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THE UNIT CELL OF MOOREITE

J. J. FINNEY, *Geology Department, Colorado School of Mines, Golden, Colorado 80401.*

ABSTRACT

Mooreite, $(Mg, Zn, Mn)_8(SO_4)(OH)_{14} \cdot 4H_2O$, is monoclinic although the space group is not $P2_1/m$ as previously reported but rather $P2_1/a$. The new unit cell has $a = 11.18$, $b = 20.28$ $c = 8.23$ Å and $\beta = 92°55'$ for which $Z = 4$. A new chemical analysis confirms the original formula except for one less H_2O molecule.

The mineral mooreite was first described by Bauer and Berman (1929) from Sterling Hill, New Jersey. A complete chemical analysis of the mineral was presented together with the morphological crystallography and optical data. Prewitt-Hopkins (1949) provided an X-ray study of mooreite and also tabulated X-ray powder data for the mineral.

Recently an excellent specimen of mooreite from Sterling Hill was sent to the author. As is the case with all rare or unusual minerals, a check was made of published data in order to verify the species. It was noted that for her unit cell Prewitt-Hopkins gave $Z = 13$, an unusual number in its own right crystallographically, but more so in view of the space group listed, $P2_1/m$, and the composition, $(Mg, Zn, Mn)_8(SO_4)(OH)_{14} \cdot 4H_2O$. Such a unit cell content in conjunction with the published formula for mooreite would necessitate a single SO^{4-} tetrahedron placed so that a sulfur would occupy a center of symmetry.

A single crystal X-ray analysis was undertaken by the precession method in order to clarify the discrepancy. The identity of the mineral has been established by a comparison of published powder data with

TABLE 1. CHEMICAL ANALYSES OF MOOREITE

	1			2		
	Wt %	Mole prop.	Units	Wt %	Mole prop.	Units
MgO	25.38	.629	8	26.26	.651	8
ZnO	24.58	.300		25.34	.311	
MnO	11.93	.167		11.34	.160	
SO_3	10.99	.136	1	11.34	.142	1
H_2O	27.12	1.506	11	25.72	1.429	10
	$\rho = 2.47$			$\rho = 2.46$		

1. Analysis by L. H. Bauer (1929). Recalculated to 100.00% less $CaCO_3$. Results in the formula: $(Mg_{4.53}Zn_{2.23}Mn_{1.23})(SO_4)(OH)_{14} \cdot 4H_2O$.
2. Analysis by H. Ochs, this paper. Recalculated to 100.00% less $CaCO_3$. Results in the formula: $(Mg_{4.64}Zn_{2.22}Mn_{1.14})(SO_4)(OH)_{14} \cdot 3H_2O$.

that of the new material and also by a complete chemical analysis. Table 1 shows a comparison of the analyses of Bauer and the present one. Note that the formula differs only in the number of water molecules.

In her paper, Prewitt-Hopkins (1949) stated that, on the basis of the only systematic extinction $0k0: k=2n$, the space group was $P2_1/m$. This cannot be the case. The $h0l$ precession photograph reveals that, for her axes, $h+l=2n$ and further that $h=2n$ and $l=2n$. Upper level b-axis photographs show also that for hkl reflections $h+l=2n$, that is B-centering. Consequently a new unit cell has been chosen. Figure 1 shows the relationship of the Prewitt-Hopkins axes to those of the present investigation and Table 2 is a tabulation of the unit-cell data for the two orien-

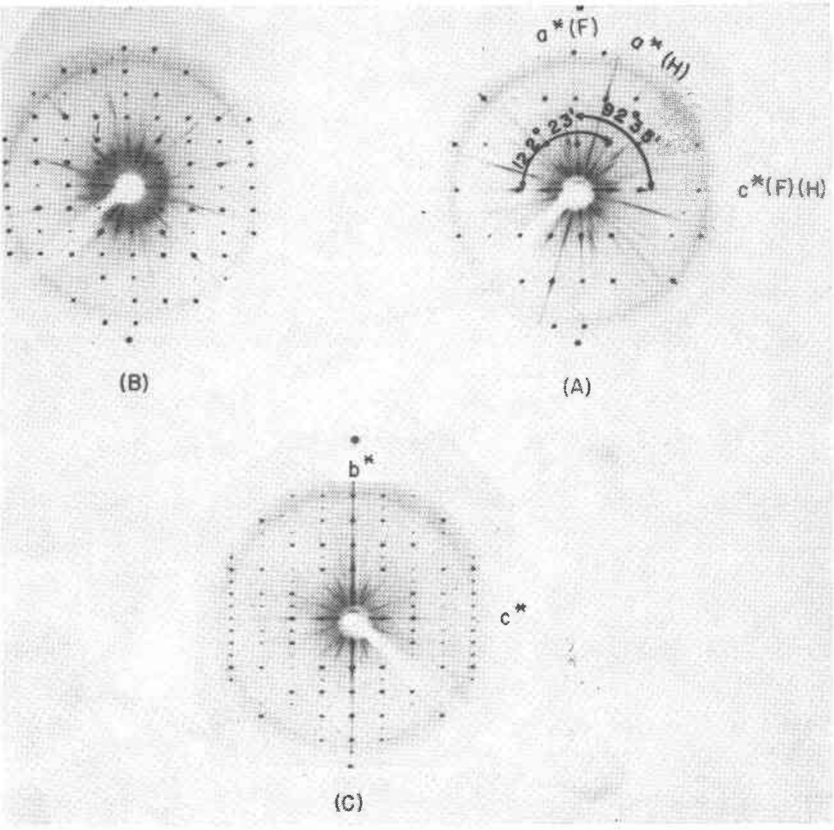

FIG. 1. Precession photographs of mooreite, Cu radiation. (A) $h0l$ photograph with H = axes of Prewitt-Hopkins (1949) and F = those of present paper. (B) $h1l$ photograph and (C) $0kl$ photograph.

TABLE 2. UNIT-CELL DATA FOR MOOREITE

	1	2
a	11.18	11.18
b	20.25	20.28
c	19.52 Kx	8.23 Å
β	122°23′	92°55′

1. Prewitt-Hopkins (1949)
2. This paper

tations. The transformation matrix, new to old is $100/010,\bar{1}0\bar{2}$ and old to new is $100/010/\frac{\bar{1}}{2}0\frac{\bar{1}}{2}$.

The space group is $P2_1/a$ with reflections obeying the systematic absences hkl: none; $h0l: h=2n$; $0k0: k=2n$. For the present cell $Z=4$ and the cell formula $(Mg, Zn, Mn)_{32}(SO_4)_4(OH)_{56}\cdot 12H_2O$ is compatible with space group requirements. The calculated density, based upon the present analysis, is 2.52.

REFERENCES

BAUER, L. H., AND H. BERMAN (1929) *Amer. Mineral.*, **14**, 165.
PREWITT-HOPKINS, J. (1949) *Amer. Mineral.*, **34**, 589.

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SILLIMANITE FROM TWO CONTACT AUREOLES

J. M. MOORE, JR., *Carleton University, Ottawa, Canada*
AND
MYRON G. BEST, *Brigham Young University, Provo, Utah 84601.*

ABSTRACT

"Fibrolite" from two contact aureoles is proved by X-ray diffraction to be sillimanite; mullite in such occurrences now seems unlikely.

In the contact metamorphism of pelitic rocks, andalusite is typically produced in spotted slates and hornfels of low grade, being accompanied (or, infrequently, entirely supplanted) by a fibrous aluminosilicate near the igneous body. This "fibrolite" is commonly in the form of fine acicular prisms which, at first appearance with increasing grade, compose mats