SOME COMPUTATIONS ON SVANBERGITE, WOODHOUSEITE AND ALUNITE

A. PABST, *University of California, Berkeley, California.*

ABSTRACT

Computations have been carried out to correct the indexing of a powder diffraction pattern of svanbergite found in the literature. Similar computations lead to the first published indexing of powder patterns of woodhouseite. Parameters are obtained for the structures of these two minerals. Less extended computations for alunite, using the parameters given by Hendricks, afford a basis for evaluating the results. They also afford a check on the reliability of standard patterns recorded on ASTM cards.

Incidentally the transformation from hexagonal to rhombohedral axes is discussed.

INTRODUCTION

Svanbergite is a rare member of the alunite-beudantite group. Its composition may be written $SrAl_3(SO_4)(PO_4)(OH)_6$. In a recent paper Ygberg[1] has reported on a powder diffraction of svanbergite and has calculated lattice dimensions and density.

Minerals of the alunite-beudantite group have been shown by Hendricks[2] to have a rhombohedral lattice. Ygberg also assigns svanbergite to a rhombohedral space group but in his indexing of part of a powder pattern, in which he gives indices for 26 planes, 8 planes fail to meet the criteria for a rhombohedral lattice. It follows that either the assignment of the space group, or the indexing of the pattern must be in error.

Specimens of svanbergite were not available, but it was found that Ygberg's observations could be checked directly without new experimental data. Once these computations had been carried out it was a simple matter to extend them to the related mineral woodhouseite, $CaAl_3(SO_4)(PO_4)(OH)_6$, for which Ygberg reported lattice dimensions and density though his tabulation of the powder pattern is not indexed, and to check them against new observations.

An alunite-like structure was assumed for these minerals and so it has seemed desirable to calculate the theoretical intensities and positions of lines in an alunite powder pattern using the parameters given by Hendricks, who did not report on such a pattern, and to compare these with published patterns and a new pattern obtained from alunite from the type locality. In the following the results on these three minerals will be reported in the order in which they have just been mentioned.

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[1] Ygberg, Erik R., Svanbergite from Horrsjöberg: *Arkiv för Kemi, Mineralogi och Geologi*, **20A,** no. 4, 1–17 (1945).

[2] Hendricks, S. B., The crystal structure of alunite and the jarosites: *Am. Mineral.*, **22,** 773–784 (1937).

SVANBERGITE

Since no new observations were made on svanbergite the cell dimensions given by Ygberg, $a_0 = 6.96 \pm 0.03$ Å and $c_0 = 16.8$ Å, were accepted. The stated dimensions correspond to an axial ratio, c/a, 2.414, which is close to twice the value assigned from goniometric measurements. The observed density is given as 3.20 and the calculated density corresponding to three formular units in the hexagonal cell as 3.18.

Ygberg correctly gives the dimensions of the corresponding rhombohedral cell as $a_{rh} = 6.89$ Å and $\alpha = 60°\ 38'$, but states that these were found to be "the dimensions of the rhombohedral unit cell $\{40\bar{4}1\}$." This is rather puzzling. A cell of the stated dimensions would, if referred to the hexagonal axes found by *x*-ray diffraction have the indices $10\bar{1}1$ or $01\bar{1}1$. If referred to axes with half the axial ratio, as chosen from the morphology, the indices would be $20\bar{2}1$ or $02\bar{2}1$.

Reports on a powder pattern of svanbergite are given by Ygberg in two tables. In the first of these (his table 2) he gives intensity, $\sin^2\theta$ (obs), $\sin^2\theta$ (calc) and hexagonal indices for 22 lines whose $\sin^2\theta_{Cu} \leqq 0.420$. In another table (his table 5) intensities and spacings (presumably observed spacings) are given for 33 lines of svanbergite together with similar data for woodhouseite. At the base of the former table the value of $\lambda^2/3a^2$ is given as 0.0162 though the calculated values of $\sin^2\theta$ given for $11\bar{2}0$, $22\bar{4}0$ and $41\bar{5}0$ correspond to 0.0160, whereas the stated length of a_h leads to 0.0163.

Disregarding these difficulties, spacings were calculated from the stated cell dimensions for all rhombohedral planes with spacings greater than 1.3. This alone was not quite sufficient for assured indexing of the pattern because many coincidences or near coincidences occur. Assuming that the structure of svanbergite is similar to that found for alunite by Hendricks, that the content of the hexagonal cell is three formular units, and that interionic distances are limited by known ionic radii, a search was made for parameters that would yield intensities accounting for Ygberg's observations.

Hendricks assigned alunite to the space group C_{3v}^5–$R3m$, having observed it to be pyroelectric. The structure he described for alunite may, however, be considered to be in the space group D_{3d}^5–$R\bar{3}m$.[3] In this structure all atoms lie in symmetry planes. For this reason it is a rather simple matter to picture possible atomic arrangements by constructing, say, a $1\bar{2}10$ section through the cell as has been done for another member of the group (woodhouseite) in Fig. 1. From such a diagram either hexag-

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[3] The group $R\bar{3}m$ arises from $R3m$ by addition of a center of symmetry at 000. From Hendricks' table of parameters it can be seen that all atoms in his structure are centrosymmetrically disposed in pairs on opposite sides of K at 000.

onal or rhombohedral coordinates of atoms may be read off directly and by a system of overlapping grids (not shown in the figure) it is possible to make a quick graphical transformation of coordinates. It will be noted that for the hexagonal cell the a_1 axis does not lie in the plane of projection but the coordinates of atoms in this plane along an axis normal to c are the same as their a_1 coordinates. For the rhombohedral cell an equally convenient situation exists. The outline of this cell in the plane in question is a parallelogram whose edges are a_{r1} and the face diagonal of the unit rhombohedron. This face diagonal is vectorially $a_{r2}+a_{r3}$. All atoms in this plane will have equal coordinates along a_{r2} and a_{r3} which will be the same as the coordinate of such an atom along the face diagonal as can be seen in the lower part of Fig. 1.

A choice of parameters was first made from ionic radii. This was then modified with the help of intensity calculations. In addition to trials for isolated planes several extended series of intensity calculations were carried out. The parameters used for the reported intensity calculations are set forth in Table 1. In this table P and S share the rhombohedral positions xxx and $\bar{x}\bar{x}\bar{x}$, leaving the structure in space group $R\bar{3}m$. If they did not share the two positions but each occupied one of them the symmetry centers would be lost and the space group would be $R3m$.

TABLE 1. PARAMETERS AND INTERATOMIC DISTANCES FOR SVANBERGITE

Parameters

All Trials	Sr		Al	
	Rh	Hex	Rh	Hex
	1: (*a*) 000	3: (*a*) 000	3: (*d*) ½00	9: (*d*) 1/6 1/6 $\overline{1/6}$

	S, P		O$_1$		O				OH			
	Rh 2: (*c*) xxx	Hex 6: (*c*) $00z$	Rh 2: (*c*) xxx	Hex 6: (*c*) $00z$	Rh 6: (*h*) zxx		Hex 18: (*h*) $x\bar{x}z$		Rh 6: (*h*) zxx		Hex 18: (*h*) $x\bar{x}z$	
Trial	x	z	x	z	x	z	x	z	x	z	x	z
A	.30	.30	.39	.39	.15	.51	.12	.27	.27	−.18	−.15	.12
B	.30	.30	.39	.39	.15	.51	.12	.27	.28	−.14	−.14	.14
C	.29	.29	.38	.38	.14	.50	.12	.253	.28	−.14	−.14	.14

Interatomic Distances

All Trials (S, P)−O$_1$=1.512 O−O=2.51

Trial C
(S, P)−O=1.57 Sr−O=2.90 Al−O=1.71
O$_1$−O=2.58 Sr−OH=2.89 Al−OH=1.97
O$_1$−OH=2.80

TABLE 2. OBSERVED AND CALCULATED SPACINGS AND INTENSITIES FOR LINES IN A POWDER DIFFRACTION PATTERN OF SVANBERGITE

Calculated from E. Ygberg's Cell Dimensions				Calculated Intensity			Quoted from E. Ygberg's Table 2				Table 5
hkil	*hkl*	$\sin^2\theta_{cu}$	d_{hkl}	Trial A	Trial B	Trial C	I	$\sin^2\theta$ (obs.)	$\sin^2\theta$ (calc.)	*HIKL*	d_{hkl}
$10\bar{1}1$	100	.0184	5.67	300	321	264	s	.018	.0181	$10\bar{1}1$	5.73
0003	111	.0189	5.60	22	1	3			.0189	0003	
$01\bar{1}2$	110	.0247	4.90	0	9	28	w−	.024	.0244	$10\bar{1}2$	4.96
$11\bar{2}0$	$10\bar{1}$	.0489	3.48	171	189	189	s	.048	.0480	$11\bar{2}0$	3.51
$10\bar{1}4$	211	.0499	3.44	61	70	56					
$02\bar{2}1$	$11\bar{1}$	.0675	2.965	54	40	37	s+	.067	.0661	$20\bar{2}1$	2.97
$11\bar{2}3$	210	.0678	2.955	725	749	750					
$01\bar{1}5$	221	.0688	2.930	2	4	9					
$20\bar{2}2$	200	.0736	2.835	22	41	46	w	.077	.0756	0006	2.77
0006	222	.0756	2.800	13	60	38					
$02\bar{2}4$	220	.0988	2.435	144	70	102	w†	†	†	†	2.47
$21\bar{3}1$	$20\bar{1}$	.1162	2.260	71	92	143	s+	.120	.1204	$21\bar{3}2$	2.22
$20\bar{2}5$	311	.1177	2.250	72	73	72					
$10\bar{1}7$	322	.1193	2.230	203	217	176					
$12\bar{3}2$	$21\bar{1}$	.1225	2.198	77	90	70					
$11\bar{2}6$	321	.1245	2.181	41	23	17					
$30\bar{3}0$	$2\bar{1}\bar{1}$	.1467	2.010	16	14	14	w	.145	.1440	$30\bar{3}0$	2.02
$21\bar{3}4$	310	.1477	2.008	12	34	17			.1456	$21\bar{3}4$	
$01\bar{1}8$	332	.1507	1.982	15	22	56					
$03\bar{3}3$	$22\bar{1}$	.1656	1.891	198	211	273	s	.163	.1629	$31\bar{3}3$‡	1.91
$30\bar{3}3$	300			19	24	24					
$12\bar{3}5$	320	.1676	1.883	14	7	3			.1645	$21\bar{3}5$	
$02\bar{2}7$	331	.1681	1.877	1	1	4					
0009	333	.1701	1.866	2	16	11					
$22\bar{4}0$	$20\bar{2}$	.1956	1.740	235	215	215	s	.193	.1920	$22\bar{4}0$	1.75
$20\bar{2}8$	422	.1996	1.723	43	19	21	w−	.202	.2004	$22\bar{4}2$*	1.71
$13\bar{4}1$	$21\bar{2}$	.2140	1.663	13	12	11					
$22\bar{4}3$	$31\bar{1}$	.2145	1.662	12	1	1					
$21\bar{3}7$	421	.2170	1.652			37					
$11\bar{2}9$	432	.2190	1.645			10	w	.220	.2196	$30\bar{3}6$	1.64
$31\bar{4}2$	$30\bar{1}$	.2203	1.640			0			.2210	000·10*	
$03\bar{3}6$	330	.2223	1.633			5					
$30\bar{3}6$	411					11					
$10\bar{1}\cdot 10$	433	.2263	1.618			4	w−	.230	.2269	$31\bar{4}3$*	1.60
$13\bar{4}4$	$32\bar{1}$	.2455	1.553			2					
$12\bar{3}8$	431	.2485	1.543			0					
$40\bar{4}1$	$3\bar{1}\bar{1}$	.2629	1.501			0					
$31\bar{4}5$	410	.2644	1.496			26					
$01\bar{1}\cdot 11$	443	.2684	1.486			24	w	.265	.2644	$40\bar{4}2$	1.49
$04\bar{4}2$	$22\bar{2}$	.2692	1.483			15					
$22\bar{4}6$	420	.2712	1.478			68	w	.276	.2749	$40\bar{4}3$*	1.46
$02\bar{2}\cdot 10$	442	.2752	1.466			108	m	.281	.2821	$21\bar{3}9$*	1.45
000·12	444	.2924	1.423			4					
$40\bar{4}4$	400	.2944	1.418			29	w	.295	.2949	$22\bar{4}7$*	1.41
$32\bar{5}1$	$30\bar{2}$	.3118	1.378			23					
$04\bar{4}5$	$33\bar{1}$	.3133	1.375			0					
$13\bar{4}7$	430	.3148	1.372			68	w	.316	.3148	$32\bar{5}2$	1.37
$03\bar{3}9$	441	.3168	1.367			3					
$30\bar{3}9$	522					21					
$23\bar{5}2$	$31\bar{2}$	.3181	1.365			1					
$20\bar{2}\cdot 11$	533	.3183	1.364			1					
$21\bar{3}\cdot 10$	532	.3251	1.350			19					
$41\bar{5}0$	$3\bar{1}\bar{2}$	.3423	1.316			28	w−	.337	.3360	$41\bar{5}0$	1.32
$32\bar{5}4$	$41\bar{1}$	.3433	1.314			7					
$31\bar{4}8$	521	.3463	1.308			19					

* Indices thus marked denote planes not conforming to rhombohedral criteria.

† Intensity and spacing for this line taken from Ygberg's Table 5. It is omitted in his Table 2.

‡ Impossible indices.

Since S^{+6} and P^{+5} have practically the same scattering power discrimination by *x*-ray diffraction is not feasible.

Intensity calculations were made by the well known formula

$$I_{calc} \sim \dot{J} \cdot F^2 \cdot \frac{1 + \cos^2 \theta}{\sin^2 \theta \cdot \cos \theta}$$

using ionic scattering factors from the ITDCS for all ions except Sr^{+2}. For Sr the atomic scattering factors of the ITDCS were slightly modified for low angles to correspond to expected ionic scattering. For the sake of simplicity intensity calculations were made from the rhombohedral parameters. In Table 1 all parameters are given for both cells.

In Table 2 the results of three series of intensity calculations are shown together with rhombohedral and hexagonal indices, calculated spacings and Ygberg's data from two of his tables for the range here covered. It can be seen that trial C for intensities best accounts for the observations, especially on 111, 200 and 222, 220 and on 422. Accordingly, calculations for this trial were extended to the first 55 planes as an additional check. The margin for choice between trials B and C is, however, not large. Comparison of calculations with observations further shows that even a number of lines to which Ygberg assigned permissible indices are to be attributed to other planes if svanbergite has an alunite structure. For instance, the strong line for spacing 2.97 to which he gave the indices $20\bar{2}1$ must be attributed largely if not entirely to $11\bar{2}3$.

In the range covered by calculations, the seven lines for which Ygberg gave indices that are non-rhombohedral or impossible have been explained as due to diffraction from planes in a rhombohedral lattice. In addition to these Ygberg also listed $32\bar{5}6$ ($\sin^2\theta$ (obs) $= .378$). No doubt this observation as well might be accounted for by rhombohedral indices but present calculations were not carried so far. It may now be asserted with greater assurance that svanbergite does indeed have a rhombohedral lattice.

As will be seen more clearly in the discussion of woodhouseite, the intensity designations w and s, as used by Ygberg each cover a wide range of intensities, whereas the designation m is but sparingly used by him. Under these circumstances no close determination of the parameters is possible but the fit of calculated intensities for trial C and reported intensities over a rather large range shows that a fair approximation has been reached.

RHOMBOHEDRAL INDEXING

Since indices of planes and coordinates of atoms in this paper are referred to both hexagonal and rhombohedral cells it is necessary to make a statement about the conventions adopted. The writer has not followed the ITDCS in these matters. It is pertinent to quote Donnay[4] in this connection. He has written:—"If the lattice is rhombohedral (hexagonal-R), and is referred to the smallest R-centered cell, there are still two alternatives. The dominant rhombohedron may have a face sloping forward, in which case it is symbolized $\{10\bar{1}1\}$, or backward, in which case it is indexed $\{01\bar{1}1\}$. The second setting may be obtained from the first by a 180° (or 60°) rotation about the c axis. In the first setting, the cell (which is here a triple cell) has its additional nodes at $\frac{2}{3}\,\frac{1}{3}\,\frac{1}{3}$ and $\frac{1}{3}\,\frac{2}{3}\,\frac{2}{3}$; in the second setting, at $\frac{2}{3}\,\frac{1}{3}\,\frac{2}{3}$ and $\frac{1}{2}\,\frac{2}{3}\,\frac{1}{3}$. The extinction criterion of the faces $(hk\bar{i}l)$ is, in the first setting $2h+k+l=3n$ or $h+i+l=3n$; in the second setting $2h+k-l=3n$ or $h+i-l=3n$. It is unfortunate that the *International Tables* should recommend the adoption of the second setting. The dominant rhombohedron has always been indexed $\{10\bar{1}1\}$ by mineralogists."

With all this the writer is in agreement except that the sign before the i in the alternative forms of the criteria should be negative in each case.[5]

This matter is taken up at two points in the ITDCS. The transformation γ given on page 74 in volume I corresponds to Donnay's "first setting," whereas in volume II under "Indices Transformations," page 471, both settings are described. In the space group tables the second setting is used consistently as indicated by Donnay.

Under "Rhombohedral centering" a transformation corresponding to the "first setting" is discussed by Buerger[6] and an equivalent transformation formula [88] is given in the new seventh edition of *Dana's System of Mineralogy.*[7] Neither of these authorities hint at the possibility of a "second setting."

The writer follows mineralogical usage in making the transformation according to the "first setting." Then $(10\bar{1}1)$ becomes (100) and the criteria for hexagonal indices which correspond to planes in the rhombohedral lattice may be taken to be:

$$h-i+l=3n,$$
$$k-h+l=3n$$
$$\text{or } i-k+l=3n.$$

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[4] Donnay, J. D. H., Rules for the conventional orientation of crystals: *Am. Mineral.,* **28,** 313–328 (1943).

[5] This slip corresponds to the statement found at the foot of page 77 in Rogers' "Introduction to the study of minerals," 3rd. ed. 1937, that $h+k=i$. Though this is stated as a conclusion from a detailed proof it is incorrect.

[6] Buerger, M. J., *X-ray Crystallography,* New York, (**1942**), pp. 68–70.

[7] Palache, Berman and Frondel, *Dana's System of Mineralogy,* 7th ed., vol. I, New York (1944), p. 25. This is taken from C. W. Wolfe's "Crystallographic Procedures," *Am. Mineral.,* **26,** 55–91 (1941), where the transformation here referred to is stated as formula [94].

These are also the transformation formulas and may be applied to the correlated indices of tables 2, 5 and 7 in this paper.

The relations of the two lattices thus chosen may be seen from Fig. 1 showing that the coordinates of atoms which give rhombohedral centering to the hexagonal lattice are $\frac{2}{3}$, $\frac{1}{3}$, —, $\frac{1}{3}$, and $\frac{1}{3}$, $\frac{2}{3}$, —, $\frac{2}{3}$.

WOODHOUSEITE

Thanks to the courtesy of Professor C. D. Woodhouse, Santa Barbara College, University of California, Santa Barbara, California, the writer was able to obtain specimens of woodhouseite from the type locality. The specimens consist of small clusters of woodhouseite crystals a millimeter or two in diameter implanted on much larger quartz crystals. It proved quite easy to detach uncontaminated material suitable for density determination or x-ray powder study.

TABLE 3. LATTICE DIMENSIONS AND DENSITY OF WOODHOUSEITE

	Hexagonal axes			Rhombohedral axes		Density	
	a_h	c_h	c/a	a_r	$\angle\alpha$	$d_{\text{obs.}}$	$d_{\text{calc.}}$
Lemmon	—	—	1.170 $(\frac{1}{2}\times 2.340)$			3.012	—
Ygberg	6.93	16.3	2.352	6.75	61° 75′*	—	3.024
Pabst	6.961	16.27	2.338	6.75	62° 4′	3.003	3.003†

* The value given for α here is quoted from Ygberg. This was obviously a misprint. The value corresponding to his dimensions for the hexagonal cell would be 61° 48′.

† The calculated density given at this point is based on the assumption of a cell content corresponding to the ideal formula. The analysis reported by Lemmon, however, shows 1.00% BaO and other contaminants. It must be assumed that these constituents enter into the lattice. On this basis the density would be 3.029 using my dimensions or 3.051 using Ygberg's dimensions.

The density of woodhouseite was determined by the Berman balance using toluene of density 0.862 at 26° C. The lattice dimensions were determined from a powder pattern made in a camera of 360 mm. circumference with copper radiation and nickel filter. The wave length of the unresolved copper K_α radiation was taken to be 1.539 kX. In calculating density from cell content the value of Avogadro's number was taken as 60.594×10^{22} for consistency with the kX units.[8] The results of these measurements and calculations are given in Table 3 together with earlier values reported by Lemmon and Ygberg.

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[8] Schlecht, Wm. G., Calculation of density from x-ray data: *Am. Mineral.*, **29**, 108–110 (1944).

If my dimensions for the woodhouseite cell are rounded off to three significant figures, like Ygberg's, they become 6.96 and 16.3. This leaves us with a correction for a_0 and so it may be well to state precisely the basis for this change. The cell dimensions were determined from 16 lines free from disturbing coincidences in the powder pattern. They are indicated by asterisks in Table 5. From these lines one obtains 14 values for each of the necessary constants. The average values are:—

$$\sin^2 \theta_{10\bar{1}0} = 0.016296 \qquad \text{and} \qquad \sin^2 \theta_{0001} = 0.002237.$$

The standard errors,

$$S_{\bar{x}} = \sqrt{\frac{\Sigma(X - \bar{x})^2}{n(n-1)}},$$

are respectively 0.00000615 and 0.00000335. They correspond to 0.0015 kX and 0.013 kX. The maximum errors calculated from the maximum values of $(X - \bar{x})$ correspond to 0.012 kX and 0.10 kX, respectively. They may be assumed to be well beyond the limits of probable error. A further check was obtained from the alunite pattern discussed below. Lattice dimensions obtained from this showed no significant difference from those given by Hendricks.

TABLE 4. PARAMETERS AND INTERATOMIC DISTANCES FOR WOODHOUSEITE

Parameters

Rh Ca 1: (*a*) 000		Hex 3: (*a*) 000	Rh Al 3: (*d*) ½00			Hex 9: (*d*) 1/6 1/6 1/6	
	2: (*c*) *xxx*	6: (*c*) 00*z*		6: (*h*) *zxx*		18: (*h*) $x\bar{x}z$	
	x	*z*		*x*	*z*	*x*	*z*
S, P	.31	.31	O	.16	.52	.12	.28
O_1	.405	.405	OH	.27	−.12	−.13	.14

Interatomic distances

(S, P)−O=1.53
(S, P)−O_1=1.55

O−O=2.51
O_1−O=2.50
O_1−OH=2.69
OH−OH=2.71

Ca−O=2.71
Ca−OH=2.77
Al−O=1.93
Al−OH=1.88

Parameters were found for woodhouseite in the same manner as described for svanbergite. Several sets of intensity calculations were made with various parameters. In Table 4 are given only the parameters finally chosen together with the corresponding interatomic distances. These are in close accord with accepted values but no great weight should be laid on this since the parameters are stated only to two figures for most atoms and a small shift may make substantial changes in interatomic distances. For instance, changing z for O_1 by only 0.005 would change the $S-O_1$ distance by a little more than 0.08 kX.

Table 5 shows the observed and calculated spacings for woodhouseite down to 1.293 kX. The observed intensities for the new woodhouseite pattern are recorded by the heights of peaks on a photometer curve. Except that the heights of the first two peaks which lie within the central halo of fog seem low (in the direct estimate of intensities made before the photometer curve was run they were assigned the same value as that of the third line) the agreement with calculated intensities is rather satisfactory, being just as good as that shown for alunite in Table 7. Even so, no high accuracy is claimed for the adopted parameters.

Records of powder patterns of woodhouseite have previously been published by Ygberg[9] and by McConnell.[10] The latter gave no cell dimensions; neither gave indices. Their data are included in Table 5. The record is carried a little farther in Table 5*a* in which are given lines of woodhouseite patterns between 1.29, the limit of intensity calculations, and 0.90, the line of smallest spacing recorded by Ygberg. McConnell's published record does not extend into this region. Measurement of my pattern was not carried beyond 0.90 kX.

Though there is substantial agreement among the several patterns some notable differences occur. The new pattern shows a few more lines. In the indexed part these are all satisfactorily accounted for except the weak line 2.56. Ygberg's pattern shows a few marked departures in spacing, for instance for his 2.99 line, whereas McConnell records two or more lines not observed by the writer and not explained by the supposed structure of woodhouseite. These discrepancies can hardly be explained by differences in material since we all worked with woodhouseite from Inyo County, the only known locality.

The structure of woodhouseite is shown in section in Fig. 1. Since all atoms lie in symmetry planes this may be considered to be a full representation of the structure. In the diagram all atoms within one rhombohedral cell are shown in the side view, whereas only atoms at the corners of such a cell are shown in the top view. The hexagonal parameters of Table 4 must be taken with x along the a_1 and a_3 axes to give correct positions corresponding to the labelled atoms or ions in the drawing.

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[9] *Op. cit.* p. 15.

[10] McConnell, Duncan, *X*-ray data on several phosphates: *Am. J. Sci.*, **240,** 649–657 (1942).

TABLE 5. CALCULATED AND OBSERVED SPACINGS AND INTENSITIES IN POWDER DIFFRACTION PATTERNS OF WOODHOUSEITE

Calculated Lines				Observed Lines					
Radiation		Cu		Pabst		Ygberg (1946)		McConnell (1942)	
				Cu		Cu		Fe	
$hk\bar{i}l$	$h_rk_rl_r$	I	d_{hkl}	I	d_{hkl}	I	d_{hkl}	I	d_{hkl}
$10\bar{1}1$	100	74	5.652	.30‡	5.66−	m	5.73	<½	5.61
0003	111	6	5.427						
$01\bar{1}2$	110	79	4.854	.40	4.84+	m	4.86	½	4.81
								<½	3.83
$11\bar{2}0$*	$10\bar{1}$	87	3.479	.90	3.48+	s	3.51	1	3.46
$10\bar{1}4$	211	0	3.373						
				.20	3.27‖			2	3.21
$02\bar{2}1$	$11\bar{1}$	0	2.963					2	2.960
$11\bar{2}3$*	210	436	2.929	2.45	2.93−	s+	2.99	6	2.908
$01\bar{1}5$	221	8	2.865	.15	2.84				
$20\bar{2}2$	200	0	2.825						
0006*	222	32	2.714	.45	2.70−	w	2.72	1	2.683
				.15	2.56§				
$02\bar{2}4$*	220	13	2.423	.40	2.42	w	2.40	1	2.418
								2	2.370
$21\bar{3}1$	$20\bar{1}$	6	2.257						
$20\bar{2}5$	311	21	2.213						
$12\bar{3}2$	$21\bar{1}$	41	2.195}	2.10†	{2.19+	s+	2.18	3	2.198
$10\bar{1}7$	322	147	2.171}		{2.16−			4	2.152
$11\bar{2}6$	321	2	2.141						
				.20	2.09+‖			2	2.068
$30\bar{3}0$	$2\bar{1}\bar{1}$	1	2.009						
$21\bar{3}4$	310	14	1.987	.20	1.99−	w−	2.01		
$01\bar{1}8$	332	0	1.930						
$03\bar{3}3$*	$22\bar{1}$	144}	1.884	2.30	1.885	s+	1.89	2	1.918
$30\bar{3}3$	300	6}						5	1.886
$12\bar{3}5$	320	1	1.867						
$02\bar{2}7$*	331	6	1.842	.10	1.844				
0009*	333	15	1.810	.20	1.804				
$22\bar{4}0$*	$20\bar{2}$	138	1.740	1.90	1.741	s	1.73	4	1.740
$20\bar{2}8$*	422	5	1.687	.20	1.685	w−	1.68		
$13\bar{4}1$	$21\bar{2}$	0	1.663						
$22\bar{4}3$	$31\bar{1}$	0	1.657						
$31\bar{4}2$*	$30\bar{1}$	4	1.638	.40} B	{1.638			1	1.638
$21\bar{3}7$	421	10	1.628			w−	1.62		
				?}	{1.621			1	1.619
$03\bar{3}6$	330	2}	1.615						
$30\bar{3}6$	411	0}							
$11\bar{2}9$*	432	18	1.605	.40	1.602	w−	1.60	1	1.600
$10\bar{1}.10$	433	4	1.572	.10	1.568			1	1.573
$13\bar{4}4$	$32\bar{1}$	4	1.547	.10	1.546				
$12\bar{3}8$*	431	13	1.521}	.45	1.519	w−	1.51	1	1.515
$40\bar{4}1$	$3\bar{1}\bar{1}$	7	1.501}						
$31\bar{4}5$	410	12	1.487}	.60	1.487	w	1.48	2	1.486
$04\bar{4}2$	$22\bar{2}$	13	1.482}						
$22\bar{4}6$*	420	49	1.464	.90	1.466	w	1.46	2	1.464
$01\bar{1}.11$	443	0	1.438						
$02\bar{2}.10$*	442	80	1.433	1.55	1.432	m	1.43	3	1.426
$40\bar{4}4$*	400	13	1.414	.25	1.416				
$32\bar{5}1$	$30\bar{2}$	5	1.378						
$04\bar{4}5$	$33\bar{1}$	2	1.367}						
$23\bar{5}2$	$31\bar{2}$	12	1.363}	.55B	1.366	w−	1.36		
$13\bar{4}7$	430	29	1.357}						
000.12	444	1	1.357}						
$03\bar{3}9$*	441	22}	1.344	.40	1.345	w−	1.34		
$30\bar{3}9$	522	2}							
$20\bar{2}.11$	533	5	1.328}						
$21\bar{3}.10$	532	3	1.325}	.40B	1.322	w	1.31		
$41\bar{5}0$	$3\bar{1}\bar{2}$	7	1.315}						
$32\bar{5}4$	$41\bar{1}$	0	1.310						
$31\bar{4}8$	521	1	1.293						

* Lines used to determine cell dimensions.

† Photometer curve shows common peak for two lines whose intensities were estimated at 4 and 8 (intensity of strongest line being 10), in agreement with calculated intensities.

‡ Observed intensities given by heights of peaks on photometer curve.

§ Unidentified line, probably due to unknown contaminant, not quartz.

‖ β lines.

Table 5a. Observed Lines in Woodhouseite Powder Diffraction Patterns for the Interval 1.29 to 0.90 kX

Pabst		Ygberg		Pabst		Ygberg	
I	d_{hkl}	I	d_{hkl}	I	d_{hkl}	I	d_{hkl}
4*	1.282	m	1.27	2	1.036		
1	1.262			2	1.031		
2	1.225			3	1.007		
5	1.192	m	1.19	3	1.003	w	1.00
4	1.164	w+	1.16	2−	0.962		
3−	1.138−	w	1.13	5	0.953	w+	0.95
2	1.124			4	0.945	w	0.94
2	1.106			5	0.935	w+	0.93
4	1.098	w−	1.10	2−	0.930		
4	1.078	w+	1.07	3+	0.913	w−	0.91
2+	1.067			5	0.903	w	0.90
2+	1.056						

* Intensities given by arbitrary serial numbers from 1 for very faint lines to 10 for the strongest line.

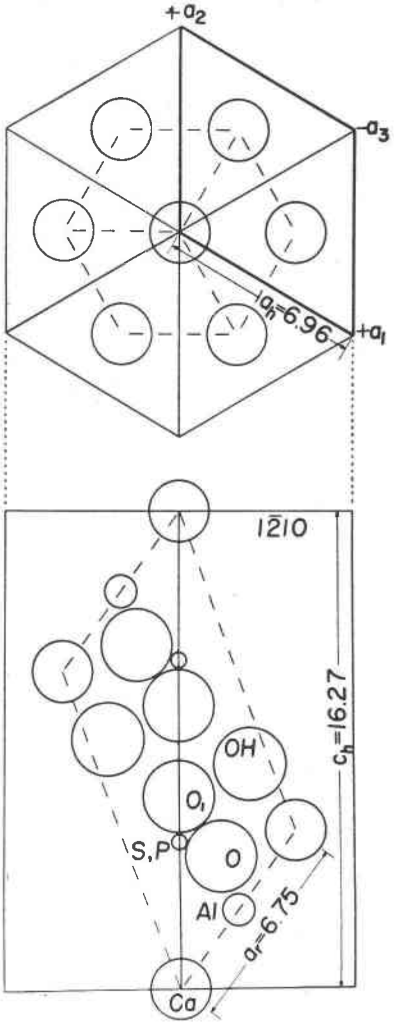

FIG. 1. Atomic arrangement of woodhouseite. Dashed lines in both views outline rhombohedral unit cell. Heavy full lines outline hexagonal unit cell in top view only.

ALUNITE

Alunite from Tolfa, Italy, taken from the collections of the Department of Geological Sciences, University of California, Berkeley, originally obtained through Ward's Natural Science Establishment, was used for a powder pattern. This may be considered to be from the type locality since the mineral was known at Tolfa from early times, before it received its present name.

The density was determined with the Berman balance on three small fragments of this material consisting of compact fine-grained crystal aggregates. Single crystals were not available. The resulting value, 2.70 is slightly lower than the observed and calculated values, 2.75 and 2.80, given by Hendricks,[11] as might be expected.

The dimensions of the hexagonal cell were determined from a powder pattern taken under just the same conditions as that of woodhouseite. The results checked closely with the dimensions given by Hendricks. These, together with the constants calculated for the corresponding rhombohedral cell, are:—

a_h	c_h	c_h/a_h	a_{rh}	α
6.96	17.35	2.492	7.058	59° 5′.

The parameters found for alunite by Hendricks are given in Table 6 in the same form in which parameters have been given for svanbergite

TABLE 6. PARAMETERS USED IN INTENSITY CALCULATION FOR ALUNITE. ADAPTED FROM HENDRICKS

Rh K 1: (a) 000		Hex 3: (a) 000	Rh Al 3: (d) ½00			Hex 9† (d) 1/6 $\overline{1/6}$ 1/6	
	2: (c) xxx	6: (c) $00z$		6: (h) zxx		18: (h) $x\bar{x}z$	
	x	z		x	z	x	z
S	.305	.305	O	.157	.512	−.213	−.058‡
O_1	.393	.393*	OH	.276	−.174	−.150	.126

* The O_1 parameter is given by Hendricks as .06. This is obviously a slip as it would make the $K-O_1$ distance only 1.04. The value given in the table herewith is obtained by adding .333 to the value given by Hendricks (*op. cit.*, p. 777). From his figure 2 it is clear that he intended the value here given.

† There are 9 aluminums in the hexagonal unit, not 3 as suggested by Hendricks' tabulation (*op. cit.*, p. 777).

‡ The hexagonal parameters for O here given are the same as tabulated by Hendricks. By adding .333 to each it will be seen that these parameters are very close to those found for svanbergite and woodhouseite stated in Tables 1 and 4.

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[11] *Op. cit.*, p. 775.

and woodhouseite. Using these parameters and the dimensions cited, the intensities and positions for the first twenty five possible lines in an alunite powder pattern were calculated. Table 7 shows the results of

TABLE 7. COMPARISON OF CALCULATED AND OBSERVED SPACINGS AND INTENSITIES FOR ALL POSSIBLE LINES IN AN ALUNITE POWDER DIFFRACTION PATTERN FOR WHICH d_{hkl} IS GREATER THAN 1.69

Calculated				Observed† (Pabst)		ASTM—ASXRED‡			
						card 2155		card II-1459	
$hk\bar{i}l$	$h_rk_rl_r$	d_{hkl}	I	d_{hkl}	I	d_{hkl}	I	d_{hkl}	I
0003	111	5.783	1						
$10\bar{1}1$	100	5.69	38	5.75	.30	5.70	.25	5.70	.2
$01\bar{1}2$	110	4.946	59	4.98	.65	4.94	.50	4.92	.4
								3.97	.$\frac{1}{2}$
$10\bar{1}4$	211	3.52	3						
$11\bar{2}0$	$10\bar{1}$	3.481	62	3.50	1.05	3.49	.41	3.50	.2
				3.33+*	.40	3.34	.03		
$01\bar{1}5$	221	3.01	16	3.00−	2.80	2.98	1.00	2.96	1.0
$11\bar{2}3$	210	2.985	424						
$02\bar{2}1$	$11\bar{1}$	2.97	138						
0006	222	2.892	23	2.89+	.55	2.88	.06	2.85	.$\frac{1}{2}$
$20\bar{2}2$	200	2.848	0						
$02\bar{2}4$	220	2.474	54	2.48+	.65	2.47	.09	2.47	.$\frac{1}{4}$
$10\bar{1}7$	322	2.292	148	2.29+	2.40	2.29	.50		
$20\bar{2}5$	311	2.276	28	2.26	.95				
$21\bar{3}1$	$20\bar{1}$	2.259	14						
$11\bar{2}6$	321	2.227	5	2.21+	.25			2.24	.5
$12\bar{3}2$	$21\bar{1}$	2.204	35			2.20	.19		
				2.11+*		2.13	.03		
$01\bar{1}8$	332	2.042	12	2.04−	.20	2.02	.03		
$21\bar{3}4$	310	2.018	0						
$30\bar{3}0$	$2\bar{1}\bar{1}$	2.010	2						
0009	333	1.928	9						
$02\bar{2}7$	331	1.914	18	1.90+	3.30	1.893	.59	1.89	.5
$12\bar{3}5$	320	1.904	0						
$03\bar{3}3$	$22\bar{1}$	1.897	133						
$30\bar{3}3$	300		4						
$22\bar{4}0$	$20\bar{2}$	1.740	145	1.750	2.90	1.74	.50	1.735	.5
$20\bar{2}8$	422	1.699	1						

* β lines. See text.

† Cu radiation. Intensities given as heights of peaks on photometer curve. The calculated intensities are also for Cu radiation.

‡ Presumably the patterns recorded on both ASTM cards were made with Mo radiation.

these calculations together with observations on the powder pattern. Included in the table are also parts of the records of alunite patterns that are available on ASTM-ASXRED cards.

The observed lines include several that do not correspond to calculated spacings. When the lines at 3.33 and 2.11 kX were noted on the pattern of alunite from Tolfa, Italy, they were at first suspected of being due to quartz contamination. Quartz has strong lines at 3.35 and 2.11.[12] Microscopic examination, however, revealed no quartz in the sample and it proved to be completely soluble upon prolonged treatment with sulphuric acid. These two lines are Cu-K_β lines corresponding to $11\bar{2}3$ and $03\bar{3}3$, the strongest α lines observed. Such Cu K_β lines ought to simulate Cu K_α lines for spacings 3.315 and 2.119, very close to the observed positions.

On card 2155 lines are also recorded near the positions just discussed, namely at 3.34 and 2.13. It may be assumed that this pattern, from the first ASTM set, was made with Mo radiation. Due to the different ratio of β to α wave lengths for this radiation the β lines for $11\bar{2}3$ and $03\bar{3}3$ would simulate α lines corresponding to spacings 3.382 and 2.152 respectively, in this case. Thus it seems probable that the alunite used for the pattern of ASTM card 2155 carried a little quartz contamination, though one might again attribute the lines to β radiation if one allowed about a one per cent error in the reporting of the positions of these particular lines.

No explanation has been found for the 3.97 line on card II—1459.

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[12] ASTM-ASXRED card II—1007.