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## Part II. Crystal structure

ROLAND C. ROUSE, DONALD R. PEACOR AND PETE J. DUNN

### Introduction

The chemical and crystallographic data presented in Part I of this study suggest that the crystal structures of fluor- and hydroxyapophyllite are identical except for the  $\text{OH}^- = \text{F}^-$  substitution. However, since cases exist in which this substitution produces a structural change, e.g. hexagonal fluorapatite vs. monoclinic hydroxyapatite (Elliot *et al.*, 1973), a structure determination of the pure hydroxyl end-member has been undertaken, the results of which are presented here. In addition, Prince (1971) has proposed that the fluorine in fluorapophyllite from Centreville, Virginia, is present as HF "molecules" rather than  $\text{F}^-$  ions. We shall examine this hypothesis in the light of new chemical data on Centreville apophyllite.

### Experimental methods and results

The X-ray diffraction study was performed on a square cleavage plate of dimensions  $0.58 \times 0.53 \times 0.12$  mm obtained from a crystal (#93040) from Kimberley, South Africa. A chemical analysis of this material is presented in Part I. Unit-cell parameters are  $a = 8.979 \text{ esd } 0.004$  and  $c = 15.83 \text{ esd } 0.01$  Å. These are essentially the same as those of the North Carolina material and were obtained by the same method. The intensities of 1409 reflections having  $\sin \theta \leq 0.460$  and constituting two asymmetric units in reciprocal

space were measured with a Supper-Pace diffractometer system employing Weissenberg equi-inclination geometry, graphite crystal monochromatized  $\text{MoK}\alpha$  radiation, a scintillation counter, and a scanning rate of  $2^\circ/\text{min}$ . The intensities were then converted to structure factor amplitudes by correction for Lorentz, polarization, and absorption effects ( $\mu_l = 14.8 \text{ cm}^{-1}$ ). Unobserved reflections were assigned intensities of  $I_{\text{min}}/3$ , where  $I_{\text{min}}$  is the minimum observable intensity. Equivalent amplitudes  $|F|_{hkl}$  and  $|F|_{\bar{h}\bar{k}l}$  showed excellent agreement, and the latter were deleted from the data set, leaving 757 reflections of which 696 are observed.

The  $N(z)$  test of Howells *et al.* (1950) indicated hydroxyapophyllite to be centrosymmetric, which is consistent with space group  $P4/mnc$ . A least-squares refinement of the structure was then carried out using the program RFINE 2 of L. W. Finger and commencing with the atomic coordinates in fluorapophyllite given by Colville *et al.* (1971). Neutral atom scattering factors for K, Ca, Si, and O (Doyle and Turner, 1968) were employed, the 0.1 weight percent Al indicated by the chemical analysis (Part I of this study) being neglected. The reciprocal variances,  $1/\sigma^2$ , of the structure-factor amplitudes were used as weights in the refinement, except for unobserved reflections which were assigned zero weight.

	H	K	L	F (OBS)	F (CAL)	H	K	L
	6	5	6	24.0	23.2	6	6	6
	7	5	6	20.1	20.1	7	6	6
	8	5	6	19.2	19.0	8	6	6
	9	5	5	20.0	20.5	9	6	6
	6	5	7	34.8	35.0	7	6	7
	7	5	7	38.3	38.8	8	6	7
	8	5	7	10.5	10.4	9	6	7
	9	5	7	12.6	11.6	6	6	8

TABLE 4. OBSERVED AND CALCULATED STRUCTURE FACTORS OF HYDROXYAPPHYLITE

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
4	0	0	38.7	37.5	8	0	10	38.5	38.4	7	1	1	13.2	14.6
6	0	0	188.3	185.1	10	0	10	31.6	29.9	8	1	1	25.4	24.7
8	0	0	65.5	65.1	1	0	11	50.3	50.9	9	1	1	6.4	3.1
10	0	0	35.7	32.6	3	0	11	58.6	57.8	10	1	1	29.1	30.8
3	0	1	129.1	128.2	5	0	11	56.8	56.7	11	1	1	34.4	33.1
5	0	1	73.0	73.2	9	0	11	46.0	44.3	1	1	2	8.0	6.2
7	0	1	41.7	39.9	9	0	11	76.3	72.7	2	1	2	116.9	115.8
9	0	1	65.0	61.7	0	0	12	131.8	131.1	3	1	1	80.6	77.1
11	0	1	16.9	16.8	2	0	12	20.6	21.4	4	1	2	26.4	29.6
4	0	2	97.9	93.4	4	0	12	15.6	16.5	5	1	2	26.7	26.3
5	0	2	9.5	9.0	6	0	12	32.3	31.6	6	1	2	51.4	50.1
9	0	2	77.9	76.8	8	0	12	74.0	73.6	7	1	2	85.9	86.0
10	0	2	16.7	15.5	1	0	13	24.2	22.9	8	1	2	4.5	1.4
3	0	3	25.4	23.5	1	0	13	17.3	16.9	9	1	2	11.9	10.4
5	0	3	34.1	33.9	5	0	13	20.6	19.2	10	1	2	11.5	10.2
7	0	3	86.4	85.5	9	0	13	53.0	51.7	11	1	2	12.9	12.0
9	0	3	20.5	20.0	0	0	13	9.2	8.4	2	1	3	6.0	3.8
11	0	3	15.4	14.6	0	0	14	27.1	25.0	3	1	3	172.5	173.3
2	0	4	2.6	1.6	2	0	14	2.2	1.7	4	1	3	12.1	13.6
4	0	4	36.8	33.9	4	0	14	13.3	14.5	5	1	3	51.3	51.2
6	0	4	1.8	1.2	6	0	14	2.3	3.2	6	1	3	4.3	2.9
8	0	4	64.5	62.6	8	0	14	20.2	17.8	7	1	3	17.0	16.2
10	0	4	10.1	10.1	1	0	15	40.5	39.6	8	1	3	12.0	13.2
1	0	5	164.1	161.9	1	0	15	20.6	22.0	9	1	3	57.0	56.4
3	0	5	56.4	55.5	5	0	15	21.2	19.9	10	1	3	26.5	26.7
5	0	5	40.5	39.0	5	0	15	37.5	35.8	11	1	3	30.1	29.5
7	0	5	109.3	108.8	7	0	16	82.3	81.2	1	1	4	69.5	69.1
9	0	5	46.8	46.1	2	0	16	21.6	21.1	2	1	4	46.8	44.8
11	0	5	9.5	8.4	4	0	16	5.0	1.8	3	1	4	10.8	10.5
0	0	6	11.0	4.0	6	0	16	49.8	49.1	4	1	4	46.3	43.2
2	0	6	4.9	1.5	1	0	17	17.0	17.5	5	1	4	65.2	64.1
4	0	6	45.6	45.7	3	0	17	2.4	1.1	6	1	4	44.4	44.7
6	0	6	59.3	57.5	5	0	17	13.7	15.9	7	1	4	26.0	26.3
8	0	6	57.4	55.0	0	0	18	35.1	33.0	8	1	4	47.8	48.0
10	0	6	23.9	23.7	2	0	18	8.7	6.4	9	1	4	23.7	23.5
1	0	7	50.7	49.5	4	0	18	2.5	0.8	10	1	4	8.7	8.4
3	0	7	39.8	35.8	1	0	19	2.4	1.2	11	1	4	10.6	12.3
5	0	7	27.7	26.1	3	0	19	2.5	2.6	11	1	5	135.6	135.6
7	0	7	52.6	52.0	0	0	20	83.4	80.9	2	1	5	114.4	110.5
9	0	7	6.7	5.8	2	0	20	22.3	21.5	3	1	5	47.6	46.0
0	0	8	6.0	5.8	2	1	20	38.5	37.1	4	1	5	23.3	23.4
2	0	8	16.3	17.5	3	1	20	35.7	31.7	5	1	5	57.9	58.6
4	0	8	22.5	22.4	4	1	21	21.1	16.3	6	1	5	6.0	6.6
6	0	8	58.9	59.0	5	1	21	50.3	48.7	7	1	5	7.4	7.8
8	0	8	72.9	72.4	6	1	21	37.4	38.7	8	1	5	11.2	12.7
10	0	8	21.3	22.5	7	1	21	27.0	26.8	9	1	5	5.0	5.7
1	0	9	50.1	47.3	8	1	21	8.0	9.1	10	1	5	42.3	43.7
3	0	9	58.2	56.7	9	1	21	35.2	33.3	11	1	6	82.9	81.5
5	0	9	40.7	39.8	10	1	21	41.0	40.5	2	2	6	26.2	23.8
7	0	9	4.3	0.4	1	0	21	12.4	13.4	4	2	6	56.2	56.2
9	0	9	15.7	14.3	2	1	21	81.4	80.2	5	2	6	54.7	53.5
10	0	10	288.9	290.8	3	1	21	46.3	43.3	6	2	6	54.0	56.5
2	0	10	52.8	53.0	4	1	21	47.0	52.2	7	2	6	21.4	21.0
4	0	10	61.9	61.6	5	1	21	64.3	63.6	8	2	6	16.1	16.1
6	0	10	132.1	130.7	6	1	21	64.3	63.6	8	2	6	16.1	16.1

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
9	1	6	51.1	52.2	7	1	12	27.5	26.1	11	2	0	13.6	14.5
19	1	6	54.5	52.6	8	1	12	2.2	1.5	3	2	1	22.0	20.2
11	1	6	28.6	28.0	9	1	12	4.6	3.0	4	2	1	34.2	34.5
2	1	7	16.0	16.4	2	1	13	4.6	9.2	5	2	1	97.8	101.1
3	1	7	124.7	124.7	3	1	13	101.7	103.3	6	2	1	7.7	8.8
4	1	7	4.0	3.9	4	1	13	12.3	11.7	7	2	1	17.9	18.4
5	1	7	46.0	44.6	5	1	13	23.8	24.9	8	2	1	7.5	7.8
6	1	7	15.9	14.9	6	1	13	3.7	2.3	9	2	1	41.1	42.6
7	1	7	2.0	2.6	7	1	13	29.6	28.1	10	2	1	2.2	1.3
9	1	7	21.4	21.0	8	1	13	5.7	3.4	11	2	1	36.1	37.2
9	1	7	32.6	30.9	8	1	14	23.4	23.6	2	2	2	59.3	59.9
10	1	7	23.9	23.1	2	1	14	70.6	72.5	3	2	2	36.6	41.1
1	1	8	3.7	3.5	3	1	14	2.4	2.2	4	2	2	37.1	39.2
2	1	8	63.3	62.8	4	1	14	49.9	51.4	5	2	2	52.3	54.6
3	1	8	59.5	59.4	5	1	14	2.3	2.6	6	2	2	5.7	8.4
4	1	8	79.5	77.1	6	1	14	47.1	46.9	7	2	2	54.9	57.6
5	1	8	3.5	5.0	7	1	14	21.3	20.7	8	2	2	12.7	12.5
6	1	8	45.1	44.9	8	1	14	25.5	25.2	9	2	2	48.7	52.6
7	1	8	38.6	37.8	2	1	15	41.0	40.6	10	2	2	8.5	6.9
8	1	8	42.1	41.6	3	1	15	29.3	31.0	11	2	2	21.9	22.9
9	1	8	17.4	19.3	4	1	15	23.1	24.7	3	2	3	30.6	29.5
10	1	8	36.1	35.0	5	1	15	27.8	27.4	4	2	3	10.1	11.8
2	1	9	43.2	41.7	6	1	15	29.1	28.8	5	2	3	56.1	58.2
3	1	9	81.7	92.3	7	1	15	2.4	1.5	6	2	3	26.7	27.6
4	1	9	12.2	13.3	1	1	16	14.0	11.8	7	2	3	29.9	31.9
5	1	9	22.5	21.0	2	1	16	11.5	11.4	8	2	3	26.1	27.4
6	1	9	22.3	22.7	3	1	16	2.6	1.2	9	2	3	34.1	36.2
7	1	9	26.3	26.7	4	1	16	43.2	43.6	10	2	3	32.3	35.5
8	1	9	2.2	2.9	5	1	16	31.6	31.7	11	2	3	53.0	51.9
9	1	9	26.5	26.9	6	1	16	6.5	5.6	2	2	4	32.3	34.6
10	1	9	14.2	14.7	7	1	16	33.1	32.9	3	2	4	110.6	108.0
1	1	10	41.3	40.3	2	1	17	26.4	25.8	4	2	4	62.9	66.0
2	1	10	16.9	18.4	3	1	17	52.4	50.2	5	2	4	54.3	58.4
3	1	10	8.6	9.4	4	1	17	20.9	15.4	6	2	4	36.3	38.4
4	1	10	21.2	19.9	5	1	17	8.9	20.1	7	2	4	24.2	25.8
5	1	10	18.5	18.6	6	1	17	20.3	15.4	8	2	4	8.4	8.0
6	1	10	7.9	6.5	1	1	18	16.4	18.8	9	2	4	13.8	15.7
7	1	10	2.1	0.1	2	1	18	58.9	56.6	10	2	4	10.9	11.0
8	1	10	17.3	16.5	3	1	18	3.0	1.6	11	2	5	17.2	20.1
9	1	10	27.4	26.5	4	1	18	43.7	41.4	3	2	5	24.7	24.9
10	1	10	41.0	40.1	5	1	18	4.5	1.7	4	2	5	36.8	39.4
1	1	11	58.8	61.4	2	1	19	6.2	7.1	5	2	5	79.9	82.4
2	1	11	79.7	80.7	3	1	19	77.7	77.1	6	2	5	34.2	36.1
3	1	11	55.5	56.2	4	1	19	2.6	0.4	7	2	5	21.8	22.7
4	1	11	40.0	40.6	1	1	20	5.4	1.2	8	2	5	38.8	42.4
5	1	11	61.1	61.0	2	1	20	2.5	0.5	9	2	5	2.2	4.7
6	1	11	10.5	8.9	2	2	0	188.0	191.8	10	2	5	39.2	42.2
7	1	11	36.7	37.5	3	2	0	20.1	19.6	11	2	5	35.9	37.1
8	1	11	27.3	24.8	4	2	0	14.0	14.3	2	2	6	49.8	47.7
9	1	12	17.0	16.1	5	2	0	105.9	110.7	3	2	6	8.5	8.4
1	1	12	48.9	9.6	6	2	0	30.8	34.3	4	2	6	64.9	68.0
2	1	12	14.5	14.1	7	2	0	24.8	25.0	5	2	6	4.8	5.5
3	1	12	2.1	5.4	8	2	0	16.4	17.0	6	2	6	32.1	35.1
4	1	12	6.4	4.4	9	2	0	34.0	34.8	7	2	6	47.1	50.8
5	1	12			10	2	0			8	2	6	9.6	9.2

#	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
9	2	5	28.5	30.2	8	2	13	21.7	22.5	5	3	3	91.9	90.2
10	2	6	27.5	28.1	2	2	14	13.4	13.5	6	3	3	24.5	25.5
3	2	7	20.5	19.4	3	2	14	61.4	63.4	7	3	3	115.8	115.5
4	2	7	31.9	33.6	4	2	14	15.8	16.1	8	3	3	31.0	30.3
5	2	7	47.1	48.7	5	2	14	21.8	22.1	9	3	3	8.0	8.4
6	2	7	2.0	0.7	6	2	14	12.5	12.7	10	3	3	16.8	17.6
7	2	7	17.0	17.5	7	2	14	22.7	22.4	11	3	3	6.2	6.8
8	2	7	9.2	9.7	8	2	14	15.4	14.8	3	3	4	6.8	4.6
9	2	7	20.3	20.9	3	2	15	2.3	1.6	4	3	4	12.6	13.1
10	2	7	10.9	12.3	4	2	15	22.7	23.5	5	3	4	37.9	37.0
2	2	8	72.8	75.3	5	2	15	32.7	34.7	6	3	4	46.4	47.0
3	2	8	114.3	119.0	6	2	15	14.3	15.9	7	3	4	45.5	45.8
4	2	8	10.7	9.8	7	2	15	4.5	1.5	8	3	4	28.8	27.7
5	2	8	76.7	80.3	2	2	16	2.3	4.2	9	3	4	12.3	12.6
6	2	8	9.4	8.6	3	2	16	8.8	10.6	10	3	4	14.6	13.6
7	2	8	36.1	38.6	4	2	16	46.7	49.3	11	3	4	23.4	21.9
8	2	8	25.3	25.6	5	2	16	23.2	25.3	4	3	5	1.8	0.4
9	2	8	28.3	29.2	6	2	16	15.4	17.4	5	3	5	40.7	41.7
10	2	8	9.2	9.3	7	2	16	25.8	28.5	6	3	5	18.8	17.6
3	2	9	6.9	7.4	3	2	17	2.8	4.7	7	3	5	15.5	14.5
4	2	9	50.2	51.4	4	2	17	19.0	20.0	8	3	5	31.1	32.3
5	2	9	38.7	38.9	5	2	17	5.2	6.0	9	3	5	16.2	15.8
6	2	9	26.7	27.9	6	2	17	9.7	10.8	10	3	5	34.4	35.6
7	2	9	10.9	10.9	2	2	18	33.5	33.3	3	3	6	5.4	3.5
8	2	9	8.4	7.4	3	2	18	59.3	57.5	4	3	6	46.9	45.7
9	2	9	14.4	14.8	4	2	18	2.6	1.0	5	3	6	63.4	61.5
10	2	9	17.6	17.8	5	2	18	19.5	19.0	6	3	6	12.5	11.5
2	2	10	78.2	80.8	6	2	18	40.9	41.1	7	3	6	8.8	8.7
3	2	10	23.5	23.5	3	2	19	9.4	9.3	8	3	6	5.2	5.7
4	2	10	111.4	115.4	4	2	0	33.1	33.7	9	3	6	24.1	23.9
5	2	10	14.4	14.8	5	2	0	4.1	4.1	10	3	7	73.3	72.7
6	2	10	61.2	62.9	6	2	0	34.7	35.4	4	3	7	20.6	21.0
7	2	10	2.1	0.3	7	2	0	64.7	66.3	5	3	7	92.2	91.5
8	2	10	16.2	15.0	8	2	0	72.3	72.6	6	3	7	29.9	30.1
9	2	10	12.2	14.4	9	2	0	2.1	0.3	7	3	7	24.5	24.7
10	2	10	19.5	20.8	10	2	0	2.2	4.0	8	3	7	9.0	9.0
3	2	11	24.4	24.1	11	2	0	21.6	20.6	9	3	8	1.9	1.9
4	2	11	79.0	81.3	4	2	1	53.7	53.8	10	3	8	15.5	15.5
5	2	11	17.9	17.7	5	2	1	45.9	45.9	3	3	8	7.5	7.5
6	2	11	9.2	9.3	6	2	1	30.7	31.1	4	3	8	5.9	5.6
7	2	11	4.7	2.5	7	2	1	21.6	21.9	5	3	8	8.5	8.1
8	2	11	28.2	28.1	8	2	1	12.3	12.4	6	3	8	13.9	14.9
9	2	11	11.5	11.5	9	2	1	9.1	9.1	7	3	8	31.0	30.2
10	2	11	27.5	27.2	10	2	1	2.4	3.1	8	3	9	25.1	23.8
3	2	12	51.5	49.8	3	2	2	68.6	65.5	4	3	9	15.6	14.4
4	2	12	47.2	49.8	3	2	2	52.9	51.3	5	3	9	19.3	19.3
5	2	12	8.8	8.4	4	2	2	7.9	6.8	6	3	9	44.1	44.8
6	2	12	18.0	18.2	5	2	2	1.9	7.1	7	3	9	12.3	11.9
7	2	12	5.1	4.7	6	2	2	23.6	25.3	8	3	9	2.3	1.6
8	2	12	7.4	9.2	7	2	2	68.0	68.8	9	3	9	5.1	6.7
9	2	13	14.8	16.1	8	2	2	11.8	11.0	10	3	10	42.4	42.1
10	2	13	48.3	50.1	9	2	2	29.8	30.8	3	3	10	2.5	2.5
4	2	13	11.3	11.8	10	2	2	33.4	33.2	4	3	10		
5	2	13	34.1	34.6	11	2	2	45.2	45.8	5	3	10		
6	2	13	21.5	22.0	4	2	3			4	3	10		



H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
5	3	10	31.7	31.7	7	4	2	43.6	44.7	7	4	11	12.5	11.7
6	3	10	17.9	16.6	8	4	2	25.0	26.1	8	4	11	31.0	30.1
7	3	10	16.1	15.7	9	4	2	10.8	9.8	4	4	12	31.9	32.3
8	3	10	36.1	35.2	10	4	2	33.4	33.6	5	4	12	2.1	0.5
9	3	10	2.3	0.9	5	4	3	19.7	20.5	6	4	12	19.6	19.4
4	3	11	24.9	35.8	6	4	3	15.7	15.0	7	4	12	20.8	20.1
5	3	11	52.3	50.8	7	4	3	5.8	7.2	8	4	12	9.9	12.1
6	3	11	20.2	20.4	8	4	3	40.1	40.1	5	4	13	10.3	11.1
7	3	11	4.1	3.3	9	4	3	22.3	21.5	6	4	13	30.0	31.0
8	3	11	11.5	11.0	10	4	4	9.5	8.8	7	4	13	7.5	6.3
9	3	11	44.0	40.6	4	4	4	17.2	16.8	8	4	14	45.7	44.0
4	3	12	8.6	8.0	5	4	4	19.8	21.1	4	4	14	23.2	23.2
5	3	12	18.9	20.3	6	4	4	5.4	3.6	5	4	14	29.2	30.9
6	3	12	12.9	12.0	7	4	4	5.8	6.9	6	4	14	26.2	27.0
7	3	12	14.5	15.5	8	4	4	2.2	6.3	7	4	14	19.9	21.4
8	3	12	9.1	9.5	9	4	4	46.1	46.1	5	4	15	43.3	43.7
9	3	12	10.7	8.4	10	4	4	102.8	104.9	6	4	15	18.1	18.4
4	3	13	29.4	29.4	5	4	5	41.2	43.1	4	4	16	40.1	40.7
5	3	13	46.2	44.9	6	4	5	6.1	6.8	5	4	16	15.2	15.3
6	3	13	2.2	0.8	7	4	5	48.6	48.2	6	4	16	2.5	2.0
7	3	13	72.1	72.1	8	4	5	18.5	18.7	5	4	17	22.2	24.0
8	3	13	14.8	14.2	9	4	5	29.9	31.0	5	4	17	68.2	69.5
9	3	14	21.2	22.5	10	4	5	79.3	79.9	6	4	0	2.0	4.5
4	3	14	9.7	10.5	4	4	6	1.9	3.1	7	4	0	30.3	28.7
5	3	14	14.0	15.0	5	4	6	26.2	26.4	8	4	0	8.6	7.7
6	3	14	7.3	3.9	6	4	6	17.8	17.4	9	4	0	2.2	0.4
7	3	14	2.4	1.4	7	4	6	10.4	11.5	10	4	0	65.1	63.3
8	3	15	4.5	5.4	8	4	6	26.9	27.8	6	4	1	27.3	27.5
9	3	15	13.1	14.5	9	4	6	43.9	44.5	7	4	1	29.2	27.5
4	3	15	32.4	33.8	10	4	6	4.8	0.1	8	4	1	53.2	51.5
5	3	15	2.3	2.8	5	4	7	10.9	12.8	9	4	1	22.6	19.8
6	3	16	2.5	3.6	6	4	7	9.8	8.0	10	4	1	16.7	18.6
7	3	16	13.1	12.1	7	4	7	7.3	7.5	5	4	2	101.4	102.5
8	3	16	59.7	59.2	8	4	7	14.9	14.5	6	4	2	7.8	6.4
9	3	17	2.5	2.1	9	4	7	19.7	19.7	7	4	2	9.0	8.5
4	3	17	22.4	20.8	10	4	8	46.3	46.8	8	4	2	36.1	35.2
5	3	18	7.5	8.8	5	4	8	41.5	41.2	9	4	2	29.8	29.8
6	3	18	2.6	3.0	6	4	8	39.8	39.6	10	4	2	19.1	19.6
7	4	0	119.4	120.2	7	4	8	15.9	15.1	6	4	3	38.0	37.2
8	4	0	54.3	56.3	8	4	8	2.3	3.5	7	4	3	45.7	45.7
9	4	0	11.4	10.6	9	4	8	33.6	33.4	8	4	3	5.1	6.6
4	4	0	17.1	17.2	5	4	9	20.0	20.2	9	4	3	25.4	24.4
5	4	0	28.4	27.4	6	4	9	2.2	3.6	10	4	3	4.2	3.7
6	4	0	7.2	8.0	7	4	9	29.3	28.7	5	4	4	28.1	29.1
7	4	0	80.8	81.5	8	4	9	29.5	30.2	6	4	4	61.9	61.7
8	4	0	78.6	78.8	9	4	9	114.1	116.0	7	4	4	20.0	20.5
9	4	0	14.3	16.4	4	4	10	25.4	24.4	8	4	4	11.1	10.5
4	4	1	8.9	9.3	5	4	10	7.1	7.8	9	4	4	2.3	4.1
5	4	1	6.3	3.1	6	4	10	11.4	8.9	10	4	4	18.6	18.5
6	4	1	32.1	32.9	7	4	10	2.3	2.6	6	4	5	36.7	36.8
7	4	1	2.3	2.4	8	4	10	71.8	72.3	7	4	5	26.0	25.4
8	4	1	48.6	48.2	9	4	10	7.6	7.6	8	4	5	40.9	40.4
9	4	2	41.3	41.6	10	4	11			9	4	5	37.1	36.7
4	4	2	62.4	62.8	6	4	11			10	4	5	30.8	29.1

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
6	5	5	24.0	23.2	6	6	6	60.8	60.5
7	5	6	20.1	20.1	7	6	6	4.0	4.9
8	5	6	19.2	19.0	8	6	6	23.0	21.2
9	5	5	20.0	20.5	9	6	6	51.1	50.0
6	5	7	34.8	35.0	7	5	7	29.4	26.3
7	5	7	38.3	38.8	8	6	7	11.2	10.3
8	5	7	10.5	10.4	9	6	7	11.4	9.4
9	5	7	12.6	11.6	6	6	9	11.0	8.8
6	5	8	64.7	64.9	7	6	8	36.3	34.9
7	5	8	55.2	55.1	8	6	8	10.9	10.7
8	5	8	8.4	8.8	7	6	9	21.3	21.5
9	5	8	21.5	20.3	8	6	9	20.7	19.8
6	5	8	31.1	31.8	6	6	10	75.6	74.1
7	5	8	6.9	6.9	7	6	10	17.3	17.6
8	5	9	33.6	33.4	8	6	10	29.5	27.2
9	5	9	20.7	20.0	7	6	11	33.6	32.0
6	5	9	7.3	7.0	6	6	12	47.5	47.9
7	5	10	29.7	30.5	7	6	12	22.1	21.2
8	5	10	17.2	18.2	6	6	14	9.6	11.7
9	5	10	11.9	11.4	7	6	0	46.8	44.9
6	5	10	10.2	9.1	8	7	7	14.6	13.9
7	5	11	39.0	39.8	9	7	7	17.8	17.0
8	5	11	14.7	15.0	8	7	1	4.2	5.8
9	5	11	55.4	54.1	9	7	2	2.2	1.6
6	5	12	35.9	35.9	7	7	2	28.6	26.1
7	5	12	13.1	12.2	8	7	2	8.7	9.3
8	5	12	15.8	15.5	9	7	2	29.8	28.8
9	5	12	9.5	9.4	8	7	3	10.5	9.0
6	5	13	18.4	18.1	9	7	3	50.8	48.1
7	5	13	34.8	34.3	7	7	4	18.3	15.8
8	5	14	8.5	9.3	8	7	4	22.1	19.7
9	5	14	20.5	20.2	9	7	4	2.3	3.5
6	5	15	7.2	6.1	8	7	5	2.2	1.1
7	5	16	30.5	30.5	7	7	6	62.5	60.9
8	6	0	106.9	104.9	8	7	6	33.3	32.1
9	6	0	13.8	13.9	8	7	7	16.4	15.5
6	6	0	20.1	20.6	7	7	8	48.7	47.0
7	6	0	17.8	18.0	8	7	8	11.8	12.4
8	6	1	10.1	10.0	7	7	10	47.3	46.3
9	6	1	6.2	7.2	8	8	0	56.6	56.8
6	6	1	46.3	44.9	8	8	2	34.9	34.5
7	6	2	26.5	26.7	8	8	4	48.5	48.7
8	6	2	43.2	43.2					
9	6	2	29.7	28.2					
6	6	2	17.2	16.2					
7	6	3	57.6	56.4					
8	6	3	26.3	25.1					
9	6	3	2.3	4.7					
6	6	4	21.4	20.8					
7	6	4	18.9	18.2					
8	6	4	5.8	5.1					
9	6	4	8.2	8.9					
6	6	5	44.3	43.4					
7	6	5	14.1	14.3					
8	6	5	54.6	52.2					
9	6	5							