THE UNIT CELL AND SPACE GROUP
OF STERNBERGITE, $AgFe_2S_3$

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Abstract

Sternbergite from Joachimsthal, Bohemia, has been studied by the equi-inclination Weissenberg method. It is evident from the results obtained in this work that the axial ratio derived by morphological study should be changed so that b has $\frac{1}{3}$ the length assigned to it by Peacock. This change also brings with it the necessity of interchanging the usual a and b axes in order to leave b the longer of the two.

The investigation leads to the following cell data, in terms of the new orientation:

Diffraction symbol: $mmmCc--$

Crystal class:	C_{2v} or D_{2h}
Crystal system:	Orthorhombic
Space group:	Ccm (C_{2v}^{12}) or $Ccmm$ (D_{2h}^{17})
Unit cell:	

Absolute		*Ratio*
$a=$ 6.61Å		0.568
$b=$ 11.64		1.
$c=$ 12.67		1.088
$Z=$ 8 $AgFe_2S_3$ per cell.		

There is no real isomorphism between sternbergite and cubanite.

Introduction

Crystals of sternbergite from Joachimsthal, Bohemia, have recently been remeasured and redescribed by Peacock.[1] Through the courtesy of Professor Palache and Doctor Peacock, specimens of this material were obtained for x-ray diffraction study. One of the purposes of this investigation was to follow out Peacock's attempt at comparing sternbergite with cubanite.

Method

Because of the very soft and plastic nature of the mineral, crystals suitable for x-ray examination cannot be handled freely without deformation. An attempt was made to overcome this difficulty by working with the cluster while it was in direct contact with carbon dioxide ice. It is believed that this cooling helped to make the material more rigid and to reduce distortion during the detachment of the separate crystals.

Rotation photographs were taken for the three crystallographic axes, and Weissenberg resolutions were made of all the equators. In addition,

[1] Peacock, M. A., On the crystal form of sternbergite: *Am. Mineral.*, vol. **21**, pp. 103–108, 1936.

equi-inclination resolutions were made for these three plane lattice stacking directions. These included the 1, 2, 3 and 4 levels about the a axis, the 1 and 2 levels about the b axis, and the 1, 2, 3, and 4 levels about the c axis. From these photographs the reciprocal lattice has been reconstructed in three different elevations.

SYMMETRY

All the photographs exhibit the plane group symmetry C_{2l}. The centro-symmetrical crystal symmetry is therefore D_{2h}. Sternbergite is accordingly orthorhombic, and may belong to any of the three crystal classes D_2, C_{2v}, or D_{2h}, so far as the symmetry of the photographs alone is concerned.

THE UNIT CELL

Space Lattice Type

Each of the c axis n-level equi-inclination Weissenberg photographs exhibits a diamond pattern. The level stacking sequence in the c direction is 7.[2] The a and b axis n-level photographs display rectangular patterns, each having a level stacking sequence 10. The space lattice type is accordingly C-centered orthorhombic.

Lattice Constants

The cell constants obtained from the reconstructed reciprocal lattice, refined by measurements from the three equatorial photographs, are as follows:

N. W. Buerger		Peacock	Haidinger[3]
Absolute	Ratio*		
$a = 11.64$Å.	1.761	.5913 ($\times 3 = 1.7739$)	.583 ($\times 3 = 1.75$)
$b = 6.61$	1.	1.	1.
$c = 12.67$	1.916	.6250 ($\times 3 = 1.8750$)	.838 ($\times 2 = 1.676$)

* It is likely that this ratio is more accurate than a ratio derived from goniometric measurements, since it is obtained from interatomic spacing measurements which are less sensitive to crystal deformation and distortion than the external surface angle measurements.

It is apparent from these values that the axial ratio derived by morphological study should be changed so that b has one-third the length

[2] Buerger, M. J., The application of plane groups to the interpretation of Weissenberg photographs: *Zeits. Krist.*, vol. **91**, Fig. 26, p. 275, 1935.

[3] Haidinger, W., Description of sternbergite, a new mineral species: *Trans. Roy. Soc. Edinburgh*, vol. **11**, pt. I, 1828, pp. 1–7.
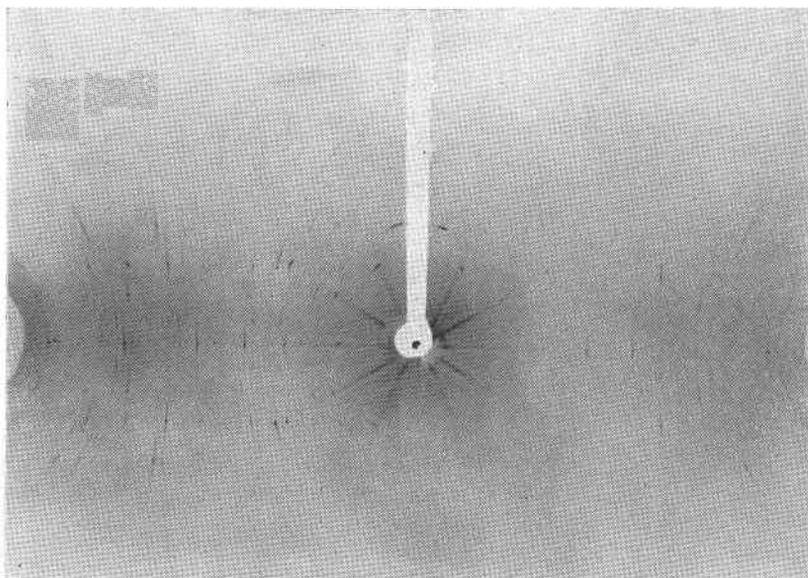
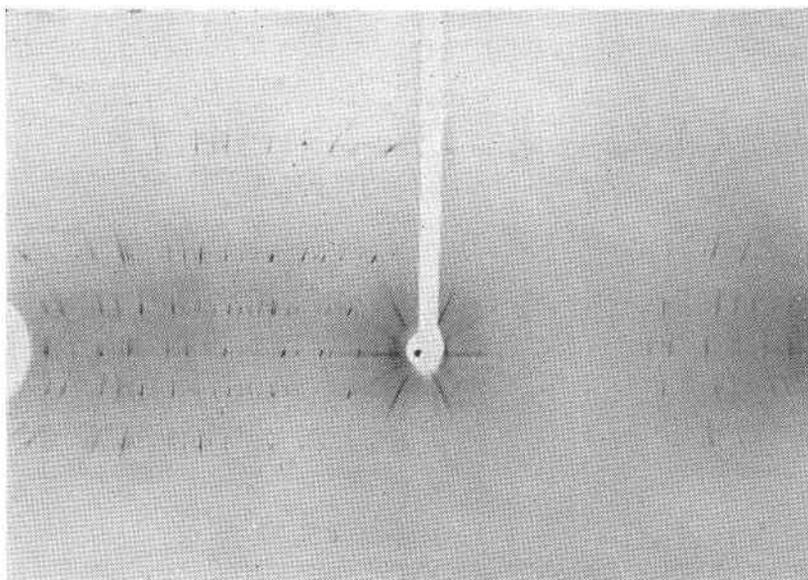FIG. 1. Sternbergite, old *a* axis (new *b* axis) oscillation photograph.

FIG. 2. Sternbergite, old *b* axis (new *a* axis) oscillation photograph.

assigned to it by Peacock. This change also necessitates the interchange of the a and b axial directions, in order to leave b the longer of the two. The need of changing the length of the c axis so that it has three times the length given it was foreseen by Peacock as a possible result of x-ray investigation.[4]

Since the proposed interchange of the a and b axes involves an important innovation in the accepted crystallography of sternbergite, photographic proof of the necessity of such an interchange is presented in Figs. 1 and 2. These are oscillation photographs about the old a and b axes, taken from portions of twins as shown in Figs. 3 and 4. A twin
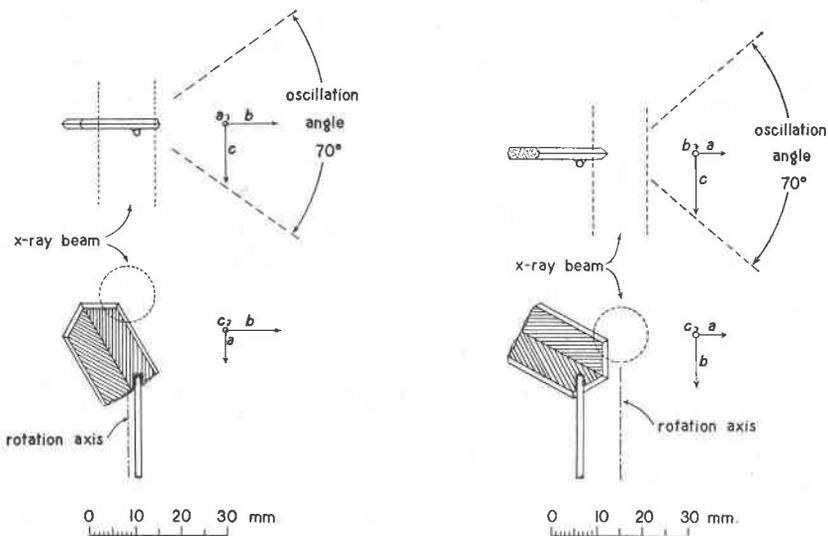

FIG. 3 (left). Method of obtaining old a axis (new b axis) oscillation photograph from individual of twin.

FIG. 4 (right). Method of obtaining old b axis (new a axis) oscillation photograph from individual of twin.

was used because twins are more resistant to deformation, and consequently provide cleaner photographs (less smeared spots) than untwined crystals. The crystal was oscillated about both the a and the b axes, through an angle of approximately 70°. The orientation was such that when the crystal was in the 35° position, the beam was normal to the crystal plate (parallel to the c axis); this allowed no portion of the other member of the twin to come within the path of the beam. The results, of course, are in harmony with the other rotation photographs. It is clear from Figs. 1 and 2 that the old reciprocal axis length, a^*, is less than the old reciprocal axis length, b^*; thus old a is greater than old b.

[4] Peacock, M. A., Op. cit., p. 104.

The new orientation results in the following cell constants:

Absolute	Ratio
$a = 6.61$Å.	0.568
$b = 11.64$	1.
$c = 12.67$	1.088

The transformations of axes are shown in Table 1. It is of interest to mention here that Haidinger's notation of axes followed Mohs' old system in which the a axis was the principal, or vertical axis, b the macroaxis, and c the brachyaxis. Thus, Haidinger's c would be designated a in present day notation, and his a would be designated c.

The transformation of the form symbols is given in Table 2. It will be noted that with the new orientation, the forms are simplified in all cases

TABLE 1. TRANSFORMATION OF AXES

Haidinger	Peacock	N. W. Buerger
b ⟶ b		
c ⟶ a		
$\frac{3}{2}a$ ⟶ c		
$3b$ ⟶ a		
c ⟶ b		
$\frac{3}{2}a$ ⟶ c		
	$3b$ ⟶ a	
	a ⟶ b	
	c ⟶ c	

TABLE 2. TRANSFORMATION OF FORMS

Haidinger to Peacock:*	300/030/002
Haidinger to Buerger:	010/300/002
Peacock to Buerger:	010/300/003

Haidinger	Peacock	N. W. Buerger
a (001)	c (001)	(001)
i (010)	b (010)	(100)
—(100)	a (100)	(010)
—(011)	d (032)	(102)
b (021)	—(031)	(101)
c (0·10·1)	—(0·15·1)	(501)
h (106)	—(104)	(014)
—(203)	e (101)	(011)
—(301)	—(902)	(092)
f (111)	q (332)	(132)
—(443)	r (221)	(263)
g (221)	s (331)	(131)
d (121)	—(362)	(232)
—(263)	t (131)	(111)
m (110)†	m (110)†	(130)†

* Transformation formulae according to Barker, *Systematic Crystallography*, p. 32, 1930.
† Twin plane only.

except Peacock's (221). A stereographic projection of the recorded forms of sternbergite, using the new orientation and axes, is given in Fig. 5.
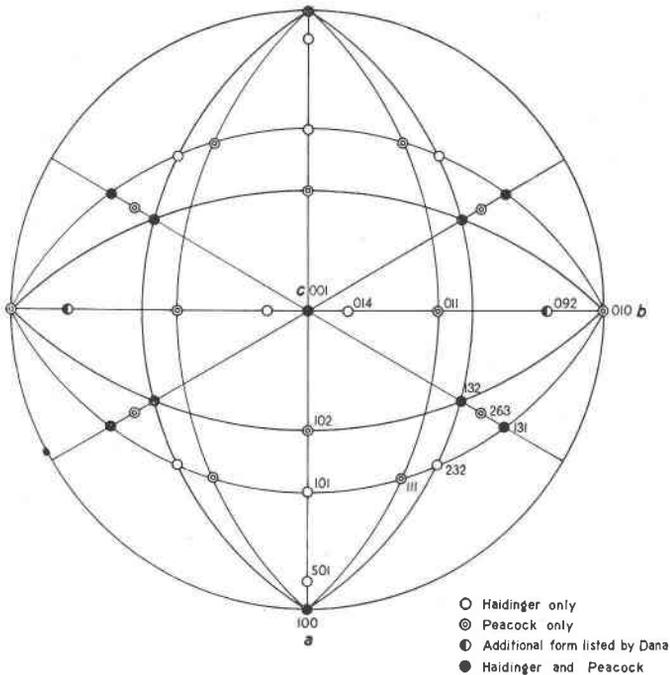

FIG. 5. Sternbergite. Stereographic projection of recorded forms, using new axes and orientation.

The cell contents may be calculated with the aid of the relation

$$\text{Measured density} = \frac{\text{cell mass}}{\text{cell volume}}$$

$$d = \frac{Z \times f \times 1.649 \times 10^{-24}}{V \times 10^{-24}}$$

where

d = measured density.
Z = number of formula weights per unit cell.
f = chemical formula weight.
V = cell volume in cubic Ångstroms.

Substituting the appropriate values of d, f, and V for sternbergite in this relation gives Z a value of $7.9 \approx 8$ formula weights per unit cell.

Space Group

Comparison of reciprocal cell translations on n-level and zero level equi-inclination Weissenberg photographs shows that in the (100) plane the c reciprocal translation is doubled, indicating a glide plane perpendicular to a, with glide component $c/2$. There are no other multiple reciprocal translations on the other zero levels. This total diffraction information may be expressed by the diffraction symbol $mmmCc--$. The only possible space groups are therefore $Ccm(C_{2v}^{12})$ and $Ccmm(D_{2h}^{17})$. The symmetrical morphological development makes it probable that sternbergite is holohedral, which indicates D_{2h}^{17} as the probable space group. Figure 6 shows the space group in three projections.
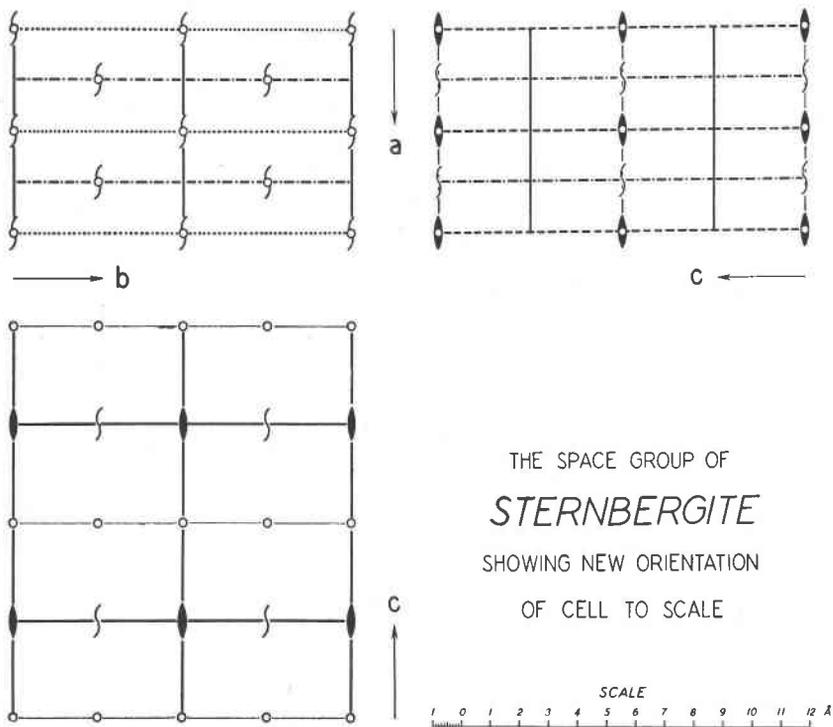

THE SPACE GROUP OF

STERNBERGITE

SHOWING NEW ORIENTATION

OF CELL TO SCALE

Fig. 6. The space group of sternbergite, showing new orientation to scale.

Comparison with Cubanite

The lattice types and dimensions give no grounds for believing that any isostructural or isomorphous relation exists between sternbergite and cubanite, despite certain similarities displayed. Table 3 shows in tabular form a structural comparison between the two minerals. The c axis of

sternbergite is about double that of cubanite. The two are certainly not strictly isostructural for sternbergite is based on a $C-$ centered lattice (C) while cubanite is based on a simple lattice (P).

TABLE 3. STERNBERGITE CELL CONSTANTS (NEW ORIENTATION) COMPARED WITH
CUBANITE CELL CONSTANTS

Sternbergite		Cubanite*
absolute $\begin{cases} a= & 6.61 \text{ Å.} \\ b= & 11.64 \\ c= & 12.67 \end{cases}$		6.43 Å. 11.04 6.19 ($\times 2 = 12.38$)
ratio $\begin{cases} a= & .568 \\ b= & 1. \\ c= & 1.088 \end{cases}$ $a/c=$ .521		$.582_5$ 1. .561 ($\times 2=$ 1.122) 1.038 ($\times \frac{1}{2}=$ .519)
lattice type	C	P
formula weights per cell	8 $AgFe_2S_3$	4 $CuFe_2S_3$

* Buerger, M. J., The crystal structure of cubanite: *Am. Mineral.*, vol. 21, p. 205, 1936.

ACKNOWLEDGMENTS