The crystallography of sartorite.

By F. A. BANNISTER, M.A., ADOLF PABST, Ph.D., and
GEORGE VAUX, B.Sc., D.I.C.

SARTORITE is one of four minerals once thought to be isomorphous. Of these only two are truly so—chalcostibite, copper antimony sulphide, $CuSbS_2$; and emplectite, copper bismuth sulphide, $CuBiS_2$—both orthorhombic minerals. The third, zinckenite, has been shown by two of the authors[1] to be hexagonal and to approach more closely the formula $Pb_6Sb_{14}S_{27} = 6PbS.7Sb_2S_3$ than $PbSb_2S_4 = PbS.Sb_2S_3$. It seemed appropriate to continue a study of the series by an X-ray investigation of sartorite, a lead arsenic sulphide formerly supposed isomorphous with zinckenite. More than usual interest was attached to such a task, since discrepant interpretations of the symmetry and setting of sartorite had been obtained by well-known crystallographers.

Indeed, the difficulties of indexing different crystals of sartorite on the same lattice proved insuperable to G. F. H. Smith and R. H. Solly,[2] so that they devised three incongruent lattices—one monoclinic and two anorthic. Also they used slightly different elements for each crystal. Their device, however, was not uniformly successful with certain crystals of sartorite previously measured by C. O. Trechmann.[3] Two crystals in particular eluded their efforts. These, they decided, could not belong to the same species, but must be another mineral, perhaps a dimorphous form of sartorite, which they then named sartorite-α.

Amongst an extremely fine collection of sartorite crystals from the Lengenbach quarry, Binn valley, Switzerland, preserved in the Department of Mineralogy of the British Museum, are fortunately the actual crystals measured by Trechmann, and by Smith and Solly. The first problem was to determine whether they would all give the same diffraction patterns. Several crystals were selected including Trechmann's nos. 1 and 2, renamed sartorite-α by Smith and Solly, and Trechmann's no. 5 on which Smith recorded over one hundred faces.

X-ray rotation photographs about the elongation axis [010] of all

[1] G. Vaux and F. A. Bannister, Min. Mag., 1938, vol. 25, p. 221.
[2] G. F. H. Smith and R. H. Solly, Min. Mag., 1919, vol. 18, p. 259.
[3] C. O. Trechmann, Min. Mag., 1907, vol. 14, p. 212.

these crystals are completely superposable. The layer-lines although not close together are packed with spots. It was considered necessary, therefore, to show that photographs of the same crystals rotating about the [100] or [001] axes are also superposable. This was only achieved by setting the crystals as accurately as possible with Lauegrams. ·These revealed orthorhombic symmetry, but owing to the high absorptive power of lead minerals for X-rays the spots probably correspond only to the pseudo-cell to which we shall refer shortly. The rotation photographs of the crystals studied proved them all to be identical and presumably sartorite. No small differences in spacing could be detected from one crystal to another and certainly nothing approaching the variability of crystal elements suggested by Smith and Solly. Moreover, no X-ray evidence exists that sartorite-α is an independent species. In all respects Trechmann's crystals nos. 1 and 2 are identical with the rest.

Long-exposure oscillation photographs of a sartorite crystal about the axes [100], [010], and [001] revealed a number of intermediate weak layer-lines not detected on the rotation photographs. These are restricted to the [100] and [001] axes, and they have different intensities above and below the equator, so that sartorite must really be monoclinic. No attempt has been made to work out the monoclinic space-group, but only the space-group of the well-marked pseudo-cell, the diffractions from which are due largely to the lead atoms. The weak spots, which are only revealed by oscillation photographs, are, on the other hand, due entirely to diffractions from the much lighter arsenic and sulphur atoms. The cell dimensions are a 58·38, b 7·79, c 83·30 Å. with β 90°. The orthorhombic pseudo-cell has the dimensions a 19·46, b 7·79, c 4·17 Å. Space-group $P2_12_12_1$.

It should be stated here that no X-ray evidence of twinning in sartorite has been found. As for zinckenite, the crystals photographed give layer-line patterns for all three axes in which: (a) all the layer-lines are exactly parallel to the equator; and (b) the layer-lines of each photograph correspond to integral sub-multiples of only one of the three cell sides a, b, or c. Twinning of the type found by Buerger[1] in mispickel cannot be detected by X-ray methods, but should be observable on polished sections in polarized light. We have examined bright striated faces of Smith and Solly's sartorite crystal no. 1, but could find no trace of twin-lamellae nor any marked anisotropy.

A thorough optical investigation of other sartorite crystals has not been carried out, so that our evidence does not contradict in any way

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[1] M. J. Buerger, Zeits. Krist., 1936, vol. 95, p. 83. [M.A. 6–409.]

H. Schneiderhöhn and Ramdohr's[1] account of twin-lamellae in the mineral. The optical and X-ray examination of crystal no. 1 show that this crystal at least is not twinned, and that the symmetry and cell-dimensions are most probably the true ones for untwinned sartorite.

Chemical analyses of sartorite, mostly prior to 1855, do not show any appreciable variations from the simple formula $PbAs_2S_4$, and the contents of the pseudo-cell are $3.95PbAs_2S_4$. Rounding this figure off to 4, the true unit cell contents are then $240PbAs_2S_4$.

The relation of sartorite to the three minerals zinckenite, chalcostibite, and emplectite is not one of isomorphism, but the elongation direction in all four minerals is close to, or a simple multiple of, the corresponding spacing 3·89 Å. for stibnite. It is hoped to undertake a crystal-structure analysis of the pseudo-cells of zinckenite and sartorite, so that the interrelations of the four minerals may be revealed in more detail. A corresponding study of jordanite[2] and dufrenoysite, two lead arsenic sulphides with which sartorite was confused by the early crystallographers, is only one of the numerous corollaries. The few crystal-structures that have so far been worked out, together with our cell measurements, suggest that in the metallic arsenic, antimony, and bismuth sulphide minerals we have a group of substances rivalling in complexity and probably as closely interrelated as the silicates.

The final portion of this study is devoted to the reconciliation of axial ratios given by former workers with the X-ray cell dimensions of sartorite and to the successful indexing of the numerous forms previously observed.

Sartorite has been assigned no less than four different sets of axial elements. G. vom Rath[3] and Victor Goldschmidt[4] considered it to be orthorhombic. Trechmann gave it monoclinic elements; and Smith and Solly actually suggested that the forms be referred to three incongruent lattices, one monoclinic and two anorthic. Table I shows that all of these elements (excluding the anorthic elements of Smith and Solly) can be reconciled with the elements that correspond to the unit cell or to the pseudo-cell.

It is desirable that the crystallographic observations on sartorite be explained by reference to the structural elements. To this end the

¹ H. Schneiderhöhn and P. Ramdohr, Lehrbuch der Erzmikroskopie, 1931, vol. 2, p. 491. [M.A. 4–434.]

² The cell dimensions of jordanite have recently been given by W. E. Richmond in a paper by C. Palache, Amer. Min., 1938, vol. 23, p. 829.

³ G. vom Rath, Ann. Phys. Chem. (Poggendorff), 1864, vol. 122, p. 373.

⁴ V. Goldschmidt, Index der Krystallformen der Mineralien, 1888, vol. 3, p. 320; Krystallographische Winkeltabellen, 1897, p. 320.

measurements of Smith and Solly's crystal no. 1 were recalculated and it was found that nearly all faces can be given simple indices, provided that some are referred to the elements of the true cell and some to the elements of the pseudo-cell. The agreement of observed and calculated angles is no worse than that obtained by Smith and Solly using three incongruent lattices. Moreover, large discrepancies or relatively high indices are found only with faces which are described by Smith and Solly as 'bad' or 'striated'.

TABLE I. Comparison of axial ratios of sartorite.

	$a:b:c$.	Transformation.	$a:b:c$.
	True cell.		
Bannister (1938) ...	58·38 7·79 83·30 Å.	—	7·49:1:10·69
vom Rath (1864) ...	0·539:1:0·619	$12c:b:20a$	7·43:1:10·78
Goldschmidt (1888) ...	0·771:1:0·956	$6c:a:\frac{100}{13}b$	7·44:1:10·82
,, (1897) ...	0·956:1:0·771	$6a:c:\frac{100}{13}b$	7·44:1:10·82
Trechmann (1907) ...	1·276:1:1·195 $\beta = 77°\ 48'$	$6a \sin \beta:b:9c \sin \beta$	7·48:1:10·52
Smith and Solly (1919)	2·574:1:2·712 $\beta = 74°\ 38'$	$3a \sin \beta:b:4c \sin \beta$	7·45:1:10·46
	Pseudo-cell.		
Bannister (1938) ...	19·46 7·79 4·17Å.	—	2·498:1:0·535
vom Rath (1864) ...	0·539:1:0·619	$4c:b:a$	2·476:1:0·539
Goldschmidt (1888) ...	0·771:1:0·956	$2c:a:\frac{5}{11}b$	2·482:1:0·541
,, (1897) ...	0·956:1:0·771	$2a:c:\frac{5}{12}b$	2·482:1:0·541
Trechmann (1907) ...	1·276:1:1·195 $\beta = 77°\ 48'$	$2a \sin \beta:b:\frac{9}{20}c \sin \beta$	2·493:1:0·526
Smith and Solly (1919)	2·574:1:2·712 $\beta = 74°\ 38'$	$a \sin \beta:b:\frac{1}{3}c \sin \beta$	2·485:1:0·523

Table II shows the results of the recalculation for the [010] zone of Smith and Solly's crystal no. 1. In this table only the simpler of the two new indices have been given in those cases where a choice was easy. This brings out a simple relation showing the influence of the pseudo-cell on the morphology. In the zone [010] both axes of the pseudo-cell differ in magnitude from those of the true cell. For faces close to (100) simpler indices are found when they are referred to the true cell elements, whereas for faces closer to (001) simpler indices are found when they are referred to the elements of the pseudo-cell.

The relations are somewhat different and possibly more striking in the [001] zone, table III. Here the ratio $a:b$ is much smaller, i.e. more nearly 'normal' for the pseudo-cell, and all faces close to (100) receive simple indices only when referred to the elements of the pseudo-cell. If the elements of the true cell were used alone, no faces making an angle

of less than 39° 47′ with (100) could receive indices with h less than 10; in other words, faces with indices in this range could only occur in a little more than half of the zone.

TABLE II. Indexing of the faces in the [010] zone of sartorite.

	Smith and Solly measured	Calculated	True cell $(a/c = 0.701)$	Pseudo-cell $(a/c = 4.672)$
$(h0l)$.	$(100):(h0l)$.	$(100):(h0l)$.	$(h0l)$.	$(h0l)$.
$(50\bar{1})$	11° 39′	11° 20′	$(70\bar{2})$	—
(301)	15° 34′	15° 39′	(502)	—
$(70\bar{2})$	15° 47′	15° 39′	$(50\bar{2})$	—
$(30\bar{1})$	18° 35′	18° 24′	$(21.0.\bar{10})$	$(14.0.\bar{1})$
(705)	29° 13′	29° 17′	(504)	—
$(50\bar{3})$	32° 31′	32° 30′	$(11.0.\bar{10})$	—
$(40\bar{3})$	42° 25′	43° 3′	$(30\bar{4})$	$(50\bar{1})$
(405)	42° 41′	43° 3′	(304)	(501)
$(60\bar{5})$	44° 4′	43° 56′	$(8.0.\bar{11})$	—
(305)	46° 23′	46° 27′	(203)	—
(102)	49° 48′	49° 26′	(305)	(401)
$(10\bar{1})$	50° 48′	50° 48′	$(40\bar{7})$	—
(207)	59° 10′	60° 17′	(205)	(803)
(104)	61° 52′	61° 51′	(308)	(502)
(105)	63° 38′	63° 28′	—	(703)
(108)	67° 14′	66° 50′	—	(201)
$(50\bar{9})$	71° 37′	71° 35′	—	$(14.0.\bar{9})$
(001)	74° 8′	74° 4′	(105)	(403)
$(10\bar{2})$	75° 25′	75° 5′	—	$(50\bar{4})$
(409)	78° 1′	77° 58′	—	(101)
$(30\bar{7})$	79° 37′	79° 41′	—	$(60\bar{7})$
$(20\bar{5})$	80° 47′	80° 53′	—	$(30\bar{4})$
$(10\bar{4})$	85° 10′	85° 6′	—	$(20\bar{5})$
$(10\bar{4})$	86° 58′	86° 56′	—	$(10\bar{3})$
$(3.0.\bar{10})$	87° 32′	87° 33′	—	(105)

A question of the validity of the so-called 'law of rational indices' does not arise. 'Rational' indices can always be found: it is merely a question of the discrepancies between measured and calculated angles that are allowable and the simplicity of indices demanded by the prejudice of the crystallographer. In the present case, only 14 forms of a total of 102 receive indices higher than 11, and of those that receive higher indices 8 are described as bad or striated, so that they should not cause concern.

Fig. 1 shows the gnomonic projection of Smith and Solly's crystal no. 1 on (010). Faces which receive simpler indices on the elements of the pseudo-lattice are limited to certain parts of the projection. Although two lattices are needed for a satisfactory indexing of the forms of sartorite, they are not incongruent lattices. In a discussion of the structure
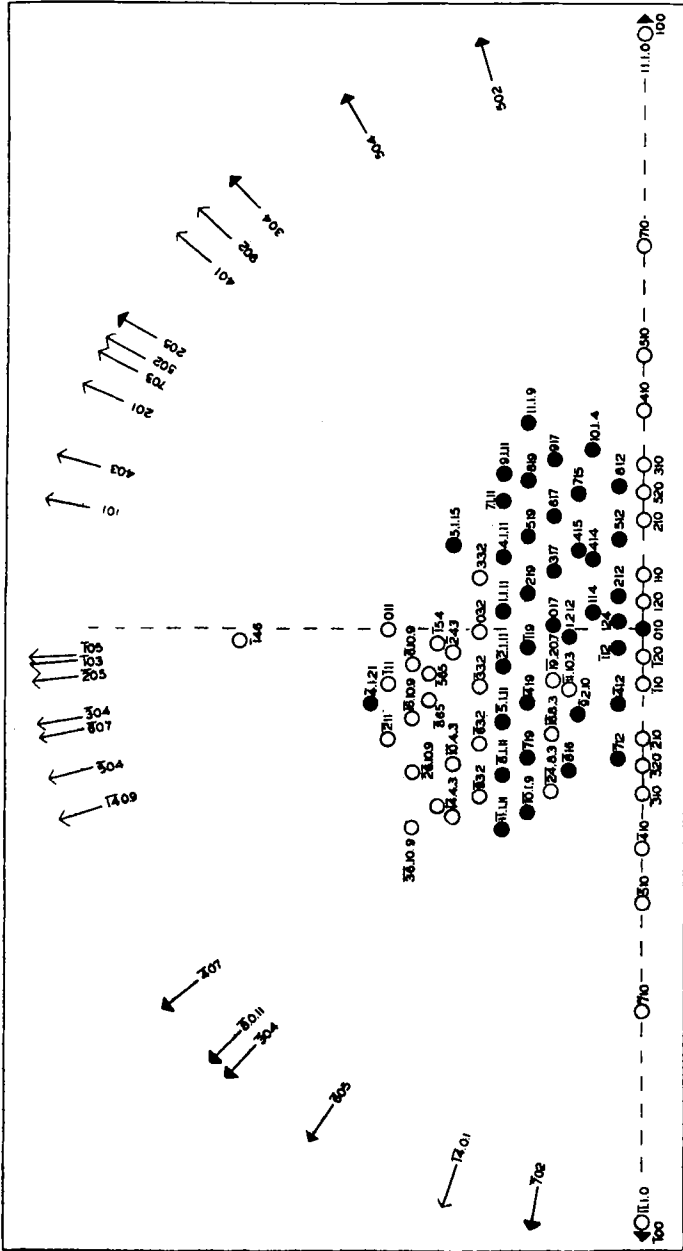
FIG. 1. Gnomonic projection of sartorite on (010). Full symbols designate forms indexed with reference to the true cell and open symbols designate forms indexed with reference to the pseudo-cell.

and morphology of calaverite, it has been pointed out by Tunell and Ksanda[1] that only some of the faces of that mineral can be simply indexed on the elements of the unit cell and that the other faces are related to 'adventive' spots found in the X-ray patterns. In the case

TABLE III. Indexing of the faces in the [001] zone of sartorite.

(hk0).	Smith and Solly measured (100):(hk0).	Calculated (100):(hk0).	True cell ($a/b = 7.494$) (hk0).	Pseudo-cell ($a/b = 2.498$) (hk0).
(11.1.0)	12° 54′	12° 48′	(33.1.0)	(11.1.0)
(710)	19° 35′	19° 38′	(21.1.0)	(710)
(510)	26° 39′	26° 33′	(15.1.0)	(510)
(310)	39° 34′	39° 47′	(910)	(310)
(520)	45° 0′	44° 59′	(15.2.0)	(520)
(210)	51° 8′	51° 19′	(610)	(210)
(110)	68° 1′	68° 11′	(310)	(110)
(120)	78° 24′	78° 41′	(320)	(120)
(010)	89° 41′	90° 00′	(010)	(010)

of sartorite, it may be said that many faces may be simply indexed on the elements of the small pseudo-cell, while others receive simpler indices when referred to the large true cell and are thus related to the spots of the X-ray patterns which indicate the existence of this larger true cell. In a recent paper on meneghinite, a sulpho-salt with one large cell dimension and an unusual ratio, Palache[2] refers to the occurrence of 'aberrant' forms possibly analogous in some measure to the forms that have caused trouble in dealing with sartorite. This may be an indication that such forms are attendant upon certain relations of the cell dimensions.

A recalculation of Trechmann's crystal no. 1 from the published measured angles showed that it may be completely indexed with reference to the structural elements found for sartorite, again using elements corresponding to either the true or pseudo-cell. The crystallographic calculations check the conclusion from the X-ray observations that sartorite-α is identical with sartorite and a comparison of the form lists for the two shows the reason for the previous uncertainty. Of twenty-five forms found in the orthodome zone [010] of sartorite, only four occur on sartorite-α. The latter, however, possesses thirteen forms not found on other sartorite crystals. This shows in a striking fashion that the elements of Trechmann and of Smith and Solly differed as they did because they were designed to fit the peculiarities of particular crystals.

¹ G. Tunell and C. J. Ksanda, Journ. Washington Acad. Sci., 1936, vol. 26, p. 509. [M.A. 7-81.]   ² C. Palache, Amer. Min., 1938, vol. 23, p. 823.