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Crystal chemistry of a metamorphic biotite and its significance in water barometry¹

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Abstract

The crystal structure of a metamorphic biotite from Au Sable Forks, New York (northeast Adirondacks) has been refined to an unweighted *R* value of 4.2%. The Au Sable biotite is a 2M₁ mica with space group symmetry C2/c. Although the biotite equilibrated near and cooled slowly from *T* = 700° ± 50°C, octahedral and tetrahedral cations are apparently disordered. There are few, if any, octahedral and interlayer cation site deficiencies. Average bond lengths are M1-O 2.106, M2-O 2.086, T1-O 1.657, T2-O 1.661, inner K-O 3.046, outer K-O 3.289 Å. The tetrahedral rotation angle (α) is 5.3°. The Au Sable biotite structure is nearly identical to the igneous 2M₁ biotite of similar composition refined by Takeda and Ross (1975).

The Au Sable biotite coexists with magnetite (Usp₃₂), ilmenite (Hm₃), perthite (Or₆₈), and plagioclase (An₂₂). This assemblage fixes *T* (700°C), *f*_{O₂} (10^{-17.2}), and *f*_{H₂O} (10²⁻¹⁰) for metamorphic pressure of 7 ± 1 kbar. Metamorphism of orthogneisses in the Au Sable area of the Adirondacks took place under quite dry (*P*_{H₂O} << *P*_{solid}) conditions.

Introduction

Although the basic mica crystal structure was solved in the early 1930's, in the past fifteen years the knowledge of the details of mica crystal chemistry has been significantly increased through numerous structure refinements. Muscovite polytypes 2M₁ and 3T have been refined by Burnham and Radoslovich (1964), Güven (1967), and Güven and Burnham (1967). 2M₁ paragonite and 2M₁ phengite have been investigated by Burnham and Radoslovich (1964) and Güven (1967) respectively. Brittle micas of various compositions have been studied by Takéuchi (1964), and Guggenheim and Bailey (1975) have discussed the details of margarite crystal structure. Lithium micas such as fluor-polyolithionite (Takeda and Burnham, 1969) and 2M₁ and 1M lepidolites (Takeda *et al.*, 1971) have also been refined.

In comparison to the numerous crystal structure refinements of these dioctahedral calcium and lithium micas, trioctahedral micas have received some-

what less attention. Steinfink (1962), Hazen and Burnham (1973), McCauley *et al.* (1973), and Takeda and Ross (1975) have refined various phlogopites, biotites, or annites. Of these micas only one, a nearly end-member phlogopite, was obtained from a metamorphic rock. Refinements of igneous biotite suggest that the octahedral and tetrahedral cations are disordered, a result which might have been predicted from our understanding of cation order-disorder in minerals equilibrating at igneous temperatures.

There may be a good reason why no refinements of metamorphic biotites have been attempted to date. Due to the nature of the rocks in which metamorphic biotites occur, it is difficult to obtain an undeformed mica sample acceptable for crystal structure analysis. Nevertheless, phlogopite and biotite are found in many metamorphic rock types and are involved in numerous important metamorphic reactions. Because mica-bearing reaction equilibria can be profoundly affected by mica cation ordering, which reduces configurational entropy, the assumption of an igneous structure model for metamorphic biotites may lead to systematic errors in calculated equilibria.

In addition to their importance in isogratic reactions, micas along the phlogopite-annite join have been used to infer equilibrium water fugacities when

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	0	57.0	52.2	4	10	1	4.8 *	0.3
6	0	0	91.0	88.8	-3	11	1	4.6 *	6.7
3	1	0	24.3	25.9	3	11	1	4.5 *	1.6
5	1	0	3.7 *	6.1	-6	0	2	175.2	170.6
2	2	0	53.4	47.8	-4	0	2	104.9	101.9
2	4	0	19.0	21.6	-2	0	2	281.4	285.8
1	5	0	43.3	45.9	2	0	2	8.0	9.5
3	5	0	18.2	19.9	4	0	2	195.6	200.1
5	5	0	3.9 *	1.1	-7	1	2	15.5	14.5
-6	6	0	57.9	49.2	-3	1	2	32.8	34.6
2	6	0	101.6	100.5	3	1	2	73.3	74.9
4	6	0	128.7	127.8	5	1	2	43.1	48.6
6	6	0	59.0	49.2	-6	2	2	3.9 *	4.1
1	7	0	32.0	35.1	-4	2	2	12.4	17.1
3	7	0	18.8	22.4	-2	2	2	41.4	40.3
5	7	0	4.6 *	4.0	2	2	2	36.6	38.4
2	8	0	3.7 *	9.5	4	2	2	19.6	21.0
5	9	0	5.5 *	5.8	-2	4	2	10.3	10.5
2	10	0	3.4 *	2.5	2	4	2	14.5	17.1
3	11	0	15.3	14.2	4	4	2	21.0	27.3
-7	1	1	4.8 *	3.3	-3	5	2	36.5	39.6
-3	1	1	28.6	29.8	-1	5	2	10.8	7.2
3	1	1	17.7	20.7	1	5	2	11.7	12.6
-4	2	1	37.0	41.2	3	5	2	60.4	63.5
-2	2	1	84.9	75.7	-6	6	2	162.9	150.5
2	2	1	81.9	80.0	-4	6	2	29.6	31.2
4	2	1	3.4 *	2.8	-2	6	2	240.3	241.5
-7	3	1	93.2	87.9	2	6	2	45.5	47.6
-5	3	1	30.2	30.9	4	6	2	155.8	154.0
-3	3	1	345.5	343.4	6	6	2	4.6 *	8.1
3	3	1	143.4	147.0	-1	7	2	22.9	26.3
5	3	1	37.4	39.8	1	7	2	33.8	32.7
7	3	1	86.6	87.0	-4	8	2	4.0 *	1.6
-6	4	1	27.6	28.9	-1	9	2	3.8 *	17.9
-4	4	1	15.6	17.0	-4	10	2	4.8 *	9.4
-2	4	1	40.1	41.3	-2	10	2	15.0	0.6
2	4	1	14.6	13.7	2	10	2	4.3 *	13.6
4	4	1	24.4	26.7	-3	11	2	4.3 *	12.0
-3	5	1	17.0	24.2	-1	11	2	4.3 *	15.4
-1	5	1	15.6	16.3	1	11	2	21.4	19.8
1	5	1	16.6	15.3	3	11	2	16.1	15.5
-1	7	1	18.7	25.1	-3	1	3	2.9 *	0.4
1	7	1	3.1 *	7.2	1	1	3	65.9	67.2
-4	8	1	3.6 *	0.6	3	1	3	51.2	54.3
-2	8	1	21.3	24.2	7	1	3	6.9 *	13.0
2	8	1	3.4 *	4.3	-6	2	3	4.2 *	4.7
-3	9	1	176.2	175.2	-2	2	3	78.9	77.4
-1	9	1	30.8	28.8	2	2	3	50.7	54.4
1	9	1	129.9	130.4	4	2	3	60.5	63.4
3	9	1	67.4	66.2	-7	3	3	21.3	22.5
5	9	1	4.8 *	17.1	-5	3	3	128.2	125.0
-2	10	1	3.4 *	0.5	-3	3	3	150.7	149.3
2	10	1	3.7 *	9.2	1	3	3	264.7	261.6

H	K	L	F(OBS)	F(CALC)
3	3	3	64.3	67.7
5	3	3	88.8	88.1
-2	4	3	43.2	44.0
0	4	3	68.0	67.2
2	4	3	63.7	64.9
4	4	3	34.2	38.4
-1	5	3	31.2	29.1
1	5	3	30.3	28.8
3	5	3	41.6	47.9
0	6	3	6.7	28.2
2	6	3	4.0 *	4.6
-5	7	3	5.8 *	18.7
-1	7	3	3.2 *	8.3
1	7	3	49.3	49.9
-4	8	3	11.2	12.4
-2	8	3	22.0	23.0
0	8	3	38.2	39.7
2	8	3	42.4	44.0
4	8	3	5.0 *	25.4
-5	9	3	95.8	92.2
-3	9	3	100.3	94.3
-1	9	3	41.9	43.1
1	9	3	158.7	158.5
3	9	3	42.0	43.6
5	9	3	75.3	72.4
-4	10	3	4.5 *	1.9
-2	10	3	24.4	22.8
0	10	3	28.3	27.0
2	10	3	20.8	23.2
4	10	3	23.0	31.1
-1	11	3	9.6	1.3
1	11	3	21.6	19.6
3	11	3	21.9	13.9
-6	0	4	63.3	64.1
-4	0	4	42.3	44.7
-2	0	4	261.8	262.6
2	0	4	124.2	135.0
4	0	4	60.0	59.9
6	0	4	51.9	51.7
-7	1	4	4.6 *	8.6
-3	1	4	37.2	40.8
-1	1	4	131.3	130.5
1	1	4	148.0	148.0
3	1	4	95.9	96.9
5	1	4	47.6	44.4
-2	2	4	36.2	38.5
2	2	4	13.9	15.5
-1	3	4	6.8	2.5
3	3	4	3.6 *	14.6
-2	4	4	60.2	58.0
0	4	4	23.6	25.4
2	4	4	54.8	53.7
-1	5	4	99.9	99.6

H	K	L	F(OBS)	F(CALC)
1	5	4	85.1	85.7
3	5	4	80.8	83.7
-6	6	4	46.1	49.7
-4	6	4	38.5	40.5
-2	6	4	206.3	206.8
0	6	4	68.4	69.8
2	6	4	168.5	172.3
4	6	4	75.6	74.9
-5	7	4	5.1 *	2.3
-1	7	4	48.1	47.7
1	7	4	88.7	92.1
3	7	4	44.9	45.3
-2	8	4	24.6	25.5
0	8	4	22.4	22.5
2	8	4	26.1	28.9
1	9	4	22.1	19.7
-4	10	4	30.8	11.2
0	10	4	24.0	22.5
2	10	4	15.0	16.1
4	10	4	11.2	11.6
-3	11	4	29.4	25.3
-1	11	4	26.6	28.2
1	11	4	50.2	50.3
3	11	4	31.9	30.4
-3	1	5	40.7	44.9
-1	1	5	94.9	91.3
1	1	5	78.2	78.2
3	1	5	41.8	42.1
-4	2	5	84.6	86.2
-2	2	5	32.9	36.2
0	2	5	153.9	147.1
2	2	5	11.3	9.5
4	2	5	45.9	48.1
-5	3	5	161.6	156.8
-3	3	5	66.8	69.2
-1	3	5	133.3	137.1
1	3	5	254.7	248.5
3	3	5	87.2	93.6
5	3	5	82.6	80.8
7	3	5	40.7	39.4
-6	4	5	32.8	31.7
-2	4	5	104.3	103.7
0	4	5	14.0	13.9
2	4	5	83.4	80.4
4	4	5	3.6 *	9.3
-5	5	5	21.3	20.9
-3	5	5	32.1	33.3
-1	5	5	64.6	62.3
1	5	5	49.3	49.3
0	6	5	11.1	33.4
-1	7	5	43.6	43.7
1	7	5	41.2	40.7
-4	8	5	29.5	34.2

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	8	5	60.0	59.5	-5	7	6	33.1	30.8
0	8	5	27.6	26.7	-1	7	6	63.4	62.3
2	8	5	44.0	42.3	1	7	6	39.5	39.3
4	8	5	3.9 *	2.2	3	7	6	16.0	15.2
-5	9	5	92.7	94.7	5	7	6	12.6	12.2
-3	9	5	13.2	15.8	0	8	6	9.2	1.9
-1	9	5	95.3	94.7	2	8	6	11.3	10.0
1	9	5	78.7	78.9	4	8	6	3.9 *	6.7
3	9	5	55.9	56.9	-1	9	6	17.2	21.8
5	9	5	47.5	46.0	1	9	6	8.2	0.6
-4	10	5	34.0	34.9	3	9	6	16.4	16.8
0	10	5	38.3	38.6	5	9	6	21.3	19.2
2	10	5	16.3	14.4	-2	10	6	6.3	5.4
4	10	5	9.8	11.3	0	10	6	21.9	18.8
-3	11	5	22.2	20.1	2	10	6	8.1	4.1
-1	11	5	22.9	23.3	4	10	6	4.1 *	5.9
1	11	5	25.6	27.2	-3	11	6	36.1	34.6
3	11	5	14.1	12.3	-1	11	6	38.3	35.3
-6	0	6	39.0	40.6	1	11	6	23.4	24.5
-4	0	6	172.2	172.7	3	11	6	3.9 *	7.5
-2	0	6	256.6	249.7	-3	1	7	44.1	42.1
0	0	6	283.5	287.4	-1	1	7	43.0	39.8
2	0	6	198.8	199.7	1	1	7	28.4	25.4
4	0	6	114.9	119.0	3	1	7	12.1	12.3
6	0	6	113.3	110.0	5	1	7	13.7	12.2
-7	1	6	31.8	27.7	7	1	7	14.4	14.7
-5	1	6	40.4	46.8	-4	2	7	61.0	63.8
-3	1	6	91.4	92.4	-2	2	7	33.2	32.4
-1	1	6	133.8	124.0	0	2	7	60.9	56.3
1	1	6	93.7	90.5	2	2	7	48.6	49.2
3	1	6	29.4	27.9	4	2	7	3.4 *	3.8
5	1	6	3.9 *	11.6	-7	3	7	74.4	72.9
7	1	6	15.5	11.1	-5	3	7	76.2	77.6
-2	2	6	2.7 *	0.7	-3	3	7	89.2	95.0
0	2	6	69.0	64.0	-1	3	7	215.0	204.4
2	2	6	24.5	23.7	1	3	7	127.6	131.2
-2	4	6	49.8	50.0	3	3	7	166.8	166.5
0	4	6	12.5	9.7	5	3	7	3.9 *	5.7
2	4	6	29.2	27.9	-4	4	7	3.8 *	5.4
4	4	6	3.8 *	9.5	-2	4	7	58.1	54.4
6	4	6	5.0 *	2.2	0	4	7	46.9	46.4
-3	5	6	68.8	70.9	2	4	7	14.6	12.6
-1	5	6	85.1	82.7	4	4	7	23.5	21.6
1	5	6	62.9	63.0	6	4	7	4.2 *	9.4
3	5	6	3.9 *	16.1	-1	5	7	22.1	19.0
5	5	6	3.9 *	7.3	1	5	7	15.0	12.0
-6	6	6	4.6 *	7.4	3	5	7	12.4	14.3
-4	6	6	91.4	93.3	5	5	7	4.2 *	10.6
-2	6	6	66.0	64.6	-2	6	7	3.5 *	0.5
0	6	6	97.8	96.8	2	6	7	3.5 *	25.0
2	6	6	68.7	65.8	-1	7	7	24.4	22.3
4	6	6	43.1	45.4	1	7	7	10.3	6.6
6	6	6	69.5	57.7	3	7	7	3.5 *	6.3

H	K	L	P(OBS)	P(CALC)	H	K	L	P(OBS)	P(CALC)
5	7	7	12.3	13.5	-3	7	8	3.8 *	3.1
-2	8	7	30.9	26.7	-1	7	8	15.4	16.3
0	8	7	20.3	18.8	1	7	8	27.6	27.5
2	8	7	7.6	0.7	3	7	8	20.3	17.3
4	8	7	19.0	18.7	5	7	8	20.3	20.6
-5	9	7	38.4	40.6	-4	8	8	4.2 *	7.5
-3	9	7	54.6	54.0	-2	8	8	7.5	5.5
-1	9	7	90.9	88.8	0	8	8	16.0	17.7
1	9	7	45.4	46.1	2	8	8	9.4	9.2
3	9	7	90.3	91.4	4	8	8	11.5	6.4
-2	10	7	8.5	0.2	-3	9	8	2.0	19.0
0	10	7	7.7	2.2	-1	9	8	11.1	29.5
2	10	7	18.5	17.8	1	9	8	20.7	21.4
4	10	7	4.1 *	4.1	3	9	8	9.4	2.6
-3	11	7	19.9	10.2	-4	10	8	4.5 *	0.7
-1	11	7	12.6	10.2	-2	10	8	7.8	5.2
1	11	7	6.8	5.3	0	10	8	14.2	9.8
3	11	7	4.0 *	6.4	2	10	8	7.5	9.5
-6	0	8	52.4	55.8	4	10	8	15.9	12.9
-4	0	8	67.1	64.5	-3	11	8	4.1 *	2.8
-2	0	8	131.9	133.2	-1	11	8	10.0	7.9
0	0	8	149.9	161.5	1	11	8	22.4	21.5
4	0	8	221.2	226.3	3	11	8	12.0	10.6
6	0	8	26.9	27.2	-7	1	9	5.0 *	3.0
-7	1	8	24.7	20.2	-3	1	9	3.1 *	2.1
-3	1	8	35.0	35.2	-1	1	9	7.2 *	7.2
1	1	8	3.0 *	3.7	1	1	9	18.2	18.0
3	1	8	36.8	36.1	3	1	9	11.5	14.4
5	1	8	20.3	17.4	5	1	9	4.1 *	4.4
-2	2	8	25.8	29.5	-6	2	9	4.4 *	12.9
0	2	8	3.3 *	0.1	-4	2	9	3.7 *	9.4
2	2	8	15.5	17.9	-2	2	9	41.4	41.1
4	2	8	11.8	8.2	0	2	9	23.7	22.1
1	3	8	15.5	15.3	4	2	9	3.5 *	7.1
-4	4	8	3.8 *	12.5	-7	3	9	47.0	47.4
-2	4	8	10.0	9.3	-5	3	9	41.4	44.3
0	4	8	30.4	30.4	-3	3	9	173.0	172.0
2	4	8	3.2 *	4.3	-1	3	9	16.0	13.8
4	4	8	14.6	14.0	1	3	9	286.3	301.0
6	4	8	4.2 *	3.4	3	3	9	38.2	39.6
-3	5	8	30.3	33.0	5	3	9	116.2	113.2
-1	5	8	9.2	2.4	-4	4	9	23.6	24.7
1	5	8	8.3	0.9	-2	4	9	30.3	27.5
3	5	8	37.3	38.4	0	4	9	20.8	18.9
5	5	8	11.6	12.8	4	4	9	3.9 *	8.3
-6	6	8	69.2	69.6	6	4	9	4.4 *	3.3
-4	6	8	84.6	86.0	-3	5	9	3.5 *	3.2
-2	6	8	118.7	123.6	-1	5	9	18.9	17.9
0	6	8	171.1	170.6	1	5	9	7.1	6.9
2	6	8	11.2	4.8	5	5	9	4.1 *	0.6
4	6	8	171.0	174.5	0	6	9	8.6	0.2
6	6	8	21.0	23.5	2	6	9	10.9	14.0
-5	7	8	31.8	29.3	-3	7	9	12.0	11.9

H	K	L	F(OBS)	F(CALC)
-1	7	9	3.7 *	1.2
1	7	9	28.3	28.1
3	7	9	3.6 *	4.5
5	7	9	8.9	8.9
-4	8	9	22.8	20.4
-2	8	9	22.2	21.2
0	8	9	21.5	20.1
2	8	9	13.8	14.1
4	8	9	7.2	6.9
-5	9	9	42.1	41.7
-3	9	9	121.2	120.4
-1	9	9	11.2	9.2
1	9	9	170.1	180.2
3	9	9	4.0 *	3.8
-4	10	9	9.1	7.4
-2	10	9	24.7	24.6
0	10	9	18.9	17.5
2	10	9	12.1	2.2
-3	11	9	4.1 *	9.0
-1	11	9	4.1 *	3.2
1	11	9	14.0	13.8
-6	0	10	90.2	90.9
-4	0	10	7.6	3.2
-2	0	10	299.7	305.4
0	0	10	152.7	144.0
2	0	10	239.2	243.5
4	0	10	35.9	35.9
6	0	10	4.5 *	1.7
-7	1	10	4.2 *	0.2
-5	1	10	11.0	13.0
-3	1	10	11.2	8.8
-1	1	10	29.2	26.3
3	1	10	3.4 *	0.0
5	1	10	16.1	16.1
-2	2	10	7.4	3.5
0	2	10	11.0	10.8
2	2	10	31.8	32.1
4	2	10	3.9 *	8.2
6	2	10	23.3	21.2
-1	3	10	12.6	12.0
1	3	10	14.6	13.6
3	3	10	3.7 *	6.6
-6	4	10	18.9	11.7
-2	4	10	25.2	24.2
0	4	10	16.0	16.1
2	4	10	3.4 *	2.4
6	4	10	9.9	7.9
-5	5	10	15.8	16.9
-3	5	10	3.3 *	4.3
-1	5	10	37.9	34.9
1	5	10	6.7	6.1
3	5	10	10.4	6.2
5	5	10	20.4	18.6

H	K	L	F(OBS)	F(CALC)
-6	6	10	71.7	71.3
-4	6	10	9.9	8.0
-2	6	10	232.4	237.3
0	6	10	42.0	38.5
2	6	10	198.7	207.4
4	6	10	62.8	62.5
-5	7	10	9.8	4.9
-3	7	10	25.6	21.2
3	7	10	8.9	10.3
5	7	10	4.2 *	2.2
-2	8	10	13.8	11.7
0	8	10	4.0 *	3.9
2	8	10	3.6 *	2.9
4	8	10	17.9	15.6
-1	9	10	13.2	16.7
1	9	10	21.1	21.0
3	9	10	4.0 *	9.6
-4	10	10	9.8	6.2
-2	10	10	16.0	14.3
0	10	10	4.2 *	5.2
2	10	10	4.0 *	4.6
-3	11	10	19.4	18.1
-1	11	10	10.8	9.5
1	11	10	19.4	17.0
-7	1	11	9.7	1.1
-3	1	11	6.7	3.0
-1	1	11	10.1	6.8
1	1	11	11.8	10.9
5	1	11	24.4	23.7
-6	2	11	13.8	12.2
-4	2	11	41.4	39.3
-2	2	11	44.6	42.6
0	2	11	3.3 *	0.9
2	2	11	92.9	94.9
4	2	11	27.2	26.1
6	2	11	45.7	41.5
-5	3	11	178.6	182.5
-3	3	11	38.9	40.0
-1	3	11	262.1	249.9
1	3	11	118.8	125.1
3	3	11	20.6	21.0
5	3	11	138.7	137.6
-6	4	11	25.0	23.8
-4	4	11	15.9	8.6
-2	4	11	22.8	19.0
0	4	11	74.8	71.5
2	4	11	19.7	18.8
4	4	11	65.2	63.5
6	4	11	14.9	13.8
-3	5	11	7.0	2.8
-1	5	11	6.9	6.1
1	5	11	9.7	9.3
3	5	11	12.4	12.9

H	K	L	F(OBS)	F(CALC)
5	5	11	21.9	20.8
-4	6	11	12.4	10.1
0	6	11	3.9 *	10.0
2	6	11	24.6	5.3
4	6	11	10.9	10.1
-5	7	11	4.0 *	8.0
-3	7	11	12.3	8.8
-1	7	11	3.9 *	4.4
1	7	11	10.8	8.1
3	7	11	16.0	15.2
5	7	11	22.2	19.3
-4	8	11	13.0	11.2
-2	8	11	11.3	9.8
0	8	11	36.5	32.9
2	8	11	22.0	22.0
4	8	11	40.4	39.7
-3	9	11	24.6	25.8
-1	9	11	128.2	122.4
1	9	11	61.4	65.7
3	9	11	9.6	7.1
-4	10	11	18.2	17.8
-2	10	11	4.1 *	4.9
0	10	11	13.0	9.6
2	10	11	25.4	28.2
-1	11	11	4.3 *	0.5
1	11	11	4.2 *	0.2
-6	0	12	4.2 *	5.8
-4	0	12	207.2	212.3
-2	0	12	128.3	128.4
0	0	12	138.9	135.7
2	0	12	260.6	272.4
3	0	12	29.9	0.7
4	0	12	11.8	9.5
6	0	12	107.0	100.8
-5	1	12	3.9 *	1.1
-3	1	12	3.3 *	3.3
-1	1	12	26.5	25.8
1	1	12	47.1	47.6
3	1	12	51.9	50.6
5	1	12	42.7	41.4
-6	2	12	11.3	1.5
-2	2	12	51.0	50.1
0	2	12	20.4	19.7
2	2	12	62.9	64.1
4	2	12	14.9	15.9
6	2	12	22.4	20.7
-3	3	12	3.6 *	4.4
1	3	12	3.6 *	12.4
-6	4	12	14.5	10.9
-4	4	12	13.6	9.1
-2	4	12	3.5 *	9.5
0	4	12	63.3	61.3
2	4	12	28.2	28.7

H	K	L	F(OBS)	F(CALC)
4	4	12	35.6	34.7
6	4	12	11.1	9.7
-5	5	12	4.1 *	3.9
-3	5	12	3.5 *	2.0
-1	5	12	26.1	23.1
1	5	12	34.7	35.9
3	5	12	44.7	45.5
5	5	12	32.7	30.8
-6	6	12	17.1	23.9
-4	6	12	116.6	122.4
-2	6	12	43.9	39.8
0	6	12	27.0	23.5
2	6	12	142.2	149.0
4	6	12	22.7	25.8
-5	7	12	9.8	1.8
-3	7	12	9.9	2.7
-1	7	12	15.9	15.0
1	7	12	33.8	34.0
5	7	12	33.9	32.8
-4	8	12	8.6	4.8
-2	8	12	3.8 *	6.4
0	8	12	31.2	30.8
2	8	12	17.5	17.8
4	8	12	23.7	20.0
-3	9	12	4.1 *	6.4
-1	9	12	25.3	6.9
1	9	12	4.0 *	17.8
-2	10	12	18.0	19.3
0	10	12	13.5	15.2
2	10	12	27.3	32.1
-1	11	12	4.6 *	9.7
1	11	12	20.3	19.4
-5	1	13	13.4	8.9
-3	1	13	14.3	14.5
-1	1	13	37.8	34.4
1	1	13	35.8	33.2
3	1	13	29.5	32.4
5	1	13	13.4	12.1
-6	2	13	16.2	18.1
-4	2	13	17.1	16.8
-2	2	13	114.2	111.2
0	2	13	62.9	60.6
2	2	13	92.1	92.6
4	2	13	20.0	20.3
6	2	13	17.5	16.1
-5	3	13	66.1	67.8
-3	3	13	20.1	20.3
-1	3	13	286.3	281.4
1	3	13	21.8	22.7
3	3	13	145.1	147.1
5	3	13	57.3	56.2
-6	4	13	4.4 *	9.0
-4	4	13	56.0	55.5

H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
-2	4	13	44.4	41.6	-1	3	14	18.2	2.5
0	4	13	112.0	108.0	3	3	14	27.1	7.7
2	4	13	45.2	45.0	5	3	14	8.6	4.7
4	4	13	39.3	35.8	-6	4	14	4.6 *	5.0
-5	5	13	4.2 *	8.7	-4	4	14	45.3	44.7
-3	5	13	10.8	8.7	-2	4	14	35.4	33.7
-1	5	13	29.1	27.1	0	4	14	54.7	51.1
1	5	13	25.1	24.4	2	4	14	15.4	14.3
3	5	13	27.4	27.1	4	4	14	8.2	6.8
5	5	13	12.4	9.3	-5	5	14	28.9	28.4
-2	6	13	3.8 *	18.0	-3	5	14	34.4	32.2
0	6	13	10.0	15.9	-1	5	14	60.5	57.7
2	6	13	11.9	6.3	1	5	14	35.9	34.3
4	6	13	4.1 *	5.0	3	5	14	32.2	34.3
-5	7	13	4.1 *	4.9	5	5	14	8.2	3.3
-3	7	13	16.5	13.4	-4	6	14	144.6	149.8
-1	7	13	25.4	22.9	-2	6	14	11.2	10.1
1	7	13	27.8	27.9	0	6	14	153.3	152.8
3	7	13	16.6	19.2	2	6	14	70.8	71.9
-4	8	13	35.5	33.8	4	6	14	36.9	33.1
-2	8	13	36.5	33.4	-3	7	14	44.6	42.4
0	8	13	72.5	68.0	-1	7	14	30.6	28.3
2	8	13	32.1	33.3	1	7	14	42.4	43.6
4	8	13	27.6	26.2	3	7	14	12.7	16.3
-3	9	13	8.1	4.3	-4	8	14	25.9	25.8
-1	9	13	156.4	149.0	-2	8	14	21.4	23.9
1	9	13	25.9	26.7	0	8	14	29.2	27.5
3	9	13	86.1	86.1	2	8	14	8.8	11.4
-2	10	13	42.4	41.2	4	8	14	4.3 *	1.6
0	10	13	30.5	33.7	-3	9	14	17.0	14.5
2	10	13	34.2	37.9	-1	9	14	16.2	4.7
-1	11	13	4.8 *	6.6	1	9	14	4.5 *	11.0
1	11	13	16.1	15.6	3	9	14	21.0	15.7
-6	0	14	4.5 *	4.1	-2	10	14	28.7	27.3
-4	0	14	150.4	154.8	0	10	14	21.9	22.4
-2	0	14	23.9	23.1	2	10	14	9.1	9.0
0	0	14	160.5	162.0	-1	11	14	20.9	16.3
2	0	14	85.1	88.3	1	11	14	25.2	29.1
4	0	14	36.1	37.0	-5	1	15	20.3	21.6
6	0	14	79.4	77.1	-3	1	15	25.4	27.4
-5	1	14	30.4	28.3	-1	1	15	26.5	26.6
-3	1	14	50.0	46.7	1	1	15	18.1	18.2
-1	1	14	66.7	60.4	5	1	15	4.3 *	1.0
1	1	14	52.9	50.1	-6	2	15	46.7	46.5
3	1	14	36.8	36.6	-4	2	15	50.1	51.0
5	1	14	9.2	5.8	-2	2	15	70.1	66.6
-6	2	14	21.3	19.1	0	2	15	37.1	36.3
-4	2	14	26.7	26.8	2	2	15	9.3	5.9
-2	2	14	62.2	59.4	4	2	15	4.1 *	2.6
0	2	14	37.0	35.0	-5	3	15	26.6	30.5
2	2	14	27.8	24.9	-3	3	15	154.1	155.4
4	2	14	4.0 *	4.2	-1	3	15	92.9	90.7
6	2	14	8.1	5.3	1	3	15	24.6	22.9

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	3	15	138.1	141.2	5	3	16	15.8	4.7
5	3	15	4.5 *	4.5	-6	4	16	24.8	24.4
-6	4	15	31.1	32.5	-4	4	16	12.2	18.4
-4	4	15	56.8	56.3	-2	4	16	17.9	20.5
-2	4	15	55.4	51.9	0	4	16	18.1	13.7
0	4	15	30.4	27.6	2	4	16	8.0	1.6
2	4	15	3.8 *	4.1	4	4	16	22.1	21.4
4	4	15	20.7	16.3	-5	5	16	27.0	28.8
-5	5	15	17.0	19.6	-3	5	16	12.3	10.7
-3	5	15	19.3	17.8	-1	5	16	19.2	22.1
-1	5	15	26.7	26.0	1	5	16	15.5	2.8
1	5	15	12.6	8.0	3	5	16	4.3 *	0.7
3	5	15	12.3	8.4	5	5	16	15.9	11.3
5	5	15	4.5 *	5.0	-4	6	16	60.6	62.7
-2	6	15	11.9	10.2	-2	6	16	42.4	40.1
0	6	15	19.1	17.2	0	6	16	145.8	149.1
2	6	15	4.0 *	12.0	2	6	16	29.3	20.8
4	6	15	11.3	1.7	4	6	16	92.7	95.5
-5	7	15	11.3	10.4	-5	7	16	14.0	13.1
-3	7	15	29.8	29.3	-3	7	16	18.4	18.7
-1	7	15	10.6	8.8	-1	7	16	4.0 *	0.5
1	7	15	18.2	19.4	3	7	16	15.0	13.7
3	7	15	7.9	3.0	-4	8	16	18.1	14.3
-4	8	15	43.8	43.1	-2	8	16	11.2	10.0
-2	8	15	38.5	36.6	0	8	16	12.1	7.1
0	8	15	19.6	19.7	2	8	16	4.3 *	6.0
2	8	15	12.9	5.2	-3	9	16	22.2	18.0
-3	9	15	116.2	115.7	-1	9	16	4.3 *	16.2
-1	9	15	64.0	61.3	1	9	16	14.9	1.9
1	9	15	39.5	36.0	-2	10	16	12.0	8.4
3	9	15	97.5	100.0	0	10	16	4.4 *	3.7
-2	10	15	30.9	30.7	-5	1	17	9.2	8.9
0	10	15	13.7	14.9	-3	1	17	6.9	3.2
2	10	15	13.0	6.4	-1	1	17	3.7 *	0.1
-6	0	16	88.5	88.5	1	1	17	4.0 *	6.0
-4	0	16	73.9	75.5	3	1	17	4.0 *	6.1
-2	0	16	26.4	22.2	5	1	17	8.4	6.5
0	0	16	159.4	164.5	-6	2	17	15.1	10.3
2	0	16	10.0	0.6	-4	2	17	19.7	23.7
4	0	16	87.1	88.0	-2	2	17	40.9	35.1
-5	1	16	28.1	27.5	0	2	17	3.7 *	0.9
-3	1	16	16.9	18.4	2	2	17	49.9	50.1
-1	1	16	20.1	18.8	4	2	17	4.1 *	0.1
3	1	16	8.9	4.1	-5	3	17	34.1	35.2
5	1	16	8.8	8.0	-3	3	17	151.7	151.6
-6	2	16	22.7	24.1	-1	3	17	4.1 *	0.1
-2	2	16	14.2	8.0	1	3	17	167.0	169.8
0	2	16	10.5	5.9	3	3	17	4.4 *	9.3
2	2	16	26.0	23.7	5	3	17	84.2	82.1
4	2	16	8.7	5.0	-4	4	17	4.1 *	1.9
-5	3	16	4.2 *	5.9	-2	4	17	4.1 *	4.1
-1	3	16	4.1 *	9.1	0	4	17	52.6	48.8
3	3	16	17.1	5.7	2	4	17	8.7	3.8

H	K	L	F(OBS)	F(CALC)
4	4	17	28.6	30.0
-5	5	17	11.5	5.2
-3	5	17	4.1 *	3.1
-1	5	17	4.1 *	1.4
1	5	17	12.8	7.2
3	5	17	4.2 *	3.8
-4	6	17	10.6	11.0
-2	6	17	4.5 *	0.4
0	6	17	8.1	11.3
2	6	17	14.1	14.6
4	6	17	17.3	9.3
-3	7	17	4.2 *	1.2
-1	7	17	4.1 *	3.0
1	7	17	4.3 *	6.9
3	7	17	9.2	5.0
-4	8	17	4.4 *	2.4
-2	8	17	4.3 *	2.6
0	8	17	30.0	28.8
2	8	17	15.1	11.7
-3	9	17	88.5	90.3
-1	9	17	4.3 *	5.2
1	9	17	100.8	101.9
0	10	17	13.2	13.6
-6	0	18	102.7	106.4
-4	0	18	31.3	30.3
-2	0	18	172.8	174.7
0	0	18	74.7	76.5
2	0	18	156.0	153.1
4	0	18	28.9	30.5
-5	1	18	9.8	10.2
-3	1	18	9.0	5.9
-1	1	18	9.8	4.1
1	1	18	4.0 *	2.3
3	1	18	6.6	0.9
5	1	18	4.4 *	2.4
-6	2	18	10.3	9.9
-4	2	18	4.1 *	1.5
-2	2	18	35.3	35.3
0	2	18	3.9 *	4.6
2	2	18	22.2	25.1
4	2	18	4.4 *	5.9
-3	3	18	18.8	6.4
-1	3	18	25.5	10.9
1	3	18	7.8	7.1
3	3	18	16.3	2.8
5	3	18	14.6	2.6
-4	4	18	17.3	15.9
-2	4	18	4.3 *	10.2
0	4	18	27.9	31.5
2	4	18	4.4 *	4.2
4	4	18	11.2	8.9
-5	5	18	16.1	7.8
-3	5	18	15.0	5.7

H	K	L	F(OBS)	F(CALC)
-1	5	18	10.0	8.4
1	5	18	4.2 *	1.5
3	5	18	4.4 *	5.8
-4	6	18	10.5	5.2
-2	6	18	94.8	97.0
0	6	18	15.5	10.9
2	6	18	83.5	83.8
4	6	18	4.6 *	2.6
-3	7	18	11.9	8.0
-1	7	18	10.4	3.8
1	7	18	4.4 *	7.0
-2	8	18	11.1	9.2
0	8	18	21.6	19.9
2	8	18	4.6 *	4.3
-1	9	18	4.7 *	20.7
1	9	18	4.7 *	15.3
-5	1	19	13.6	12.4
-3	1	19	4.1 *	4.1
-1	1	19	4.0 *	4.3
1	1	19	8.8	5.4
3	1	19	4.2 *	3.1
5	1	19	4.6 *	9.1
-4	2	19	4.3 *	7.5
-2	2	19	44.4	46.1
4	2	19	20.6	20.7
-5	3	19	101.2	104.9
-3	3	19	4.3 *	10.0
-1	3	19	159.5	159.2
1	3	19	12.7	14.3
3	3	19	95.3	95.6
-4	4	19	40.6	36.5
-2	4	19	4.4 *	5.8
0	4	19	28.7	30.9
2	4	19	13.8	10.1
4	4	19	4.7 *	6.4
-5	5	19	13.9	12.2
-3	5	19	11.9	2.3
-1	5	19	4.2 *	4.9
1	5	19	4.4 *	4.2
3	5	19	9.6	0.1
-4	6	19	9.1	13.5
-2	6	19	12.2	11.1
0	6	19	11.6	3.4
2	6	19	13.4	7.7
-3	7	19	4.6 *	6.7
-1	7	19	4.1 *	2.4
1	7	19	4.4 *	0.2
3	7	19	4.6 *	5.1
-2	8	19	4.8 *	9.8
0	8	19	21.2	24.1
2	8	19	4.8 *	5.0
-1	9	19	91.8	89.8
1	9	19	8.2	4.4

H	K	L	F(OBS)	F(CALC)
-4	0	20	91.1	87.8
0	0	20	114.8	110.0
2	0	20	47.5	47.9
-5	1	20	4.5 *	4.6
-3	1	20	4.3 *	3.8
-1	1	20	14.9	11.7
1	1	20	21.2	19.4
3	1	20	16.3	15.6
-4	2	20	7.7	7.1
-2	2	20	9.1	12.6
0	2	20	10.4	9.2
2	2	20	13.6	13.6
4	2	20	16.5	17.3
-5	3	20	15.9	4.8
-3	3	20	22.4	0.7
-1	3	20	16.1	4.2
1	3	20	18.1	6.2
3	3	20	24.6	4.1
-4	4	20	16.8	20.7
-2	4	20	4.4 *	2.1
0	4	20	4.1 *	1.9
2	4	20	15.2	19.5
4	4	20	10.0	16.1
-3	5	20	14.1	7.1
-1	5	20	9.0	3.1
1	5	20	20.1	20.5
3	5	20	9.9	11.3
-4	6	20	92.2	90.4
-2	6	20	32.4	35.5
0	6	20	101.6	99.2
2	6	20	49.9	47.6
-3	7	20	4.7 *	5.7
-1	7	20	16.5	15.7
1	7	20	4.3 *	5.3
-2	8	20	4.6 *	1.8
0	8	20	11.7	0.0
2	8	20	4.9 *	10.0
-1	9	20	21.0	9.7
-5	1	21	10.1	3.2
-3	1	21	9.8	11.4
-1	1	21	14.3	19.0
1	1	21	16.7	20.9
3	1	21	16.8	19.7
-2	2	21	4.5 *	5.9
0	2	21	26.3	27.9
2	2	21	42.6	46.0
4	2	21	24.6	27.0
-5	3	21	4.7 *	2.0
-3	3	21	107.0	102.5
-1	3	21	51.5	49.8
1	3	21	24.7	25.1
3	3	21	112.9	107.3
-4	4	21	10.4	7.9

H	K	L	F(OBS)	F(CALC)
-2	4	21	10.6	8.9
0	4	21	24.8	28.1
2	4	21	27.9	33.5
-3	5	21	8.6	10.9
-1	5	21	12.8	10.5
1	5	21	14.6	19.6
3	5	21	11.2	12.0
-4	6	21	23.6	6.5
-2	6	21	4.6 *	10.9
0	6	21	18.9	8.2
2	6	21	4.7 *	0.6
-3	7	21	4.7 *	1.7
-1	7	21	15.3	21.8
1	7	21	4.4 *	11.1
-2	8	21	4.7 *	5.8
0	8	21	17.3	20.8
-2	0	22	23.6	24.5
0	0	22	125.1	116.9
2	0	22	29.0	22.4
4	0	22	72.1	69.3
-5	1	22	4.9 *	12.6
-3	1	22	26.8	30.5
-1	1	22	31.6	34.7
1	1	22	32.9	35.8
3	1	22	27.0	25.8
-4	2	22	4.5 *	7.3
-2	2	22	23.2	24.3
0	2	22	17.7	23.1
2	2	22	31.3	33.4
4	2	22	9.4	10.2
-3	3	22	26.9	4.6
-1	3	22	8.5	1.0
1	3	22	24.7	4.1
3	3	22	11.2	3.1
-4	4	22	14.6	12.4
-2	4	22	4.5 *	14.8
0	4	22	31.6	35.2
2	4	22	18.9	17.0
-3	5	22	28.4	30.5
-1	5	22	21.8	25.0
1	5	22	32.7	35.2
3	5	22	17.9	18.5
-2	6	22	24.4	32.6
0	6	22	117.7	113.6
2	6	22	4.6 *	3.8
-1	7	22	29.3	30.8
1	7	22	14.8	17.7
0	8	22	16.2	21.9
-3	1	23	17.6	24.7
-1	1	23	17.8	19.4
1	1	23	14.9	14.8
3	1	23	8.5	4.9
-4	2	23	16.2	15.9

H	K	L	F(OBS)	F(CALC)
-2	2	23	52.7	60.6
0	2	23	26.7	30.7
2	2	23	46.7	47.2
-3	3	23	126.8	118.0
-1	3	23	25.1	22.6
1	3	23	128.8	123.9
3	3	23	32.4	26.9
-4	4	23	29.0	31.6
-2	4	23	24.9	29.2
0	4	23	57.7	58.5
2	4	23	17.6	14.1
-3	5	23	15.6	19.6
-1	5	23	14.4	16.1
1	5	23	4.8 *	13.5
-2	6	23	10.8	6.5
0	6	23	15.4	8.5
2	6	23	4.9 *	4.4
-1	7	23	11.9	14.4
1	7	23	15.6	10.8
-4	0	24	4.7 *	2.8
-2	0	24	123.6	129.4
0	0	24	79.3	73.6
2	0	24	28.2	33.4
-3	1	24	25.4	27.5
-1	1	24	21.1	19.5
1	1	24	10.4	4.4
3	1	24	10.6	7.7
-4	2	24	4.9 *	11.1
-2	2	24	34.4	33.4
0	2	24	9.9	5.3
2	2	24	18.1	11.8
-3	3	24	15.0	4.0
-1	3	24	4.4 *	1.6
-2	4	24	13.1	14.9
0	4	24	22.3	21.6
2	4	24	8.6	2.5
-3	5	24	21.6	22.8
-1	5	24	21.5	18.9
1	5	24	4.8 *	0.7
-2	6	24	75.9	77.9
0	6	24	32.3	28.5
-3	1	25	4.5 *	3.3
-1	1	25	4.3 *	0.5
1	1	25	10.7	10.7
-2	2	25	30.3	31.8
0	2	25	4.4 *	10.3
2	2	25	4.7 *	2.3
-3	3	25	34.9	29.3
-1	3	25	29.3	35.4
1	3	25	117.0	111.1
-2	4	25	15.3	4.2
0	4	25	16.1	11.2
-1	5	25	4.7 *	0.9

H	K	L	F(OBS)	F(CALC)
1	5	25	10.9	10.9
-2	0	26	115.4	117.0
0	0	26	39.1	39.5
2	0	26	99.6	99.7
-3	1	26	11.6	12.7
-1	1	26	22.0	20.6
-2	2	26	8.5	0.8
2	2	26	12.3	10.4
-1	3	26	24.2	4.0
1	3	26	10.2	1.0
-2	4	26	14.3	7.4
0	4	26	4.6 *	3.3