

nism. The presence of minerals such as portlandite and ettringite indicates an extremely high alkalinity, in excess of $\text{pH}=11$, which also remains unexplained. Water of such high alkalinity is most unusual, but has been observed, although not explained, in at least one case: the spring of Aqua de Ney, California. (Feth *et al.* 1961).

The data presented here are the result of a preliminary study of this interesting rock sequence. Further unusual mineral assemblages are under investigation.

ACKNOWLEDGMENT

We are grateful to Dr. M. Fleischer for drawing our attention to some of the references listed below.

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THE AMERICAN MINERALOGIST, VOL. 48, JULY-AUGUST, 1963

THE PROBABLE CHEMICAL FORMULA OF AKSAITE, A NEW HYDRATED MAGNESIUM BORATE¹

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Aksaite, a new hydrated magnesium borate, has recently been described by Blazko *et al.* (1962). Crystallographic, optical and chemical data were given, but these authors stated that the chemical composition of aksaite remains in doubt. The two chemical formulas suggested by them as most probable are: $2\text{MgO} \cdot 5\text{B}_2\text{O}_3 \cdot 8\text{H}_2\text{O}$ and $3\text{MgO} \cdot 7\text{B}_2\text{O}_3 \cdot 10\text{H}_2\text{O}$.

¹ Publication authorized by the Director, U. S. Geological Survey.

Lehmann and Papenfuss (1959) described the synthesis of $\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ and gave x -ray powder data for that compound. Crystals were kindly supplied to us for examination through the courtesy of Prof. Dr. H.-A. Lehmann, Institut für anorganische Chemie der TH für Chemie, Leuna-Merseburg, to whom we are indebted. The crystallographic and optical data obtained by us for the synthetic magnesium

TABLE 1. CRYSTALLOGRAPHIC AND OPTICAL DATA COMPARED FOR $\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ AND FOR AKSAITE

	$\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ Present Study ¹	Aksaite Blazko <i>et al.</i> (1962) ²	
		(1)	(2)
Symmetry	Orthorhombic	Orthorhombic	Orthorhombic
a	$12.54 \pm 0.04 \text{ \AA}$	$12.54 \pm 0.01 \text{ kX}$	$12.52 \pm 0.01 \text{ kX}$
b	24.35 ± 0.08	24.28 ± 0.02	24.27 ± 0.03
c	7.484 ± 0.025	7.49 ± 0.01	7.47 ± 0.01
Cell Volume	2285 \AA^3	2280.49 kX^3	$[2270 \text{ kX}^3]^3$
Space Group	<i>Pbca</i>	<i>Pbca</i>	<i>Pbca</i>
Cell Contents	$8[\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}]$	$5[2\text{MgO} \cdot 5\text{B}_2\text{O}_3 \cdot 8\text{H}_2\text{O}]$	$4[3\text{MgO} \cdot 7\text{B}_2\text{O}_3 \cdot 10\text{H}_2\text{O}]$
Specific Gravity			
(calc.)	1.972	2.072	2.293
(obs.)	1.99 ± 0.01	2.066	2.367
Optical Classification	Biaxial negative	Biaxial negative	
α	1.472 ± 0.002	1.473 ± 0.001 , X = a	
β	1.503 ± 0.002 , Y = c	1.508 ± 0.001 , Y = c	
γ	1.526 ± 0.002	1.528 ± 0.001 , Z = b	
2V (calc.)	80°	$88^\circ [73^\circ]^3$	

¹ Synthetic crystals (Lehmann and Papenfuss, 1959). Precession camera, Zr-filtered Mo radiation, λ (MoK α) = 0.7107 Å; film measurements corrected for shrinkage.

² Sample (1) collected by Blazko *et al.*, locality not given; sample (2) collected by V. V. Lobanova, locality not given. The samples are said to be identical in morphology and in optical properties. Single-crystal data obtained from Laue, rotation, oscillation and Weissenberg photographs using Ni-filtered Cu radiation, λ (CuK α) = 1.539 kX.

³ Calculated by present authors from data given by Blazko *et al.* (1962).

borate crystals are compared in Table 1 with the data given by Blazko *et al.* (1962) for aksaite. The x -ray powder data, calculated by us from the cell constants found from single-crystal examination, are given in Table 2 together with the observed lines measured by us and by Lehmann and Papenfuss (1959) for the synthetic crystals. The measured lines for aksaite reported by Blazko *et al.* (1962) are also given in Table 2 for comparison.

The evidence of the two tables is sufficient to show that the mineral crystals of aksaite are the same compound as the synthetic crystals of $\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$, thus confirming the suggestion made by M. E. Mrose, quoted by Fleischer (1963). The chemical analyses and specific gravity determinations for aksaite were apparently made from impure samples, a possibility suggested by Blazko *et al.* (1962).

TABLE 2. X-RAY POWDER DATA COMPARED FOR $MgO \cdot 3B_2O_3 \cdot 5H_2O$ AND AKSAITE

Calculated ¹		Observed						
		Synthetic $MgO \cdot 3B_2O_3 \cdot 5H_2O$					Aksaite	
		Present Study ²		Lehmann and Papefuss (1959) ³			Blazko <i>et al.</i> (1962) ⁴	
<i>hkl</i>	d_{hkl} (Å)	d_{hkl} (Å)	I	$\theta/2$	d_{hkl} (Å)	I	d_{hkl} (kX)	I
020	12.18	12.2	10					
		7.2 ⁵	2					
021	6.38	6.4	100	—				
200	6.27	6.3	35	7.0	6.3	st	6.36	10
111	6.21							
040	6.09	6.1	50				6.00	8
210	6.07			7.6	5.8	ss	5.63	3
121	5.68	5.7	2					
220	5.57							
131	5.04	5.03	10	8.8	5.04	s		
230	4.96	4.98	10	—			4.98	6
201	4.81							
041, 211	4.72	4.72	50	9.4	4.72	m	4.68	9
221	4.47	4.48	2					
141	4.42	4.37	25	10.1	4.40	s	4.33	6
240	4.37							
231	4.14	4.15	5	10.8	4.11	ss	4.10	r 3
060	4.06							
151	3.88	3.86	2					
250	3.85							
241	3.77	3.74	20	11.6	3.83	ss	3.70	4
002	3.74							
311	3.61							
102	3.59	3.59	35	12.3	3.62	m	3.54	9
022	3.58							
061	3.57							
112	3.55							
321	3.50							
122	3.44	3.44	10	—			3.43	3
161	3.43							
251	3.42							
260	3.41							
331	3.33	3.34	10	13.2	3.38	ss	3.31	4
132	3.28	3.28	2	—				
202	3.21							
212, 042	3.19	3.19	50	14.0	3.19	st	3.19	9
400	3.14							
341	3.13							
222, 410	3.11	3.11	50	14.2	3.14	m	3.09	7
261	3.10							
142	3.09							

¹ Interplanar spacings (d_{hkl}) calculated from single-crystal data given in Table 1 for synthetic $MgO \cdot 3B_2O_3 \cdot 5H_2O$. All possible lines are listed for $d \geq 2.200$ Å.

² Film no. 17198; camera diameter 114.59 mm; Ni-filtered Cu radiation, $\lambda(CuK\alpha) = 1.5418$ Å; film measurements corrected for shrinkage; b = broad. Lower limit of 2θ measurable, approximately 7° (13 Å).

³ Camera diameter 57.4 mm; Ni-filtered Cu radiation; $\theta/2$ corresponds to Bragg θ ; d_{hkl} obtained from $\theta/2$ value by present authors; significance of intensity notations apparently as follows: st = very strong, m = strong, s = medium strong, and ss = medium.

⁴ Camera diameter 57.29 mm; Mn-filtered Fe radiation; NaCl used as an internal standard. Sample may have contained anhydrite (strongest line 3.50 Å); r = diffuse. ⁵ CuK β line of 021.

TABLE 2—(continued)

Calculated ¹		Observed						
		Synthetic MgO·3B ₂ O ₃ ·5H ₂ O					Aksuïte	
		Present Study ²		Lehmann and Papenfuss (1959) ³			Blazko <i>et al.</i> (1962) ⁴	
<i>hkl</i>	d_{hkl} (Å)	d_{hkl} (Å)	I	$\theta/2$	d_{hkl} (Å)	I	d_{hkl} (kX)	I
171	3.06	3.05	5b	—			3.02	r 1
270, 080, 420	3.04							
232	2.988	2.92	5					
430	2.924							
351	2.920	2.88	10	15.3	2.92	ss	2.90	r 2
152	2.887							
411	2.871	2.82	20	15.9	2.81	st		
242	2.842							
081	2.819	2.79	20	16.2	2.76	ss	2.78	8
271	2.818							
421	2.813	2.74	2					
302	2.788							
440	2.787	2.69	2	—			2.69	r 3
312	2.770							
181, 062	2.751	2.52	2					
280	2.738							
431	2.724	2.48	10	17.9	2.51	s	2.470	5
322	2.718							
361	2.714	2.44	2					
162	2.687							
252	2.682	2.40	5	—			2.393	1
332	2.637							
450	2.636	2.36	15	18.9	2.38	m	2.348	6
441	2.612							
281	2.571	2.40	5					
342	2.535							
262	2.519	2.48	10	17.9	2.51	s	2.470	5
371	2.518							
172	2.497	2.44	2					
191	2.494							
451	2.486	2.40	5	—			2.393	1
290	2.484							
460	2.481	2.36	15	18.9	2.38	m	2.348	6
023	2.444							
0, 10, 0	2.435	2.40	5	—			2.393	1
113	2.434							
352	2.420	2.36	15	18.9	2.38	m	2.348	6
402	2.403							
123	2.399	2.36	15	18.9	2.38	m	2.348	6
412	2.391							
511	2.367	2.36	15	18.9	2.38	m	2.348	6
082	2.361							
272	2.360	2.36	15	18.9	2.38	m	2.348	6
291, 422	2.358							
461	2.355	2.36	15	18.9	2.38	m	2.348	6
133	2.343							
381	2.337	2.36	15	18.9	2.38	m	2.348	6
521	2.334							
470	2.329	2.36	15	18.9	2.38	m	2.348	6

TABLE 2—(continued)

Calculated ¹		Observed						
		Synthetic MgO·3B ₂ O ₃ ·5H ₂ O					Aksaitite	
		Present Study ²		Lehmann and Papenfuss (1959) ³			Blazko <i>et al.</i> (1962) ⁴	
<i>hkl</i>	<i>d</i> <i>hkl</i> (&)	<i>d</i> <i>hkl</i> (&)	I	$\theta/2$	<i>d</i> <i>hkl</i> (&)	I	<i>d</i> <i>hkl</i> (kX)	I
182	2.320	2.31	10	19.5	2.31	m	2.300	5
540	2.319							
0, 10, 1	2.316							
213, 043	2.308							
432	2.304							
362	2.298	2.27	10	20.5	2.20	ss	2.215	1
531	2.282							
223; 1, 10, 1	2.277							
2, 10, 0, 143	2.270	2.23	2	21.4	2.11	s	2.115	4
442	2.235							
233	2.229	2.18	5b)	—	2.04	s	2.074	5
471	2.224							
541	2.215	2.13	10	22.2	2.02	—	2.013	6
28	2.210							
		2.11	5	22.9	1.98	m	1.970	7
		2.09 ₂	10	Plus additional lines, all with I ≤ 5		Plus additional lines, all with I ≤ 6		
		2.07 ₆	2					
		2.04 ₂	2					
		2.02 ₄	5					

Other considerations provide additional evidence that the formulas given by Blazko *et al.* are implausible. First, the space group *Pbca* contains only fourfold and eightfold positions, so that the total number per cell for each atomic species may be expected to be an integral multiple of four or eight. Five formula units of $MgO \cdot 3B_2O_3 \cdot 8H_2O$ per cell requires that 10 Mg, 125 O and 50 B be assigned positions, yet none of these numbers is an integral multiple of four or eight. On these grounds, the first formula is unlikely. The second formula, $3MgO \cdot 7B_2O_3 \cdot 10H_2O$, violates the second rule governing hydrated borates (Christ, 1960), *i.e.* a borate polynuclear anion of low to medium negative charge is expected. On the other hand, the formula for the synthetic $MgO \cdot 3B_2O_3 \cdot 5H_2O$ is analogous to that of the mineral gowerite, $CaO \cdot 3B_2O_3 \cdot 5H_2O$ (Erd *et al.* 1959). The structural possibilities associated with this $1 \cdot 3 \cdot x$ formula have been discussed by Christ (1960) and, with particular reference to

gowerite, by Christ and Clark (1960). A similar discussion may be expected to be valid for the $1 \cdot 3 \cdot 5$ Mg compound by analogy to the relationship between the $2\text{CaO} \cdot 3\text{B}_2\text{O}_3 \cdot x\text{H}_2\text{O}$ series and the $2\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot x\text{H}_2\text{O}$ series. The prediction by Christ (1960) that the mineral inderite, $2\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 15\text{H}_2\text{O}$ (= lesserite; Schaller and Mrose, 1960) would have the structural formula, $\text{Mg}[\text{B}_3\text{O}_3(\text{OH})_5]_5 \cdot 5\text{H}_2\text{O}$, has recently been confirmed by a crystal structure analysis (Ashirov *et al.*, 1962). All evidence therefore points to the chemical formula $\text{MgO} \cdot 3\text{B}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$, and a probable structural formula $\text{Mg}[\text{B}_3\text{O}_3(\text{OH})_4]_2 \cdot \text{H}_2\text{O}$ for the mineral aksaite.

We wish to thank four of our colleagues for their contributions to this study. Daniel E. Appleman calculated the d-spacings on a digital computer using a program written by him; Mary E. Mrose took x-ray powder patterns of the synthetic crystals, and she and M. Fleischer translated the Russian article on aksaite into English; C. L. Christ gave valuable discussion on the structural principles.

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THE AMERICAN MINERALOGIST, VOL. 48, JULY-AUGUST, 1963

X-RAY DATA FOR HYDROTUNGSTITE

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In the original description of hydrotungstite by Kerr and Young (1944) x-ray powder data were given for the more intense reflections, but the values were not indexed and the unit cell constants were lacking. Recently the writer noticed a similarity between the x-ray patterns for hydrotungstite (tungstic acid, $\text{H}_2\text{WO}_4 \cdot \text{H}_2\text{O}$) and molybdic acid ($\text{H}_2\text{MoO}_4 \cdot \text{H}_2\text{O}$). This similarity is quite reasonable since the ionic radii