

# RULES FOR THE CONVENTIONAL ORIENTATION OF CRYSTALS

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## ABSTRACT

The following rules are recommended for the conventional orientation of a crystal. They are intended to apply to all systematic descriptions, either morphological or structural.

1. The cell chosen to express *the* lattice should be the smallest cell having full lattice symmetry; to be defined by the shortest three non-coplanar translations, unless otherwise prescribed by the symmetry.

2. The axial cross should be right-handed.

3. The cell edges should be named  $c, a, b$  so that  $c < a < b$ , unless otherwise prescribed by the symmetry (in the monoclinic system, *e.g.*, the rule becomes  $c < a$ ).

4. The coordinate axes should be directed by the following conventions: (a) In the triclinic system,  $\alpha$  and  $\beta$  obtuse; (b) in the monoclinic system,  $\beta$  obtuse. Letting  $\phi(010) = 0$ , these conditions are respectively equivalent to: (a)  $\phi(001) < \phi(100)$ ; (b)  $\phi(001) = \phi(100) = 90^\circ$ .

Alternative rules ( $a < b < c$ , with  $\beta$  and  $\gamma$  obtuse; or  $b < c < a$ , with  $\gamma$  and  $\alpha$  obtuse) are provided for special problems, where the standard rules ( $c < a < b$ , with  $\alpha$  and  $\beta$  obtuse) would prove unsuitable.

Rules for the triclinic system, recently proposed by others, are discussed. The rule " $\alpha, \beta, \gamma$  all obtuse" contains a superabundant condition and hence cannot be applied in all cases. The rule " $\phi(001) < 90^\circ$ " is less natural than " $\phi(001) < \phi(100)$ ."

## INTRODUCTION

In 1933 Mélon and I published an attempt to systematize the conventions for the orientation of a triclinic crystal. The proposed rules were restated in a more precise form, shortly afterwards, in a joint paper (Donnay, Tunell, and Barth, 1934), which also included rules for the orientation of monoclinic and orthorhombic crystals. At that time the distinction had to be drawn between the *morphological lattice*, for which the Law of Haüy-Bravais held true, and the *structural lattice*, which defined the true periodicity of the crystal architecture as revealed by x-ray diffraction. The two lattices were not in agreement for all crystalline species, and it was recognized that different sets of conventional rules might have to be used in morphology and in structure. The rules proposed at that time were intended for morphological descriptions only.

Since then progress has been made in the field of the relationships between external form and internal structure of crystals. Present day morphological methods of crystal analysis usually lead to a lattice strictly proportional to the structural lattice; in favorable cases the latter can even be predicted in absolute dimensions, provided the chemical formula

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and the density of the compound be known. In other words, the two concepts of *morphological lattice* and *structural lattice* have now been unified—there is only one lattice, the same one for both the morphologist and the leptomorphologist. These concepts, which had been readily accepted in mineralogical circles, may have already outlived their usefulness. A single set of rules for the conventional orientation of crystals, to be used in structural as well as in morphological descriptions, now appears extremely desirable.

#### THE CRYSTAL LATTICE

Morphologists seem to have rallied to the idea that the crystal lattice should provide the coordinate system to be used—the lattice, that is to say the expression of the crystalline tri-periodicity. Except for very special reasons, a former *morphological lattice* will usually be discarded if different from that obtained by *x*-rays. Conversely, structural results in disagreement with morphological findings should be scrutinized anew, and either confirmed or invalidated.<sup>1</sup>

#### THE CHOICE OF THE UNIT CELL

The first condition imposed on the unit cell chosen to define the lattice is that it should possess the full symmetry of the lattice. This condition must be considered in all systems except the triclinic.

The second rule is to choose the smallest cell that fulfills the first condition. Exceptions to this rule are as follows: In the monoclinic and orthorhombic systems, the Miller cell is used rather than the Lévy cell;<sup>2</sup> in the hexagonal system, a rhombohedral lattice should preferably be referred to the *R*-centered hexagonal cell.<sup>3</sup>

Morphologists, I believe, would be prepared to adhere to this rule, even though it may entail the reorientation of numerous minerals as, for exam-

<sup>1</sup> This has happened. Tourmaline was first assigned a simple hexagonal lattice on the basis of *x*-ray work, in contradiction to remarkable morphological extinctions that proclaimed the *R*-centering; on re-examination, the error was discovered (Buerger and Parrish, 1937). A mistake in the determination of the unit cell of aramayoite by *x*-ray work was found by morphological analysis (Berman and Wolfe, 1939). In the case of stephanite an aberrant spot on a Weissenberg picture had led to a space-group different from that indicated by the good morphological development of the crystals; additional photographs confirmed the morphological result (Taylor, 1940). The polemics about chalcopyrite too could have been settled by the morphological evidence, which leads to the correct indices {112} for the pseudo-tetrahedron, long erroneously symbolized as {111}.

<sup>2</sup> In other words: The *b* axis of a monoclinic crystal must be the 2-axis of the lattice; the *c* and *a* axes must lie in the plane of symmetry of the lattice. The cell edges of an orthorhombic crystal must be the 2-axes of the lattice.

<sup>3</sup> A statement of the rhombohedral axial elements should, however, accompany the description in terms of the *R*-centered hexagonal cell.

ple, in the tetragonal system, where body-centered species were often described in the face-centered setting.

As to structural crystallographers, one will notice that the *International Tables* (1935) make an exception to this rule in the case of crystals belonging to the class  $\bar{4}2m$ , the multiple cell being preferred whenever necessary to avoid the orientation  $\bar{4}m2$ . Thus, their conventional setting<sup>4</sup> of the space group  $D_{2d}^5$  is not  $P\bar{4}m2$ , but  $C\bar{4}2m$ ; likewise,  $D_{2d}^9$  is not written  $I\bar{4}m2$ , but  $F\bar{4}2m$ . The same policy is again followed in classes  $\bar{6}m2$ ,  $\bar{3}2/m$ ,  $32$ ,  $3m$ , in order to obviate the necessity of using the orientation  $\bar{6}2m$ ,  $\bar{3}12/m$ ,  $312$ ,  $31m$ . This probably was a concession to some old conventions governing the setting in such classes. They may well be discarded now, for the sake of uniformity, as was done by Buerger in his recent book (1942).

In cases where the cell is not imposed by the symmetry (triclinic and monoclinic systems), the cell with the shortest translations is chosen. This convention offers no disadvantage whatsoever in the triclinic system, where it seems to be universally accepted. In the monoclinic system, the rule must apply only to the choice of the  $c$  and  $a$  axes. It may conflict with two conventions of the *International Tables*, which in case of centering propose to make the lattice base-centered ( $C$ ), and in case of glide advise to make the glide-direction the  $c$  axis. The advantages of the rule of the shortest translations should outweigh all other considerations in most instances. Examples of difficulties have been encountered in sylvanite, realgar, lorandite, lanarkite (see appendix).

#### NAMING THE AXES

The naming of the axes is imposed by the symmetry of the lattice, in all except the trimetric systems. Two axes ( $c$ ,  $a$ ) in the monoclinic system and all three axes ( $c$ ,  $a$ ,  $b$ ) in the triclinic and orthorhombic systems need be conventionally labelled.

The time-honored morphological rule was to set the axis of the *main zone* vertical (making it the  $c$  axis). It must be abandoned, at least in that form, as it cannot be applied by structural workers who may be dealing with crystals devoid of faces. The concept of the main zone always lacked clarity; it has been construed to mean a zone of elongation, a zone perpendicular to a tabular habit, a zone rich in faces, etc. Donnay, Tunell, and Barth (1934) defined it as the direction of elongation in all cases except that of tabular orthorhombic crystals. Peacock (1937a) added another exception, namely that in tabular, pseudo-dimetric crystals, the plane of flattening should become the base (001).

<sup>4</sup> For the conventional orientation of the *International Tables*, the space-group symbol is shown in italics in Donnay and Harker's *Tables* (1940).

Clearly, if the new conventional rules are to be adopted by structural crystallographers, they must be expressed in terms of lengths of axial translations. Naumann's old rule to take  $a < b$ , first proposed for orthorhombic crystals, is now widely accepted for triclinic crystals as well; it should be retained, but it does not suffice. According to the Law of Bravais,<sup>5</sup> if a crystal is set with its direction of elongation vertical,  $c$  should be the smallest translation. The morphologists' rules as to the naming of the axes can thus be interpreted as:  $c < a < b$ . This convention is applicable to both the triclinic and orthorhombic systems, if the provisos concerning tabular habits be abandoned. In the monoclinic system, the rule reduces to  $c < a$ .

The monoclinic rule ( $c < a$ ) was proposed by Barker (1930), albeit for other purposes, and by Donnay, Tunell, and Barth (1934, p. 446). The rule  $c < a < b$ , proposed by Peacock (1937*a*, p. 596) for usually elongated triclinic crystals, has been used in orthorhombic cases too. In fact this convention has been rather generally adopted by mineralogists in the past five years; Buerger (1942, p. 366) admits that the custom "prevails."

Buerger (1942) proposes to replace the prevailing custom ( $c < a < b$ ) by the rule  $a < b < c$ . His case against the convention  $c < a < b$  is not convincing: (1) He writes (p. 367) that the ultimate explanation of crystal habit depends upon packing and bonding of atoms rather than identity periods. I do not wish to question this statement, but it so happens that, in most cases, the packing and bonding explanation coincides with that based on identity periods.<sup>6</sup> (2) He says (p. 366) that "though it is true that the choice of labels is arbitrary, the same arguments can be advanced against the choice of this order ( $c < a < b$ ) as against the choice of the order  $\gamma < \alpha < \beta$  for refractive indices." The question then becomes one of pure formalism. While it is true that the ordinal arrangement is very simple, it may be pointed out that any one of the three cyclic permutations ( $cab$ ,  $abc$ ,  $bca$ ) is just as elegant as any other; in fact the rule  $c < a < b$  could be preferred, on formalistic grounds alone, because it reduces to  $c < a$  in the monoclinic system.

<sup>5</sup> This aspect of the Law of Bravais is not commonly known, or appreciated: a crystal is usually elongated parallel to the lattice row of highest *linear density* (number of nodes per unit of length on the row). A statement of this law may be found in Mauguin's book on crystal structure (1924).

<sup>6</sup> Although the Law of Bravais is not perfect and, even in its generalized form, remains susceptible of refinements, it nevertheless embodies a mass of observed facts which—as such—cannot be lightly dismissed. Friedel's imposing evidence (1904, 1907) established the empirical character of the law, experimentally valid regardless of any of the speculations that led Bravais to formulate it. The accumulated x-ray data on crystals have confirmed the relation of habit to lattice periods in the majority of cases.

## DIRECTING THE AXES

Most modern crystallographers use the right-handed system of coordinates; the axial cross being conventionally so oriented that the  $c$  axis is positive upward, the  $a$  axis toward the observer, the  $b$  axis to the right of the observer.

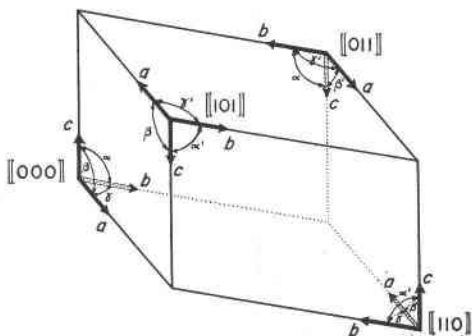


FIG. 1. The four ways of directing the named axes so as to obtain a right-handed axial cross.

A triclinic cell having been chosen, and its axes named (according to any convention) but not directed, there are four ways of choosing a right-handed system of coordinates. This can be visualized (Fig. 1) by placing axial crosses at the cell corners  $[[000]]$ ,  $[[011]]$ ,  $[[101]]$ ,  $[[110]]$ . These four axial crosses differ by the values of their interaxial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  (respectively between the axes  $bc$ ,  $ca$ ,  $ab$ ). If at any corner of the cell, say  $[[000]]$ , the interaxial angles are  $\alpha$ ,  $\beta$ ,  $\gamma$ ; then they will be  $\alpha$ ,  $\beta'$ ,  $\gamma'$ , at  $[[011]]$ ;  $\alpha'$ ,  $\beta$ ,  $\gamma'$ , at  $[[101]]$ ;  $\alpha'$ ,  $\beta'$ ,  $\gamma$ , at  $[[110]]$ ; where the primed letters designate supplementary angles ( $\alpha' = 180^\circ - \alpha$ ,  $\dots$ , etc.). At any corner, say  $[[000]]$ , the interaxial angles may have any values, in general different from  $90^\circ$ , acute or obtuse. All the possibilities are summarized in Table 1, where an acute angle is represented by a + sign and an obtuse one by a - sign.

The tabulation shows that only in one half of the cases (possibilities Nos. 1, 2, 3, 4) will one be able to find an axial cross with all three interaxial angles obtuse. In every case, on the other hand, the choice of the axial cross is uniquely determined by the condition that two stated angles, say  $\alpha$  and  $\beta$ , be obtuse. The only convention necessary for directing the axes (assuming a right-handed system of coordinates) is thus that the interaxial angles  $\alpha$  and  $\beta$  be both obtuse. This rule was recommended by Donnay, Tunell, and Barth in 1934. It can be variously stated: by saying that the  $a$  axis should slope to the front ( $\beta > 90^\circ$ ) and the  $b$  axis to the right ( $\alpha > 90^\circ$ ), or, more simply, that the base (001) should slope

TABLE 1. ACUTE OR OBTUSE CHARACTER OF THE INTERAXIAL ANGLES IN THE FOUR RIGHT-HANDED AXIAL CROSSES FOR EACH OF THE EIGHT POSSIBILITIES

Possi- bilities	Corner [[000]]			Corner [[011]]			Corner [[101]]			Corner [[110]]		
	$\alpha$	$\beta$	$\gamma$	$\alpha$	$\beta'$	$\gamma'$	$\alpha'$	$\beta$	$\gamma'$	$\alpha'$	$\beta'$	$\gamma$
1	-	-	-	-	+	+	+	-	+	+	+	-
2	-	+	+	-	-	-	+	+	-	+	-	+
3	+	-	+	+	+	-	-	-	-	-	+	+
4	+	+	-	+	-	+	-	+	+	-	-	-
5	-	-	+	-	+	-	+	-	-	+	+	+
6	-	+	-	-	-	+	+	+	+	+	-	-
7	+	-	-	+	+	+	-	-	+	-	+	-
8	+	+	+	+	-	-	-	+	+	-	-	+

N.B.—The character of an angle is indicated by the sign of its cosine: acute angle, +; obtuse angle, -.

forward and to the right of (100). In terms of the usual azimuthal angles of face poles, letting  $\phi(010)=0$ , it is also equivalent to the condition  $\phi(001) < \phi(100)$ .

Buerger proposes (1942, p. 366) to "take  $+a$ ,  $+b$ , and  $+c$  in such directions that the interaxial angles  $\alpha$ ,  $\beta$ , and  $\gamma$  are all obtuse." The interesting corollary of this rule, he points out, is that "the interaxial angles  $\alpha^*$ ,  $\beta^*$ , and  $\gamma^*$ , of the reciprocal cell are acute." The corollary is true, but the rule unfortunately implies a superabundant condition and, as has been shown above, will lead to no solution in 50 *per cent* of the cases. It must therefore be amended.

Other crystallographers in the past had proposed the same fallacious rule of three obtuse interaxial angles. Bauer (1886, p. 99) writes: "Man stellt die Krystalle gerne so auf dass die Winkel  $\alpha$ ,  $\beta$ ,  $\gamma$  im vorderen, oberen, rechten Oktanten stumpf sind." Walker (1914, p. 137) says that "the crystal is usually so oriented that the obtuse angles formed by the three axes are all enclosed by the positive ends of the axes." Niggli (1920, p. 50) records the usual practice that one axis ( $c$ ) is placed vertically, another ( $b$ ) sloping slightly from left to right, the third one ( $a$ ) sloping relatively slightly forward; and he adds: "Alle drei Achsen bilden dann hier im vorderen rechten  $+$ -Oktanten . . . stumpfe Winkel  $\alpha$ ,  $\beta$ ,  $\gamma$  miteinander." Yet (p. 123) he gives axinite with  $\alpha$  acute and albite with  $\gamma$  acute.

In the matter of directing the axes, Peacock (1937*a*, p. 594) stated the rule that the base should slope front-right, in the belief (which I shared at the time) that it was equivalent to the condition  $\alpha$  and  $\beta$  obtuse. He

soon corrected the error (1937*b*), but decided to discard the rule in favor of the  $0 < \phi(001) < 90^\circ$  condition. Although this condition, equivalent to  $\beta$  obtuse and  $\alpha^*$  acute, does give a unique setting and has several advantages (simplicity of statement, easy recognition in gnomonic projection or on a model), it introduces into the triclinic system an artificial orthogonality concept and entails complicated consequences. Professor Peacock has now agreed<sup>7</sup> to revert to the rule  $\alpha$  and  $\beta$  both obtuse, equivalent to  $0 < \phi(001) < \phi(100)$ .

Hurlbut (1941, p. 57) adopts the rule (taken from Peacock) that the base should slope forward and to the right. If, after the words "to the right," be added "of the front pinakoid (100)," then the statement is brought in agreement with the convention  $\alpha$  and  $\beta$  both obtuse.<sup>8</sup>

It is of interest to recall that Barker (1930), in his work on goniometric determination of (non-isometric) crystalline substances, encountered the problem of determining a unique conventional orientation. For directing previously named axes in the triclinic system, he stated rules that are equivalent to taking  $\alpha$  and  $\beta$  both obtuse. Although, as Peacock pointed out (1937*b*), the Barker method was only intended as a determinative tool and not a general system of morphological descriptions, it remains true that when one reaches the stage of selecting arbitrary rules in order to attain a unique orientation (after a cell has been chosen and the axes named) no question of propriety from the morphological point of view is involved any more. It is then simply a matter of choosing rules on the sole merit of their convenience. The fact that Barker's choice was the convention " $\alpha$  and  $\beta$  both obtuse" is undeniably an argument in its favor.

Finally it remains to be stated that the rule for directing the axes reduces to  $\beta$  obtuse in the monoclinic system. This is equivalent to saying that the base should slope forward. In terms of the usual azimuthal angles of face poles, letting  $\phi(010) = 0$ , the rule is expressed:  $\phi(001) = \phi(100) = 90^\circ$ . This convention has long enjoyed universal recognition.

### CONCLUSIONS

From the foregoing considerations, it seems that the recommended set of conventional rules ( $c < a < b$ ;  $\alpha$  and  $\beta$  both obtuse) is probably as good as any other arbitrary set. It has already won wide acceptance among mineralogists.

<sup>7</sup> Private communication.

<sup>8</sup> Incidentally, note that axinite, given by Hurlbut to illustrate his rule, is still oriented as in the Dana System (1892), namely  $a:b:c=0.492:1:0.480$ ,  $\alpha=82^\circ54'$ ,  $\beta=91^\circ52'$ ,  $\gamma=131^\circ32'$ . With these elements the base does not slope to the right, but slopes considerably to the left, as  $\phi(001)$  is approximately equal to  $166^\circ$ .

In certain special problems, however, it may happen that this set of rules becomes unsatisfactory; for example, in cases of unusual habit, pseudosymmetry, homeomorphism between related species, imperfect morphological development (in the absence of *x*-ray data), etc. It is well, therefore, not to make the rule too rigid. Any orientation that can be derived from the standard one (recommended above) by cyclic permutations of the unit-lengths and the interaxial angles, should prove acceptable in such special problems. The rules could be enlarged<sup>9</sup> as follows: The axes will be named so as to satisfy the condition  $c < a < b$ , or a cyclic permutation thereof (either  $a < b < c$ , or  $b < c < a$ ). In any case the axes will be directed so as to render obtuse the interaxial angles opposite the largest two unit-lengths. (If one angle has to be acute, it will always be that opposite the smallest unit-length.)<sup>10</sup>

The choice is thus limited to the three alternatives: (1)  $c < a < b$ ,  $\alpha$  and  $\beta$  obtuse; (2)  $a < b < c$ ,  $\beta$  and  $\gamma$  obtuse; (3)  $b < c < a$ ,  $\gamma$  and  $\alpha$  obtuse.

Posnjak and Tunell (1929) gave a morphological description of the compound  $3\text{CuO} \cdot 2\text{SO}_3 \cdot 5\text{H}_2\text{O}$ , in which the elements were

$$a:b:c = 0.7805:1:1.0760, \alpha = 103^\circ 4', \beta = 99^\circ 7', \gamma = 104^\circ 48',$$

thus obeying the rule  $a < b < c$ . (The lattice was not determined by *x*-rays; therefore the above elements do not necessarily express the true periodicity.) The zone placed vertically is a zone rich in faces; the crystals are somewhat equant, tabular on {010}. This is an example of a difficult case in finding the lattice by morphology alone.

Richmond (1942) has recently reoriented inosite, with the following elements:

$$a_0 = 8.89, b_0 = 9.14, c_0 = 12.14, \alpha = 87^\circ 38\frac{1}{2}', \beta = 132^\circ 30', \gamma = 97^\circ 5\frac{1}{2}',$$

which also illustrates the rule  $a < b < c$ . The transformation matrix 010/001/100 would lead to the elements:

$$a_0 = 9.14, b_0 = 12.14, c_0 = 8.89, \alpha = 132^\circ 30', \beta = 97^\circ 5\frac{1}{2}', \gamma = 87^\circ 38\frac{1}{2}',$$

directly comparable with the former (by cyclic permutation).

#### ACKNOWLEDGMENTS

My best thanks are due to the following gentlemen, with whom I discussed the conventional rules proposed in this paper: Dr. Harry Berman (Harvard University), Dr. M. J. Buerger (Massachusetts Institute of

<sup>9</sup> Professor Harry Berman has agreed (private communication) to follow these rules as far as possible in the work he is doing on the revision of the *Dana System*.

<sup>10</sup> Professor M. J. Buerger has agreed (private communication) that, if one angle must be acute, the angle opposite the smallest unit-length should be the acute one.



Technology), Dr. David Harker (General Electric Co.), Dr. W. J. Kirkpatrick (Hercules Experiment Station), Dr. M. A. Peacock (University of Toronto), Dr. Franco Rasetti (Université Laval), Dr. G. Tunell (Geophysical Laboratory).

The treatment of the four monoclinic species (Appendix I) is based on the work I did at Harvard University, during the summer of 1937, in connection with the revision of Dana's *System*. It is a pleasure to recall the fruitful discussions I had at the time with Professor Charles Palache and his co-workers.

## APPENDIX I MONOCLINIC CRYSTAL SYSTEM

### *Sylvanite*

Schrauf (1878) chose the following axial elements:  $a:b:c=1.6339:1:1.1265$ ,  $\beta=90^{\circ}25'$ , intended to bring out a remarkable orthorhombic pseudo-symmetry.

Friedel (1904b, p. 410) found that the lattice defined by the Schrauf elements would, provided it be centered on  $\{010\}$ , give the Law of Bravais an adequate expression.

The structural lattice (Tunell and Ksanda, 1937), however, can only be obtained by a halving of the  $b$  unit-length in addition to the  $\{010\}$ -centering. The  $x$ -ray investigation revealed the fact that the plane of monoclinic symmetry is a glide-plane, with glide-component in the direction of Schrauf's  $a$  axis. Following the recommendations of the *International Tables for the Determination of Crystal Structures*, Tunell and Ksanda adopted the direction of the glide-component as their  $c$  axis and chose the smallest translation in the  $(010)$  net as their  $a$  axis.

Peacock (unpublished) proposed to take the shortest translation in the  $(010)$  plane as the  $c$  axis and the next short one as the  $a$  axis ( $c < a$ ).

The relationships between the three settings are shown in a projection of the direct lattice on the  $(010)$  plane (Fig. 2) and in the transformation matrices (Table 2).

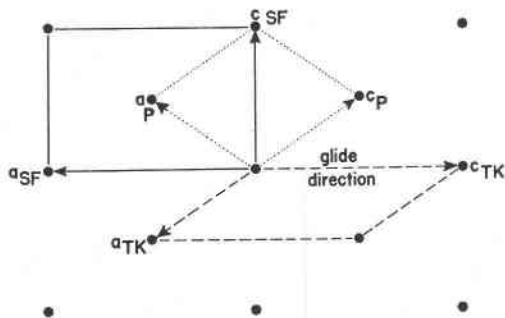


FIG. 2. Direct lattice of sylvanite projected on  $(010)$ . Solid line, Schrauf-Friedel; dashed line, Tunell-Ksanda; dotted line, Peacock. The  $b$  unit-length of Schrauf is twice that of the other two settings; the negative  $b$  of Tunell-Ksanda is the positive  $b$  of the other settings.

TABLE 2. TRANSFORMATION MATRICES FOR SYLVANITE SETTINGS

From \ To	Schrauf-Friedel	Tunell & Ksanda	Peacock
Schrauf-Friedel ( <i>B</i> -centered) (1878-1904)	1 0 0 0 1 0 0 0 1	$\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\bar{1}$ 0 0	$\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$
Tunell & Ksanda (1937)	0 0 $\bar{1}$ 0 $\bar{2}$ 0 $\bar{2}$ 0 $\bar{1}$	1 0 0 0 1 0 0 0 1	$\bar{1}$ 0 $\bar{1}$ 0 $\bar{1}$ 0 $\bar{1}$ 0 0
Peacock (unpublished)	1 0 $\bar{1}$ 0 2 0 1 0 1	0 0 $\bar{1}$ 0 $\bar{1}$ 0 $\bar{1}$ 0 1	1 0 0 0 1 0 0 0 1

N.B.—This table gives face-to-face transformations, which also serve to transform lattice vectors (hence the fractional values of some of the matrix elements).

The influence of the glide-plane of symmetry on the morphology is expressed in the space-group criterion:

$$\{h0l\} \text{ with } l \text{ even,}$$

in the case of the Tunell-Ksanda setting ( $P2/c$ ). Twelve forms have been observed in that zone; they are:

$$\bar{1}02. 100. \bar{2}02. 002. \bar{3}04. \bar{1}04. 102. \bar{5}06. 202. \bar{4}02. \bar{5}04. 104.$$

Eight out of twelve already had  $l$  even without the artifice of the "multiple indices." The forms whose indices have to be doubled are either important forms, with very small indices, which remain among the first of the theoretical sequence even after the symbols are doubled ( $\bar{1}01 = \bar{2}02$ ,  $001 = 002$ ), or uncommon forms, which are appropriately made to recede in the theoretical list of decreasing importance ( $101 = \bar{2}02$ ,  $\bar{2}01 = \bar{4}02$ ). The space-group restriction is seen to be remarkably obeyed. The setting of Tunell and Ksanda permits writing both the space-group symbol ( $P2/c$ ) and criterion ( $h0l$ , with  $l$  even) in the simplest way.

In the Peacock setting, the space-group criterion becomes

$$\{p0r\} \text{ with } (p-r) \text{ even.}$$

This is seen immediately from the transformation "Tunell-Ksanda to Peacock," since  $\{h0l\}$  to T.-K. becomes  $\{p0r\} = \{h+l. 0. h\}$ , in which  $l$  must be even. The space-group symbol must be written  $P2/n$ . The glide-component is  $\frac{1}{2}(c+a)$ . The forms in the  $[010]$  zone are written:

$$\bar{1}01. 101. 002. 200. \bar{1}03. \bar{3}01. 301. \bar{1}05. 402. 204. 105. 501.$$

The space-group symbol and criterion are a little less simply expressed than in the Tunell-Ksanda setting, but this is hardly a compelling reason for rejecting the conventions followed by Peacock.

In the Schrauf setting,  $\{h0l\}$  of Tunell-Ksanda becomes  $\{e0g\} = \{l. 0. 2h+l\}$ . This shows immediately that  $(e+g)$  must be even ( $B$ -centering criterion) and that  $e$  must be even (space-group criterion). It follows that  $g$  must also be even; so that, in the symbols  $\{e0g\}$ , all three indices must be even. Morphologically, this is the equivalent of no condition at

all, and the forms  $\{e0g\}$  should constitute a *simple zone*. They can be written as follows (all indices divided by 2):

$$100.201.101.203.102.103.001.103.203.101.302.201.$$

All other forms must obey the *B*-centering criterion:  $\{efg\}$  with  $(e+g)$  even.

#### Realgar

The case of realgar is similar.

Goldschmidt (1904) referred it to a set of axial elements,

$$a:b:c = 0.7203:1:0.4858; \beta = 113^{\circ}44',$$

which were later found to correspond to a unit cell of the structural lattice (Buerger, 1935).

The glide-component  $\frac{1}{2}a$  is directed along the *a* axis of Goldschmidt, and the space-group could be symbolized  $P2_1/a$  if the Goldschmidt cell were retained. Buerger prefers to select another unit cell, defined by the shortest two identity periods in the (010) plane. The translation  $[101]$  of Goldschmidt is smaller than his  $a[100]$  unit length; Buerger chooses it accordingly for his own *a* axis. The transformations are as follows: Goldschmidt to Buerger = Buerger to Goldschmidt =  $\bar{1}0\bar{1}/0\bar{1}0/001$ .

In Buerger's setting the glide-component is  $\frac{1}{2}(c+a)$  and the space-group is accordingly written  $P2_1/n$ .

The space-group criterion for  $\{h0l\}$  is "*h* even" in the Goldschmidt, " $(h+l)$  even" in the Buerger, setting. The conventional setting of the *International Tables* would make the glide direction that of the *c* axis, the space-group would be written  $P2_1/c$ , and the space-group criterion would be, for  $\{h0l\}$ , "*l* even." An additional criterion, for  $\{0k0\}$ , is common to all settings: "*k* even."

The relationship between the three settings is shown in Fig. 3.

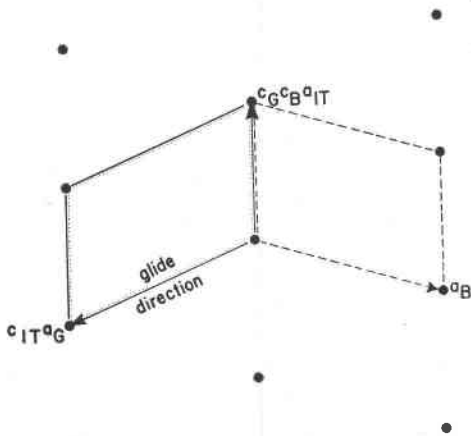


FIG. 3. Direct lattice of realgar projected on (010). Solid line, Goldschmidt; dashed line, Buerger; dotted line, *International Tables*. The negative *b* of Buerger is the positive *b* of the other settings.

Only five forms are known in the  $[010]$  zone. They are, in Goldschmidt's setting,  $202.200.201.001.\bar{2}01$ ; in Buerger's setting,  $002.200.101.\bar{1}01.501$ . Three out of the five obey the space-group criterion without multiplication of indices.

## Lorandite

The case of lorandite is perhaps the most instructive of the four considered here.

Lorandite was referred by Krenner (1894) to a set of elements that bring out the orthorhombic pseudo-symmetry, namely:

$$a:b:c = 0.8534:1:0.6650; \beta = 90^\circ 17'.$$

Goldschmidt (1898) obtained a simplification of the indices by abandoning the pseudo-orthorhombic elements and choosing the following:

$$a:b:c = 1.3291:1:1.0780; \beta = 127^\circ 33'.$$

The half diagonal of Krenner's  $ca$  mesh became the new  $c$ , the negative  $c$  was made the new  $a$ , and the  $b$  unit length was halved. The new cell was not the smallest cell of the lattice, however, as later investigation showed.

Ungemach (1923, p. 155) proposed another set of axial elements, also chosen on morphological grounds, but which corresponded to the unit cell of the lattice, as was proved nine years later (Hofmann, 1932). Goldschmidt's  $c$  was halved and became the new  $a$ , the negative  $b$  was taken as the new  $b$ , and the new  $c$  was the vectorial sum of Goldschmidt's  $a$  and  $\frac{1}{2}c$ . Ungemach's elements are:

$$a:b:c = 0.5396:1:1.0867; \beta = 104^\circ 38'.$$

The structural investigation of lorandite, made by Hofmann (1932), confirmed Ungemach's lattice. Hofmann, however, described it by means of the axial directions of Goldschmidt, whose  $c$  unit length had to be halved. The plane of symmetry was found to be a glide-plane, with glide-component  $\frac{1}{2}a$ . The space-group symbol was written  $P2/a$ ; its criterion,  $\{h0l\}$  with  $h$  even. The only forms observed in the  $[010]$  zone are, in Krenner's notation:

$$001.200.\bar{4}01.\bar{2}01.\bar{4}05.$$

TABLE 3. TRANSFORMATION MATRICES FOR LORANDITE SETTINGS

From \ To	Krenner	Goldschmidt	Ungemach	Hofmann	Peacock
Krenner 1894	1 0 0 0 1 0 0 0 1	0 0 $\bar{1}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$	$\frac{1}{4}$ 0 $\frac{1}{4}$ 0 $\frac{1}{2}$ 0 $\frac{1}{4}$ 0 $\frac{3}{4}$	0 0 $\bar{1}$ 0 $\frac{1}{2}$ 0 $\frac{1}{4}$ 0 $\frac{1}{4}$	$\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{2}$ 0 $\frac{1}{4}$ 0 $\frac{1}{4}$
Goldschmidt 1898	1 0 2 0 2 0 $\bar{1}$ 0 0	1 0 0 0 1 0 0 0 1	0 0 $\frac{1}{2}$ 0 $\bar{1}$ 0 1 0 $\frac{1}{2}$	1 0 0 0 1 0 0 0 $\frac{1}{2}$	$\bar{1}$ 0 $\bar{1}$ 0 $\bar{1}$ 0 0 0 $\frac{1}{2}$
Ungemach 1923	3 0 1 0 $\bar{2}$ 0 1 0 $\bar{1}$	$\bar{1}$ 0 1 0 $\bar{1}$ 0 2 0 0	1 0 0 0 1 0 0 0 1	$\bar{1}$ 0 1 0 $\bar{1}$ 0 1 0 0	$\bar{1}$ 0 $\bar{1}$ 0 1 0 1 0 0
Hofmann 1932	1 0 4 0 2 0 $\bar{1}$ 0 0	1 0 0 0 1 0 0 0 2	0 0 1 0 $\bar{1}$ 0 1 0 1	1 0 0 0 1 0 0 0 1	$\bar{1}$ 0 $\bar{2}$ 0 $\bar{1}$ 0 0 0 1
Peacock (unpublished)	$\bar{1}$ 0 2 0 $\bar{2}$ 0 1 0 2	$\bar{1}$ 0 $\bar{2}$ 0 $\bar{1}$ 0 0 0 2	0 0 1 0 1 0 $\bar{1}$ 0 $\bar{1}$	1 0 $\bar{2}$ 0 $\bar{1}$ 0 0 0 1	1 0 0 0 1 0 0 0 1

The choice of axes in the monoclinic system is limited to that of  $a$  and  $c$ , since  $b$  is fixed by the symmetry. The rule is to choose the shortest two lattice translations in the  $(010)$  net, the shorter of the two being taken as  $c$ . Now, neither Ungemach's nor Hofmann's cell was chosen according to that convention. Ungemach's unit length  $a$  is indeed the shortest lattice translation in the net; his  $c$ , however, is not the next shorter, but one slightly longer. Hofmann took the shortest translation for his  $c$ , but preferred to retain Goldschmidt's  $a$ , probably on account of it being the glide direction.

Peacock (unpublished) proposes to adhere to the morphologists' convention and adopts the smallest two translations: the shortest one as  $c$  and the next one as  $a$ ; this is the diagonal of Goldschmidt's mesh  $-(a+c)$ . Peacock's elements are:

$$a:b:c = 1.0873:1:0.5390; \beta = 104^{\circ}16'$$

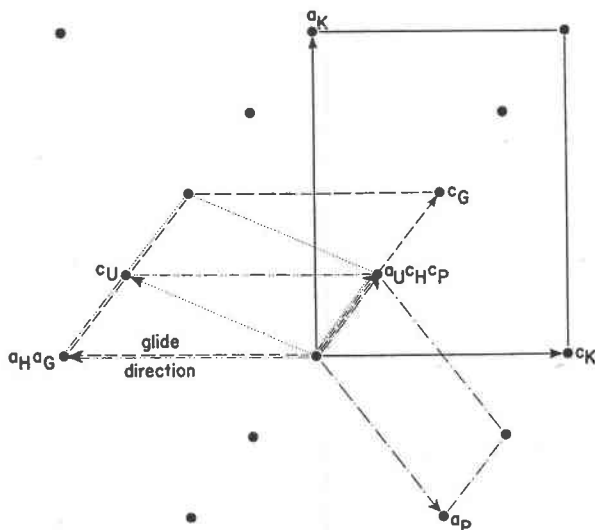


FIG. 4. Direct lattice of lorandite projected on  $(010)$ . Solid line, Krenner; dashed line, Goldschmidt; dotted line, Ungemach; dash-and-dot, Peacock; dash-and-double-dot, Hofmann. The  $b$  unit-length of Krenner is twice that of the other settings. The negative  $b$  of Ungemach and Peacock is the positive  $b$  of the other settings.

The relationships between the various settings are illustrated in Fig. 4. The transformation matrices are collected in Table 3.

What is the space-group symbol and how will the space-group criterion be expressed in the various settings?

The Krenner and the Goldschmidt settings may be left out since they do not correspond to unit cells of the lattice (the Goldschmidt cell being double; the Krenner cell, octuple).

Hofmann's setting is the simplest. Space-group  $P2/a$ . Glide-component:  $\frac{1}{2}a$ . Criterion:  $\{h0l\}$  with  $h$  even.

The setting advocated by the *International Tables*, in which the glide direction is made the  $c$  axis, would be equally simple. Space-group:  $P2/c$ . Glide-component:  $\frac{1}{2}c$ . Criterion:  $\{h0l\}$  with  $l$  even.

The Ungemach setting leads to symbols which are a little more complicated, but which are provided for in the Hermann-Mauguin system of notation. Space-group:  $P2/n$ . Glide-component:  $\frac{1}{2}(c-a)$ . Criterion:  $\{h0l\}$  with  $(l-h)$  even.

In the Peacock setting the glide direction is such that a special Mauguin symbol must be devised. The space-group can be represented by  $P2/x$ , provided the glide-component be explicitly indicated as  $\frac{1}{2}(a+2c)$ . The criterion becomes  $\{h0l\}$  with  $(h+2l)$  even. The application of the convention of the shortest translations leads here to some difficulties: impossibility to take advantage of the Mauguin notation in its simplest form for the space-group symbol, with the resulting necessity of expressing the glide-component; a complicated space-group criterion, which is apt to conceal rather than bring out the systematic "morphological extinctions" of crystal forms. The forms in the zone  $[010]$  are written, in Peacock's notation:

$$\bar{2}01. \bar{2}00. 201. 001. \bar{6}05,$$

with the criterion " $(h+2l)$  even."

#### *Lanarkite*

In all three preceding examples, the lattice is monoclinic primitive ( $P$ ). The only other monoclinic lattice mode is usually made one-face centered, either  $C$  (base centered) or  $A$  (front pinakoid centered).

Compliance to the rule of the shortest two lattice translations in the  $(010)$  plane may lead to a unit cell that is not referable to any of these modes. Lanarkite is a case in point. The unit cell defined by the shortest translations turns out to be body centered (Richmond and Wolfe, 1938), with space-group  $I2/m$  (no glide-plane). This case is provided for by the Hermann-Mauguin symbols.

## APPENDIX II

### CRYSTAL SYSTEMS OTHER THAN MONOCLINIC

#### *Tridinic system*

The question of space-group symmetry does not enter into consideration. There is never any systematic extinction of  $x$ -ray spectra on the photographic film, nor of crystal forms in the morphological development.

#### *Orthorhombic system*

The structure investigators have devised conventions of their own, in which the relative lengths of the three unit lengths play no part, the setting being governed by the recognition of screw-axes or glide-plane (*International Tables*). Perusal of the recent literature on structural descriptions will show that the structural conventions as to setting are freely disregarded. The rules proposed in this paper entail no inconvenience, since the Hermann-Mauguin space-group notation provides a symbol for any one of the six possible settings. Note that the old convention of orienting antihemihedral crystals with the 2 axis vertical ( $mm2$ ) will be disregarded if the rule  $c < a < b$  is adopted. The symmetry symbol may have to be written  $2mm$  or  $m2m$ , which is not objectionable.

#### *Tetragonal system*

The choice is always limited to two settings, at  $45^\circ$  to each other, the  $c$  axis being imposed by point-group symmetry. One setting corresponds to the smallest cell, either primitive ( $P$ ) or body-centered ( $I$ ); the other, to a multiple cell, either base-centered ( $C$ ) or all-face centered ( $F$ ). The logical course is to adopt the smallest cell in all cases. This procedure will remove the ambiguity that existed in the choice of a setting for the following classes:

$4/m\ 2/m\ 2/m$ ,  $4\ 2\ 2$ ,  $4\ m\ m$ ,  $4/m$ ,  $4$ , and  $\bar{4}$ . In the case of the chalcopyrite class, the morphologists have used the rule that the 2-axes should be taken as coordinate axes. This implies that the symmetry of the class should always be written  $\bar{4}\ 2\ m$ , in which case the unit cell may or may not be the smallest one. The proposal of adopting the smallest cell may then, in some cases, lead to the necessity of writing the symmetry  $\bar{4}\ m\ 2$ , which entails no drawback. In the setting  $\bar{4}\ 2\ m$ , the forms  $\{hhl\}$  are tetragonal disphenoids and the forms  $\{hOl\}$  are tetragonal dipyramids. In the setting  $\bar{4}\ m\ 2$ , the forms  $\{hhl\}$  become dipyramids, while the forms  $\{hOl\}$  become disphenoids. The two cases are well recognized in Friedel's *Leçons* (1926).

#### Hexagonal system (sensu vasto).

The choice, here as in the tetragonal system, is restricted to two settings. One of them is turned  $30^\circ$  (or  $90^\circ$ ) with respect to the other.

If the lattice is hexagonal (designated by  $C$  in the *International Tables*), the point-group symmetry may be one out of twelve. If the horizontal axes of coordinates  $a_1$ ,  $a_2$ ,  $a_3$ , are taken parallel to the horizontal edges of the smallest hexagonal cell, there will never be any ambiguity. The point-group symmetry of a crystal belonging to the antihemihedry with a  $\bar{6}$ -axis, may be written either  $\bar{6}\ m\ 2$  or  $\bar{6}\ 2\ m$ . The same situation exists for the parahemihedry with a  $\bar{3}$ -axis ( $\bar{3}\ 2/m\ 1$  or  $\bar{3}\ 1\ 2/m$ ), the holoaxial tetartoedry ( $3\ 2\ 1$  or  $3\ 1\ 2$ ), and the antitetartoedry ( $3\ m\ 1$  or  $3\ 1\ m$ ). In each one of these classes, the first setting was the one imposed by former morphological conventions, namely that the 2-axes or the normals to the planes of symmetry be chosen as coordinate axes. This case is similar to that of the class  $\bar{4}2m-\bar{4}m2$ .

If the lattice is rhombohedral (hexagonal- $R$ ), and is referred to the smallest  $R$ -centered hexagonal 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  $180^\circ$  (or  $60^\circ$ ) rotation about the  $c$  axis. In the first setting, the cell (which is here a triple cell) has its additional nodes located at  $\frac{2}{3}\frac{1}{3}\frac{2}{3}$  and  $\frac{1}{3}\frac{2}{3}\frac{2}{3}$ ; in the second setting, at  $\frac{2}{3}\frac{2}{3}\frac{2}{3}$  and  $\frac{1}{3}\frac{2}{3}\frac{1}{3}$ . The extinction criterion of the faces ( $hki\bar{l}$ ) 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.

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