

# ON THE CRYSTALLOGRAPHY OF AXINITE AND THE NORMAL SETTING OF TRICLINIC CRYSTALS

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## PRESENT STATUS OF THE PROBLEM OF CHOOSING MORPHOLOGICAL ELEMENTS

The problem of choosing morphological crystallographic elements reaches full generality in the triclinic system, in which the mutual intersections of any three non-tautozonal crystal planes may be taken as axes of reference with the intercepts of any crystal plane cutting all the axes to define the parameters. If the indices of the observed planes are to be small numbers only a moderate number of morphological lattices come under consideration; but since a triclinic lattice may be defined by any one of numerous cells, and any triclinic cell can be oriented in twenty-four different ways, the number of sets of geometrical elements that can be chosen for any one triclinic species is still very considerable.

Is there a single solution to the problem of choosing triclinic elements in a given case, a solution which can justly be claimed as the correct one?

The question is of fundamental theoretical interest; and anyone who has attempted to correlate the crystallographic work on a much studied triclinic species will appreciate its practical importance.

Many serious studies have been directed toward finding the "correct" elements from purely morphological data. The more important principles that have been used are the following: the Principle of Simplest Cleavages,<sup>1</sup> which claims a closed cleavage form as the true primitive form, and cleavage planes in general as fundamental (simplest) lattice planes; the Principle of Simplest Indices,<sup>2</sup> according to which the proper elements are those resulting in the simplest face-symbols; the Law of Bravais,<sup>3</sup> by which elements are properly chosen when the relative importance of the observed crystal planes corresponds best with their respective reticular densities in the inferred Bravais lattice; the Law of Complication<sup>4</sup> and other number rules,<sup>5</sup> by which the principal crystal planes are determined and indexed so that the symbol series in the main zones approach most closely the particular number series believed to represent normal zonal development; the Principle of Highest Pseudo-Symmetry,<sup>6</sup> by which elements are chosen to exhibit the highest apparent or presumed pseudo-symmetry; and the Principle of Homeomorphism or morphological analogy,<sup>7</sup> according to which elements are chosen so as to bring out geometrical similarities between species believed to be more or less closely related.

None of these procedures has brought a satisfying general solution of

<sup>1</sup> This principle originated in Haiüy's conception of crystal structure. It is also accordant with the Law of Bravais, since cleavage planes are commonly lattice planes with the greatest spacings and, therefore, the highest reticular densities.

<sup>2</sup> This is the most widely used criterion; it has been particularly emphasized in recent years by Ungemach (1923) and Barker (1930).

<sup>3</sup> Logically developed and applied to a large number of species by Friedel (1904).

<sup>4</sup> Developed by Victor Goldschmidt (1897) and applied by him and many of his pupils to numerous species. The law is connected with Goldschmidt's theory of the development of crystal faces normal to principal crystal forces and their resultants, believed to reside in the crystal particle. In effect, the Law of Complication is an expression of the Law of Bravais in the special case a simple cubic lattice.

<sup>5</sup> Other number rules are the "Zielreihen" of Haag (1913) and the "Séries" of Ungemach (1935).

<sup>6</sup> Fundamental in the ideas of Fedorov and Barker, much used by Schrauf and Tschermak, and generally more or less recognized. Closely related to the Principle of Highest Pseudo-Symmetry is what may be called the Principle of Simplest Twinning Planes of Wallerant (1899); the Principle of Least Anorthism, which demands sub-rectangular axes in preference to axes more inclined; and the Sub-Cubic Rule, by which one chooses a parametral plane that slopes like the cubic octahedron in preference to one which is inclined much more or much less steeply to the vertical axis.

<sup>7</sup> Successfully used by the systematists, Dana and Hintze, but sometimes carried to extremes by Groth and others.

the problem of selecting crystallographic elements; and the reason is that the principles on which they depend are not laws but hypothetical principles based on empirical generalizations which are only more or less true. Proceeding deductively from an adopted principle, such as the Principle of Simplest Indices or the Law of Bravais, a unique solution can always be reached, albeit indirectly and laboriously; but when the unique solutions from different postulates sometimes agree and sometimes differ, and the result of rigorous  $x$ -ray analysis gives still another solution which is entirely acceptable, it becomes increasingly clear that none of the morphological principles at present in use leads consistently to geometrical elements which can fairly be claimed as correct.

Since the analysis of crystal structures by means of  $x$ -rays has provided the means of directly determining the unique physical lattice, and this lattice always proves to be either geometrically similar to the well-chosen morphological lattice, or simply related to it, and in most cases eminently suitable for morphological purposes, it appears that morphological crystallographers have, in effect, been striving to find the physical lattice, with more or less success but never with certainty. It is not surprising that the empirical principles have proved uncertain; it is rather a matter of wonder that morphologists have in so many cases been led to adopt the lattice which has subsequently proved to be geometrically similar to the translation lattice of the crystal structure.

At this stage in the development of crystallography two courses are open: either we decide that  $x$ -ray analysis is bringing the solution of a problem which cannot be solved satisfactorily from morphological data; or, realizing that the physical lattices of only a small proportion of the known crystallized substances have been determined, we may approach the problem afresh by studying the relations of crystal forms to known structural lattices, thus learning to recognize these relations and to infer the structural lattice in other cases by choosing elements which most nearly result in similar relations. In this way the old problem of choosing geometrical elements is redefined as the problem of finding the geometrical equivalent of the structural lattice from the external geometry of the crystal; and instead of speaking of "correct elements," a vague phrase which has hitherto meant "elements which agree best with a preferred hypothetical principle," we shall consider "normal elements," meaning thereby unique geometrical elements which correspond to a cell of the structural lattice, selected and oriented according to widely accepted conventions. The "normal setting" is thus the setting which gives normal elements. These terms will be more sharply defined later, when the conventions involved have been severally stated.

The suggested course offers considerable promise of success in all but

two situations. If the crystals have very few forms, or if they are very imperfectly developed, it may be impossible to discern the structural lattice or indeed any crystallographic lattice whatever. Again, if the crystal forms show the influence of two or more related lattices it may not be possible to select the structural lattice; but in such cases, which may properly be regarded as exceptions requiring special study, there may also be valid reasons for departing from the structural lattice for morphological description.<sup>8</sup> Experience with a fair number of crystallized minerals in the triclinic, monoclinic and orthorhombic systems indicates that, with proper criteria, it will be possible in most cases except those mentioned above, to discern the structural lattice, usually by simple inspection of the gnomonic projection of the known forms.

Before attempting to formulate the criteria which promise to solve the old problem of choosing crystallographic elements, it will be necessary to examine a sufficient number of special cases. In the present paper one example is studied with due consideration of the many variables which must be taken into account in the general case of the triclinic system. The course of such an examination having been established, other cases can be rapidly treated; and eventually, if the investigation is successful, it will be possible to formulate a simple general procedure for selecting normal elements from morphological data.

#### COURSE OF THE PRESENT STUDY

As an example of the most general case, axinite has been chosen, since it is triclinic, notably oblique and somewhat variable in habit, and free from obvious pseudo-symmetry and twinning which might prejudice the choice of morphological elements. Axinite appears the more suitable for the present purpose since it has been oriented in many different ways according to the particular principles preferred by the several responsible authors. Furthermore, the only published determination of the structural lattice gives yet another setting. But this determination is manifestly faulty; and therefore, apart from the theoretical problem in hand, a redetermination is desirable.

A well-developed crystal of axinite was sketched, measured on the two-circle goniometer and projected in gnomonic projection. Using criteria which in previously studied cases had led to the structural lattice, and a few well-known and generally accepted conventions governing the choice and setting of the representative lattice cell, unique geometrical elements were obtained by inspection and direct measurement of the gnomonic projection. These elements, which fulfil all the reasonable re-

<sup>8</sup> See Ungemach (1935, p. 198) on calcite and other cases of multiple periods.

quirements of a good morphological setting, were found to differ in some respect from all those previously proposed.

The same crystal was then used for a rigorous determination of the structure lattice with the Weissenberg  $x$ -ray goniometer, by means of which the necessary six lattice elements were found directly, without reliance on the known geometry. Employing the above-used conventions to select and orient the representative cell in the determined structural lattice, unique absolute elements were obtained. These elements, which differ from the published structural elements, were found to be proportional to the elements determined from the external geometry within narrow limits of experimental error. This agreement showed that in the chosen example of the most general case it was possible to infer the proportional elements of the structure lattice from the relations of the external crystal planes, and that, therefore, the provisional criteria used for this purpose were so far adequate.

From the determined structural elements and the known composition and specific gravity of axinite the atomic content of the unit cell was obtained. Using the same crystal, a redetermination of the optical orientation in relation to the new setting was also made. Recognizing the propriety of the new setting, Professor Charles Palache contributed a definitive presentation of the crystallography of axinite, one which will, it is believed, commend itself to those who look forward to a closer correlation of the results of morphological and structural investigations.

Finally, the existing orientations of axinite are reviewed and related to the new orientation by the appropriate transformation determinants. This correlation has practical value; and the review is of interest in affording a brief history of the development of ideas on the choice of geometrical elements.

#### SEVERAL STEPS IN CHOOSING NORMAL TRICLINIC ELEMENTS

The problem of choosing crystallographic elements, morphologically or röntgenographically, resolves into three parts: (1) determination of the specific lattice; (2) choice of the representative lattice cell; (3) choice of orientation of the representative lattice cell. Thus resolved, the full problem with its many variables is easily envisaged.

*Determination of the Specific Lattice.* By specific lattice we mean the system of lattice points established by successive identity points in the crystal structure. The specific direct lattice is completely defined by any three non-coplanar identity periods in the structure of the crystal, together with the three angles made by the respective lattice rows. Similarly, the specific reciprocal lattice is defined by the reciprocals of the spacings of any three sets of non-tautozonal planes in the direct lattice,

together with the three angles made by the respective normals to the three sets of lattice planes. Both in morphological and structural practice it is convenient to work with the reciprocal lattice and derive the direct lattice by calculation.

The specific reciprocal lattice is determined directly by *x*-ray analysis; the morphological problem centers on finding the geometrically similar lattice from the relations of the observed crystal planes. The problem is solved if we can recognize the points of the first layer of the reciprocal lattice in the gnomonic projection of the known forms. This, I believe, can usually be done; but since we are proceeding inductively, it will be better to defer the necessary argument and details until later.

*Choice of the Representative Lattice Cell.* Out of the unlimited number of lattice cells which may be used to define a given space lattice, structural crystallographers have agreed to use the smallest cell with the highest symmetry of the lattice. This entirely natural and proper convention should be equally binding in morphological crystallography. In the triclinic system every simple cell has the full symmetry of the lattice; and since all simple cells have the same volume, the "smallest cell" is understood to mean the cell whose edge-lengths are the three shortest non-coplanar lattice periods, and whose axial planes are, consequently, the three non-tautozonal lattice planes with the greatest spacings. Usually this unique cell can be found immediately by inspecting a construction of the direct or reciprocal lattice; its correctness can always be tested by showing that all the ten diagonals of the direct lattice cell are longer than its edges, or that all the ten diagonal planes have smaller spacings than the axial planes.

In the gnomonic projection in which the first layer reciprocal lattice points have been distinguished and missing points in the central region restored, the desired lattice cell is simply obtained by finding the three non-tautozonal first-layer points which are nearest the center of the projection. Take the point nearest center as an axial plane, provisionally (001); name the others provisionally (011), (101). The remaining axial planes (010), (100), and all the indices are thus provisionally determined, and the chosen cell is the cell whose axial planes have the three greatest non-tautozonal spacings in the direct lattice since the respective reciprocal lattice points are the three non-tautozonal points nearest the origin.

*Orientation of the Representative Lattice Cell.* To the structural crystallographer any one orientation of a determined triclinic lattice cell will serve as well as any other. The morphological crystallographer, on the other hand, is much concerned with the orientation of a crystal with respect to fixed space directions; and in this matter it is desirable that

the structural worker consider the simple and reasonable requirements of good conventional morphological orientation.

As already stated, there are twenty-four possible orientations of a given triclinic cell. This number is readily verified: with either end of any of the three axes directed vertically upward (six possibilities) either end of either of the two remaining axes may be directed toward the observer in the vertical fore-and-aft plane (four possibilities), giving twenty-four orientations in all. If we agree to use right-handed axial systems, now in universal use, the twenty-four orientations give a like number of sets of unlike elements; if we admit left-handed axial systems, the possible number of sets of unlike elements which may be used to describe a triclinic lattice cell is raised to forty-eight.

Excluding left-handed axial systems, a unique good conventional morphological orientation of a triclinic lattice cell is reached in three steps: 1. Select the appropriate vertical axis without fixing its sense; when this has been done eight settings are possible, four with one end of the vertical axis directed upward, and four in the inverted position. 2. Let the base slope to the front and the right ( $\phi_{001}$  between  $0^\circ$  and  $90^\circ$ ;  $\alpha$  and  $\beta$  both obtuse), a condition which admits two of the eight available settings. 3. Of these two positions take the one in which the athwart axis  $b[010]$  is longer than the fore-and-aft axis  $a[100]$ . These rules express generally accepted conventions of long standing, conventions designed to place a triclinic crystal in a favorable position as seen from the usual viewpoint, in which the eye is raised about  $10^\circ$  above the crystal centre and moved about  $20^\circ$  to the right of the vertical plane containing the fore-and-aft axis.

The judicious selection of the vertical axis is of prime importance; and if this axis is properly chosen at the very outset of a morphological or röntgenographic study the final desired orientation is quickly reached. The vertical axis is properly selected from a consideration of the normal crystal habit. If a crystal species is habitually acicular or columnar, the axis of the acicular or columnar zone is almost certainly an edge of the properly chosen lattice cell; and most morphologists will set this axis vertical for the sake of appearance alone. But aside from the matter of appearance, it is highly desirable for practical reasons that the axis of habitual morphological elongation be taken as the vertical axis, since this axis is the most convenient, sometimes the only practical axis of adjustment on the Goldschmidt reflecting goniometer and the Weissenberg  $x$ -ray goniometer, instruments which have a great advantage in giving complete lattice determinations with one crystal adjustment.

In the case of crystals which are habitually elongated and tabular to a plane in the elongated zone, morphologists are less consistent in setting

the edge of the elongated zone vertical. But here the practical consideration mentioned above is equally valid and it is equally desirable that the edge of an elongated table be set upright.<sup>9</sup>

Crystals which are tabular without pronounced elongation are likely to have pseudo-dimetric lattices, clino-quadratic or clino-hexagonal, to use Schrauf's appropriate terms. Such lattices are properly set with the axis of dimetric pseudo-symmetry vertical, the plane of tabular development thus becoming the base.

Finally there is the possible but, in the triclinic system, infrequent case of habitual equant development, without consistent flattening or elongation. In such cases a study of all the available drawings of crystals of the species, assembled in Goldschmidt's *Atlas der Krystallformen*, might reveal a tendency toward elongation or flattening in certain directions, which would indicate the proper vertical axis. In a few cases, which might be expected among lattices of pseudo-cubic type, the crystal habit might give no indication of the proper vertical axis; in such cases one of the edges of the lattice cell, preferably the shortest, must be arbitrarily chosen as the vertical axis. Once this has been done, it would be frivolous for another worker to depart from this choice on the basis of one or two crystals which showed fortuitous departure from equant habit.

Once the vertical axis has been determined the only difficulty attending the unique orientation of a triclinic cell has been overcome. The two remaining rules can be immediately applied if the gnomonic projection of the external planes or the reciprocal lattice construction of the internal planes has been made on a plane normal to the adopted vertical axis. Either projection is simply turned about the vertical axis until the point (001) falls into the first quadrant ( $\phi_{001}$  between  $0^\circ$  and  $90^\circ$ ) when a vertical axial plane lies fore-and-aft. The base then slopes to the front and to the right where it is visible from the normal viewpoint. This rule is a logical extension of the inflexible rule in the monoclinic system which requires the base to slope to the front. If now the athwart axis (the macrodiagonal) is longer than the fore-and-aft axis (the brachydiagonal), and therefore the corresponding reciprocal lattice periods are in the converse relation, the desired orientation has been found. If not, the projection is inverted and viewed through the paper, and again turned

<sup>9</sup> Ungemach, in particular, has frequently departed from the rule of setting the axis of columnar or elongated tabular development vertical, often setting such an axis fore-and-aft. The only possible advantage of such a position is that an entire termination can be seen from the usual viewpoint of an inclined drawing. But this is surely unimportant as against the advantage of obtaining a projection in normal position after mounting and measuring a crystal, known or unknown, in the usual manner. In the conventional setting a view of an entire termination is always given by a plan, the simplest and clearest of drawings.



about the vertical axis until the pole of the base lies in the first quadrant; then the macrodiagonal and brachydiagonal are necessarily in their proper relation and the required orientation has been attained. The macrobrachy rule, borrowed from the orthorhombic system, originates in the fact that an orthorhombic prism presents a more favorable aspect when viewed in the general direction of the shorter diagonal.

Morphological elongation commonly takes place along the shortest lattice period, while habitual flattening, often associated with cleavage, usually follows the greatest lattice spacing, therefore transversely to the longest lattice period. Consequently the conventional orientation of habitually elongated crystals usually results in the shortest cell-edge becoming the vertical axis with the longest edge as the athwart axis; if the elongation is associated with tabular development and cleavage, these will almost certainly become side-pinacoidal. In the case of pseudodimetric crystals which are tabular to the plane containing the quasi-equivalent axes, the conventional setting places the longest cell-edge vertical.

Although the above rules are severally well recognized, they have not often been applied together to determine the desirable unique orientation of a triclinic lattice cell. One reason for this is probably the fact that although the rules are singly designed to place a crystal in a favorable position, some triclinic crystals of unusual or even typical habit may seem to present a better appearance in some other position. Since a good unique orientation is the main object, it is better in such cases not to depart from the conventional orientation but to shift the viewpoint, as is commonly done in the case of monoclinic crystals tabular to the plane of symmetry.

In review, we see that the core of the problem of finding normal triclinic elements from geometrical data may be reduced to the problem of distinguishing the first-layer points of the reciprocal structure lattice in the gnomonic projection of the external crystal planes. The proper vertical axis is chosen from a consideration of the normal crystal habit. The remaining variables are fixed by accepted rules, to which I have purposely added nothing beyond some elucidation which may serve to emphasize their validity. In the matter of the conventional orientation of a triclinic cell the recommendations given are in general agreement with those made by Donnay and Mélon (1933, p. 241) and Donnay, Tunell & Barth (1934, p. 445).

Having discussed the considerations which govern the reasoned choice of unique triclinic elements, we may proceed rapidly to their application to the chosen case of axinite.

DETERMINATION OF NORMAL ELEMENTS FROM  
THE EXTERNAL GEOMETRY

All the observations in this paper were made on a single well-developed crystal of axinite detached from a specimen from near Easton, Pennsylvania, probably the same locality as "near Bethlehem, Pennsylvania," which yielded the axinite described by Frazier (1882). The crystal is 1.3 mm. in greatest dimension, and has a light-clove color; it is bounded by twenty-one faces, all but two of which give good reflections. One zone stands out prominently as the main zone, by virtue of the size and number of its faces; the axis of this zone was therefore taken provisionally as the vertical axis on the assumption, later proved, that it is an edge of the smallest cell of the structure lattice. The crystal was sketched, measured on the two-circle goniometer, and projected gnomonically on a radius of 10 cms. The plan of the crystal on the plane normal to the axis of the main zone and the corresponding projection are shown in figure 2; an inclined view of the crystal, with the lower termination symmetrically restored, is given in figure 4.

Elements believed to correspond to the normal setting of axinite were obtained from the gnomonic projection by means of the following considerations. If it is true that planes with simple indices in the proper lattice are more probable as crystal faces than planes with complex indices, then we will expect the reciprocal lattice representation of the forms of a triclinic crystal to be a system of points which can be referred to properly chosen reciprocal lattice axes  $PQR$  by co-ordinates  $hkl$  which are simple multiples, 0, 1, 2 . . . , of properly chosen reciprocal lattice parameters,  $p_0 q_0 r_0$ . The degree of complication of the numbers  $hkl$  will be determined by the complexity of the face development and by the relative lengths of the reciprocal lattice parameters; and the likelihood of occurrence of the numbers will be roughly proportional to their simplicity. Thus on the zero-layer of the reciprocal lattice  $|h\ k\ 0|$  we shall expect the points (100), ( $\bar{1}00$ ), (010), ( $0\bar{1}0$ ), then (110), ( $\bar{1}\bar{1}0$ ), ( $\bar{1}\bar{1}0$ ), ( $\bar{1}10$ ), then symbols containing 2, 3 . . . , in order of decreasing probability, according to the already mentioned limitations. On the first layer of the reciprocal lattice  $|h\ k\ 1|$  we expect (001), (011), ( $0\bar{1}1$ ), (101), ( $\bar{1}01$ ), then symbols containing 2, 3 . . . . On the second layer of the reciprocal lattice  $|h\ k\ 2|$ , all points are already less probable since the third index is always 2; the points to be expected are those with the smallest indices, namely (012), ( $0\bar{1}2$ ), (102), ( $1\bar{0}2$ ), etc. The third and higher reciprocal lattice layers will be still more weakly occupied.

Now the gnomonic projection is a two-dimensional representation of the reciprocal lattice. The direction lines to the vertical faces are parallel

to lines joining the origin of the reciprocal lattice (000) to the corresponding reciprocal lattice points on the zero-layer. Let the plane of the gnomonic projection be the first layer of the reciprocal lattice; then the points in the plane of the gnomonic projection are either first-layer points ( $h k 1$ ) in their true position in the reciprocal lattice, or projections of higher layer points ( $h k n$ ), as given by the points of intersection of the plane of the gnomonic projection with lines joining the origin (000) to the corresponding reciprocal lattice points in the higher layers.

As already stated our problem is solved if we can distinguish the first-layer points from those on higher layers. The foregoing considerations lead us to expect the first layer will be occupied at all its points up to limits determined by the complexity of the face-development and the relative lengths of the lattice parameters. The first-layer points should therefore form a plane lattice in which the distances of the points in any row make an arithmetic series when measured from any point in that row. All points not at the nodes of this plane lattice are necessarily projections of reciprocal lattice points on higher layers, a point lying midway between two first-layer points representing a point on the second layer, a point lying one third of the way between two first-layer points representing a third-layer point, and so forth. Experience shows that there may be erratic omissions of reciprocal lattice points within the region of probability, and these constitute frequent and serious exceptions to the Law of Bravais; but we do not find systematic omissions in a simple triclinic lattice.

Since we have reason to believe that the first layer will be more fully represented by face-points than any higher layer, the first-layer points will be those points which fall on the plane lattice accommodating most of the points on the gnomonic projection without systematic omissions. Inspection of figure 2 shows that there is only one plane lattice that meets this requirement, namely that which has the points  $c r e v y n Y x s$  as nodal points. Only two terminal planes remain,  $z \delta$ , obviously second layer points. Any other choice of first layer lattice points results in systematic omissions which are inadmissible.

The first-layer points being fixed, the reciprocal lattice is fixed, and it only remains to select the cell whose axial planes are the three non-tautozonal planes with the greatest spacings, and set it in the conventional position. Taking the first-layer point which is nearest the centre of the projection, namely  $c$ , as an axial plane, provisionally (001), the next nearest,  $r$ , provisionally as (011), and the next nearest,  $v$ , provisionally as (101), the desired lattice cell is completely defined;  $a, b, n$ , receive the symbols (100), (010), (111), respectively, and all the remaining points are immediately indexed by inspection.

The chosen vertical axis proves to be the axis of the zone which is habitually the main zone of axinite and the one which has been chosen as the vertical zone by most previous workers. The base  $c(001)$  slopes to the front and to the right ( $\phi = 89^\circ 55'$ , calc.) and the reciprocal lattice period  $cv$  ( $p_0' = 1.303$ ) is greater than the period  $cr$  ( $q_0' = 0.999$ ), and consequently the direct period  $b[010]$  is greater than the direct period  $a[100]$ , as required by the macro-brachy rule. The direct lattice cell is thus oriented in the one position out of twenty-four which satisfies the stated conventions; and the problem of finding normal elements for the given triclinic crystal appears to be solved, in less time than it takes to describe the procedure.

At this juncture it will be well to emphasize an important difference between the mode of discussion developed here and any procedure that accepts the Law of Bravais as strictly true. On the crystal used the faces  $c(001)$ ,  $a(100)$ , and  $a'(\bar{1}00)$  are small and they are habitually among the weaker planes of axinite. On a smaller crystal these planes might well have been absent; and anyone believing that axial planes, whose reticular densities are among the highest in any lattice are necessarily important crystal planes, would be forced to take planes other than  $c$  and  $a$  as axial planes. This is probably the reason why the French orientations take the large steep plane  $r$  as the base, giving highly oblique lattices. With the present mode of discussion the final result would have been the same even if  $c$  and  $a$  were entirely absent; the remaining points are more than sufficient to establish the reciprocal lattice with complete certainty.

With the chosen elements the faces on the crystal are, on the zero layer:  $b(010)$ ,  $b'(0\bar{1}0)$ ,  $a(100)$ ,  $a'(\bar{1}00)$ ,  $m(110)$ ,  $m'(\bar{1}\bar{1}0)$ ,  $M(\bar{1}\bar{1}0)$ ,  $M'(\bar{1}\bar{1}0)$ ,  $l(\bar{1}\bar{2}0)$ ,  $l'(\bar{1}\bar{2}0)$ ; first layer:  $r(011)$ ,  $e(0\bar{1}\bar{1})$ ,  $v(101)$ ,  $\gamma(\bar{1}01)$ ,  $n(111)$ ,  $Y(\bar{1}\bar{1}\bar{1})$ ,  $x(\bar{1}\bar{1}\bar{1})$ ,  $s(\bar{1}\bar{2}\bar{1})$ ; on the second layer:  $z(012)$ ,  $\delta(112)$ .

By direct measurement on the gnomonic projection the normal projection elements of the axinite crystal were read off as follows:

$$p_0' = 1.303, q_0' = 0.999; x_0' = 0.143, y_0' = 0.000; \nu = 102^\circ 35'.$$

By simple calculation these elements give the following polar elements, which are the geometrical elements of the chosen reciprocal lattice cell:

$$p_0 : q_0 : r_0 = 1.290 : 0.989 : 1; \lambda = 90^\circ 00', \mu = 82^\circ 07', \nu = 102^\circ 35'$$

#### DETERMINATION OF NORMAL ELEMENTS FROM X-RAY MEASUREMENTS

A precise determination of the structure lattice of axinite was made in the x-ray laboratory of the Geophysical Laboratory in Washington, with the instructive assistance of Dr. Barth, Dr. Tunell and Mr. Ksanda.

The instrument that was used is a Weissenberg  $x$ -ray goniometer built in the Fysisk Institutt of Norges Tekniske Høyskole at Trondheim, Norway, and improved by Tunell and Ksanda.<sup>10</sup> The effective radius of the camera is 35.0 mm., and the translation of the film carriage corresponding to 180° of rotation is 111.5 mm. The films were discussed by preparing two-fold enlargements with a precision pantograph made by Ksanda (1931), and projecting a sufficient number of reciprocal lattice layers by the construction of Schneider (1928), care being taken to plot lengths and angles in the proper sense. With these provisions, reciprocal lattice projections from Weissenberg photographs about a given axis are comparable with the corresponding gnomonic projection of the external planes, both in position with respect to the axis and meridian of reference, and in aspect; and the six absolute elements of the triclinic lattice are obtained by  $x$ -ray measurements alone, without reliance on the known external geometry of the crystal.

The photographs were made with Cu-K radiation which gave three to five layer-lines about the equator in rotation photographs and seven to eleven orders of diffractions from the more widely-spaced lattice planes on the Weissenberg photographs. The final values of the spacings of the axial planes were obtained by applying a small correction to allow for the crystal thickness, and placing most reliance on the higher order spots in which the  $\alpha_1$  and  $\alpha_2$  diffractions were clearly resolved and the effect of crystal thickness is at a minimum. Reciprocal axial angles were obtained by measuring the distances between rows of diffraction spots representing successive orders of diffraction from the axial planes, using a light box provided with a long glass cursor riding on a scale reading to a tenth of a millimeter by means of a vernier.

A rigorous although not highly accurate determination of a triclinic lattice is obtained from a rotation photograph about any zone edge and a first-layer Weissenberg photograph about the same axis. Better values are obtained if a zero-layer Weissenberg photograph is also made about the axis of reference; and with care this method gives excellent values,

<sup>10</sup> The improvements are the adaptation of the instrument to the equi-inclination method of Buerger (1934); and the addition of a graduated circle and two graduated arcs on the goniometer head, whereby a precision transfer of the head can be made from the  $x$ -ray goniometer to the Goldschmidt two-circle reflection goniometer suitably modified to receive the head in a precision bearing. Both the  $x$ -ray goniometer and the Goldschmidt reflection goniometer were fitted with verniers for reading the position of the head about its own axis on the new small circle permanently attached to the head. This circle lies in a plane perpendicular to the axis of the head. These additions permit a precision correlation of the external faces of a crystal with its structural (diffraction) planes, by the use of a direct beam spot made on each film when the external faces of the crystal are oriented in a defined manner. The method of carrying out this correlation between form and structure was worked out by Tunell and Ksanda and has been applied by them in their investigations of calaverite and krennerite" (*personal communication from Dr. George Tunell*).

as shown by the lattice determination of chalcantite by Barth and Tunell (1933). But even with this method two of the lattice constants, namely the two reciprocal axial angles not included by planes in the zone of reference, are not very sharply defined since they are measured by the small horizontal shear of the first layer of the reciprocal lattice with respect to the zero-layer. The greatest accuracy is obtained by making additional zero-layer Weissenberg photographs about two further lattice rows; and subsequent calculations are greatly simplified if the three chosen axes of rotation are also the three non-coplanar lattice rows with the shortest periods. In this way each of the three reciprocal axial angles can be accurately measured on a zero-layer photograph, and three pairs of accurate values are obtained for the spacings of the axial planes. The less accurate values of the principal lattice periods obtained from rotation photographs about the three axes can then be neglected. This was done in the case of axinite with little difficulty, since the axis of the main zone of the crystal proved to correspond to one of the three shortest lattice periods, and both the remaining principal lattice rows were easily recognized as zone-edges on the crystal.

From the rotation photograph and the zero- and first-layer photographs about the axis of the main zone [001] the following values were obtained as the preliminary reciprocal elements of the simple translation cell with the shortest edges. Below are given for comparison the normal reciprocal elements previously obtained from the external geometry of the measured crystal.

$$a^* = 0.2225, \quad b^* = 0.1714, \quad c^* = 0.1733; \quad \alpha^* = 90^\circ 00', \quad \beta^* = 80^\circ 04', \quad \gamma^* = 102^\circ 33'$$

$$a^* : b^* : c^* = 1.284 : 0.988 : 1;$$

$$p_0 : q_0 : r_0 = 1.290 : 0.989 : 1; \quad \lambda = 90 \ 00, \quad \mu = 82 \ 07, \quad \nu = 102 \ 35$$

Except for the difference of  $2^\circ$  between the angles  $\beta^*$  and  $\mu$ , an insensitive angle when measured by reciprocal lattice shear, the agreement is good, and we have satisfying proof that the morphological discussion led to the smallest cell of the structure lattice. This result is gratifying, not on account of any difficulty in the morphological determination, but rather on account of the ease with which it was made, there being apparently no reasonable alternative to the adopted choice of elements.

The lattice constants obtained from rotation and Weissenberg photographs about the principal lattice axes are as follows:

| Axis of rotation       | From rotation photographs | From Weissenberg photographs |                   |                    |                           |
|------------------------|---------------------------|------------------------------|-------------------|--------------------|---------------------------|
|                        |                           | $d_{100}$                    | $d_{010}$         | $d_{001}$          |                           |
| [100]                  | $a_0 = 7.1 \text{ \AA}$   | —                            | 8.95 $\text{\AA}$ | 8.84 $\text{\AA}$  | $\alpha^* = 89^\circ 55'$ |
| [010]                  | $b_0 = 9.1$               | 6.91 $\text{\AA}$            | —                 | 8.85               | $\beta^* = 82 \ 04$       |
| [001]                  | $c_0 = 9.0$               | 6.91                         | 8.97              | —                  | $\gamma^* = 102 \ 33$     |
| Adopted mean spacings: |                           | 6.91 $\text{\AA}$            | 8.96 $\text{\AA}$ | 8.845 $\text{\AA}$ |                           |

The Weissenberg values give the following final structural lattice elements for axinite, with which are given for comparison Palache's geometrical elements subsequently deduced from numerous old and new measurements referred to the normal setting:

$$\begin{array}{llll}
 a_0=7.151 \text{ \AA}, & b_0=9.184 \text{ \AA}, & c_0=8.935 \text{ \AA}; & \alpha=91^\circ 52', \quad \beta=98^\circ 09', \quad \gamma=77^\circ 19' \\
 a_0:b_0:c_0=0.7787:1:0.9729; & & & \text{(Peacock)} \\
 a:b:c=0.7789:1:0.9763; & & \alpha=91 \text{ } 51\frac{1}{2} & \beta=98 \text{ } 04, \quad \gamma=77 \text{ } 14 \\
 & & & \text{(Palache)}
 \end{array}$$

The excellent agreement confirms the belief of Barth and Tunell (1933) that careful *x*-ray goniometer measurements yield lattice elements comparable in accuracy with those obtained with the reflecting goniometer. With the additional Weissenberg photographs about two more axes the *x*-ray elements seem to be better than those obtained from the external planes of a single good crystal.

The volume of the unit cell is  $V_0=566.8$  cub.  $\text{\AA}$ ; the molecular weight of the established formula of axinite,  $\text{HBA}_2\text{Ca}_2(\text{Mn, Fe})\text{Si}_4\text{O}_{16}$ , is 569.5, assuming that Mn and Fe are present in equal atomic proportions. With two formula weights in the unit cell we obtain a calculated density which lies near the upper end of the range of measured densities, as shown by comparison with the values taken from Dana (1892):

Density of axinite

|       |   |
|-------|---|
| 3.271 | Haidinger                                 |
| 3.294 | Rammelsberg                               |
| 3.299 | Genth                                     |
| 3.306 | Genth                                     |
| 3.316 | Peacock (from <i>x</i> -ray measurements) |
| 3.358 | Genth                                     |

The unit cell of axinite therefore contains  $\text{H}_2\text{B}_2\text{Al}_4\text{Ca}_4(\text{Mn, Fe})_2\text{Si}_8\text{O}_{32}$ , in which either Mn or Fe may preponderate and small proportions of Mg and other metals may enter.

RELATION OF THE NEW LATTICE ELEMENTS TO THOSE OF  
GOSSNER AND REICHEL

Gossner and Reichel (1932) made a determination of the structural lattice of axinite on a crystal from Bourg d'Oisans, combining measurements on a reflecting goniometer to determine an axial ratio, with *x*-ray measurements of the identity periods in a number of lattice rows whose angular relations were known from the external geometry. To show that their cell edges are the three shortest identity periods in the lattice the authors list five further measured and calculated periods all of which are greater than their axial periods. The cell elements of Gossner and Reichel are related to ours as follows:

| Gossner & Reichel                        | Peacock  |
|--|--|
| $a = T[100] = 12.87 \text{ \AA}$         | $T[110] = 12.819 \text{ \AA}$ (calc.)                    |
| $b = T[010] = 7.15 \text{ \AA}$          | $T[\bar{1}00] = 7.151 \text{ \AA} = a_0$                 |
| $c = T[001] = 8.91 \text{ \AA}$          | $T[001] = 8.935 \text{ \AA} = c_0$                       |
| $\alpha = [010]:[001] = 82^\circ 26'$    | $[\bar{1}00]:[001] = 81^\circ 51' = 180^\circ - \beta$   |
| $\beta = [001]:[100] = 95 \text{ } 20$   | $[001]:[110] = 95 \text{ } 52\frac{1}{2}$ (calc.)        |
| $\gamma = [100]:[010] = 135 \text{ } 35$ | $[110]:[\bar{1}00] = 135 \text{ } 39\frac{1}{2}$ (calc.) |

Two of Gossner and Reichel's axial periods,  $b$ ,  $c$ , are thus the shortest and second shortest periods in the axinite lattice while their third axial period,  $a$ , is the longer diagonal of our basal plane, as shown by the dotted cell in figure 3, and is the sixth shortest period in the lattice. It is difficult to understand this error since the roughest construction of Gossner and Reichel's lattice, which is essentially the same as ours as far as the lattice points are concerned, shows at once which are the shortest lattice periods. Gossner and Reichel also obtain a cell content with two formula weights which they write as follows:  $2\{(\text{SiO}_4)_4\text{Al}_2\text{B Ca}_2\text{MgH}\}$ ; but this formula is not acceptable since it admits Mg as an essential constituent, whereas it is only an accessory, and neglects Mn and Fe which are always present in important amounts.

#### DETERMINATION OF THE OPTICAL ELEMENTS

In view of the many existing crystallographic orientations of axinite, the possibility of real variations in the optical orientations in different axinites, and the chances of error in the published optical orientations, it seemed better to redetermine the optical orientation with reference to the new crystal setting rather than to transform an existing orientation. This was done on the Fedorov stage using the same crystal that was used for morphological and röntgenographic study. The orientation of the crystal was found by the satisfactory method of bringing a sufficient number of recognized crystal faces into the vertical fore-and-aft plane of the microscope and plotting the circle readings on the stereographic net. After bringing the three mutually rectangular planes of continuous extinction likewise into the vertical fore-and-aft plane of the microscope, plotting their poles,  $X$ ,  $Y$ ,  $Z$ , and determining the positions of the optic axes, the combined projection was turned into the adopted position giving the relations shown in figure 5. The diagram shows that the optical ellipsoid is strongly tilted in all directions to the crystallographic axes, with  $X$ , the acute bisectrix of the large optic axial angle, nearly normal to the crystal plane  $x(\bar{1}11)$ , as stated in the handbooks.

The optical orientation and the remaining measured optical elements are given in the following table, in which the two-circle angles of the principal ellipsoid axes,  $X$ ,  $Y$ ,  $Z$ , refer to the vertical crystallographic



axis as pole and the vertical great circle through (010) as prime meridian. For comparison are given the optical elements of Des Cloizeaux (1862) and Berman, in Palache (1935), transformed to the new crystal setting.

## OPTICAL ELEMENTS OF AXINITE

| Peacock:       | (Na)   |        | $n(\text{Na})$  |                  |                   |
|----------------|--------|--------|-----------------|------------------|-------------------|
|                | $\phi$ | $\rho$ |                 |                  |                   |
| X (colorless)  | -42°   | 56°    | 1.683           |                  | } ±0.002          |
| Y (colorless)  | 59     | 75     | 1.688           |                  |                   |
| Z (colorless)  | 168    | 39     | 1.692           |                  |                   |
|                |        |        |                 |                  | Negative          |
|                |        |        |                 |                  | 2V = 81°          |
|                |        |        |                 |                  | r < v weak        |
| Des Cloizeaux: |        |        | $n(\text{red})$ | $n(\text{blue})$ |                   |
|                | $\phi$ | $\rho$ |                 |                  |                   |
| X.....         | -42°   | 60°    | 1.6720          | 1.6850           | Negative          |
| Y.....         | 54     | 81     | 1.6779          | 1.6918           | 2V = 71°38' (red) |
| Z.....         | 158    | 32     | 1.6810          | 1.6954           | 71 49 (blue)      |
| Berman:        | (Na)   |        | $n(\text{Na})$  |                  |                   |
|                | $\phi$ | $\rho$ |                 |                  |                   |
| X (yellow)     | -24°   | 55°    | 1.684           |                  | } ±0.001          |
| Y (yellow)     | 79     | 72     | 1.692           |                  |                   |
| Z (colorless)  | 180    | 42     | 1.696           |                  |                   |
|                |        |        |                 |                  | Negative          |
|                |        |        |                 |                  | 2V = 74°          |
|                |        |        |                 |                  | r < v strong      |

The three determinations agree sufficiently well to show that none contains gross errors; and the differences are not greater than might be expected from real variations in different materials combined with expected experimental errors. On the whole the writer's determination agrees more closely with that of Des Cloizeaux, which is to be expected if, as seems probable, both were made on ferro-axinite. Berman's measurements refer to a mangan-axinite from Franklin, N. J., in which a sensibly different orientation is probable.

The symbols and arrangement used in presenting the optical data are those which the writer has reached after studying the optics of several triclinic species and carefully considering the manner of presenting the results. In this arrangement the data are given in a logical order which is also approximately the order in which they are found, using accepted symbols: XYZ, the principal axes of the refractive index ellipsoid; the absorption colors of white light in these directions;  $\phi\rho$ , the co-ordinate angles precisely defining the orientation of ellipsoid axes with respect to the crystallographic axes, in this case for monochromatic light (Na);  $n(\text{Na})$ , the special lengths of the ellipsoid axes (refractive indices) for monochromatic light; and finally the dependent characters, optic sign and optic axial angle, and the nature of the dispersion of the optic axes.

A consistent optical statement in the monoclinic system has been used by the author (1936). In the orthorhombic system the corresponding statement is still simpler since the principal axes of the optical ellipsoid coincide with the crystallographic axes.

Many mineralogists use a single symbol to express a principle axis of the optical ellipsoid and its specific magnitude, the commonest symbols being  $\alpha\beta\gamma$  for biaxial crystals and  $\omega\epsilon$  for uniaxial crystals. Such compression of meaning may be justified when extreme

economy of space is the object; but the writer finds it undesirable in principle and specially unfortunate in the triclinic system where  $\alpha\beta\gamma$  mean axial angles in the intimately related field of geometrical crystallography. The suggested way of listing the refractive indices avoids this difficulty. If one wishes to write the refractive indices separately the logical symbols are  $nX$ ,  $nY$ ,  $nZ$  for biaxial crystals,  $nO$ ,  $nE$  for uniaxial, crystals,  $n$  for isotropic crystals, as suggested by Dr. W. T. Scaller in a personal communication.

#### DEFINITIVE PRESENTATION OF THE CRYSTALLOGRAPHY OF AXINITE

The crystallography of axinite in the normal setting is here presented in a form which has been developed in the Harvard Mineralogical Laboratory, approved by a number of interested mineralogists in this country and abroad, and adopted in the preparation of crystallographic material for a projected volume of crystallographic angle-tables and the new edition of Dana's System of Mineralogy. The preparation of this statement is largely the work of Professor Charles Palache, who undertook the considerable labor of deriving the new geometrical elements, critically revising the form-list, and computing the co-ordinate and interfacial angles.

The statement aims at combining the data required by single-circle and two-circle crystallographers with those röntgenographic data that seem at the present time to have direct bearing on mineralogy as a branch of natural history. The symbolism and contractions are for the most part self-explanatory; those relating to the geometrical crystallography are explained in full in a paper by the writer (1934). The angles apply to the particular plane given by the Miller symbol in the form-list. The form-letters are, as far as possible, the classical letters, only those for  $\{100\}$ ,  $\{010\}$ ,  $\{001\}$ ,  $\{110\}$ ,  $\{1\bar{1}0\}$ , being changed to  $a b c m M$  respectively. For the uncertain forms letters are omitted as superfluous. The statement given is actually that planned for the projected Angle-Tables; in the System the list of calculated angles will of necessity be reduced to save space.

#### SOME OF THE EXISTING SETTINGS OF AXINITE AND THE UNDERLYING PRINCIPLES

*Neumann (1825).*<sup>11</sup> The first geometrically correct presentation of the morphology of axinite was given by Neumann (1825), soon after the appearance of his remarkable treatise (1823) proposing to use the gnomonic projection in crystallography and co-ordinates in this projection as face-symbols. In his axinite study, however, Neumann uses the stereographic projection—also a novelty in crystallography at that time—and Weiss

<sup>11</sup> Haüy's determination of the primitive form of axinite contains errors which later workers have been unable to resolve.

AXINITE<sup>1</sup>—HBAI<sub>2</sub>Ca<sub>2</sub> (Mn, Fe) Si<sub>4</sub>O<sub>16</sub>Triclinic; pinacoidal— $\bar{1}$ 

$a:b:c=0.7789:1:0.9763$ ;  $\alpha=91^\circ 51\frac{1}{2}'$ ,  $\beta=98^\circ 04'$ ,  $\gamma=77^\circ 14\frac{1}{2}'$   
 $p_0:q_0:r_0=1.2845:0.9911:1$ ;  $\lambda=89\ 55$ ,  $\mu=82\ 09$ ,  $\nu=102\ 38$   
 $p_0'=1.2973$ ,  $q_0'=1.0010$ ;  $x_0'=0.1418$ ,  $y_0'=0.0016$

| Forms <sup>2</sup>               | $\phi$  | $\rho$ | $A$     | $B$     | $C$    |
|----------------------------------|---------|--------|---------|---------|--------|
| <i>c</i> 001                     | 89°23'  | 8°04'  | 82°09'  | 89°55'  | 0°00'  |
| <i>b</i> 010                     | 0 00    | 90 00  | 102 38  | 0 00    | 89 55  |
| <i>a</i> 100                     | 102 38  | 90 00  | 0 00    | 102 38  | 82 09  |
| $\sigma$ : 130                   | 24 58   | 90 00  | 77 40   | 24 58   | 86 31½ |
| $\gamma$ 120                     | 36 23   | 90 00  | 66 16   | 36 22   | 85 09  |
| <i>m</i> 110                     | 60 28   | 90 00  | 42 10½  | 60 27½  | 82 56½ |
| <i>X</i> 2 $\bar{1}$ 0           | 121 46½ | 90 00  | 19 08½  | 121 46½ | 83 11½ |
| <i>I</i> 540                     | 130 35  | 90 00  | 27 57   | 130 35  | 83 56½ |
| <i>M</i> 1 $\bar{1}$ 0           | 135 25½ | 90 00  | 32 47½  | 135 25½ | 84 24½ |
| <i>K</i> 9. $\bar{1}\bar{1}$ .0  | 139 58½ | 90 00  | 37 20½  | 139 58½ | 84 53½ |
| $\alpha$ 340                     | 141 58  | 90 00  | 39 20   | 141 58  | 85 06½ |
| <i>T</i> 11. $\bar{1}\bar{6}$ .0 | 143 57½ | 90 00  | 41 19½  | 143 57½ | 85 20  |
| <i>H</i> 230                     | 144 39½ | 90 00  | 42 01½  | 144 39½ | 85 25  |
| $\beta$ 350                      | 147 01  | 90 00  | 44 23   | 147 01  | 85 41½ |
| <i>l</i> 120                     | 151 01½ | 90 00  | 48 23½  | 151 01½ | 86 11  |
| <i>h</i> 130                     | 158 56  | 90 00  | 56 18   | 158 56  | 87 11½ |
| <i>z</i> 012                     | 15 46   | 27 33  | 88 33   | 63 34   | 26 21  |
| <i>j</i> 035                     | 13 15   | 31 44½ | 89 40½  | 59 11½  | 30 43½ |
| $\phi$ : 034                     | 10 40½  | 37 26½ | 91 11½  | 53 19   | 36 36  |
| <i>L</i> 045                     | 10 01½  | 39 10½ | 91 39   | 51 32   | 38 23  |
| <i>r</i> 011                     | 8 03    | 45 21½ | 93 15½  | 45 12½  | 44 42½ |
| $\pi$ 021                        | 4 03    | 63 32  | 97 40½  | 26 45   | 63 10  |
| $\phi$ 031                       | 2 42    | 71 36½ | 99 25½  | 18 35   | 71 20  |
| $\Delta$ 061                     | 1 21    | 80 33  | 101 07½ | 9 32½   | 80 22½ |
| <i>e</i> 0 $\bar{1}$ 1           | 171 55½ | 45 16  | 75 27   | 134 42  | 44 47  |
| $\Delta$ 021                     | 175 56½ | 63 30  | 75 06½  | 153 12½ | 63 17½ |
| <i>Z</i> 041                     | 177 58½ | 75 59  | 75 47   | 165 50  | 75 55  |
| <i>v</i> 101                     | 101 20  | 55 08½ | 34 53   | 99 16½  | 47 16  |
| $\mu$ 201                        | 101 57  | 69 54  | 20 06½  | 101 12½ | 62 02½ |
| <i>R</i> 401                     | 102 08  | 79 22  | 10 43   | 101 55  | 71 26  |
| <i>F</i> 104                     | -67 27½ | 10 42½ | 100 33  | 85 55   | 18 24  |
| <i>g</i> 103                     | -71 03  | 16 30  | 106 24  | 84 42½  | 24 15  |
| $\Pi$ 205                        | -72 28½ | 20 55  | 110 50  | 83 49½  | 28 41½ |
| <i>f</i> 102                     | -73 43  | 27 06  | 117 02½ | 82 40   | 34 53½ |
| <i>y</i> 101                     | -75 45½ | 49 13½ | 139 12  | 79 15½  | 57 03  |
| $\epsilon$ 201                   | -76 36½ | 67 51  | 157 50½ | 79 37   | 75 41½ |
| $\delta$ 112                     | 65 03½  | 40 30½ | 58 59½  | 74 06   | 33 15½ |
| <i>n</i> 111                     | 62 51   | 57 41  | 49 26   | 67 24   | 50 32½ |
| <i>k</i> 221                     | 61 45½  | 71 46  | 44 06   | 63 17½  | 64 40  |
| $\psi$ 113                       | -130 17 | 20 10  | 102 00  | 102 53  | 26 51½ |
| <i>o</i> 112                     | -126 01 | 31 16  | 110 00½ | 107 46  | 38 06  |
| <i>Y</i> 111                     | -122 29 | 53 07  | 124 21½ | 115 26½ | 60 04  |
| <i>V</i> 112                     | 129 35½ | 45 09  | 50 48½  | 116 52  | 39 16  |
| <i>x</i> 111                     | -41 09  | 59 39½ | 134 07½ | 49 28   | 65 04  |

AXINITE— $\text{HBA}_2\text{Ca}_2(\text{Mn, Fe})\text{Si}_4\text{O}_{16}$  (Concluded)

| Forms           | $\phi$   | $\rho$ | <i>A</i> | <i>B</i> | <i>C</i> |
|-----------------|----------|--------|----------|----------|----------|
| $\xi$ 163       | 16 27    | 63 19½ | 86 35½   | 31 01    | 61 14    |
| $\tau$ 183      | 12 20½   | 69 14  | 90 16½   | 24 01    | 67 38½   |
| $\zeta$ 215     | -103 09½ | 20 31  | 108 24   | 94 34½   | 28 26½   |
| $\epsilon$ 132  | 29 39    | 57 26½ | 75 43½   | 42 54    | 53 40    |
| $\lambda$ 325   | -110 19  | 33 22½ | 117 29½  | 101 00½  | 41 03    |
| $\Sigma$ 213    | -101 30½ | 35 37½ | 122 06½  | 96 40    | 43 34    |
| <i>Q</i> 587    | -29 29   | 57 09  | 124 17½  | 43 00½   | 61 18½   |
| <i>d</i> 121    | 39 18    | 65 46½ | 65 50½   | 45 07    | 60 46    |
| $\Omega$ 414    | -64 31½  | 51 14  | 139 28½  | 70 24½   | 58 33    |
| $\Theta$ 323    | -49 43   | 55 50  | 137 07½  | 57 39½   | 62 04½   |
| $\Phi$ 454      | -36 11   | 62 17½ | 131 47   | 44 23½   | 67 09½   |
| <i>W</i> 232    | -32 10½  | 64 39  | 129 33½  | 40 06    | 69 03    |
| <i>s</i> 121    | -26 10   | 68 34½ | 125 41   | 33 20    | 72 13½   |
| <i>i</i> 131    | -18 52½  | 73 57  | 120 08½  | 24 35    | 76 36½   |
| $\sigma$ 121    | -146 47  | 64 01  | 108 25½  | 138 46   | 68 41    |
| <i>p</i> : 735  | -97 03½  | 58 40½ | 143 32½  | 96 11½   | 66 41½   |
| $\theta$ 312    | 87 51    | 63 54½ | 29 43½   | 88 04    | 55 51    |
| <i>X</i> : 322  | 74 12½   | 64 45  | 37 18    | 75 45    | 56 59½   |
| $\lambda$ : 312 | -92 23½  | 60 22½ | 147 05½  | 92 04½   | 68 26½   |
| $\Gamma$ 322    | -50 53½  | 66 10½ | 144 58   | 54 45½   | 72 28    |
| <i>t</i> 231    | 47 39    | 74 33  | 56 25½   | 49 30½   | 68 36½   |
| $\nu$ 211       | -56 42   | 70 43½ | 152 02   | 58 47    | 77 28½   |
| <i>q</i> 211    | -100 14½ | 67 37½ | 148 25½  | 99 28    | 75 35    |
| $\rho$ 231      | -135 31½ | 73 39½ | 120 29½  | 133 12½  | 79 27    |

Structure cell: Triclinic;  $a_0=7.151$ ,  $b_0=9.184$ ,  $c_0=8.935$ ;  $\alpha=91^\circ 52'$ ,  $\beta=98^\circ 09'$ ,  $\gamma=77^\circ 19'$ ;  $a_0:b_0:c_0=0.7787:1:0.9729$ . Contains:  $\text{H}_2\text{B}_2\text{Al}_4\text{Ca}_4(\text{Mn, Fe})_2\text{Si}_8\text{O}_{32}$ .<sup>4</sup>

Habit: Oblique tabular {010} or {011}, rarely {111}; rarely columnar [001]. Common forms: *brMlsxay*; *bM* often striated [001]; *r* often striated [010]. Also lamellar, massive, granular.

Cleavage: {100} distinct; also {001}, {110}, {011} interrupted; {010}, {101} traces.<sup>5</sup>

<sup>1</sup> Haüy (*Jour. Mines*, 5, 264, 1799).

<sup>2</sup> Palache (1937), from previous measurements and new observations, in the orientation of Peacock (1937). The adopted setting differs from that of Dana (*System*, 1892) and Goldschmidt (*Winkeltabellen*, 1897; *Atlas*, 1, 1913).

Transformations: Dana to Palache—Peacock:  $\bar{1}\bar{1}0/200/002$ ; Goldschmidt to P.—P.:  $\bar{1}00/0\bar{1}0/001$ .

<sup>3</sup> Goldschmidt (1913), Flink (*Ark. Kemi*, 6, 111, 1917); Aminoff (*Ark. Kemi*, 7, 45, 1919); Poitevin (*Amer. Min.*, 4, 32, 1919; Buttgenbach (*Bull. Acad. Roy. Belge*, 10, 141, 1924).

Uncertain: {210}, {14.1.0}, {21.1.0}, {720}, {940}, {430}, {970}, {12.13.0}, {10.11.0}, {9.10.0}, {15.17.0}, {780}, {450}, {9.16.0}, {18.17.0}, {290}, {1.13.0}, {1.13.0}, {1.26.0}, {1.34.0}, {058}, {056}, {091}, {059}, {078}, {0.27.28}, {203}, {301}, {221}, {13.46. 11}, {641}.

<sup>4</sup> Peacock (1937), on a crystal from near Easton, Northampton Co., Penn. The structure cell of Gossner & Reichel (*Centralb. Min.*, 1932, 225) defines nearly the same lattice, but its edges are not the three shortest identity periods in the lattice.

<sup>5</sup> Dana (1892).

symbols, which are the intercepts of the crystal planes on the direct axes.

Using a simple reflecting goniometer, provided with an auxiliary device which appears to have been a peep-sight, Neumann measured the following five interfacial angles on a typical crystal of axinite from the Dauphiny. These angles, which are astonishingly close to the corresponding calculated angles taken from Palache's new angle-table, were used as the basis of calculation.

| Neumann                         | Palache                   | Diff.          |
|---------------------------------|---------------------------|----------------|
| $vy = 139^{\circ}29'$           | $ay = 139^{\circ}12'$     | 3'             |
| $ux = 149\ 26$                  | $Mx = 149\ 28\frac{1}{2}$ | $2\frac{1}{2}$ |
| $xy = 150\ 08\ (29^{\circ}52')$ | $xy = 29\ 47\frac{1}{2}$  | $4\frac{1}{2}$ |
| $vu = 147\ 05\ (32\ 55)$        | $aM = 32\ 47\frac{1}{2}$  | $7\frac{1}{2}$ |
| $vx = 134\ 02$                  | $ax = 134\ 07\frac{1}{2}$ | $5\frac{1}{2}$ |

Although the existence of oblique axial systems was clearly recognized in Neumann's time, some crystallographers still followed Weiss in his belief that all form systems could be referred to rectangular axes with reasonable rational symbols. To demonstrate this in the case of axinite Neumann assumed that the angle  $PM$  ( $89^{\circ}55'$  Neumann;  $bc = 89^{\circ}55'$  Palache) is exactly a right-angle and denoted the sixteen known forms of axinite with rational but complicated symbols on the orthorhombic axes:

$$a:b:c = \sqrt{51}:\sqrt{49}:\sqrt{1}.$$

The axial planes and parametral plane of Neumann and the present writer are interrelated as follows:

| Neumann    | Peacock           | Peacock    | Neumann        |
|------------|-------------------|------------|----------------|
| $-(100) =$ | $-(720)$          | $a(100) =$ | $v(9\bar{2}0)$ |
| $P(010) =$ | $b(010)$          | $b(010) =$ | $P(010)$       |
| $-(001) =$ | $-(7.\bar{2}.63)$ | $c(001) =$ | $M(101)$       |
| $-(111) =$ | $-(017)$          | $n(111) =$ | $n(10.5.1)$    |

and the determinant<sup>12</sup> for transforming Neumann's symbol for any plane to the symbol which that plane receives in our lattice is:

$$\text{Neumann to Peacock: } 707/29\bar{2}/0.0.63.$$

Neumann's symbols are, of course, intolerably complicated and his choice of lattice is entirely unacceptable; but this ingenious *tour de force* is of interest in showing the Principle of Least Anorthism, or Highest Pseudo-Symmetry, in its earliest and most uncompromising form. Even

<sup>12</sup> Derived in the simple Fedorov manner, as described by Barker (1930), and written in Barker's convenient linear style. This and the following determinants give the strict plane to plane transformations, not just form to form.

when tempered with some regard for simplicity of indices this principle has led to many crude settings. To-day one may rightly insist that a multiple lattice with high pseudo-symmetry should never be taken in preference to a simple lattice, unless the crystals habitually exhibit the pseudo-symmetry of the multiple lattice.<sup>13</sup>

*Lévy (1838)—Des Cloizeaux (1862)*: Des Cloizeaux (1862) adopted the setting of L'vy whose numerous excellent drawings of axinite have established the familiar and most satisfactory aspect of the crystals. Des Cloizeaux took three of the most important (common and large) crystal faces as the faces of his primitive form, namely  $p\ m\ t$ ,<sup>14</sup> which are respectively our  $r(011)$ ,  $b(010)$ ,  $M'(\bar{1}10)$ , his axial planes and parametral plane having the following symbols in our lattice:

|               |   |                      |
|---------------|---|----------------------|
| Des Cloizeaux | = | Peacock              |
| $h'$ (100)    | = | $l'$ ( $\bar{1}20$ ) |
| $g'$ (010)    | = | $a'$ ( $\bar{1}00$ ) |
| $p$ (001)     | = | $r$ (011)            |
| — (111)       | = | — (231)              |

Des Cloizeaux to Peacock:  $\bar{1}10/201/001$

Des Cloizeaux' vertical axis is thus the same as ours, but his elementary lattice cell is highly oblique and his parametral plane is not among the known forms of axinite. It is not surprising therefore that Des Cloizeaux' symbols are systematically more complicated than the simplest that can be found.

The practice of taking the most prominent planes in the vertical zone as "prisms" rather than as "pinacoids" has a sound basis in the higher symmetries when the lattices are appropriately centered; but in the triclinic system this procedure generally leads to a double (base-centered) cell and systematic complication of the indices. E. S. Dana (1892) often worked on this principle, as may be seen from his settings of rhodonite, babingtonite and aenigmatite, in each of which elements corresponding to those of the smallest cell of the structure lattice are obtained when Dana's unit "prisms" are taken as the vertical axial planes.

*Miller (1852)*: Miller's writings are noteworthy for their brevity and elegance, admired and successfully emulated by Dana (1892). His presentation of the crystallography of axinite is a model of clarity and condensation. Whether guided by the Principle of Simplest Indices, or sim-

<sup>13</sup> In this connection see the author (1936).

<sup>14</sup> It will be remembered that the vertical faces of the "forme primitive" of the early French School are the vertical diagonal planes of the conventional lattice cell, and *vice versa*; furthermore Lévy's axes, like Miller's, read right—front—up, in the opposite order to that generally used today.

ply by a sense of propriety, we cannot tell; but the fact is that Miller chose as his primitive parallelepiped the same cell that we have found from morphological and structural study, with the same edge set vertical. That our orientation of this cell about the vertical axis is different from Miller's is of no consequence in the present connection; that is merely a matter of convention which might well have been waived in the present case, were it not for the fact that Miller's indices could not in any case be retained unchanged since they refer to a left-handed axial system. Below are given the equivalent planes in Miller's lattice and in ours, and the transformation determinant, Miller's order of indices being retained.

| Miller    | = | Peacock              |
|-----------|---|----------------------|
| $v$ (100) | = | $a'$ ( $\bar{1}00$ ) |
| $p$ (010) | = | $b$ (010)            |
| $m$ (001) | = | $c$ (001)            |
| $x$ (111) | = | $x$ ( $\bar{1}11$ )  |

Miller to Peacock:  $\bar{1}00/010/001$

With Miller's satisfying presentation available, giving the simplest possible indices to the crystal planes then known and subsequently found and the most desirable aspect to the crystals, it is a matter of surprise and regret that the crystallography of axinite should have been later complicated by numerous re-orientations, the reasons for which now seem totally inadequate.

*Vom Rath* (1866): In his monographic study of the morphology of axinite—a fine example of the master's incomparable skill in crystal measurement and drawing—vom Rath (1866) described axinite crystals from many localities, using Quenstedt's linear projection and Weiss symbols in his geometrical treatment. After reviewing the previous orientations of axinite and discoursing on the wide range of choice of elements in the triclinic system, vom Rath indicates that one should reduce the choice by seeking a subrectangular axial system among the zone-edges made by the intersections of observed crystal planes. Vom Rath's choice, according to this limitation, is expressed as follows:

| Vom Rath  | = | Peacock                    |
|-----------|---|----------------------------|
| $s$ (100) | = | $s$ ( $\bar{1}21$ )        |
| $b$ (010) | = | $v'$ ( $\bar{1}0\bar{1}$ ) |
| $c$ (001) | = | $Y$ ( $\bar{1}11$ )        |
| $-$ (111) | = | $\iota$ ( $\bar{2}01$ )    |

Vom Rath to Peacock:  $\bar{1}12/202/1\bar{1}2$

While the guiding principle indicated by vom Rath is a useful one, it was poorly applied in the present case. Actually vom Rath's axes are on

the whole more inclined than ours; and since they are defined by the intersections of planes with relatively complicated indices in the structure lattice, the tenor of vom Rath's face symbols is more complex than that of most of the previous and subsequent settings. This has been noticed by several later workers and vom Rath himself seems to have regretted his choice of elements as the work progressed; but by then he was too deeply involved in his elaborate calculations and drawings to undertake a change.

The infelicity of vom Rath's orientation is already apparent in the attitude of his drawings, of which twenty-eight complicated but clear examples are reproduced on a single plate measuring 11 by 14 inches. One is struck at once by the absence of a prominent vertical zone and the large development of zones whose axes are inclined to the crystal axes. Apart from the inelegance and practical inconvenience of a feeble vertical zone, such a condition points to a false choice of vertical axis, since the axial zones of a normally developed triclinic crystal are usually the strongest on the crystal, the strongest of all being best taken as the vertical zone to ensure that the vertical axis is an edge of the smallest cell of the structure lattice.

*Schrauf (1870)*: Schrauf's avowed morphological procedure was to choose as symmetrical a setting as possible, and at the same time bring out morphological analogies which seemed to exist between different species. In the case of axinite, after reviewing the eight existing orientations and stating that he would gladly refrain from proposing another setting, were it not for the fact that a better one was to be found, Schrauf proceeds to a new choice of elements which purports to give axinite a desirable pseudo-monoclinic aspect, to exhibit a morphological and optical analogy with sphene, and to result in a simplification of indices. In this attempt Schrauf is singularly unsuccessful. In his setting the forms of axinite are less markedly pseudo-monoclinic than they are in ours; the angles which he tabulates as comparable in axinite and sphene differ by  $6^\circ$  to  $23^\circ$  while the optical analogy is vague; and his indices, certainly simpler than the unhappy symbols of vom Rath, are notably more complicated than those of Miller, which he also gives for comparison. The correlation and transformation of Schrauf's symbols are given by the following:

|           |   |                      |
|-----------|---|----------------------|
| Schrauf   | = | Peacock              |
| $a$ (100) | = | $y'$ ( $10\bar{1}$ ) |
| $b$ (010) | = | $v$ (101)            |
| $c$ (001) | = | $b'$ ( $0\bar{1}0$ ) |
| $u$ (111) | = | $M$ ( $1\bar{1}0$ )  |

Schrauf to Peacock:  $110/00\bar{2}/\bar{1}10$



Schrauf's own transformation formulas relating his setting to those of Miller, Des Cloizeaux and vom Rath, are all in error in that the signs should be reversed throughout; and all later writers have repeated this error. This has far-reaching effects in Hintze, who used Schrauf's setting as the basis of his presentation and correlation. Schrauf's beautiful drawings representing fully developed crystals from several localities all lack prominent vertical edges; this mars the appearance of the figures and points to the poor choice of vertical axes.

On the ill-considered use of the principle of highest pseudo-symmetry we have spoken in this paper and elsewhere (author, 1936); even greater crudities have been committed in the name of morphological analogy or homeomorphism. Before the means were available for determining absolute lattice parameters it was reasonable to assume that isogeometrical crystals are related; and in many cases this presumption has been brilliantly confirmed by *x*-ray study, the species believed to be related proving to be isodimensional or isostructural.<sup>15</sup> Such confirmation of presumed structural similarity and systematic relationship has followed in cases of chemically similar species with similar naturally chosen lattices, usually accompanied with similarities of habit and cleavage. But when geometrical similarities have been forced by taking lattices which result in relatively complicated indices for one or both of the species, admitting gross differences in axial lengths and angles and differences of lattice symmetry, and ignoring important differences of cleavage, habit and chemical constitution, the imagined systematic relationship has found no confirmation in the absolute dimensions of the structure lattices and the arrangement of the cell contents. Frazier's setting of axinite (1882), intended to bring out geometrical and systematic similarity with the pseudo-orthorhombic monoclinic species datolite, is another case in point. Considerations of morphological analogy should be allowed to influence only the arbitrary factors in choosing elements, namely those which control the orientation of the properly chosen lattice cells; and such analogies can hardly be expected to have systematic significance except when accompanied by chemical and physical similarities.

*Goldschmidt (1886)*: In the *Index* (1886) Goldschmidt founded his setting of axinite on that of Miller, in which the symbol series approach normal complication series most closely. His position of the lattice cell, however, is different from Miller's and ours.

<sup>15</sup> *Isogeometrical* describes crystal species whose forms can be referred to like morphological lattices. *Isodimensional* (with like absolute lattice elements) may also be a useful term, as distinct from *isostructural* (with like structures), to describe the similarity between such species as rhodonite and babingtonite, which have like structural lattices, but can hardly be isostructural in view of their unlike chemical compositions. Isogeometrical, isodimensional and isostructural species are all *homeomorphous*.

| Goldschmidt (1886) |   | Peacock              |
|--------------------|---|----------------------|
| $M$ (100)          | = | $a'$ ( $\bar{1}00$ ) |
| $m$ (010)          | = | $c$ (001)            |
| $c$ (001)          | = | $b$ (010)            |
| $x$ (111)          | = | $x$ ( $\bar{1}11$ )  |

Goldschmidt (1886) to Peacock:  $\bar{1}00/001/010$

Goldschmidt thus turned Miller's lattice cell so that Miller's vertical axis, which is the axis of the main zone, became the athwart axis and the weakest axial zone became the vertical zone. In thus resetting axinite Goldschmidt followed a peculiar principle which ignored tradition, appearance and convenience and aroused much opposition; this was to set the weakest axial zone of a crystal vertical, thus bringing as many as possible of the gnomonic face-poles into finite positions on the gnomonic projection where their serial relations could be most easily viewed and discussed.

In the *Winkeltabellen* (1897) Goldschmidt recognized the objection to many of his settings in the *Index* and reverted to classical orientations which he retained in the *Atlas* (1913-1924). In the case of axinite he again took Miller's lattice cell and set it in yet another position which agrees with ours when the crystal is turned  $180^\circ$  about the vertical axis.

| Goldschmidt (1897) |  | Peacock                   |
|--------------------|--|---------------------------|
| $M$ (100)          |  | $a'$ ( $\bar{1}00$ )      |
| $c$ (010)          |  | $b'$ ( $0\bar{1}0$ )      |
| $m$ (001)          |  | $c$ (001)                 |
| $Y$ (111)          |  | $Y$ ( $\bar{1}\bar{1}1$ ) |

Goldschmidt (1897) to Peacock:  $\bar{1}00/0\bar{1}0/001$

In transforming the elements Goldschmidt unfortunately gave values for the axial angles  $\alpha$  and  $\gamma$  which are the supplements of the true values; the incorrect angles have been copied by other writers.

*Dana (1892)*: Dana was usually fortunate in his choice of orientations; but in the case of axinite he adopted Naumann's position, giving a cell which is more oblique and indices more complicated than those of Miller.

| Dana      |  | Peacock              |
|-----------|--|----------------------|
| $a$ (100) |  | $l'$ ( $\bar{1}20$ ) |
| $b$ (010) |  | $a'$ ( $\bar{1}00$ ) |
| $c$ (001) |  | $c$ (001)            |
| $x$ (111) |  | $x$ ( $\bar{1}11$ )  |

Dana to Peacock:  $\bar{1}\bar{1}0/200/002$

*Friedel (1926)*: The last setting of axinite we need consider is that of Friedel (1926), the most consistent and persuasive exponent of the Law

of Bravais. As Friedel does not discuss his orientation we cannot be sure that he found the unique lattice cell which gives the best correspondence between the relative importance of the forms and their reticular densities, a very laborious process in the triclinic system if the reticular densities are calculated from the elements. It is certain, however, that Friedel's orientation is intended to express the Law of Bravais, at least in first approximation. His cell is highly oblique and his indices are not simple, a condition which Friedel regarded as less significant than good expression of the Law of Bravais.

| Friedel    | Peacock              |
|------------|----------------------|
| $h'$ (100) | $b$ (010)            |
| $g'$ (010) | $M'$ ( $\bar{1}$ 10) |
| $p$ (001)  | $r$ (011)            |
| $-$ (111)  | $i$ ( $\bar{1}$ 31)  |

Friedel to Peacock:  $0\bar{1}0/111/001$

Further orientations of axinite are those of Haüy (1822), Mohs-Haidinger (1825), Rose (1843), Hessenberg (1873), Frazier (1882), Franck (1893), and Gossner and Reichel (1932); but since these settings illustrate no principle other than those already considered they need not be discussed in detail. The selected orientations, all by eminent crystallographers of the past, illustrate the more important principles which have guided morphologists in choosing triclinic elements. If we use the normal setting, in our sense, as the criterion, then the Principle of Simplest Indices stands out as the most successful morphological principle, although it must be recognized that this principle is less useful in directly finding the desired elements than in choosing between several possible orientations. In this case also the Law of Complication leads to the proper result. On the other hand, the Law of Bravais, which often indicates the proper solution, fails to give a satisfactory setting for axinite. The Principle of Least Anorthism in its extreme form is unsuccessful and the Principle of Highest Pseudo-Symmetry likewise fails, since the structure lattice of axinite possesses no simple multiple lattice with pronounced pseudo-symmetry. Attempts to exhibit morphological analogies between axinite and other species have miscarried; and settings in which a weak zone is taken as an axial zone have proved unfortunate. Since the reported cleavages in normal setting are  $\{100\}$ ,  $\{001\}$ ,  $\{110\}$ ,  $\{011\}$ ,  $\{010\}$ ,  $\{\bar{1}01\}$ , the Principle of Simplest Cleavages would lead in this case to normal elements; but none of the previous authors appears to have been guided exclusively by this principle. In another case the score would undoubtedly be different in detail, with the Principle of Simplest Indices still leading as the most reliable of the older methods of choosing between alternative settings.

## PROPRIETY OF THE NORMAL SETTING OF TRICLINIC CRYSTALS

The proposed setting of axinite, based on the smallest structure cell, fulfils all reasonable morphological requirements. The cleavages have the simplest possible indices; the face-symbols are likewise the simplest that can be obtained; the crystal axes approach rectangularity and the lattice cell tends to orthorhombic pseudo-symmetry as closely as is consistent with simplest indices; and the lattice cell is oriented according to existing morphological conventions. The normal setting is therefore the proper setting of axinite. The fact that there is little correspondence between the relative importance of the forms and their relative reticular densities is no argument against the normal setting, especially since no lattice will give the desired agreement. The case is one in which the Law of Bravais is inadequate, and I feel sure that both Friedel and Ungemach would have freely admitted this and accepted the normal setting with the structural evidence before them.

Conversely, if we accept the normal setting of axinite as the proper setting, the fulfillment of most of the usual morphological requirements indicates that the principles which underlie them are true, and suggests that these principles should therefore give the normal setting. But, as we have seen, these principles have led to a dozen different orientations, which show in the most convincing manner that the old rules are but partial truths leading to a variety of results according to the particular compromise struck between their variously conflicting terms.

Is the normal setting equally appropriate to triclinic species in general? A number of well-developed triclinic species have been examined with this question in mind, in each case an unprejudiced determination of the normal elements from the gnomonic projection of the observed forms being compared with the elements of the structural cell, if known. In two cases, copiapite and rosenbuschite, for which the lattice determinations were lacking, rigorous determinations were made with the Weissenberg  $x$ -ray goniometer. Some of the details of these studies may be given another time; suffice it here to say that the following species were examined: wollastonite, pectolite, schizolite, vogtite, rosenbuschite, rhodonite, babingtonite, aenigmatite, cyanite, chalcantinite, copiapite and plagioclase feldspar. In all but one, namely plagioclase, the smallest cell of the structure lattice proves to be eminently suitable for morphological purposes, and this cell was easily found, as in the case of axinite, by simple inspection of the gnomonic projection of the known forms. In the case of plagioclase the classical morphological lattice, which properly exhibits the marked monoclinic pseudo-symmetry of the species, corresponds to a base-centered, therefore double structural cell. In rosenbuschite the external forms are not sufficient to determine a lattice. The

morphology of three further triclinic species, roemerite, quenstedtite and anapaite also clearly shows the structural lattice, but lattice determinations for these species are still lacking.

The cases examined constitute a large proportion of the known triclinic minerals occurring in well-developed crystals, a number sufficient to warrant the conclusion that the normal setting, based on the smallest structure cell, is the proper setting for triclinic crystals except when well-marked pseudo-symmetry of habit points definitely to a simple multiple lattice of the structure lattice as the better morphological framework.

All that has been said in the general case of the triclinic system applies with appropriate simplifications in the higher symmetries, in which the addition of symmetry elements progressively reduces the number of variables in the morphological elements to zero. But with increasing symmetry lattice centering becomes increasingly frequent; and since the effect of lattice centering on form development still remains to be systematically studied, the application of the normal setting will not be formally extended here beyond the triclinic system. Enough has been done, however, to indicate that the principle of normal setting will be perfectly general, and that a general procedure can be devised for distinguishing the structural lattice in the majority of cases in the gnomonic projection of the external crystal planes.

#### SUMMARY

Hitherto the choice of triclinic elements has been governed by various morphological principles, which prove to be imperfect expressions of the relations of the forms of a crystal to its structural lattice, together with certain rules regulating the orientation of the chosen lattice cell. The goal uncertainly approached and sometimes reached by these principles and rules is the *normal setting*. In this setting the geometrical elements correspond to those of the simple lattice cell defined by the three shortest non-coplanar identity periods in the structural lattice; and the orientation is the unique conventional one in which  $c[001]$  is the axis of the main zone of the crystal or an axis of dimetric pseudo-symmetry,  $\alpha$  and  $\beta$  are both obtuse, and  $b[010]$  is longer than  $a[100]$ .

The normal elements of axinite were sought by inspecting the gnomonic projection of a single crystal; the method provisionally used involved accepting the principle of simplest indices as an approximate truth, recognizing the gnomonic projection as a two-dimensional representation of the reciprocal lattice, and taking as the first layer of the reciprocal lattice the plane lattice which accommodates most of the gnomonic projection points without systematic omissions. A direct determination of the normal elements, based on a rigorous röntgenographic

study, gave a result comparable to that obtained by the morphological method.

Eight of the existing settings of axinite are described and discussed and related to the new setting; only Miller, and after him, Victor Goldschmidt, took settings corresponding to the simple structural cell with the shortest edges.

A definitive presentation of the crystallography of axinite in the new setting is given by Palache, in a considered form which strives to meet the requirements of single-circle and two circle goniometry and introduces essential  $x$ -ray data.

A determination of the optical orientation of axinite agrees with published orientations. But an examination of the existing structure elements shows that they do not, as purported, define the cell with the shortest edges; the published cell-formula is also unacceptable.

It was found that the structural lattice could be discerned in the gnomonic projections of the known forms of twelve further triclinic species, and that in each case except plagioclase, the normal setting is eminently suitable for morphological description. It appears, therefore, that this setting is the proper setting for triclinic crystals, except, as in plagioclase, when well-marked pseudo-symmetry of habit demands a simple multiple lattice of the structural lattice.

The following constants were measured on a crystal of axinite from near Easton, Pennsylvania:

Elements of the structural lattice in normal setting:

$$a_0 = 7.151 \text{ \AA}, b_0 = 9.184 \text{ \AA}, c_0 = 8.935 \text{ \AA}; \alpha = 91^\circ 52', \beta = 98^\circ 09', \gamma = 77^\circ 19'$$

$$a_0 : b_0 : c_0 = 0.7787 : 1 : 0.9729;$$

Elements of the morphological lattice of axinite (Palache):

$$a : b : c = 0.7789 : 1 : 0.9763; \quad \alpha = 91^\circ 51\frac{1}{2}', \beta = 98^\circ 04', \gamma = 77^\circ 14'$$

The unit cell containing  $H_2B_2Al_4Ca_4(Mn, Fe)_2Si_8O_{32}$ , with  $Mn = Fe$ , has the calculated density 3.316.

Optical elements (Na):

|   | $\phi$      | $\rho$     | $n$                 |   |
|---|-------------|------------|---------------------|---|
| X | $-42^\circ$ | $56^\circ$ | 1.683               | Negative<br>$2V = 81^\circ$<br>$r < v$ , weak |
| Y | 59          | 75         | 1.688 } $\pm 0.002$ |   |
| Z | 168         | 39         | 1.692               |   |

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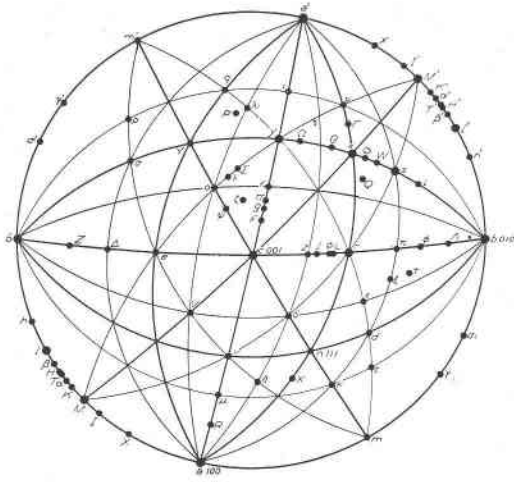
work in the  $x$ -ray laboratory of the institution; to Professor Tom. F. W. Barth, Dr. George Tunell and Mr. Charles Ksanda for friendly instruction and assistance in preparing and discussing the  $x$ -ray photographs; to Dr. Tunell and Mr. Ksanda for critically reading the manuscript; and to Professor J. D. H. Donnay of Johns Hopkins University for verifying all the transformation determinants by independent study of the original literature, and suggesting some improvements to the text.

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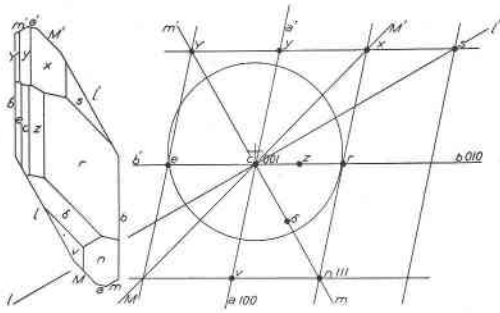
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## EXPLANATION OF THE FIGURES

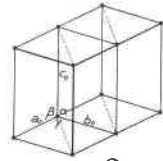
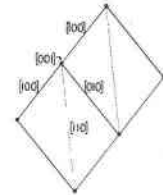
- FIG. 1. Axinite. Stereographic projection of the accepted forms in normal setting.  
 FIG. 2. Axinite from near Easton, Pennsylvania; plan and gnomonic projection of the crystal used for geometrical, structural and optical study.  
 FIG. 3. Axinite. Plan and inclined view of the structure lattice showing two properly chosen cells (full lines), and one cell as given by Gossner & Reichel (dotted).  
 FIG. 4. Axinite. Inclined view of the studied crystal which presents the familiar aspect when viewed from the direction of (010). The greatest dimension of the crystal is 1.3 mm. The lower half of the crystal, which was attached, has been restored according to the known pinacoidal symmetry.  
 FIG. 5. Axinite. Relation of the axes of the optical ellipsoid ( $XYZ$ ) and the optic axes (circles with brushes) to the principal crystal planes.



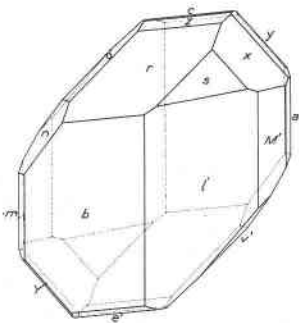
1



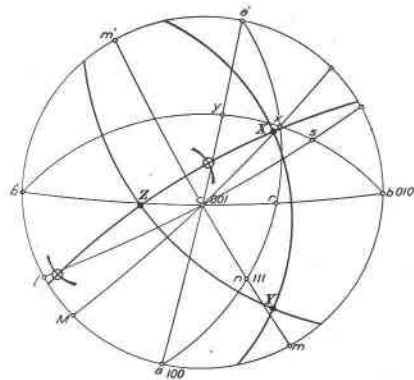
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3



4



5



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APPENDIX: TRANSFORMATION OF CO-ORDINATES

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The following table of transformations enables one to pass from any setting to any other setting. It gives the face-to-face transformation (some authors only give the form-to-form transformation). The complete transformation formulae to pass from the face symbol ( $hkl$ ) in the "old" setting to the face symbol ( $pqr$ ) in the "new" setting are:

$$\begin{aligned} p &= u h + v k + w l \\ q &= u' h + v' k + w' l \\ r &= u'' h + v'' k + w'' l \end{aligned}$$

Only the coefficients need be known; they are given in matrix form in the table:

$$\begin{pmatrix} u & v & w \\ u' & v' & w' \\ u'' & v'' & w'' \end{pmatrix}$$

In a text it is preferable to use the form proposed by T. V. Barker:

$$u \ v \ w / u' \ v' \ w' / u'' \ v'' \ w''$$

Such a tabular arrangement as is presented here is compact, typographically more elegant than one giving the complete formulae. The rows and columns of the transformation matrix have known meanings: the rows  $[u \ v \ w]$ ,  $[u' \ v' \ w']$ ,  $[u'' \ v'' \ w'']$ , represent the "new" axes in the "old" notation; the columns  $(u \ u' \ u'')$ ,  $(v \ v' \ v'')$ ,  $(w \ w' \ w'')$ , represent the "old" axial planes in the "new" notation. The tabular arrangement (in the form of a matrix of matrices) lends itself to matrix calculations, affording convenient verifications.

*Multiplication of Matrices.* If the matrix "Rath to Mohs" is multiplied by the matrix "Mohs to Peacock" the resulting matrix gives the transformation "Rath to Peacock." The rule may be recalled here: in the resulting matrix the element that lies at the intersection of the  $n$ th column and the  $m$ th row is obtained by multiplying each element of the  $n$ th column in the first matrix by the corresponding element of the  $m$ th row in the second matrix and adding the three products. Matrix multiplication, in general, is not commutative.

Example:

$$\begin{pmatrix} 114 \\ 310 \\ 112 \end{pmatrix} \cdot \begin{pmatrix} 002 \\ 110 \\ 110 \end{pmatrix} = \begin{pmatrix} 1.0+3.0+1.2 & 1.0+1.0+1.2 & 4.0+0.0+2.2 \\ 1.1+3.1+1.0 & 1.1+1.1+1.0 & 4.1+0.1+2.0 \\ 1.1+3.1+1.0 & 1.1+1.1+1.0 & 4.1+0.1+2.0 \end{pmatrix} = \begin{pmatrix} 112 \\ 202 \\ 112 \end{pmatrix}$$

TABLE OF AXINITE TRANSFORMATIONS

| From \ To                                | Neumann<br>1825             | Hausmann 1847<br>Mohs 1824<br>Zippe 1839 | Miller ( <i>hkl</i> )*<br>1852 | Lévy 1838<br>Des Cloizeaux 1862 | vom Rath<br>1866           | Schrauf<br>1870           | Hessenberg<br>1873        |
|--|-----------------------------|--|--------------------------------|---------------------------------|----------------------------|---------------------------|---------------------------|
| Neumann<br>1825                          | 100<br>010<br>001           | 2.9.65<br>2.9.61<br>7.0.7                | 2.9.2<br>7.0.7<br>0.0.63       | 2.9.65<br>16.9.79<br>0.0.126    | 1.6.22<br>7.0.56<br>3.3.24 | 7.0.70<br>7.0.56<br>2.9.2 | 2.9.2<br>7.0.56<br>7.0.70 |
| Hausmann 1847<br>Mohs 1824<br>Zippe 1839 | 1.1.18<br>774<br>110        | 100<br>010<br>001                        | 110<br>002<br>110              | 100<br>102<br>110               | 132<br>336<br>202          | 112<br>112<br>110         | 110<br>112<br>112         |
| Miller ( <i>hkl</i> )*<br>1852           | 091<br>720<br>001           | 101<br>101<br>010                        | 100<br>010<br>001              | 101<br>121<br>002               | 211<br>033<br>111          | 011<br>011<br>100         | 100<br>011<br>011         |
| Lévy 1838 Des<br>Cloizeaux 1862          | 9.9.1<br>16.2.7<br>0.0.1    | 200<br>202<br>110                        | 201<br>110<br>001              | 100<br>010<br>001               | 513<br>333<br>110          | 111<br>111<br>201         | 201<br>111<br>111         |
| vom Rath<br>1866                         | 8.10.16<br>16.2.10<br>1.1.2 | 114<br>310<br>112                        | 202<br>112<br>112              | 114<br>118<br>224               | 100<br>010<br>001          | 102<br>010<br>101         | 101<br>010<br>102         |
| Schrauf<br>1870                          | 8.10.0<br>2.2.14<br>1.1.0   | 112<br>112<br>110                        | 002<br>110<br>110              | 112<br>312<br>220               | 102<br>030<br>101          | 100<br>010<br>001         | 001<br>010<br>100         |
| Hessenberg<br>1873                       | 0.10.8<br>14.2.2<br>0.1.1   | 211<br>211<br>011                        | 200<br>011<br>011              | 211<br>213<br>022               | 201<br>030<br>101          | 001<br>010<br>100         | 100<br>010<br>001         |
| Frazier<br>1882                          | 0.9.4<br>14.2.0<br>0.0.4    | 204<br>204<br>010                        | 200<br>010<br>004              | 102<br>112<br>004               | 414<br>0.3.12<br>214       | 014<br>014<br>200         | 200<br>014<br>014         |
| V. Goldschmidt<br>1886                   | 910<br>207<br>010           | 011<br>011<br>100                        | 001<br>100<br>010              | 011<br>211<br>020               | 112<br>330<br>111          | 110<br>110<br>001         | 001<br>110<br>110         |
| Dana<br>1892                             | 9.9.2<br>16.2.0<br>0.0.2    | 202<br>202<br>110                        | 200<br>110<br>002              | 101<br>011<br>002               | 512<br>336<br>112          | 112<br>112<br>200         | 200<br>112<br>112         |
| V. Goldschmidt<br>1897-1913              | 901<br>270<br>001           | 011<br>011<br>100                        | 010<br>100<br>001              | 011<br>211<br>002               | 121<br>303<br>111          | 101<br>101<br>010         | 010<br>101<br>101         |
| Friedel<br>1926                          | 091<br>797<br>001           | 110<br>112<br>010                        | 111<br>010<br>001              | 110<br>110<br>002               | 233<br>033<br>100          | 011<br>011<br>111         | 111<br>011<br>011         |
| Gossner-Reichel<br>1932                  | 091<br>790<br>001           | 111<br>111<br>010                        | 110<br>010<br>001              | 111<br>111<br>002               | 231<br>033<br>101          | 011<br>011<br>110         | 110<br>011<br>011         |
| Peacock<br>1937                          | 901<br>270<br>001           | 011<br>011<br>100                        | 010<br>100<br>001              | 011<br>211<br>002               | 121<br>303<br>111          | 101<br>101<br>010         | 010<br>101<br>101         |

TABLE OF AXINITE TRANSFORMATIONS (Concluded)

| From \ To                                | Frazier<br>1882                   | V. Goldschmidt<br>1886         | Dana<br>1892                     | V. Goldschmidt<br>1897-1913    | Friedel<br>1926                 | Gossner-Reichel<br>1932        | Peacock<br>1937                |
|--|-----------------------------------|--------------------------------|----------------------------------|--------------------------------|---------------------------------|--------------------------------|--------------------------------|
| Neumann<br>1825                          | 4. 18. 4<br>28. 0. 28<br>0. 0. 63 | 7. 0. 7<br>0. 0. 63<br>2. 9. 2 | 2. 9. 2<br>16. 9. 16<br>0. 0. 63 | 7. 0. 7<br>2. 9. 2<br>0. 0. 63 | 9. 9. 72<br>7. 0. 7<br>0. 0. 63 | 9. 9. 9<br>7. 0. 7<br>0. 0. 63 | 7. 0. 7<br>2. 9. 2<br>0. 0. 63 |
| Hausmann 1847<br>Mohs 1824<br>Zippe 1839 | 220<br>008<br>110                 | 002<br>110<br>110              | 110<br>114<br>110                | 002<br>110<br>110              | 202<br>002<br>110               | 112<br>002<br>110              | 002<br>110<br>110              |
| Miller ( <i>khl</i> )*<br>1852           | 200<br>040<br>001                 | 010<br>001<br>100              | 100<br>120<br>001                | 010<br>100<br>001              | 111<br>010<br>001               | 110<br>010<br>001              | 010<br>100<br>001              |
| Lévy 1838<br>Des Cloizeaux 1862          | 402<br>440<br>001                 | 110<br>001<br>201              | 201<br>021<br>001                | 110<br>201<br>001              | 110<br>110<br>001               | 111<br>110<br>001              | 110<br>201<br>001              |
| vom Rath<br>1866                         | 404<br>448<br>112                 | 112<br>112<br>202              | 202<br>026<br>112                | 112<br>202<br>112              | 006<br>112<br>112               | 114<br>112<br>112              | 112<br>202<br>112              |
| Schrauf<br>1870                          | 004<br>440<br>110                 | 110<br>110<br>002              | 002<br>222<br>110                | 110<br>002<br>110              | 202<br>110<br>110               | 112<br>110<br>110              | 110<br>002<br>110              |
| Hessenberg<br>1873                       | 400<br>044<br>011                 | 011<br>011<br>200              | 200<br>122<br>011                | 011<br>200<br>011              | 202<br>011<br>011               | 211<br>011<br>011              | 011<br>200<br>011              |
| Frazier<br>1882                          | 100<br>010<br>001                 | 010<br>004<br>200              | 100<br>110<br>002                | 010<br>200<br>004              | 214<br>010<br>004               | 210<br>010<br>004              | 010<br>200<br>004              |
| V. Goldschmidt<br>1886                   | 002<br>400<br>010                 | 100<br>010<br>001              | 001<br>201<br>010                | 100<br>001<br>010              | 111<br>100<br>010               | 101<br>100<br>010              | 100<br>001<br>010              |
| Dana<br>1892                             | 200<br>220<br>001                 | 110<br>002<br>200              | 100<br>010<br>001                | 110<br>200<br>002              | 112<br>110<br>002               | 110<br>110<br>002              | 110<br>200<br>002              |
| V. Goldschmidt<br>1897-1913              | 020<br>400<br>001                 | 100<br>001<br>010              | 010<br>210<br>001                | 100<br>010<br>001              | 111<br>100<br>001               | 110<br>100<br>001              | 100<br>010<br>001              |
| Friedel<br>1926                          | 222<br>040<br>001                 | 010<br>001<br>111              | 111<br>111<br>001                | 010<br>111<br>001              | 100<br>010<br>001               | 101<br>010<br>001              | 010<br>111<br>001              |
| Gossner-Reichel<br>1932                  | 220<br>040<br>001                 | 010<br>001<br>110              | 110<br>110<br>001                | 010<br>110<br>001              | 101<br>010<br>001               | 100<br>010<br>001              | 010<br>110<br>001              |
| Peacock<br>1937                          | 020<br>400<br>001                 | 100<br>001<br>010              | 010<br>210<br>001                | 100<br>010<br>001              | 111<br>100<br>001               | 110<br>100<br>001              | 100<br>010<br>001              |

*Remark.* The product of any transformation matrix (say "Rath to Peacock") by the matrix of its inverse transformation ("Peacock to Rath") gives the unit matrix E, symbol of the identical transformation:

$$\begin{pmatrix} \overline{112} \\ 20\overline{2} \\ 1\overline{12} \end{pmatrix} \cdot \begin{pmatrix} \overline{121} \\ 30\overline{3} \\ \overline{111} \end{pmatrix} = \begin{pmatrix} 100 \\ 010 \\ 001 \end{pmatrix} = E$$

*Inverse Matrix.* Any transformation being given (say "Rath to Peacock") the matrix of the inverse transformation ("Peacock to Rath") is the inverse matrix. The rule may be recalled here: any element  $B_{ij}$  of the inverse matrix B is given by the value of the co-factor of the element  $A_{ji}$  which, in the direct matrix A, is symmetrical of  $A_{ij}$  with respect to the main diagonal (upper left-lower right).

Example:

$$\begin{array}{cc} \text{(Rath to Peacock)} & \text{(Peacock to Rath)} \\ A = \begin{pmatrix} \overline{112} \\ 20\overline{2} \\ 1\overline{12} \end{pmatrix} & B = \begin{pmatrix} \overline{121} \\ 30\overline{3} \\ \overline{111} \end{pmatrix} \end{array}$$

Matrix calculations are of great value to crystallography. Although their use has been advocated by various authors they have not received the recognition they deserve. The purpose of this appendix is to show their simplicity and illustrate their usefulness.

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\* Miller uses a left-handed system of coordinates, *i.e.*, in his symbol (*hkl*) the first index *h* refers to the axis that slopes to the right (the *b*-axis of a right-handed system) and the second index *k* refers to the axis that slopes forward (the *a*-axis of a right-handed system). Hence the rules: (1) Before applying any transformation "Miller to N . . ." interchange the first two indices in the Miller symbols. (2) After having applied any transformation "N . . . to Miller" interchange the first two indices of the obtained symbols.