1	3	4	2.5	0.1
1	3	5	18.8	16.2
1	4	0	4.8	10.2
1	4	1	10.9	12.2
1	4	2	5.8	0.2
1	4	3	11.3	11.9
1	4	4	14.1	11.4
1	4	6	10.0	10.7
1	4	7	6.4	7.9
1	5	1	12.2	10.6
1	5	2	10.9	9.5
1	5	3	19.2	17.0
1	5	4	21.0	19.4
1	5	5	11.5	9.7
1	5	6	13.5	12.5
1	5	7	1.7	2.3
1	6	0	30.9	27.6
1	6	1	15.1	19.5
1	6	2	15.7	13.6
1	6	3	10.9	12.4
1	6	4	1.7	1.3
1	6	5	3.9	2.7
1	6	6	3.4	3.1
1	6	7	9.5	9.3
1	7	1	15.1	14.2
1	7	2	11.7	9.7
1	7	3	21.7	21.1
1	7	4	14.2	12.8
1	7	5	8.5	7.8
1	7	6	7.6	6.9
1	8	0	30.2	32.4
1	8	1	14.8	17.1
1	8	2	13.6	15.2
1	8	3	5.0	6.3
1	8	4	7.8	7.2
1	8	6	10.2	10.6
1	9	1	12.6	11.8
1	9	2	4.5	5.5
1	9	3	21.5	20.2
1	9	4	8.8	9.2
1	9	5	10.6	10.1
1	9	6	7.6	7.0
1	10	0	10.0	13.3
1	10	1	2.0	1.9
1	10	2	5.1	7.1
1	10	3	2.1	1.9
1	10	4	2.9	2.8
1	10	5	3.2	2.9
1	11	1	1.4	1.0
1	11	2	10.9	10.8
1	11	3	3.3	0.6
1	11	4	13.7	14.0
1	11	5	3.1	1.4
1	12	0	16.9	15.7
1	12	1	11.4	12.7
1	12	2	9.3	8.7
1	12	3	5.1	5.3
1	12	4	2.5	1.2
1	13	1	4.4	5.7
1	13	2	4.7	5.7
1	13	3	8.5	9.5
1	13	4	5.3	5.4
1	14	0	19.7	21.1
1	14	1	5.0	2.8
1	14	2	11.8	12.9
1	14	3	2.4	0.7
1	15	1	3.0	3.2
1	15	2	2.7	1.8
2	0	2	52.3	56.0
2	0	4	8.9	10.9
2	0	6	10.9	10.9
2	1	1	52.6	50.1
2	1	2	47.0	44.5
2	1	3	73.1	75.5
2	1	4	30.8	30.4
2	1	5	35.0	36.3
2	1	6	4.9	4.7
2	1	7	1.9	3.9
2	2	0	105.5	108.3
2	2	1	70.0	62.9
2	2	2	66.2	59.5

h	k	l	F_{obs}	F_{calc}
2	2	3	25.7	22.2
2	2	4	2.8	0.3
2	2	5	23.5	22.8
2	2	6	16.1	16.0
2	2	7	27.4	28.5
2	3	1	59.3	57.1
2	3	2	5.1	7.0
2	3	3	90.1	91.7
2	3	4	17.0	18.2
2	3	5	49.9	49.4
2	3	6	13.1	13.0
2	3	7	10.1	10.5
2	4	0	52.4	52.9
2	4	1	48.9	52.8
2	4	2	38.3	37.5
2	4	3	6.8	9.2
2	4	4	[illegible].4	9.6
2	4	5	10.2	9.4
2	4	6	5.6	5.2
2	4	7	5.4	4.9
2	5	1	7.9	7.0
2	5	2	54.3	55.4
2	5	3	6.3	6.4
2	5	4	48.0	49.4
2	5	5	3.4	2.1
2	5	6	15.7	16.3
2	5	7	4.5	4.8
2	6	0	148.3	150.2
2	6	1	23.6	22.2
2	6	2	90.5	86.6
2	6	3	11.6	9.8
2	6	4	2.2	2.5
2	6	5	2.8	2.8
2	6	6	29.9	30.1
2	7	1	15.8	14.9
2	7	2	31.7	31.1
2	7	3	28.8	27.4
2	7	4	34.3	34.4
2	7	5	19.5	18.5
2	7	6	14.5	15.3
2	8	0	2.7	3.2
2	8	1	23.9	26.3
2	8	2	1.9	0.2
2	8	3	2.8	0.3
2	8	4	3.9	3.8
2	8	5	10.7	10.3
2	8	6	3.5	3.1
2	9	1	15.8	15.9
2	9	2	19.1	19.9
2	9	3	31.0	31.7
2	9	4	20.9	22.0
2	9	5	22.2	23.0
2	9	6	8.9	9.9
2	10	0	64.1	62.8
2	10	1	32.4	30.6
2	10	2	37.0	36.1
2	10	3	8.5	7.5
2	10	4	3.8	5.0
2	10	5	10.5	10.4
2	11	1	12.7	12.7
2	11	2	19.3	18.9
2	11	3	21.8	22.4
2	11	4	19.1	18.5
2	11	5	12.1	11.8
2	12	0	23.8	24.3
2	12	1	2.9	1.4
2	12	2	16.3	16.6
2	12	3	5.1	4.6
2	12	4	5.0	3.1
2	13	1	14.4	14.6
2	13	2	6.5	5.1
2	13	3	26.3	28.7
2	13	4	3.5	2.7
2	14	0	3.9	1.4
2	14	1	31.1	31.9
2	14	2	3.2	0.4
2	14	3	11.0	10.8
2	15	1	11.4	11.8
2	15	2	2.6	1.6
3	0	1	4.8	9.3
3	0	3	10.0	11.1
3	0	5	3.3	2.4
3	0	7	8.6	9.2
3	1	1	23.1	20.8
3	1	2	10.7	8.8
3	1	3	30.7	29.1
3	1	4	19.6	18.4
3	1	5	14.4	12.8
3	1	6	12.5	12.3
3	2	0	8.3	13.1
3	2	1	29.1	29.8
3	2	2	5.4	0.3
3	2	3	14.1	14.1
3	2	4	15.0	13.2
3	2	5	2.0	0.2
3	2	6	10.0	10.9
3	2	7	4.6	5.5
3	3	1	26.5	24.2
3	3	2	10.5	10.8
3	3	3	37.4	35.3

h	k	l	F_{obs}	F_{calc}
3	3	4	12.0	12.4
3	3	5	16.7	14.8
3	3	6	7.9	8.3
3	3	7	1.4	0.5
3	4	0	29.5	33.2
3	4	1	6.6	3.6
3	4	2	12.3	14.9
3	4	3	3.0	2.6
3	4	4	8.9	7.8
3	4	5	2.6	1.8
3	4	6	12.0	11.7
3	4	7	5.2	5.6
3	5	1	3.8	1.8
3	5	2	6.4	5.9
3	5	3	4.4	3.5
3	5	4	14.2	13.3
3	5	5	3.0	1.8
3	5	6	9.7	8.8
3	6	0	19.9	18.4
3	6	1	34.1	36.3
3	6	2	10.5	9.0
3	6	3	18.0	19.3
3	6	4	2.8	1.8
3	6	5	2.0	1.3
3	6	6	3.4	2.8
3	7	1	8.3	7.5
3	7	2	5.0	3.1
3	7	3	10.6	10.6
3	7	4	6.3	4.9
3	7	5	1.5	2.0
3	7	6	3.5	1.8
3	8	0	38.0	40.9
3	8	1	8.8	11.0
3	8	2	21.1	21.9
3	8	3	3.8	4.0
3	8	4	4.8	4.6
3	8	5	4.7	0.6
3	8	6	10.7	11.1
3	9	1	10.5	9.5
3	9	2	2.9	1.0
3	9	3	17.5	16.4
3	9	5	8.6	7.9
3	10	0	2.3	4.0
3	10	1	10.6	10.1
3	10	2	2.1	1.3
3	10	3	5.5	6.2
3	10	4	5.6	3.1
3	10	5	2.8	1.7
3	11	1	2.4	1.9
3	11	2	10.3	10.2
3	11	3	6.0	5.0
3	11	4	12.7	13.2
3	11	5	5.1	5.4
3	12	0	15.7	15.8
3	12	1	3.3	4.2
3	12	2	9.7	9.3
3	12	3	1.6	0.8
3	13	1	8.2	6.6
3	13	2	7.6	7.9
3	13	3	10.6	11.6
3	14	0	12.4	13.2
3	14	1	2.1	2.5
3	14	2	7.2	7.6
3	15	1	3.7	3.2
4	0	2	89.2	88.5
4	0	4	2.8	4.0
4	0	6	29.2	30.4
4	1	1	4.6	4.7
4	1	2	46.4	47.8
4	1	3	13.7	11.9
4	1	4	46.2	47.4
4	1	5	13.0	11.4
4	1	6	18.3	19.0
4	2	0	12.0	14.4
4	2	1	49.0	51.9
4	2	2	8.5	10.1
4	2	3	7.8	7.6
4	2	4	1.8	1.2
4	2	5	12.4	11.7
4	2	6	5.1	3.5
4	3	1	28.3	28.0
4	3	2	15.5	16.8
4	3	3	51.0	51.3
4	3	4	22.2	22.9
4	3	5	31.6	32.0
4	3	6	12.3	13.0
4	4	0	77.3	77.9
4	4	1	53.1	51.0
4	4	2	45.9	43.6
4	4	3	16.2	14.8
4	4	4	5.1	4.6
4	4	5	16.9	16.1
4	4	6	18.0	17.8
4	5	1	23.8	23.9
4	5	2	30.9	30.5
4	5	3	39.2	39.5
4	5	4	27.5	26.6
4	5	5	18.5	19.1
4	5	6	8.0	7.9
4	6	0	31.3	34.0
4	6	1	1.8	1.0
4	6	2	22.1	23.7

h	k	l	F_{obs}	F_{calc}
4	6	3	4.9	4.5
4	6	4	5.0	4.7
4	6	5	5.8	4.8
4	6	6	6.2	5.8
4	7	1	23.2	23.6
4	7	2	20.4	21.2
4	7	3	41.5	42.7
4	7	4	15.0	15.1
4	7	5	24.0	25.1
4	7	6	2.2	2.2
4	8	0	22.3	20.7
4	8	1	55.0	54.0
4	8	2	15.6	14.3
4	8	3	18.8	17.8
4	8	4	3.2	2.6
4	8	5	13.3	13.9
4	9	1	22.4	22.9
4	9	2	1.7	0.1
4	9	3	40.2	41.2
4	9	4	2.4	3.5
4	9	5	24.4	24.0
4	10	0	23.3	22.8
4	10	1	12.3	14.5
4	10	2	17.7	17.4
4	10	3	4.0	5.0
4	10	4	6.2	6.4
4	10	5	2.7	1.7
4	11	1	7.2	7.8
4	11	2	21.8	23.5
4	11	3	14.7	13.8
4	11	4	19.9	22.0
4	12	0	41.5	40.0
4	12	1	14.9	15.8
4	12	2	26.0	24.5
4	12	3	6.6	6.9
4	13	1	4.7	6.1
4	13	2	11.5	11.8
4	13	3	11.8	11.7
4	14	0	3.3	1.3
4	14	1	5.1	5.5
5	0	1	36.6	39.9
5	0	3	22.3	22.8
5	0	5	1.0	0.8
5	1	1	5.8	5.1
5	1	2	3.0	1.1
5	1	3	7.1	7.2
5	1	4	6.9	5.8
5	1	6	4.9	3.9
5	2	0	34.8	37.2
5	2	1	5.7	7.3
5	2	2	17.1	18.3
5	2	3	3.2	3.6
5	2	4	7.3	6.8
5	2	5	0.9	1.3
5	2	6	11.1	11.3
5	3	1	15.8	15.4
5	3	2	6.6	5.2
5	3	3	25.6	24.6
5	3	4	4.9	5.2
5	3	5	11.5	10.7
5	3	6	3.4	3.6
5	4	0	1.9	3.9
5	4	1	14.7	16.0
5	4	2	5.0	1.1
5	4	3	10.0	10.6
5	4	4	9.5	7.7
5	4	5	3.0	0.2
5	4	6	6.5	6.6
5	5	1	8.3	7.9
5	5	2	9.7	9.0
5	5	3	15.9	14.6
5	5	4	14.9	14.3
5	5	5	12.5	9.6
5	5	6	9.9	9.8
5	6	0	15.9	15.5
5	6	1	3.8	6.7
5	6	2	9.4	8.8
5	6	3	3.1	3.2
5	6	5	4.6	3.1
5	7	1	10.6	10.0
5	7	2	10.7	9.3
5	7	3	17.0	16.5
5	7	4	12.7	12.1
5	7	5	8.2	7.4
5	8	0	13.5	14.9
5	8	1	9.8	10.8
5	8	2	5.1	6.3
5	8	3	4.1	4.6
5	8	4	7.9	5.7
5	8	5	1.4	0.2
5	9	1	8.5	8.0
5	9	2	6.0	6.0
5	9	3	14.5	14.4
5	9	4	8.7	9.6
5	10	0	10.4	11.8
5	10	1	3.4	2.7
5	10	2	6.1	6.8
5	10	3	3.7	1.5
5	10	4	2.0	1.7
5	11	1	3.7	1.9
5	11	2	8.1	7.7
5	11	3	2.8	3.0

h	k	l	F_{obs}	F_{calc}
5	12	0	10.1	9.3
5	12	1	11.2	11.9
5	12	2	5.6	5.0
5	12	3	6.4	5.8
5	13	1	3.5	3.3
5	13	2	2.8	2.4
6	0	0	18.5	20.0
6	0	2	14.0	14.8
6	0	4	3.3	3.5
6	0	6	5.0	4.4
6	1	1	20.0	19.9
6	1	2	26.3	25.8
6	1	3	34.3	34.5
6	1	4	21.4	21.4
6	1	5	17.3	17.8
6	2	0	40.0	38.5
6	2	1	51.4	50.1
6	2	2	24.8	23.1
6	2	3	18.2	16.7
6	2	4	2.3	0.7
6	2	5	13.2	13.3
6	3	1	21.6	21.3
6	3	2	4.7	5.8
6	3	3	38.6	38.5
6	3	4	9.3	10.5
6	3	5	23.0	22.6
6	4	0	15.4	15.5
6	4	1	28.0	30.8
6	4	2	12.1	11.9
6	4	3	7.0	8.2
6	4	4	4.9	4.1
6	4	5	5.6	5.4
6	5	1	5.7	5.0
6	5	2	32.3	33.4
6	5	3	7.4	7.1
6	5	4	31.7	32.8
6	5	5	2.2	1.1
6	6	0	64.0	63.9
6	6	1	12.8	12.8
6	6	2	39.5	37.9
6	6	3	6.0	6.0
6	6	4	5.1	3.0
6	6	5	3.4	1.4
6	7	1	6.3	5.4
6	7	2	20.1	21.0
6	7	3	12.0	10.8
6	7	4	22.6	23.8
6	8	0	2.9	1.2
6	8	1	17.7	19.4
6	8	2	2.4	2.1
6	8	3	5.6	3.0
6	8	4	2.3	2.6
6	9	1	6.3	6.3
6	9	2	12.3	12.1
6	9	3	13.0	13.1
6	9	4	12.6	14.0
6	10	0	31.5	30.9
6	10	1	21.8	21.4
6	10	2	18.5	17.5
6	10	3	7.2	6.2
6	11	1	6.0	7.0
6	11	2	13.2	13.5
6	12	0	8.7	9.1
6	12	1	3.1	1.5
7	0	1	5.1	7.8
7	0	3	3.5	3.8
7	0	5	3.8	2.8
7	1	1	8.1	7.5
7	1	2	6.5	5.7
7	1	3	13.9	12.8
7	1	4	10.6	9.7
7	1	5	7.8	6.5
7	2	0	7.6	9.6
7	2	1	11.3	11.6
7	2	2	2.2	2.7
7	2	3	6.8	6.7
7	2	4	8.5	6.5
7	2	5	2.9	0.6
7	3	1	10.8	10.1
7	3	2	4.1	3.8
7	3	3	17.5	17.2
7	3	4	7.9	6.3
7	3	5	8.6	8.2
7	4	0	13.8	14.3
7	4	1	2.6	0.0
7	4	2	6.9	7.0
7	4	3	3.3	0.3
7	4	4	4.1	4.0
7	5	1	2.3	1.2
7	5	2	5.4	4.9
7	5	3	4.4	2.2
7	5	4	7.7	7.7
7	6	0	7.2	7.5
7	6	1	16.6	17.7
7	6	2	3.6	3.9
7	6	3	10.8	10.7
7	7	1	4.2	3.9
7	7	2	4.3	1.7
7	7	3	5.1	6.1
7	7	4	2.5	1.8
7	8	0	19.1	20.2
7	8	1	7.0	6.6
7	8	2	11.4	11.4
7	8	3	2.2	2.5

h	k	l	F_{obs}	F_{calc}
7	9	1	4.6	4.7
7	9	2	2.4	0.1
7	9	3	8.1	8.4
7	10	0	1.9	2.7
7	10	1	7.0	6.6
7	10	2	2.8	1.1
8	0	0	51.4	49.8
8	0	2	31.0	29.3
8	0	4	3.0	3.4
8	1	1	4.0	0.2
8	1	2	21.4	21.9
8	1	3	3.4	1.6
8	1	4	23.4	24.1
8	2	0	1.8	2.0
8	2	1	22.1	22.8
8	2	2	2.6	1.3
8	2	3	6.2	5.7
8	2	4	0.6	0.2
8	3	1	8.6	8.6
8	3	2	8.3	8.2
8	3	3	16.2	16.8
8	3	4	10.6	11.1
8	4	0	26.6	26.2
8	4	1	26.1	25.5
8	4	2	16.5	14.8
8	4	3	8.9	8.6
8	5	1	11.0	9.2
8	5	2	14.7	14.7
8	5	3	15.2	16.3
8	6	0	7.9	6.8
8	6	1	3.1	1.1
8	6	2	4.5	4.9
8	6	3	2.0	1.6
8	7	1	8.8	9.0
8	7	2	10.1	10.5
8	8	0	7.9	8.1
8	8	1	28.1	27.8
8	8	2	5.4	5.8
9	0	1	12.6	12.7
9	1	1	2.9	2.9
9	1	2	2.5	1.9
9	2	0	11.1	11.1
9	2	1	3.7	4.4
9	2	2	5.9	5.3
9	3	1	5.7	5.9
9	3	2	1.0	0.1
9	4	0	3.8	4.5
9	4	1	6.0	5.6
9	5	1	3.8	2.4