

## The crystal structure of kolicite, $\text{Mn}_7(\text{OH})_4[\text{As}_2\text{Zn}_4\text{Si}_2\text{O}_{16}(\text{OH})_4]^1$

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### Abstract

Kolicite,  $\text{Mn}_7(\text{OH})_4[\text{As}_2\text{Zn}_4\text{Si}_2\text{O}_{16}(\text{OH})_4]$ , is orthorhombic, space group *Cmca*,  $a = 18.59(3)$ ,  $b = 8.789(5)$ ,  $c = 12.04(1)\text{\AA}$ , with  $Z = 4$ . The structure is based on cubic-closest-packing of anions with As, Zn, and Si tetrahedra linked to form a continuous vertex-sharing slab oriented normal to  $c$ , with composition  $\text{As}_2\text{Zn}_4\text{Si}_2\text{O}_{16}(\text{OH})_4$ . These link units of seven edge-sharing Mn octahedra to form a three-dimensional structure. A basic unit of structure is common to the structure of holdenite,  $\text{Mn}_6\text{Zn}_3(\text{OH})_8(\text{AsO}_4)_2(\text{SiO}_4)$ .

### Introduction

Kolicite is a rare mineral present in a few specimens from the Sterling Hill mine, Ogdensburg, Sussex County, New Jersey (Dunn *et al.*, 1979). Dr. Akira Kato pointed out (personal communication) that it appeared to be closely related to some other unusual Franklin and Sterling Hill minerals. These complex manganese-containing phases have structures with tetrahedrally-coordinated Zn, As, and/or Si and are generally based on anion closest-packing. Two such phases with cubic closest-packed structures are holdenite,  $\text{Mn}_6\text{Zn}_3(\text{OH})_8(\text{AsO}_4)_2(\text{SiO}_4)$ , and gerstmannite,  $(\text{Mn},\text{Mg})\text{Mg}(\text{OH})_2[\text{ZnSiO}_4]$ , as determined by Moore and Araki (1977a,b). They pointed out that these orthorhombic "structures involve one axis which is some integral multiple of twice the octahedral M-O distance, a second axis which is some integral multiple of an octahedral edge, and a third which is also a multiple of an octahedral edge. The simplest unit for oxygen cubic close-packing has metrical properties ( $m \times 4.2\text{\AA}$ ,  $n \times 3.0\text{\AA}$ ,  $p \times 3.0\text{\AA}$ )" (Moore and Araki, 1977a). The lattice parameters of kolicite are consistent with these relations. Its crystal structure thus appeared to represent yet another in a complex series of related Franklin and Sterling Hill phases, and the solution of the structure was carried out in order to further clarify the apparently complex relations among these minerals.

### Experimental

As reported in Dunn *et al.* (1979), single-crystal analysis showed that kolicite is orthorhombic with extinctions consistent with either space group *C2cb* or *Cmca*. Space group *Cmca* was eventually confirmed through statistical analysis of intensities and structure analysis. The lattice parameters, as obtained using least-squares refinement of powder diffraction data, are  $a = 18.59(3)$ ,  $b = 8.789(5)$  and  $c = 12.04(1)\text{\AA}$ . This unit cell has  $Z = 4$ .

The intensities of 1052 symmetry-independent reflections were measured with a Supper-Pace diffractometer, which uses Weissenberg equi-inclination geometry.  $\text{MoK}\alpha$  radiation, monochromated by a flat crystal of graphite, was used and intensities of reflections having  $\sin \theta \leq 0.46$  were measured, although the restrictions on upper levels were more severe due to mechanical limitations of the diffractometer. The data were corrected for Lorentz, polarization, and absorption effects. The latter was significant as the crystal was approximately 0.13 mm in diameter, and  $\mu_1 = 131.0 \text{ cm}^{-1}$ . The set of 1052 structure factors included 159 which were less intense than minimum observable values.

### Structure solution and refinement

An attempt was first made to solve the structure by direct methods using the program MULTAN (Main *et al.*, 1971), but this led to an unreasonably large number of possible solutions, which was attributable to the pseudo-symmetry due to cubic closest-packing of

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Table 1

H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
12	2	0	93.3	91.7	19	3	1	86.1	78.2
14	2	0	35.5	41.8	0	4	1	148.0	133.5
16	2	0	177.0	161.7	2	4	1	97.4	85.0
18	2	0	24.6	26.8	4	4	1	162.7	152.9
0	4	0	273.8	228.3	5	4	1	156.9	161.0
2	4	0	177.6	149.9	8	4	1	140.7	130.6
4	4	0	143.4	144.8	10	4	1	94.0	88.1
5	4	0	457.2	439.4	12	4	1	52.1	47.7
8	4	0	165.0	159.2	14	4	1	27.4	20.4
10	4	0	212.3	198.6	16	4	1	75.0	67.8
12	4	0	50.8	18.2	18	4	1	83.8	79.0
14	4	0	31.3	38.2	1	5	1	101.4	97.6
16	4	0	67.3	61.7	3	5	1	135.9	127.1
18	4	0	240.3	229.3	5	5	1	315.9	307.0
0	6	0	135.8	137.8	7	5	1	228.5	222.8
2	6	0	51.9	45.6	9	5	1	117.1	112.8
4	6	0	117.6	115.7	11	5	1	132.9	128.9
5	6	0	260.2	242.7	13	5	1	31.6	18.8
8	6	0	10.5 *	13.8	15	5	1	43.4	38.4
10	6	0	35.9	32.5	17	5	1	191.4	180.0
12	6	0	89.1	88.1	19	5	1	67.8	64.6
15	6	0	132.5	121.3	0	6	1	415.6	385.8
18	6	0	138.6	134.0	2	6	1	36.2	38.4
0	8	0	611.2	634.0	4	6	1	97.3	80.3
2	8	0	44.2	49.3	5	6	1	313.2	308.3
4	8	0	64.3	64.3	8	6	1	71.2	67.7
6	8	0	316.1	315.3	10	6	1	116.2	118.5
8	8	0	11.5 *	8.7	12	6	1	279.7	258.6
10	8	0	36.1	29.5	14	6	1	10.6 *	12.1
12	8	0	457.9	445.0	16	6	1	52.0	50.6
14	8	0	77.6	76.7	18	6	1	162.4	154.7
15	8	0	94.5	84.0	1	7	1	11.2 *	14.0
0	10	0	58.2	65.9	3	7	1	11.2 *	2.1
2	10	0	97.5	102.6	5	7	1	140.0	137.9
4	10	0	27.5	22.3	7	7	1	143.3	141.9
5	10	0	93.6	96.5	9	7	1	42.9	39.9
8	10	0	12.2 *	11.9	11	7	1	47.7	50.2
10	10	0	60.0	60.7	13	7	1	51.0	47.6
17	1	1	9.1 *	15.2	15	7	1	10.6 *	4.9
19	1	1	58.2	54.6	17	7	1	93.2	85.7
12	2	1	200.0	203.8	0	8	1	314.2	328.6
14	2	1	70.1	61.4	2	8	1	78.6	84.0
16	2	1	9.5 *	1.0	4	8	1	54.3	56.8
18	2	1	262.7	249.7	6	8	1	11.4 *	24.6
1	3	1	515.0	468.3	8	8	1	47.4	49.0
3	3	1	199.1	166.6	10	8	1	104.2	98.3
5	3	1	330.0	312.3	12	8	1	230.3	224.7
7	3	1	242.6	239.0	14	8	1	31.4	25.6
9	3	1	83.3	80.5	15	8	1	28.1	22.7
11	3	1	436.2	409.5	1	9	1	70.0	72.8
13	3	1	193.7	184.2	3	9	1	12.0 *	7.9
15	3	1	86.5	83.1	5	9	1	120.8	119.4
17	3	1	179.6	170.0	7	9	1	63.9	76.2

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
9	9	1	22.1	15.5	5	5	2	121.4	117.0
11	9	1	47.7	42.2	7	5	2	113.2	120.0
13	9	1	61.1	65.8	9	5	2	41.6	35.4
0	10	1	39.7	30.4	11	5	2	376.4	366.1
2	10	1	12.6 *	26.0	13	5	2	255.5	246.5
4	10	1	36.4	12.7	15	5	2	129.6	125.2
6	10	1	223.6	230.4	17	5	2	78.7	71.8
8	10	1	48.7	46.8	19	5	2	71.2	71.0
10	10	1	12.4 *	13.1	0	6	2	151.0	144.1
1	11	1	202.7	220.2	2	6	2	10.9 *	0.4
3	11	1	68.8	73.1	4	6	2	36.5	38.2
5	11	1	114.7	125.9	6	6	2	68.1	67.0
12	0	2	29.6	28.9	8	6	2	10.1 *	4.8
14	0	2	27.5	27.2	10	6	2	54.8	51.6
16	0	2	18.3	13.2	12	6	2	95.6	90.5
13	0	2	113.6	119.5	14	6	2	32.9	34.1
11	1	2	30.9	36.2	16	6	2	62.4	54.0
13	1	2	56.3	67.6	18	6	2	10.9 *	16.9
15	1	2	9.0 *	8.9	1	7	2	11.5 *	14.7
17	1	2	313.9	313.7	3	7	2	77.3	71.7
19	1	2	174.2	175.5	5	7	2	159.4	158.8
0	2	2	254.5	264.9	7	7	2	129.5	131.3
2	2	2	30.3	24.1	9	7	2	59.2	55.4
4	2	2	8.7 *	4.1	11	7	2	11.0 *	19.6
6	2	2	174.3	176.6	13	7	2	11.1 *	17.8
8	2	2	72.9	75.7	15	7	2	45.9	46.0
10	2	2	113.5	119.5	17	7	2	102.5	95.1
12	2	2	127.2	131.5	0	8	2	61.0	68.4
14	2	2	45.2	40.4	2	8	2	12.1 *	16.6
16	2	2	46.6	47.5	4	8	2	47.4	45.7
18	2	2	52.9	48.0	6	8	2	164.4	171.9
1	3	2	443.2	435.1	8	8	2	82.7	83.5
3	3	2	156.6	145.7	10	8	2	54.6	57.9
5	3	2	8.9 *	0.7	12	8	2	36.5	35.3
7	3	2	17.6	12.9	14	8	2	11.0 *	6.7
9	3	2	72.7	72.7	16	8	2	11.2 *	8.6
1	3	2	328.7	333.9	1	9	2	173.7	172.7
3	3	2	217.1	214.9	3	9	2	39.0	49.6
5	3	2	111.0	103.6	5	9	2	225.9	229.4
7	3	2	25.3	16.7	7	9	2	139.3	195.3
9	3	2	10.9 *	29.0	9	9	2	68.4	79.5
0	4	2	309.6	289.3	11	9	2	143.0	139.4
2	4	2	119.9	106.4	13	9	2	120.0	119.0
4	4	2	74.1	73.0	0	10	2	29.6	37.2
6	4	2	202.6	200.5	2	10	2	26.7	37.7
8	4	2	25.5	14.6	4	10	2	12.5 *	5.6
0	4	2	41.1	34.5	6	10	2	77.9	82.6
2	4	2	186.5	181.2	8	10	2	27.2	25.5
4	4	2	94.8	88.6	10	10	2	48.8	53.7
6	4	2	92.2	88.9	1	11	2	12.7 *	13.7
8	4	2	77.5	70.1	3	11	2	42.6	42.7
1	5	2	467.7	442.7	5	11	2	13.1 *	25.4
3	5	2	163.2	143.9	1	1	3	404.0	435.2

	K	L	F(OBS)	F(CALC)		K	L	F(OBS)	F(CALC)
3	1	3	174.2	182.5	3	6	3	88.0	86.9
5	1	3	311.5	344.3	10	6	3	27.2	10.0
7	1	3	168.1	184.3	12	6	3	232.3	231.8
9	1	3	129.9	140.4	14	6	3	41.3	44.3
11	1	3	286.6	311.5	15	6	3	10.6	16.5
3	1	3	174.3	190.7	18	6	3	70.0	63.4
5	1	3	63.0	66.6	1	7	3	192.8	189.1
7	1	3	221.1	219.7	3	7	3	111.9	101.0
9	1	3	42.6	46.5	5	7	3	405.3	410.4
0	2	3	476.0	492.9	7	7	3	285.8	292.5
2	2	3	77.5	68.7	9	7	3	119.0	113.8
4	2	3	81.1	96.0	11	7	3	165.6	164.5
6	2	3	281.9	312.1	13	7	3	103.9	105.1
8	2	3	34.7	37.5	15	7	3	11.0	18.4
0	2	3	36.3	33.1	17	7	3	298.4	279.3
2	2	3	290.3	302.9	0	8	3	149.5	148.6
4	2	3	50.7	49.7	2	8	3	126.9	128.5
6	2	3	91.6	90.6	4	8	3	81.4	80.4
8	2	3	143.5	143.5	6	8	3	29.3	31.8
1	3	3	142.8	144.1	8	8	3	39.2	47.0
3	3	3	46.5	51.8	10	8	3	95.3	99.2
5	3	3	45.1	31.6	12	8	3	104.4	110.3
7	3	3	66.9	76.0	14	8	3	82.4	75.4
9	3	3	8.9	10.1	16	8	3	59.7	61.7
1	3	3	115.6	122.1	1	9	3	176.5	183.9
3	3	3	115.1	116.0	3	9	3	95.7	99.0
5	3	3	73.5	71.7	5	9	3	12.1	13.6
7	3	3	46.2	34.9	7	9	3	39.2	40.5
9	3	3	82.4	81.2	9	9	3	38.2	45.4
0	4	3	24.8	11.3	11	9	3	171.5	179.3
2	4	3	73.1	67.9	13	9	3	81.2	85.0
4	4	3	84.2	87.6	0	10	3	142.9	151.2
6	4	3	241.9	244.3	2	10	3	40.8	40.7
8	4	3	33.1	37.8	4	10	3	41.7	49.7
0	4	3	28.2	25.0	6	10	3	155.8	149.6
2	4	3	9.2	8.5	8	10	3	25.7	6.5
4	4	3	24.8	24.2	10	10	3	43.2	39.7
6	4	3	64.2	59.5	1	11	3	126.1	126.9
8	4	3	109.6	98.8	3	11	3	32.3	26.4
0	5	3	106.9	102.7	0	0	4	538.4	577.6
2	5	3	10.2	7.0	2	0	4	239.5	258.7
4	5	3	117.3	125.2	4	0	4	238.2	245.3
6	5	3	154.1	160.6	6	0	4	279.6	274.6
8	5	3	43.5	40.7	8	0	4	79.6	88.8
0	5	3	94.5	85.9	10	0	4	111.9	126.2
2	5	3	10.0	20.0	12	0	4	335.0	384.8
4	5	3	10.1	1.9	14	0	4	120.0	135.9
6	5	3	52.9	48.3	16	0	4	174.7	186.5
8	5	3	104.3	91.3	18	0	4	27.7	22.0
0	6	3	318.4	298.4	1	1	4	9.3	9.4
2	6	3	46.4	39.2	3	1	4	47.6	42.0
4	6	3	59.1	62.0	5	1	4	108.3	116.8
6	6	3	92.9	101.3	7	1	4	75.3	85.4

H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
9	1	4	51.4	56.0	14	6	4	31.7	23.7
11	1	4	9.8 *	10.7	15	6	4	90.1	90.0
13	1	4	21.6	1.9	13	6	4	71.9	66.8
15	1	4	26.1	4.7	1	7	4	11.5 *	22.1
17	1	4	55.7	61.6	3	7	4	32.4	14.0
19	1	4	20.3	25.9	5	7	4	65.1	62.0
0	2	4	64.5	81.5	7	7	4	51.2	51.2
2	2	4	114.8	118.3	9	7	4	11.4 *	13.6
4	2	4	140.1	139.0	11	7	4	26.3	14.2
6	2	4	24.6	5.3	13	7	4	21.0	11.0
8	2	4	43.3	45.7	15	7	4	23.3	6.6
10	2	4	177.2	182.0	17	7	4	36.2	35.6
12	2	4	111.7	120.9	0	8	4	174.0	167.3
14	2	4	9.6 *	12.7	2	8	4	51.2	48.8
16	2	4	85.7	85.2	4	8	4	64.3	64.2
18	2	4	10.2 *	9.6	6	8	4	87.8	88.7
1	3	4	91.1	88.6	8	8	4	30.8	30.9
3	3	4	26.1	21.9	10	8	4	26.2	24.2
5	3	4	50.7	66.0	12	8	4	133.9	131.7
7	3	4	47.5	48.9	14	8	4	41.3	36.4
9	3	4	9.0 *	4.8	1	9	4	24.1	27.2
11	3	4	63.2	65.9	3	9	4	24.7	20.7
13	3	4	35.7	43.0	5	9	4	12.0 *	15.4
15	3	4	10.2 *	23.8	7	9	4	11.2 *	10.4
17	3	4	10.7 *	28.3	9	9	4	26.0	27.2
19	3	4	24.8	10.8	11	9	4	11.8 *	20.4
0	4	4	411.2	413.2	13	9	4	35.6	18.9
2	4	4	31.6	24.9	0	10	4	213.0	221.7
4	4	4	78.0	86.7	2	10	4	12.6 *	12.3
6	4	4	1005.3	1074.1	4	10	4	27.4	27.0
8	4	4	64.5	54.2	6	10	4	149.1	149.8
0	4	4	70.5	74.6	8	10	4	12.5 *	3.4
2	4	4	268.3	274.1	1	11	4	13.0 *	12.0
4	4	4	27.7	34.1	1	1	5	244.0	256.5
6	4	4	136.1	133.8	3	1	5	116.1	115.0
8	4	4	505.0	475.0	5	1	5	286.8	315.8
1	5	4	49.6	44.4	7	1	5	173.2	197.5
3	5	4	27.2	28.1	9	1	5	83.4	89.4
5	5	4	24.9	6.9	11	1	5	205.1	221.3
7	5	4	17.6	12.4	13	1	5	99.5	110.0
9	5	4	9.7 *	3.8	15	1	5	38.1	36.0
1	5	4	39.6	44.3	17	1	5	178.1	189.7
3	5	4	26.3	24.1	19	1	5	48.4	52.3
5	5	4	21.0	29.6	0	2	5	474.6	492.7
7	5	4	10.4 *	1.2	2	2	5	101.4	92.3
9	5	4	10.6 *	9.3	4	2	5	80.8	89.2
0	6	4	71.9	67.9	6	2	5	364.5	401.2
2	6	4	42.3	39.5	8	2	5	21.7	21.4
4	6	4	144.3	136.7	10	2	5	56.5	56.5
6	6	4	100.8	97.7	12	2	5	302.0	325.3
8	6	4	104.2	105.4	14	2	5	55.4	61.6
0	6	4	91.6	94.3	16	2	5	99.7	96.7
2	6	4	44.6	46.0	18	2	5	189.8	192.2

#	K	L	F (OBS)	F (CALC)	#	K	L	F (OBS)	F (CALC)
1	3	5	96.3	102.0	8	8	5	47.2	53.6
3	3	5	20.1	4.9	10	8	5	174.0	125.0
5	3	5	50.2	50.8	12	8	5	144.1	152.4
7	3	5	28.7	26.5	14	8	5	149.6	85.3
9	3	5	9.2 *	17.0	1	9	5	121.9	123.8
11	3	5	63.1	62.7	3	9	5	70.6	68.0
13	3	5	90.5	96.0	5	9	5	12.0 *	25.0
15	3	5	28.1	27.1	7	9	5	12.0 *	3.2
17	3	5	33.8	37.6	9	9	5	43.6	41.2
19	3	5	51.6	51.7	11	9	5	120.5	126.3
1	4	5	31.3	34.0	1	10	5	135.7	141.1
2	4	5	98.6	89.5	2	10	5	67.8	62.1
4	4	5	87.0	89.1	4	10	5	62.7	64.9
5	4	5	238.3	255.0	6	10	5	228.4	231.6
3	4	5	37.8	38.2	8	10	5	12.1 *	0.4
10	4	5	48.0	48.8	1	0	6	348.0	362.7
12	4	5	9.8 *	22.6	2	0	6	65.0	64.2
14	4	5	36.5	35.8	4	0	6	39.1	94.0
16	4	5	67.3	65.0	5	0	6	193.7	211.7
13	4	5	114.0	109.8	8	0	6	101.6	109.0
1	5	5	55.9	56.2	10	0	6	93.8	105.9
3	5	5	19.9	16.2	12	0	6	194.5	214.7
5	5	5	9.9 *	10.5	14	0	6	8.9 *	7.4
7	5	5	51.9	52.8	16	0	6	33.4	30.4
9	5	5	9.9 *	2.1	18	0	6	108.4	110.7
11	5	5	66.3	62.8	1	1	6	23.2	36.5
13	5	5	10.0 *	2.3	3	1	6	114.0	113.0
15	5	5	10.0 *	1.4	5	1	6	395.9	431.7
17	5	5	10.2 *	7.8	7	1	6	311.0	342.1
19	5	5	57.1	48.4	9	1	6	141.6	148.7
1	6	5	409.3	399.0	11	1	6	18.3	35.8
2	6	5	11.5 *	27.1	13	1	6	38.9	46.6
4	6	5	19.5	15.0	15	1	6	21.9	11.2
5	6	5	39.3	92.1	17	1	6	239.6	248.9
8	6	5	60.4	60.6	19	1	6	134.4	135.4
10	6	5	10.5 *	17.4	1	2	6	88.9	85.7
12	6	5	292.6	301.8	2	2	6	74.9	72.9
14	6	5	45.6	53.1	4	2	6	97.7	106.8
16	6	5	30.0	20.4	6	2	6	194.1	213.2
18	6	5	65.9	63.0	8	2	6	21.1	16.4
1	7	5	171.1	166.4	10	2	6	9.5 *	10.2
3	7	5	70.8	64.3	12	2	6	27.9	31.2
5	7	5	276.9	281.3	14	2	6	40.2	45.6
7	7	5	194.3	200.0	15	2	6	126.2	118.2
9	7	5	65.3	64.7	18	2	6	85.5	79.4
11	7	5	152.4	155.8	1	3	6	332.5	334.2
13	7	5	85.2	83.3	3	3	6	68.2	68.3
15	7	5	11.2 *	10.6	5	3	6	16.8	22.4
17	7	5	207.1	195.2	7	3	6	22.3	37.1
1	8	5	205.2	205.6	9	3	6	26.8	28.1
2	8	5	152.7	152.0	11	3	6	260.3	264.9
4	8	5	86.2	92.8	13	3	6	176.6	184.4
6	8	5	33.3	37.2	15	3	6	62.8	67.1

H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
17	3	6	23.5	21.0	11	9	6	118.5	116.5
19	3	6	35.3	35.7	0	10	6	12.7 *	16.4
0	4	6	232.8	235.3	2	10	6	40.5	38.1
2	4	6	45.1	40.2	4	10	6	12.4 *	6.0
4	4	6	55.8	55.1	5	10	6	48.4	48.1
5	4	6	56.3	63.8	1	1	7	133.0	130.1
3	4	6	31.3	30.7	3	1	7	14.0	13.0
10	4	6	9.6 *	11.0	5	1	7	9.7 *	4.1
12	4	6	140.6	144.3	7	1	7	32.9	24.0
14	4	6	53.1	52.9	9	1	7	38.1	40.9
15	4	6	57.5	55.3	11	1	7	50.0	52.1
13	4	6	45.0	43.0	13	1	7	118.7	111.3
1	5	6	357.7	362.0	15	1	7	33.2	14.1
3	5	6	65.7	67.2	17	1	7	25.6	22.0
5	5	6	115.8	120.4	19	1	7	33.4	40.0
7	5	6	113.1	124.7	0	2	7	146.0	151.4
9	5	6	10.0 *	0.2	2	2	7	104.7	102.0
11	5	6	292.7	302.4	4	2	7	35.5	27.1
13	5	6	207.7	218.0	6	2	7	229.2	250.7
15	5	6	76.0	79.6	8	2	7	33.1	30.2
17	5	6	79.4	72.4	10	2	7	77.1	78.3
19	5	6	74.8	73.4	12	2	7	99.4	108.5
0	6	6	114.6	110.1	14	2	7	67.3	64.9
2	6	6	55.3	51.2	16	2	7	10.1 *	9.7
4	6	6	74.6	83.6	18	2	7	140.2	144.3
6	6	6	108.9	119.4	1	3	7	348.9	356.4
8	6	6	21.9	16.6	3	3	7	152.4	148.4
10	6	6	26.5	13.5	5	3	7	252.5	267.3
12	6	6	68.9	68.5	7	3	7	205.3	219.0
14	6	6	39.5	42.8	9	3	7	74.1	79.7
15	6	6	96.0	90.5	11	3	7	329.2	346.5
18	6	6	53.8	51.1	13	3	7	151.6	158.3
1	7	6	34.2	21.2	15	3	7	88.5	89.6
3	7	6	79.5	79.8	17	3	7	155.6	153.8
5	7	6	126.0	134.2	19	3	7	90.2	95.7
7	7	6	98.0	104.8	0	4	7	44.7	43.1
9	7	6	64.4	62.6	2	4	7	24.0	28.9
11	7	6	10.8 *	27.3	4	4	7	70.4	70.7
13	7	6	10.2 *	14.4	5	4	7	65.2	55.6
15	7	6	49.9	49.1	8	4	7	66.1	68.8
0	8	6	187.4	179.5	10	4	7	36.8	40.2
2	8	6	26.9	4.7	12	4	7	33.3	14.3
4	8	6	55.8	57.4	14	4	7	10.0 *	6.1
6	8	6	164.0	169.5	16	4	7	32.5	32.6
8	8	6	95.4	86.2	18	4	7	37.7	34.2
10	8	6	53.8	52.5	1	5	7	30.9	38.5
12	8	6	123.5	120.2	3	5	7	106.5	107.6
14	8	6	12.0 *	23.0	5	5	7	273.1	284.1
1	9	6	140.9	142.9	7	5	7	204.0	216.4
3	9	6	59.8	62.5	9	5	7	99.9	108.6
5	9	6	174.1	187.9	11	5	7	70.2	76.9
7	9	6	148.8	157.2	13	5	7	25.1	6.0
9	9	6	79.9	82.4	15	5	7	30.8	32.1

J	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
17	5	7	180.7	175.7	0	2	8	59.6	73.1
0	6	7	154.0	152.4	2	2	8	96.2	91.7
2	6	7	44.3	36.3	4	2	8	103.6	104.5
4	6	7	19.6	25.7	6	2	8	29.9	22.3
6	6	7	196.9	212.3	8	2	8	23.6	21.8
8	6	7	26.8	36.3	10	2	8	98.6	101.5
10	6	7	57.7	65.1	12	2	8	57.3	54.7
12	6	7	105.0	106.2	14	2	8	34.4	33.9
14	6	7	10.5 *	11.2	16	2	8	104.7	103.2
15	6	7	11.0 *	8.3	18	2	8	24.9	21.5
1	7	7	11.3 *	10.4	1	3	8	159.9	157.6
3	7	7	27.5	23.5	3	3	8	61.6	54.2
5	7	7	154.4	162.2	5	3	8	34.5	41.2
7	7	7	143.8	149.9	7	3	8	10.6 *	32.7
9	7	7	59.6	59.9	9	3	8	23.5	23.6
11	7	7	41.9	46.0	11	3	8	126.4	128.4
13	7	7	47.8	41.5	13	3	8	76.2	80.1
15	7	7	11.2 *	2.1	15	3	8	46.8	46.9
0	8	7	187.4	183.2	17	3	8	10.8 *	19.0
2	8	7	39.2	41.0	19	3	8	10.2 *	8.6
4	8	7	12.0 *	2.8	0	4	8	32.0	28.7
6	8	7	11.7 *	16.1	2	4	8	80.6	74.0
8	8	7	11.2 *	4.1	4	4	8	98.3	105.8
10	8	7	55.0	52.9	6	4	8	238.6	252.3
12	8	7	131.1	130.8	8	4	8	102.5	114.7
1	9	7	101.8	99.0	10	4	8	112.0	114.9
3	9	7	35.9	14.7	12	4	8	25.0	27.8
5	9	7	107.5	110.4	14	4	8	23.4	17.1
7	9	7	72.9	72.1	16	4	8	51.5	44.7
9	9	7	26.0	16.4	18	4	8	153.6	151.4
0	10	7	35.6	39.7	1	5	8	82.3	81.3
2	10	7	46.7	45.9	3	5	8	64.8	62.2
4	10	7	12.7 *	24.2	5	5	8	25.7	20.0
0	0	8	991.3	1065.0	7	5	8	23.2	20.9
2	0	8	10.6 *	16.4	9	5	8	10.9 *	24.9
4	0	8	10.2 *	23.1	11	5	8	80.7	77.9
6	0	8	285.8	319.1	13	5	8	44.7	42.7
8	0	8	44.6	45.0	15	5	8	50.9	58.9
10	0	8	122.4	131.3	17	5	8	11.0 *	8.5
12	0	8	635.7	678.4	0	6	8	103.6	100.8
14	0	8	65.8	62.1	2	6	8	11.3 *	13.6
15	0	8	76.0	79.2	4	6	8	76.8	71.1
18	0	8	152.6	156.8	5	6	8	175.1	179.5
1	1	8	51.7	51.4	8	6	8	10.6 *	8.8
3	1	8	19.2	20.1	10	6	8	24.3	4.6
5	1	8	109.5	119.7	12	6	8	68.4	68.0
7	1	8	85.1	93.6	14	6	8	20.0	4.7
9	1	8	51.8	51.1	1	7	8	55.2	52.2
11	1	8	38.6	44.5	3	7	8	26.4	19.6
13	1	8	22.7	15.0	5	7	8	65.5	67.3
15	1	8	10.0 *	9.3	7	7	8	51.1	56.7
17	1	8	74.8	74.5	9	7	8	11.2 *	20.2
19	1	8	36.4	36.5	11	7	8	55.4	40.9



H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
13	7	8	27.6	29.3	9	5	9	37.5	42.5
0	8	8	443.8	434.5	11	5	9	104.0	110.8
2	8	8	42.1	33.4	13	5	9	41.0	39.7
4	8	8	53.2	52.7	15	5	9	30.8	25.1
6	8	8	229.4	232.7	0	6	9	357.4	371.3
8	8	8	11.7 *	11.0	2	6	9	48.6	42.2
10	8	8	22.8	20.3	4	6	9	81.2	79.9
1	9	8	47.9	47.9	6	6	9	208.4	208.9
3	9	8	13.5 *	22.2	3	6	9	61.3	65.1
5	9	8	40.9	32.5	10	6	9	100.7	101.6
7	9	8	29.4	23.3	12	6	9	242.0	240.1
1	1	9	33.4	26.9	14	6	9	11.0 *	12.9
3	1	9	38.5	34.3	1	7	9	12.3 *	10.0
5	1	9	22.7	5.1	3	7	9	32.5	28.3
7	1	9	40.1	40.5	5	7	9	38.3	26.1
9	1	9	20.8	16.8	7	7	9	50.3	50.6
11	1	9	49.2	44.8	9	7	9	11.5 *	13.1
13	1	9	21.4	21.9	11	7	9	31.6	13.3
15	1	9	9.7 *	9.7	0	8	9	247.0	239.7
17	1	9	10.3 *	6.4	2	8	9	57.5	53.5
19	1	9	37.4	44.0	4	8	9	49.7	56.3
0	2	9	215.1	212.2	6	8	9	27.6	20.4
2	2	9	50.2	47.1	3	8	9	43.1	48.3
4	2	9	10.6 *	19.8	1	9	9	13.1 *	6.9
6	2	9	358.2	372.9	3	9	9	30.7	8.5
8	2	9	45.4	45.0	0	0	10	171.5	173.1
10	2	9	26.1	31.6	2	0	10	44.9	42.8
12	2	9	150.3	158.1	4	0	10	23.3	18.3
14	2	9	33.2	35.7	6	0	10	145.9	158.5
16	2	9	9.8 *	6.2	8	0	10	10.6 *	15.2
18	2	9	217.3	213.3	10	0	10	31.1	36.5
1	3	9	216.6	209.9	12	0	10	116.3	122.7
3	3	9	49.6	48.2	14	0	10	35.6	35.3
5	3	9	148.3	158.8	16	0	10	34.7	34.6
7	3	9	105.2	106.8	13	0	10	74.1	70.3
9	3	9	31.1	25.0	1	1	10	76.0	75.7
11	3	9	196.7	196.5	3	1	10	10.8 *	12.4
13	3	9	96.6	100.5	5	1	10	269.7	282.9
15	3	9	10.7 *	18.6	7	1	10	226.0	242.5
17	3	9	112.4	108.9	9	1	10	43.6	46.0
0	4	9	53.6	45.9	11	1	10	51.2	55.9
2	4	9	53.7	42.3	13	1	10	61.3	65.3
4	4	9	99.4	101.4	15	1	10	10.2 *	14.3
6	4	9	114.0	120.3	17	1	10	186.5	179.3
8	4	9	85.8	86.5	0	2	10	207.8	198.3
10	4	9	52.8	54.4	2	2	10	53.8	52.8
12	4	9	10.9 *	19.1	4	2	10	74.6	72.3
14	4	9	26.5	9.4	6	2	10	44.4	41.1
16	4	9	62.2	57.7	3	2	10	71.3	73.5
1	5	9	100.8	104.9	10	2	10	122.0	124.1
3	5	9	63.5	57.5	12	2	10	122.8	127.3
5	5	9	123.2	127.4	14	2	10	10.5 *	20.9
7	5	9	76.3	81.0	15	2	10	31.3	24.9

	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
	3	10	203.5	194.2	4	2	11	59.0	62.1
	3	10	34.0	82.8	5	2	11	68.7	71.2
	3	10	24.0	27.8	3	2	11	48.9	48.0
	3	10	26.0	23.6	10	2	11	11.0 *	1.6
	3	10	44.3	49.5	12	2	11	128.0	130.0
	3	10	151.2	171.2	14	2	11	29.9	18.6
	3	10	110.0	108.9	15	2	11	45.0	48.2
	3	10	59.3	61.5	1	3	11	108.4	99.8
	3	10	27.8	21.8	3	3	11	43.2	34.3
	4	10	158.1	159.5	5	3	11	21.3	19.5
	4	10	94.4	88.8	7	3	11	57.2	65.8
	4	10	52.6	59.6	9	3	11	11.1 *	12.5
	4	10	239.7	241.7	11	3	11	85.4	86.4
	4	10	11.2 *	9.8	13	3	11	78.6	78.0
	4	10	50.5	51.4	15	3	11	50.5	49.6
	4	10	119.7	119.8	5	4	11	35.3	26.0
	4	10	73.2	69.8	2	4	11	11.9 *	4.2
	4	10	76.5	75.0	4	4	11	21.4	18.1
	5	10	226.4	218.9	5	4	11	70.9	72.9
	5	10	83.9	82.5	3	4	11	11.2 *	4.9
	5	10	90.2	85.9	10	4	11	21.3	15.2
	5	10	72.2	77.1	12	4	11	30.5	16.0
	5	10	35.7	36.9	14	4	11	11.5 *	0.1
	5	10	201.0	196.0	1	5	11	59.0	53.3
	5	10	138.3	133.9	3	5	11	12.1 *	11.8
	5	10	75.3	73.5	5	5	11	93.3	103.4
	6	10	97.0	97.8	7	5	11	118.6	117.9
	6	10	31.6	23.4	9	5	11	31.8	34.3
	6	10	11.9 *	13.4	11	5	11	52.9	51.4
	6	10	10.3 *	4.0	13	5	11	11.5 *	13.5
	6	10	23.5	20.3	0	6	11	92.7	94.1
	6	10	65.5	65.8	2	6	11	12.4 *	16.0
	6	10	61.9	65.7	4	6	11	72.7	72.3
	7	10	21.9	15.5	5	6	11	48.8	49.9
	7	10	26.1	22.5	3	6	11	67.5	68.3
	7	10	35.7	78.1	10	6	11	25.0	21.8
	7	10	66.5	70.0	1	7	11	125.3	120.0
	7	10	12.0 *	18.5	3	7	11	73.5	66.2
	7	10	12.2 *	12.7	5	7	11	278.8	272.1
	8	10	43.4	50.5	7	7	11	201.1	201.1
	8	10	32.2	22.4	0	8	11	13.1 *	16.4
	8	10	12.3 *	16.7	0	0	12	182.4	180.8
	8	10	38.1	40.0	2	0	12	109.2	113.6
	1	11	236.7	231.3	4	0	12	68.6	64.8
	1	11	97.6	96.6	5	0	12	11.0 *	6.2
	1	11	159.3	166.3	3	0	12	10.7 *	14.1
	1	11	90.1	98.0	10	0	12	67.4	66.9
	1	11	77.0	77.4	12	0	12	143.3	145.6
	1	11	197.5	197.3	14	0	12	82.6	80.1
	1	11	128.6	128.5	1	1	12	35.1	12.1
	1	11	44.2	48.5	3	1	12	51.1	50.1
	2	11	190.4	178.1	5	1	12	140.9	143.1
	2	11	11.8 *	16.0	7	1	12	108.6	110.9

H	K	L	F (OBS)	F (CALC)	H	K	L	F (OBS)	F (CALC)
9	1	12	58.9	73.1	7	3	13	11.3 *	4.2
11	1	12	11.1 *	12.5	9	3	13	22.2	25.4
13	1	12	10.4 *	1.6	11	3	13	11.3 *	6.9
15	1	12	10.6 *	9.9	0	4	13	12.9 *	9.0
0	2	12	101.5	92.0	2	4	13	47.8	36.5
2	2	12	43.7	42.6	4	4	13	30.6	33.3
4	2	12	23.6	29.5	5	4	13	117.6	113.4
5	2	12	11.2 *	11.8	8	4	13	11.6 *	10.6
8	2	12	11.0 *	15.7	10	4	13	23.3	26.1
10	2	12	73.8	71.8	1	5	13	12.8 *	8.3
12	2	12	64.4	71.7	3	5	13	13.2 *	24.4
14	2	12	19.4	0.5	5	5	13	39.5	46.9
1	3	12	114.0	106.8	7	5	13	12.3 *	21.4
3	3	12	27.9	31.0	0	6	13	281.0	247.6
5	3	12	68.8	67.4	0	0	14	249.7	237.2
7	3	12	56.5	51.4	2	0	14	37.5	40.3
9	3	12	11.2 *	7.1	4	0	14	57.4	65.5
11	3	12	90.7	93.1	5	0	14	100.4	98.9
13	3	12	64.2	62.4	8	0	14	64.7	64.3
0	4	12	242.0	224.4	10	0	14	65.3	67.1
2	4	12	12.6 *	16.0	1	1	14	51.8	43.3
4	4	12	35.8	26.3	3	1	14	43.0	42.2
6	4	12	457.7	448.3	5	1	14	137.3	140.6
8	4	12	26.3	32.7	7	1	14	114.6	115.0
10	4	12	59.3	58.7	9	1	14	50.7	50.0
1	5	12	77.3	74.2	0	2	14	31.1	8.2
3	5	12	45.3	38.9	2	2	14	68.0	57.4
5	5	12	11.9 *	10.2	4	2	14	68.9	67.8
7	5	12	11.6 *	16.2	5	2	14	119.4	118.1
9	5	12	11.7 *	7.8	8	2	14	11.5 *	1.5
11	5	12	72.3	72.7	1	3	14	128.1	112.5
0	6	12	34.8	27.5	3	3	14	12.4 *	7.1
2	6	12	12.8 *	8.9	5	3	14	42.8	33.2
4	6	12	61.9	56.8	7	3	14	44.8	37.3
6	6	12	45.4	38.6	0	4	14	106.6	89.7
8	6	12	53.0	54.1	2	4	14	12.6 *	0.8
1	7	12	27.8	24.0	4	4	14	12.9 *	33.6
3	7	12	34.2	21.0	6	4	14	123.7	118.7
1	1	13	75.7	71.5	1	1	15	33.5	72.3
3	1	13	11.7 *	23.0	3	1	15	12.0 *	16.1
5	1	13	125.9	123.2	5	1	15	11.9 *	12.5
7	1	13	31.1	87.8	0	2	15	25.5	27.0
9	1	13	23.2	19.0	2	2	15	64.0	61.4
1	1	13	32.1	81.4	4	2	15	12.3 *	7.6
0	2	13	256.9	239.0					
2	2	13	42.4	48.0					
4	2	13	58.9	54.6					
5	2	13	221.0	216.1					
8	2	13	27.7	20.8					
0	2	13	25.3	31.8					
1	3	13	33.7	15.7					
3	3	13	43.5	33.9					
5	3	13	24.3	18.2					