gowerite, by Christ and Clark (1960). A similar discussion may be expected to be valid for the 1·3·5 Mg compound by analogy to the relationship between the $2CaO \cdot 3B_2O_3 \cdot xH_2O$ series and the $2MgO \cdot 3B_2O_3 \cdot xH_2O$ series. The prediction by Christ (1960) that the mineral inderite, $2MgO \cdot 3B_2O_3 \cdot 15H_2O$ (=lesserite; Schaller and Mrose, 1960) would have the structural formula, $Mg[B_3O_3(OH)_5] \cdot 5H_2O$, has recently been confirmed by a crystal structure analysis (Ashirov *et al.*, 1962). All evidence therefore points to the chemical formula $MgO \cdot 3B_2O_3 \cdot 5H_2O$, and a probable structural formula $Mg[B_3O_3(OH)_4]_2 \cdot H_2O$ 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.

References

Ashirov, A., I. M. Rumanov, and N. V. Belov (1962) Crystal structure of lesserite, $Mg[B_3O_3(OH)_5] \cdot 5H_2O$. *Doklady Akad. Nauk SSSR* **143,** 331–334 (in Russian).

Blazko, L. N., V. V. Kondrat'eva and Ya. Ya. Yarzhemskii (1962) Aksaite, a new hydrous magnesium borate. *Zapiski Vses. Mineralog. Obshch.* **91,** 447–454 (in Russian).

Christ, C. L. (1960) Crystal chemistry and systematic classification of hydrated borate minerals. *Am. Mineral.* **45,** 334–340.

——— and J. R. Clark (1960) *X*-ray crystallography and crystal chemistry of gowerite, $CaO \cdot 3B_2O_3 \cdot 5H_2O$. *Am. Mineral.* **45,** 230–234.

Erd, R. C., J. F. McAllister and H. Almond (1959) Gowerite, a new hydrous calcium borate from the Death Valley region, California. *Am. Mineral.* **44,** 911–919.

Fleischer, M. (1963) New mineral names: aksaite. *Am. Mineral.* **48,** 209–210.

Lehmann, H.-A. and H.-J. Papenfuss (1959) Über ein wasserhaltiges Magnesiumhexaborat der Formel $MgB_6O_{10} \cdot 5H_2O$. *Zeit. anorg. allgemein. Chemie,* **301,** 228–232.

Schaller, W. T. and M. E. Mrose (1960) The naming of the hydrous magnesium borate minerals from Boron, California—a preliminary note. *Am. Mineral.* **45,** 732–734.

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

X-RAY DATA FOR HYDROTUNGSTITE

Richard S. Mitchell, *University of Virginia, Charlottesville, Virginia.*

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, $H_2WO_4 \cdot H_2O$) and molybdic acid ($H_2MoO_4 \cdot H_2O$). This similarity is quite reasonable since the ionic radii

of W^{6+} and Mo^{6+} are approximately equal (0.62 Å). Using *x*-ray data reported for molybdic acid by Lindqvist (1950) (ASTM powder data card #6-0205), the writer was able to index *x*-ray powder data for hydrotungstite and derive the unit cells constants. Although the solution presented here should be considered somewhat tentative until single crystal data are at hand, it seems entirely tenable.

The specimens (#2769, #2770) used in this study were donated to Lewis Brooks Museum, University of Virginia, by Dr. Frank L. Hess. They were incorrectly labeled, tungstite, and the locality was given as Taborga, Bolivia. The mineral is probably from the San Antonio mine of Sr. Rafael Taborga, about nineteen miles north of Oruro, Bolivia (Hess, 1921). The greenish yellow mineral occurs as dull earthy coatings on ferberite and quartz. A semiquantitative spectrographic analysis showed the principal metal to be tungsten. Visually, *x*-ray powder films compare well with photographs of films of tungstic acid published by Morley (1930) and Kerr and Young (1944). Although the agreement between measured *x*-ray data and values published by Kerr and Young (1944) is not completely satisfactory, there is an almost perfect agreement with data obtained from samples of the type material secured from the U. S. National Museum (#104901). The material was further checked by heating it between 100° C. and 150° C. for nine days. *X*-ray patterns showed the mineral had lost water to become tungstite (H_2WO_4) mixed with minor amounts of anhydrous monoclinic tungsten trioxide. Another sample heated for five hours at 580° C. became pure monoclinic tungsten trioxide.

The measured interplanar spacings given in Table 1 represent the average of values obtained from five *x*-ray powder films, of five different samples, made with CuKα radiation in cameras with 11.46 cm diameters. Assuming a monoclinic (pseudo-orthorhombic) structure similar to that for molybdic acid the values were partially indexed using the Hesse-Lipson procedure (Azároff and Buerger, 1958). The following unit cell constants were determined: $a=7.45$ Å, $b=6.92$ Å, and $c=3.72$ Å (all ± 0.02 Å); $\beta \cong 90°$; $a:b:c=1.077:1:0.538$. Using these values, all possible interplanar spacings allowed by the fullest symmetry ($P2/m$) were calculated down to 1.30 Å. An excellent correlation with the observed data is evident from Table 1. Using a molecular weight of 267.892, and a specific gravity of 4.60 (Kerr and Young, 1944), the value for Z is 2 (1.98, calculated). A unique determination of the space group was not achieved, because there is no way to tell if a specific reflection should be present or absent in those cases where several planes have similar interplanar spacings. For example, an examination of Table 1 shows that in most cases *hkO* reflections are absent when *h* is odd, yet it is uncertain

TABLE 1. *X*-RAY POWDER DATA FOR HYDROTUNGSTITE FROM ORURO, BOLIVIA

hkl	d(calc.)Å	d(obs.)Å	I(obs.)
100	7.45		
010	6.92	6.95	vs+
110	5.07		
200	3.73	3.73	s
001	3.72		
020	3.46	3.46	ms
101	3.33		
210, 011	3.28	3.27	s+
120	3.14		
111	3.00	3.02	w
201	2.63	2.63	m
220	2.54	2.54	m
021	2.53		
300	2.48		
211	2.46	2.46	m
121	2.40		
310	2.34		
030	2.31	2.31	m
130	2.20		
221	2.09	2.09	m
301	2.07		
320	2.02		
311	1.98		
230, 031	1.96	1.96	ms
131	1.90	1.88	w
400, 002	1.86	1.85	w+
102, 410, 012	1.80	1.81	w
321	1.77	1.78	w+
112	1.75		
231, 040	1.73	1.73	m
330, 140	1.69		
401	1.67		
420, 022	1.64	1.65	w
411	1.62	1.61	m
122	1.60		
240, 041	1.57	1.57	m
331, 141	1.54	1.54	vw
421	1.50	1.50	mw
500, 302	1.49		
510, 312	1.46		
430, 032, 241	1.45	1.45	mw+
132, 340	1.42		
050, 501	1.38	1.38	w
520, 322	1.37		
150, 511	1.36		
431	1.35	1.35	w
341	1.33		
402	1.32		
250, 051	1.30	1.30	w

TABLE 2. COMPARISON OF DATA FOR HYDROTUNGSTITE AND MOLYBDIC ACID

	Hydrotungstite	Molybdic Acid[1]
Composition	$H_2WO_4 \cdot H_2O$	$H_2MoO_4 \cdot H_2O$
Cell values	$a = 7.45$ Å	$a = 7.34$ Å
	$b = 6.92$ Å	$b = 6.91$ Å
	$c = 3.72$ Å	$c = 3.77$ Å
	$\beta \cong 90°$	$\beta = 90°40'$
$a:b:c$	1.077:1:0.538	1.062:1:0.546
Z	2	2
Lattice	P	P
Space group	$P2/m$ (?)	$P2/m$

[1] From Lindqvist (1950). The unit cell values for a and c are reversed in the original paper and on ASTM card #6-0205. This misprint has been corrected by Bijvoet (1954).

whether the 510, 520 and 150 planes are present or absent since their interplanar spacings are so close to observed values. The lattice is definitely primitive (P), and the space group is probably P2/*m*. A comparison between the proposed data for hydrotungstite and those reported for molybdic acid is given in Table 2.

Whether or not hydrotungstite is truly monoclinic is still a matter of conjecture. It is here considered to be monoclinic because of optical data reported by Kerr and Young (1944), and because of its relationship to molybdic acid which is monoclinic (pseudo-orthorhombic). However, unlike molybdic acid, the writer did not observe a doubling of any *hOl* and *hkl* reflections due to a departure of β from 90°. Lindqvist (1950) reported very close but separate reflections for the pairs 201, $20\bar{1}$ and 211, $21\bar{1}$. In some respects hydrotungstite may also be considered pseudo-tetragonal since a is approximately equal to $2c$. With the exception of a few lines the powder data can be indexed quite satisfactorily using tetragonal constants such as $a = 3.72$ Å, $c = 6.92$ Å, or $a = 3.72$ Å, $c = 13.84$ Å. Here again the writer chose the monoclinic cell for the reasons outlined above.

The writer is grateful to Mr. Stanley S. Johnson, University of Virginia, who purified samples for *x*-ray study.

REFERENCES

AZÁROFF, L. V. AND M. J. BUERGER (1958) *The Powder Method in X-ray Crystallography.* McGraw-Hill Book Company, Inc., New York.

BIJVOET, J. M. (Sect. editor) (1954) Yellow molybdic acid. *Structure Reports (for 1950)* **13,** 257–259.

HESS, F. L. (1921) Some unique Bolivian tungsten deposits. *Eng. Min. Jour.* **112,** 492–499.

KERR, P. F. AND F. YOUNG (1944) Hydrotungstite, a new mineral from Oruro, Bolivia. *Am. Mineral.* **29,** 192–210.

LINDQVIST, I. (1950) The crystal structure of the yellow molybdic acid, $MoO_3 \cdot 2H_2O$. *Acta Chem. Scand.* **4**, 650–657.

MORLEY, A. M. (1930) The structure of the tungstic acids. *Jour. Chem. Soc. London* (*Trans.*) 1930 (II), 1987–1999.

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

THE UNIT CELL OF ETTRINGITE

L. G. BERRY, *Queen's University, Kingston, Ontario, Canada.*

In the course of a review of the published x-ray powder data for ettringite, $Ca_6Al_2(SO_4)_3(OH)_{12} \cdot 24H_2O$, a difference was noted in the length of the a axis as reported by several writers. Bannister *et al.* (1936) obtained $a = 11.26$ Å, $c = 21.48$ Å, using rotation photographs about $[10\bar{1}0]$, $[11\bar{2}0]$ and c. Feitknecht and Buser (1949) give $a = 11.2$, $c = 21.4$, and Swanson *et al.* (1959) obtained $a = 11.23$, $c = 21.44$ for synthetic material. Hurlbut and Baum (1960), on the other hand, give $a = 22.28$ Å, $c = 21.29$ Å for crystal from Franklin, New Jersey. These authors also remeasured a on crystals from Scawt Hill and Ettringen, concluding that a should be double the value previously reported. Murdoch and Chalmers (1960) give $a = 22.49$ for Ettringen material and $a = 22.33$ for material from Crestmore, California. This larger value for a is also quoted by McConnell and Murdoch (1962).

The powder data of Swanson *et al.* (1959) indexes fully to $d = 1.768$ using $a = 11.23$, $c = 21.44$. The powder data given by Murdoch and Chalmers (1960) may be indexed using $a = 11.23$ except for two weak lines with $d = 10.5$ and 4.55 which are not present in the Swanson pattern and do not index when a is doubled.

Hurlbut and Baum (1960) obtained their cell dimensions from rotation and Weissenberg films about the c axis and about "a horizontal axis normal to the $\{10\bar{1}0\}$ cleavage." Their rotation films about c yield $c = 21.29$, which corresponds closely to other determinations. Their rotation film about the normal to $[10\bar{1}0] = [10\bar{1}0]$ gives 19.27 Å. The identity period in an hexagonal net normal to an a axis is the long diagonal of the 60° rhomb and thus the correct a is $19.27/\sqrt{3} = 11.13$ Å, not 22.25 as deduced by Hurlbut and Baum. The new doubled value of a for materials from Ettringen and Scawt Hill are based on the same method. Murdoch and Chalmers (1960) based their determination of $a = 22.4$ on rotation films about $[10\bar{1}0]$. From a rotation film about $[10\bar{1}0]$ Murdoch and Chalmers also obtain $a = 22.12$ Å for thaumasite, double the value given by Welin (1956).