

AM-87-332

Petrologic and crystal-chemical implications of cation order-disorder
in kutnahorite [CaMn(CO₃)₂]

Peacor, et al.

To be deposited: Table 4

American Mineralogist, 72, 3-4, 319-328

Table 4.

Structure factors for Sterling Hill kutnahorite

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
7	-5	0	33.4	34.1	2	3	2	45.2	45.1
5	-4	0	48.5	49.5	0	4	2	10.6	9.2
8	-4	0	39.1	37.3	3	4	2	16.5	17.1
6	-3	0	38.5	37.7	1	5	2	34.5	35.3
4	-2	0	54.7	56.0	7	-5	3	10.0	9.3
7	-2	0	27.9	28.3	5	-4	3	4.0	3.3
2	-1	0	73.3	77.1	8	-4	3	3.8	0.7
5	-1	0	55.1	55.9	6	-3	3	5.0	3.8
3	0	0	95.7	102.8	4	-2	3	4.4	4.5
6	0	0	28.1	27.7	7	-2	3	13.2	12.5
1	1	0	73.9	77.1	2	-1	3	65.7	69.5
4	1	0	48.5	49.5	5	-1	3	8.1	7.0
2	2	0	55.7	56.0	3	0	3	5.5	5.3
5	2	0	32.8	34.1	6	0	3	1.7 *	2.8
0	3	0	98.1	102.8	1	1	3	55.1	55.2
3	3	0	39.0	37.7	4	1	3	5.6	4.9
1	4	0	56.2	55.9	2	2	3	13.3	14.9
4	4	0	38.1	37.3	5	2	3	1.9 *	4.9
2	5	0	27.9	28.3	0	3	3	12.0	10.7
0	6	0	28.6	27.7	3	3	3	9.6	9.8
7	-6	1	1.9 *	3.4	1	4	3	1.3 *	1.3
8	-5	1	4.5	3.6	4	4	3	2.2 *	4.6
6	-4	1	3.7	1.3	2	5	3	8.7	8.2
4	-3	1	12.4	13.5	0	6	3	7.3	7.1
7	-3	1	1.8 *	3.0	7	-6	4	26.5	25.9
5	-2	1	19.4	20.0	6	-4	4	34.0	35.6
3	-1	1	27.2	27.2	4	-3	4	68.4	69.7
6	-1	1	9.9	9.5	7	-3	4	39.4	38.4
4	0	1	4.6	3.3	5	-2	4	43.3	44.0
7	0	1	2.1 *	0.9	3	-1	4	65.0	68.1
2	1	1	46.8	46.1	6	-1	4	27.8	27.1
5	1	1	18.3	18.4	4	0	4	80.0	84.8
0	2	1	2.2	2.7	2	1	4	63.4	64.6
3	2	1	19.0	20.1	5	1	4	28.8	29.7
1	3	1	4.0	1.2	0	2	4	71.4	71.2
4	3	1	4.0	3.6	3	2	4	35.9	36.3
2	4	1	12.6	12.5	1	3	4	80.9	83.1
0	5	1	2.8	2.3	4	3	4	45.2	45.3
3	5	1	3.7	2.9	2	4	4	33.3	32.0
1	6	1	3.9	6.6	0	5	4	41.3	41.5
6	-5	2	36.2	36.0	1	6	4	30.4	30.9
7	-4	2	11.1	10.7	6	-5	5	12.2	12.6
5	-3	2	48.6	48.7	7	-4	5	1.9 *	1.3
3	-2	2	76.4	80.3	5	-3	5	23.9	25.6
6	-2	2	35.6	37.2	3	-2	5	27.7	28.0
4	-1	2	24.5	21.7	6	-2	5	6.9	6.9
7	-1	2	19.3	19.5	4	-1	5	5.0	5.1
2	0	2	93.5	97.1	7	-1	5	1.9 *	3.3
5	0	2	30.5	31.8	2	0	5	15.8	15.7
3	1	2	37.8	37.0	5	0	5	6.3	6.8
6	1	2	23.0	23.5	0	1	5	0.8 *	0.4
1	2	2	70.2	68.7	3	1	5	10.7	5.6
4	2	2	33.6	32.2	6	1	5	5.7	6.4

4

Structure factors for Sterling Hill kutnahorite (cont.)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
1	2	5	34.8	34.7	2	3	8	37.2	36.4
4	2	5	4.4	3.4	0	4	8	72.1	73.7
2	3	5	11.1	11.3	3	4	8	36.2	35.7
0	4	5	1.2 *	0.7	1	5	8	27.8	27.9
3	4	5	4.2	5.1	7	-5	9	6.1	5.0
1	5	5	13.5	13.5	5	-4	9	2.7	1.5
7	-5	6	20.4	20.6	6	-3	9	6.3	6.9
5	-4	6	31.9	32.0	4	-2	9	9.2	10.6
6	-3	6	30.7	30.5	7	-2	9	8.3	7.6
4	-2	6	50.7	51.2	2	-1	9	28.6	30.7
2	-1	6	89.4	97.8	5	-1	9	4.6	1.6
5	-1	6	26.3	26.3	3	0	9	3.6	1.6
3	0	6	28.4	27.3	6	0	9	5.3	5.8
6	0	6	27.8	28.6	1	1	9	42.7	43.8
1	1	6	85.5	87.0	4	1	9	1.3 *	0.2
4	1	6	31.1	31.6	2	2	9	2.5	3.5
2	2	6	53.3	53.1	5	2	9	7.5	7.0
0	3	6	28.8	27.4	0	3	9	2.1	2.2
3	3	6	32.1	32.2	3	3	9	1.6 *	4.1
1	4	6	25.8	25.8	1	4	9	4.9	3.0
0	6	6	29.5	28.8	2	5	9	11.2	9.9
7	-6	7	5.2	6.9	0	6	9	1.8 *	2.6
6	-4	7	4.4	3.8	6	-4	10	28.0	27.7
4	-3	7	2.9	0.2	4	-3	10	28.5	28.9
7	-3	7	9.5	8.0	7	-3	10	14.9	15.7
5	-2	7	11.0	10.3	5	-2	10	32.7	32.8
3	-1	7	29.6	31.0	3	-1	10	52.2	53.5
6	-1	7	12.6	12.4	6	-1	10	30.8	31.9
1	0	7	9.5	9.8	1	0	10	40.1	41.8
4	0	7	8.8	8.6	4	0	10	11.2	10.3
2	1	7	24.3	23.9	2	1	10	51.4	51.2
5	1	7	11.8	12.1	5	1	10	27.3	27.3
0	2	7	13.6	13.3	0	2	10	64.2	64.2
3	2	7	22.5	23.5	3	2	10	40.7	41.9
1	3	7	8.9	10.0	1	3	10	20.8	20.0
4	3	7	1.8 *	2.3	4	3	10	10.7	9.6
2	4	7	6.6	6.2	2	4	10	28.3	29.7
0	5	7	8.0	8.0	0	5	10	26.1	26.8
1	6	7	1.9 *	1.9	6	-5	11	13.7	13.3
6	-5	8	24.5	24.6	7	-4	11	6.0	5.7
7	-4	8	41.4	40.8	5	-3	11	13.0	13.7
5	-3	8	35.6	37.0	3	-2	11	24.7	25.3
3	-2	8	50.2	49.9	6	-2	11	9.2	9.3
6	-2	8	27.8	28.3	4	-1	11	5.8	5.1
4	-1	8	68.0	72.3	2	0	11	2.6	0.3
7	-1	8	26.2	27.4	5	0	11	1.5 *	0.4
2	0	8	58.6	59.9	0	1	11	12.8	12.5
5	0	8	37.8	38.0	3	1	11	10.6	12.2
0	1	8	110.2	112.5	1	2	11	12.7	12.9
3	1	8	59.0	59.5	4	2	11	4.2	1.5
6	1	8	25.3	25.0	2	3	11	13.4	13.3
1	2	8	61.8	63.5	0	4	11	7.9	8.4
4	2	8	32.7	33.6	1	5	11	7.0	7.1

Structure factors for Sterling Hill kutnahorite (cont.)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
7	-5	12	25.5	25.3	1	1	15	15.5	15.5
5	-4	12	35.4	36.3	4	1	15	4.9	4.3
6	-3	12	30.5	30.4	2	2	15	6.5	7.0
4	-2	12	39.7	40.8	0	3	15	8.7	8.6
7	-2	12	20.6	21.0	3	3	15	7.8	6.2
2	-1	12	43.0	41.5	1	4	15	3.2	2.3
4	1	12	36.6	36.9	6	-4	16	24.3	23.2
5	-1	12	39.8	40.5	4	-3	16	40.6	39.3
3	0	12	60.1	63.0	5	-2	16	30.3	30.1
6	0	12	22.2	22.3	3	-1	16	35.3	34.1
1	1	12	52.4	52.9	6	-1	16	17.5	17.2
2	2	12	38.6	38.3	1	0	16	56.2	55.4
5	2	12	27.6	28.1	4	0	16	46.8	46.9
0	3	12	62.2	62.9	2	1	16	38.0	37.8
3	3	12	28.0	27.9	5	1	16	21.9	22.2
1	4	12	41.5	41.3	0	2	16	38.1	36.6
2	5	12	23.6	23.9	3	2	16	23.1	21.9
0	6	12	21.3	22.0	1	3	16	45.4	44.5
6	-4	13	3.4	0.3	2	4	16	23.3	22.5
4	-3	13	4.3	3.5	0	5	16	26.6	26.7
7	-3	13	5.2	4.5	5	-3	17	12.0	11.5
3	-1	13	11.8	11.9	3	-2	17	10.0	10.1
6	-1	13	6.4	6.0	6	-2	17	1.7 *	4.0
1	0	13	1.9	0.7	4	-1	17	3.3	1.2
4	0	13	1.3 *	4.1	2	0	17	5.3	4.5
2	1	13	20.4	19.9	5	0	17	1.5 *	2.4
5	1	13	11.6	12.1	0	1	17	1.9	2.7
0	2	13	1.0 *	0.2	3	1	17	5.0	5.4
3	2	13	10.3	12.3	1	2	17	11.0	10.7
1	3	13	3.0	3.3	4	2	17	2.7	1.1
4	3	13	1.8 *	0.4	2	3	17	6.6	5.7
2	4	13	8.1	7.8	0	4	17	4.6	4.3
0	5	13	5.0	3.1	5	-4	18	20.0	19.6
6	-5	14	27.3	27.4	6	-3	18	16.8	18.0
5	-3	14	29.8	29.0	4	-2	18	25.8	25.6
3	-2	14	43.8	45.5	2	-1	18	39.5	40.4
6	-2	14	25.8	26.8	5	-1	18	16.5	16.8
4	-1	14	17.1	16.5	3	0	18	17.6	17.5
2	0	14	45.5	46.7	1	1	18	32.6	31.7
5	0	14	21.3	22.3	4	1	18	19.0	19.1
0	1	14	32.9	32.9	2	2	18	27.3	27.9
3	1	14	25.1	25.5	0	3	18	17.6	17.5
1	2	14	35.9	34.5	3	3	18	20.3	20.5
4	2	14	22.4	22.2	1	4	18	15.3	16.1
2	3	14	30.7	31.8	4	-3	19	1.4 *	2.0
0	4	14	10.9	10.4	5	-2	19	4.0	4.1
1	5	14	22.7	22.9	3	-1	19	10.0	10.3
5	-4	15	3.0	3.3	1	0	19	5.2	5.4
6	-3	15	1.6 *	1.4	4	0	19	6.7	7.0
4	-2	15	2.9	1.6	2	1	19	8.0	6.9
2	-1	15	20.8	21.5	0	2	19	3.8	4.3
5	-1	15	6.3	5.5	3	2	19	10.3	10.2
3	0	15	6.4	6.2	1	3	19	6.0	6.1
					0	5	19	1.8 *	4.8

Structure factors for Bald Knob kutnahorite

H	K	L	F (OBS)	F (CALC)	0	4	2	10.1	9.3
					3	4	2	14.8	14.3
7	-5	0	31.7	30.9	1	5	2	34.3	35.9
5	-4	0	51.2	53.6	7	-5	3	9.1	9.0
8	-4	0	38.0	37.9	5	-4	3	2.9	1.3
6	-3	0	37.5	38.0	8	-4	3	2.7	1.3
4	-2	0	53.9	56.4	6	-3	3	6.9	7.5
7	-2	0	31.1	30.9	4	-2	3	8.0	9.6
5	-1	0	51.0	53.3	7	-2	3	9.0	9.0
3	0	0	93.7	103.5	2	-1	3	63.0	61.7
6	0	0	27.2	28.0	5	-1	3	2.7	1.0
1	1	0	72.8	78.5	3	0	3	0.7 *	0.2
4	1	0	52.4	53.6	6	0	3	2.0	0.1
2	2	0	54.3	56.4	1	1	3	65.9	62.9
5	2	0	29.8	30.9	4	1	3	0.9 *	1.1
0	3	0	101.5	103.5	2	2	3	7.8	9.1
3	3	0	38.3	38.0	5	2	3	8.1	8.9
1	4	0	51.3	53.3	0	3	3	0.8 *	0.3
4	4	0	38.1	37.9	3	3	3	7.6	7.4
2	5	0	32.0	30.9	1	4	3	1.8	1.1
0	6	0	29.2	28.0	4	4	3	1.3 *	1.8
7	-6	1	5.3	5.0	2	5	3	9.0	8.7
8	-5	1	3.6	2.8	0	6	3	2.3	0.0
6	-4	1	6.2	5.2	7	-6	4	27.7	27.9
4	-3	1	5.0	5.7	6	-4	4	35.4	34.3
7	-3	1	3.7	3.2	4	-3	4	73.2	76.8
5	-2	1	19.2	20.0	7	-3	4	43.3	42.0
3	-1	1	37.4	37.4	5	-2	4	43.2	41.1
6	-1	1	14.2	14.0	3	-1	4	69.2	66.8
4	0	1	0.8 *	0.2	6	-1	4	27.4	28.3
7	0	1	1.2 *	0.3	4	0	4	80.5	86.0
2	1	1	37.6	36.5	2	1	4	70.5	67.1
5	1	1	14.5	14.3	5	1	4	27.6	28.7
0	2	1	0.6 *	0.7	0	2	4	73.3	72.9
3	2	1	19.7	20.7	3	2	4	40.6	40.8
1	3	1	5.1	5.7	1	3	4	77.3	77.3
4	3	1	4.5	3.4	4	3	4	42.0	42.4
2	4	1	6.0	5.4	2	4	4	35.5	33.5
0	5	1	1.8	0.6	0	5	4	44.2	42.6
3	5	1	2.7	3.4	1	6	4	27.9	28.8
1	6	1	5.7	5.7	6	-5	5	13.4	13.3
6	-5	2	34.3	35.9	7	-4	5	2.3	3.2
7	-4	2	13.7	13.9	5	-3	5	17.8	18.7
5	-3	2	50.3	47.1	3	-2	5	31.5	32.1
3	-2	2	72.0	76.3	6	-2	5	6.0	5.1
6	-2	2	35.8	35.5	4	-1	5	4.6	4.6
4	-1	2	33.2	29.7	7	-1	5	5.4	5.2
7	-1	2	21.2	21.5	2	0	5	1.5	0.1
2	0	2	94.9	98.4	5	0	5	1.0 *	0.3
5	0	2	30.2	31.7	0	1	5	1.5	1.4
3	1	2	30.8	30.3	3	1	5	8.3	6.2
6	1	2	20.6	22.2	6	1	5	4.9	4.7
1	2	2	73.1	75.3	1	2	5	33.7	31.7
4	2	2	35.0	34.6					
2	3	2	46.5	47.6					

Structure factors for Bald Knob kutnahorite (cont.)

H	K	L	F (OBS)	F (CALC)	4	2	8		
								32.5	32.1
								38.3	36.8
4	2	5	5.0	4.9	0	4	8	74.8	75.0
2	3	5	17.9	18.5	3	4	8	39.9	38.5
0	4	5	1.5	0.8	1	5	8	27.7	27.0
3	4	5	2.6	2.8	7	-5	9	6.8	7.4
1	5	5	14.3	13.2	5	-4	9	2.3	1.5
7	-5	6	23.6	23.2	6	-3	9	6.9	6.1
5	-4	6	30.6	28.9	4	-2	9	6.8	6.6
6	-3	6	33.1	31.4	7	-2	9	7.5	7.6
4	-2	6	51.7	53.0	2	-1	9	36.0	37.4
7	-2	6	22.3	23.1	5	-1	9	0.9 *	1.0
5	-1	6	30.2	29.0	3	0	9	0.8 *	0.9
3	0	6	29.0	28.4	6	0	9	3.3	0.0
6	0	6	28.8	29.0	1	1	9	36.8	37.0
1	1	6	87.2	92.5	4	1	9	0.9 *	0.4
4	1	6	28.5	28.7	2	2	9	6.4	7.0
2	2	6	51.5	53.1	5	2	9	6.5	7.7
5	2	6	22.8	22.7	0	3	9	0.7 *	0.6
0	3	6	30.1	28.1	3	3	9	6.3	6.1
3	3	6	31.0	31.7	1	4	9	2.2	0.7
1	4	6	29.4	29.2	2	5	9	7.1	7.3
2	5	6	23.5	22.8	0	6	9	1.1 *	0.1
0	6	6	27.8	28.6	6	-4	10	29.9	29.0
7	-6	7	3.9	4.7	4	-3	10	25.7	25.1
6	-4	7	5.0	4.5	7	-3	10	13.0	12.9
4	-3	7	4.5	4.4	5	-2	10	39.2	36.9
7	-3	7	3.1	3.2	3	-1	10	53.0	53.8
5	-2	7	17.9	17.2	6	-1	10	29.7	30.3
3	-1	7	29.8	27.3	1	0	10	41.3	42.5
6	-1	7	12.8	12.3	4	0	10	10.1	10.2
1	0	7	1.3	0.2	2	1	10	52.2	52.9
4	0	7	0.9 *	0.5	5	1	10	29.0	29.6
2	1	7	28.8	27.8	0	2	10	63.5	64.4
5	1	7	13.5	12.6	3	2	10	36.8	37.6
0	2	7	1.9	0.3	1	3	10	24.7	24.9
3	2	7	17.5	17.4	4	3	10	12.0	12.4
1	3	7	4.4	4.3	2	4	10	28.3	29.6
4	3	7	3.8	2.9	0	5	10	25.3	26.1
2	4	7	5.1	4.7	6	-5	11	11.3	10.5
0	5	7	1.8	0.6	7	-4	11	1.2 *	2.7
1	6	7	5.1	5.0	5	-3	11	13.3	13.8
6	-5	8	27.9	26.6	3	-2	11	19.1	19.3
7	-4	8	38.6	38.7	6	-2	11	4.1	4.0
5	-3	8	38.5	37.7	4	-1	11	3.8	3.3
3	-2	8	57.3	57.1	2	0	11	0.7 *	0.6
6	-2	8	31.3	31.2	5	0	11	1.0 *	0.1
4	-1	8	64.4	67.4	0	1	11	0.7 *	0.5
7	-1	8	26.6	26.5	3	1	11	3.2	4.5
2	0	8	59.8	61.0	1	2	11	18.8	19.9
5	0	8	40.4	38.7	4	2	11	3.9	3.9
0	1	8	105.6	114.9	2	3	11	13.4	13.4
3	1	8	65.5	66.8	0	4	11	0.9 *	0.9
6	1	8	24.6	26.2					
1	2	8	59.7	58.7					

Structure factors for Bald Knob kutnahorite (cont.)

H	K	L	F (OBS)	F (CALC)	2	-1	15	18.7	18.3
3	4	11	3.2	1.9	5	-1	15	0.9 *	0.7
1	5	11	10.2	10.3	3	0	15	1.7	0.6
7	-5	12	24.9	24.5	1	1	15	18.1	18.8
5	-4	12	39.7	40.0	4	1	15	2.3	0.1
6	-3	12	31.4	30.2	2	2	15	4.5	4.2
4	-2	12	40.4	40.8	0	3	15	0.8 *	0.4
7	-2	12	25.3	24.7	3	3	15	4.3	4.3
2	-1	12	49.2	48.4	1	4	15	1.9	0.4
5	-1	12	39.8	40.0	6	-4	16	23.5	23.6
3	0	12	61.7	64.2	4	-3	16	43.0	43.2
6	0	12	22.6	22.6	5	-2	16	27.6	28.0
1	1	12	49.6	50.0	3	-1	16	37.5	37.0
4	1	12	39.5	40.1	6	-1	16	20.0	20.1
2	2	12	43.2	40.6	1	0	16	57.2	57.6
5	2	12	24.0	25.2	4	0	16	47.5	48.6
0	3	12	63.2	64.5	2	1	16	37.6	37.9
3	3	12	30.0	29.8	5	1	16	20.4	20.8
1	4	12	39.8	39.7	0	2	16	39.4	39.0
2	5	12	25.1	25.0	3	2	16	27.7	27.2
0	6	12	23.7	23.2	1	3	16	42.9	43.3
6	-4	13	3.9	3.3	2	4	16	23.6	23.2
4	-3	13	3.2	2.2	0	5	16	28.4	28.5
7	-3	13	2.5	2.6	5	-3	17	8.6	8.7
5	-2	13	12.0	11.9	3	-2	17	10.8	10.9
3	-1	13	16.5	16.1	6	-2	17	2.9	2.7
6	-1	13	9.0	9.1	4	-1	17	0.9 *	1.7
1	0	13	0.7 *	1.0	2	0	17	0.8 *	0.0
4	0	13	0.8 *	0.9	5	0	17	1.0 *	0.0
2	1	13	16.4	15.6	0	1	17	0.7 *	0.9
5	1	13	9.6	9.4	3	1	17	0.9 *	3.2
0	2	13	0.7 *	0.3	1	2	17	10.9	10.7
3	2	13	11.7	12.3	4	2	17	2.3	2.6
1	3	13	3.1	3.1	2	3	17	8.9	8.6
4	3	13	3.2	2.2	0	4	17	0.9 *	1.0
2	4	13	2.8	3.4	5	-4	18	18.3	17.8
0	5	13	1.8	0.6	6	-3	18	19.3	19.0
6	-5	14	26.8	25.4	4	-2	18	27.4	26.9
5	-3	14	30.6	30.3	2	-1	18	36.5	36.8
3	-2	14	39.8	41.1	5	-1	18	17.0	17.7
6	-2	14	24.4	24.6	3	0	18	17.8	17.7
4	-1	14	21.3	20.8	1	1	18	36.5	35.6
2	0	14	46.8	47.7	4	1	18	17.4	17.7
5	0	14	21.1	22.6	2	2	18	26.9	27.1
0	1	14	32.5	33.1	0	3	18	17.9	17.5
3	1	14	21.4	21.2	3	3	18	18.6	19.4
1	2	14	40.0	39.6	1	4	18	17.8	18.0
4	2	14	24.2	24.0	4	-3	19	0.9 *	1.1
2	3	14	31.2	31.4	5	-2	19	7.6	7.4
0	4	14	10.9	10.2	3	-1	19	8.6	8.6
1	5	14	24.5	24.8	1	0	19	0.8 *	0.4
5	-4	15	1.0 *	1.2	4	0	19	2.7	0.8
6	-3	15	4.6	4.2	2	1	19	8.7	8.6
4	-2	15	4.4	4.2					

Structure factors for Bald Knob kutnahorite (cont.)

H	K	L	F (OBS)	F (CALC)
0	2	19	0.8 *	0.0
3	2	19	7.5	7.6
1	3	19	2.0	1.9
0	5	19	1.0 *	0.5